

THE REDUCED DENSITY MATRIX

PROSEMINAR IN THEORETICAL PHYSICS
INSTITUT FÜR THEORETISCHE PHYSIK
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FS12

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CHAPTER 1

THE SET OF DENSITY OPERATORS

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*The main question treated in the talk is the following: **What is the most general state a quantum system can have?** The answer to this question is given by density operators. In this sense density operators generalize the concept of wave functions. In a first part we will follow two different approaches leading to the same mathematical concept of density operators. After giving the formal definition of the set of density operators we will investigate the spectral properties. Further we focus on general structural properties of the set and identify extremal states. We will introduce a measure of mixedness and talk about the non-uniqueness of spectral decompositions into pure states. Finally, we introduce the Bloch representation and investigate the geometry of the set as well as its boundary.*

1.1 INTRODUCTION

We will take two conceptually different paths.

1.1.1 MIXING OF PREPARATION PROCEDURES

The concept of a state can be understood as an ensemble of similarly prepared systems. In the following we will denote states by ρ and the set of states by $\mathcal{S} \ni \rho$. To determine a system's state one can perform measurements on the system. A statistical theory, such as quantum theory, does not predict the outcomes of the

1.1 Introduction

measurements but their probabilities. From the axioms of quantum mechanics we know that in the Hilbert space formalism measurements are described by observables, which are self-adjoint operators on our Hilbert space \mathcal{H} . The outcomes are eigenvalues of this specific operator. If our system is in the state $|\psi\rangle$ we can calculate the probability to get the outcome q by

$$\Pr(q, |\psi\rangle) = \langle\psi|Q|\psi\rangle \equiv \text{tr}(Q|\psi\rangle\langle\psi|), \quad (1.1)$$

where Q is the projection onto the eigenspace $\text{Eig}(q)$.

What if we cannot assign one particular state $|\psi\rangle$ to our quantum system but for example two? This can be achieved through a preparation procedure that chooses randomly between two different states $|\psi_1\rangle$ and $|\psi_2\rangle$ with probability λ and $(1 - \lambda)$, respectively. In general we call such a configuration a statistical ensemble of quantum states and denote it by $\{|\psi_i\rangle, p_i\}$ where the p_i are the probabilities to find the system in the state $|\psi_i\rangle$. Of course the probabilities must fulfil $\sum_i p_i = 1$.

Example 1.1.1. It is important that one does not confuse a superposition with an ensemble of states. For instance, the following two expressions, written in different notations, do not describe the same state:

$$\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \neq \left\{|\uparrow\rangle, \frac{1}{2}; |\downarrow\rangle, \frac{1}{2}\right\} \quad (1.2)$$

Suppose now that we perform the same measurement on the ensemble of states $\{|\psi_1\rangle, \lambda; |\psi_2\rangle, 1 - \lambda\}$. To be able to calculate the probabilities of the possible outcomes we have to make a basic assumption.

Assumption. For an ensemble of states the following equation must hold:

$$\Pr(q, \{|\psi_1\rangle, \lambda; |\psi_2\rangle, 1 - \lambda\}) = \lambda\Pr(q, |\psi_1\rangle) + (1 - \lambda)\Pr(q, |\psi_2\rangle) \quad (1.3)$$

The basic assumption is nothing less than the demand for consistency. It is only natural that we expect the probability for the occurrence of an event given an ensemble of states equals to the sum of probabilities for each state weighted with the probability to find the system in a particular state. Making a few manipulations on the assumption tells us that we can interpret an ensemble of states as a new state.

$$\begin{aligned} \Pr(q, \{|\psi_1\rangle, \lambda; |\psi_2\rangle, 1 - \lambda\}) &\stackrel{\text{Ass.}}{=} \lambda\Pr(q, |\psi_1\rangle) + (1 - \lambda)\Pr(q, |\psi_2\rangle) & (1.4) \\ &= \lambda\text{tr}(Q|\psi_1\rangle\langle\psi_1|) + (1 - \lambda)\text{tr}(Q|\psi_2\rangle\langle\psi_2|) \\ &= \text{tr}(Q[\lambda|\psi_1\rangle\langle\psi_1| + (1 - \lambda)|\psi_2\rangle\langle\psi_2|]) \end{aligned}$$

If we interpret a state given by a wave function $|\psi\rangle$ as the projector $|\psi\rangle\langle\psi|$ we find that an ensemble of states is simply the convex combination of these projectors. This is an extended concept of state as states are now represented by Hilbert space operators. The question is: By which operators?

Suggestion: Density operators.

Definition 1.1.1. A **density operator** ρ on a Hilbert space \mathcal{H} is a normalized, positive operator on \mathcal{H} , i.e. $\rho \geq 0$ and $\text{tr}(\rho) = 1$.

The **set of density operators** is denoted by $\mathcal{S}(\mathcal{H})$.

In other words density operators are trace class operators¹ which are positive and of unit trace. This will allow us to use the spectral theorem later on.

Remark. Positivity of a linear operator ρ means: $\forall \phi \in \mathcal{H} : \langle \phi | \rho | \phi \rangle \geq 0$.

The following general definitions help to understand an important property of density operators.

Definition 1.1.2. Let V be a vector space, $M \subset V$. M is a **convex** subset if

$$\forall v, w \in M, 0 \leq \lambda \leq 1 : \lambda v + (1 - \lambda)w \in M. \quad (1.5)$$

Definition 1.1.3. A **convex combination** of vectors $v_i \in V$, where V is a vector space, is a linear combination

$$\sum_i a_i v_i \text{ with } 0 \leq a_i \leq 1 \text{ and } \sum_i a_i = 1. \quad (1.6)$$

Remark. By construction $\mathcal{S}(\mathcal{H})$ is convex. One could say that mixing introduces the convex structure.

Proof. To see this we need to show that convex combinations of density operators are again density operators. W.l.o.g. we show it only for the convex combination of two density operators.

Let $\rho_1, \rho_2 \in \mathcal{S}(\mathcal{H})$, $\lambda \in [0, 1]$ and $\phi \in \mathcal{H}$. Consider $\rho = \lambda\rho_1 + (1 - \lambda)\rho_2$. Then:

$$\langle \phi | \rho | \phi \rangle = \underbrace{\lambda}_{\geq 0} \underbrace{\langle \phi | \rho_1 | \phi \rangle}_{\geq 0} + \underbrace{(1 - \lambda)}_{\geq 0} \underbrace{\langle \phi | \rho_2 | \phi \rangle}_{\geq 0} \geq 0 \quad (1.7)$$

and

$$\begin{aligned} \text{tr}(\rho) &= \lambda \underbrace{\text{tr}(\rho_1)}_{=1} + (1 - \lambda) \underbrace{\text{tr}(\rho_2)}_{=1} \\ &= \lambda + 1 - \lambda = 1. \end{aligned} \quad (1.8)$$

So the convex combination of normalized and positive operators is normalized and positive. This is what we wanted to show. \square

¹Operators for which the trace is well-defined.

1.1 Introduction

Remark. For a finite dimensional system positivity implies hermiticity.

Proof.

$$\rho \geq 0 \Rightarrow \langle \phi | \rho | \phi \rangle \in \mathbb{R}_{\geq 0} \forall \phi \in \mathcal{H} \quad (1.9)$$

$$\Rightarrow \langle \rho \phi | \phi \rangle = \langle \phi | \rho \phi \rangle^* \stackrel{\in \mathbb{R}}{=} \langle \phi | \rho \phi \rangle \quad (1.10)$$

$$\Rightarrow \rho^\dagger = \rho \quad (1.11)$$

□

In retrospective, (1.4) can be seen as the defining property of density operators.

1.1.2 IGNORING A SYSTEM'S ENVIRONMENT

The second approach to density operators arises due to the need to describe a system interacting with its environment. To illustrate this we make an example.

Example 1.1.2. Suppose we are given two qubits, one in room A and one in room B. We have only access to room A, meaning that we can only perform measurements on the qubit in room A. The qubits shall be in the state

$$|\psi_{AB}\rangle = a|0\rangle \otimes |0\rangle + b|1\rangle \otimes |1\rangle, \quad (1.12)$$

where a and b must fulfil $|a|^2 + |b|^2 = 1$. It is immediately clear that the qubits are correlated, meaning that the outcomes of measurements in room A and room B are not independent.

We are now looking for a compact way to characterize the observations that can be made in room A without having access to room B. In order to do this we have to know how to formulate a measurement made in room A only. One can show that it must be expressed by $M_A \otimes \mathbb{1}$ where M_A is a self-adjoint operator acting on A. Therefore we find

$$\langle M_A \rangle = \langle \psi_{AB} | M_A \otimes \mathbb{1} | \psi_{AB} \rangle \equiv \text{tr}((M_A \otimes \mathbb{1}) |\psi_{AB}\rangle \langle \psi_{AB}|), \quad (1.13)$$

i.e.

$$\rho_{AB} = |\psi_{AB}\rangle \langle \psi_{AB}|. \quad (1.14)$$

We would like to write $\langle M_A \rangle = \text{tr}(M_A \rho_A)$ so we need a function that gives us ρ_A from ρ_{AB} . More generally: Assuming that $\rho_{AB} = \sum_j A_j \otimes B_j$,

$$\langle M_A \rangle = \text{tr} \left(\sum_j (M_A \otimes \mathbb{1}) (A_j \otimes B_j) \right) = \sum_j \text{tr} (M_A A_j) \text{tr} (B_j) = \text{tr} (M_A \rho_A), \quad (1.15)$$

where $\rho_A = \sum_j \text{tr} (B_j) A_j = \text{tr}_B (\rho_{AB})$ is a partial trace as defined in

Definition 1.1.4. The **partial trace over system B** of an operator $S \otimes T$ acting on a Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ is an operator acting on \mathcal{H}_A given by

$$\text{tr}_B (S \otimes T) := \text{tr}(T)S \text{ and linear.} \quad (1.16)$$

$\rho_A := \text{tr}_B (\rho_{AB})$ is called the **reduced density operator**.

One can show that the partial trace is the unique function that fulfils

$$\text{tr} ((M_A \otimes \mathbb{1}) \rho_{AB}) = \text{tr} (M_A \text{tr}_B (\rho_{AB})) \quad (1.17)$$

for all measurements that can be made on subsystem A.

Example 1.1.3. As before, let our two-qubit world be in the state $|\psi_{AB}\rangle = a|0\rangle \otimes |0\rangle + b|1\rangle \otimes |1\rangle$. We find

$$\begin{aligned} \rho_{AB} = |\psi_{AB}\rangle \langle \psi_{AB}| &= |a|^2 \cdot |0\rangle \langle 0| \otimes |0\rangle \langle 0| + ab^* \cdot |0\rangle \langle 1| \otimes |0\rangle \langle 1| \\ &\quad + a^*b \cdot |1\rangle \langle 0| \otimes |1\rangle \langle 0| + |b|^2 \cdot |1\rangle \langle 1| \otimes |1\rangle \langle 1| \end{aligned} \quad (1.18)$$

$$\begin{aligned} \Rightarrow \rho_A = \text{tr}_B (\rho_{AB}) &= |a|^2 \cdot |0\rangle \langle 0| + 0 + 0 + |b|^2 \cdot |1\rangle \langle 1| \\ &= |a|^2 \cdot |0\rangle \langle 0| + |b|^2 \cdot |1\rangle \langle 1|, \end{aligned} \quad (1.19)$$

where we used $\text{tr} (|\phi_1\rangle \langle \phi_2|) = \langle \phi_1 | \phi_2 \rangle$.

Remark. ρ_A can be interpreted as an ensemble $\{|0\rangle, |a|^2; |1\rangle, |b|^2\}$. But one has to pay attention: This is not the only ensemble that leads to the state ρ_A as we will see soon.

So far we have seen that density operators give us the possibility to include missing knowledge in the state of a system. From now on we are able to describe a system A correlated with another system B only by results gotten from system A.

1.2 SPECTRAL PROPERTIES

As mentioned, positive operators are hermitian. By using the spectral decomposition theorem we can make a canonical convex decomposition for every $\rho \in \mathcal{S}(\mathcal{H})$:

$$\rho = \sum_i p_i P_i, \quad (1.20)$$

where $0 \leq p_i \leq 1$, $\sum_i p_i = 1$ and the P_i are one-dimensional orthogonal projections.

In general this decomposition is not unique. It is called *canonical* because the projectors must be *orthogonal*. The spectral properties will become important for proofs of propositions later on.

1.3 STRUCTURAL PROPERTIES OF THE SET

For convex sets one can define extremal points.

Definition 1.3.1. $\rho \in \mathcal{S}(\mathcal{H})$ is **extremal** if $\rho = \lambda\rho_1 + (1 - \lambda)\rho_2$ with $0 < \lambda < 1$ implies $\rho_1 = \rho_2 = \rho$ i.e. if the only convex decomposition is trivial.

Extremal states are called **pure**, non-extremal states are called **mixed**.

The following proposition helps to find out what pure, i.e. extremal, states are.

Proposition 1.1. *The following are equivalent:*

- (i) ρ is pure,
- (ii) ρ is a one-dimensional projection,
- (iii) $\text{tr}(\rho^2) = 1$.

Proof. We will show (i) \Rightarrow (ii) \Rightarrow (iii) \Rightarrow (i).

(i) \Rightarrow (ii): For ρ pure the only convex decomposition is

$$\rho = p_1 P_1. \quad (1.21)$$

Since $\text{tr}(\rho) = 1$ and $\text{tr}(P) = 1 \forall$ projections P , it must be $p_1 = 1$.

(ii) \Rightarrow (iii): Every projection fulfils $P^2 = P$. If $\rho = P$ we find

$$\text{tr}(\rho^2) = \text{tr}(\rho) = 1. \quad (1.22)$$

(iii)⇒(i): We can always write $\rho = \sum_i p_i P_i$. This yields

$$1 \stackrel{!}{=} \text{tr}(\rho^2) = \text{tr}\left(\sum_{i,j} p_i p_j P_i P_j\right) = \sum_i p_i^2 \cdot \text{tr}(P_i) = \sum_i p_i^2. \quad (1.23)$$

We made use of the fact that the P_i are orthogonal projections. Since $0 \leq p_i \leq 1$ it follows: $p_i = \delta_{ij}$ for some j . Per construction this is the only convex decomposition [1].

□

Remark. We used the spectral decomposition theorem to prove the proposition. Notice that this is not necessary.

The next step is to find an easily applicable instrument to decide whether a given state is pure or not. The proposition above already gives us

Definition 1.3.2. Given a state $\rho \in \mathcal{S}(\mathcal{H})$ the **purity** of ρ is

$$\mathcal{P}(\rho) := \text{tr}(\rho^2). \quad (1.24)$$

Not only can we now decide whether we are dealing with a pure state, but we also have a measure for mixedness. The following proposition lists two important properties of the purity which will be used afterwards to make statements about the boundary of the state space.

Proposition 1.2. *Important properties of \mathcal{P} are:*

- (i) \mathcal{P} is a convex map, i.e. $\mathcal{P}(\lambda\rho_1 + (1-\lambda)\rho_2) \leq \lambda\mathcal{P}(\rho_1) + (1-\lambda)\mathcal{P}(\rho_2)$.
- (ii) If $\dim(\mathcal{H}) = d$ then for all states $\rho \in \mathcal{S}(\mathcal{H})$: $\frac{1}{d} \leq \mathcal{P}(\rho) \leq 1$.

Remark. The proof of this proposition is technical and not too difficult. We leave it to the reader. It can be found in [1].

With this we are now able to harvest the fruits of our labour. It is easy to see that in the finite dimensional case $\mathcal{P}\left(\frac{\mathbb{1}}{d}\right) = \text{tr}\left(\frac{\mathbb{1}^2}{d^2}\right) = \frac{d}{d^2} = \frac{1}{d}$. So we found a maximally mixed state with $\frac{1}{d}$. But a minimum of a convex function on a convex set is automatically a global minimum. Therefore we conclude that $\frac{1}{d}$ is the unique maximally mixed state.

Remark. One can also see this easily by using Lagrange multipliers to find the minimum of \mathcal{P} .

1.4 Decomposition into Pure States

We now know the unique minimum of \mathcal{P} . But what about the maximum? From the proposition we know that \mathcal{P} is always less than or equal to 1. We also know that pure states have purity equal to 1. We conclude that the maximum of \mathcal{P} is 1. And since the state space is convex, as well as the function \mathcal{P} , the maximum, i.e. the pure states, must lie on the boundary of $\mathcal{S}(\mathcal{H})$. But in general the pure states are not the only states lying on the boundary.

To talk about the boundary properly we need to have a measure of distance. In this case we take the trace distance.

Definition 1.3.3. The **trace norm** of an operator ρ is defined as

$$\|\rho\|_{\text{tr}} := \text{tr}|\rho|. \quad (1.25)$$

The **trace distance** between two operators ρ and σ is then

$$\delta(\rho, \sigma) := \frac{1}{2}\|\rho - \sigma\|_{\text{tr}}. \quad (1.26)$$

Remark. Of course these definitions are only valid if the expressions (1.25) and (1.26) exist. This is the case for trace class operators.

Definition 1.3.4. We say that a state ρ belongs to the **boundary** of $\mathcal{S}(\mathcal{H})$ if for each $\epsilon > 0$, there exists an operator $\xi_\epsilon \in \mathcal{T}_s(\mathcal{H})$ such that $\delta(\rho, \xi_\epsilon) < \epsilon$ but $\xi_\epsilon \notin \mathcal{S}(\mathcal{H})$. Here, $\mathcal{T}_s(\mathcal{H})$ is the space of all hermitian operators on \mathcal{H} .

Proposition 1.3. *If a state $\rho \in \mathcal{S}(\mathcal{H})$ has 0 as an eigenvalue it belongs to the boundary.*

Proof. Let $\rho \in \mathcal{S}(\mathcal{H})$ be a state with eigenvalue 0 and let $\varphi \in \mathcal{H}$ be a corresponding normalized eigenvector. Fix $\epsilon > 0$.

The operator $\xi_\epsilon := \rho - \epsilon|\varphi\rangle\langle\varphi|$ is trace class and self adjoint, but not positive, as $\langle\varphi|\xi_\epsilon\varphi\rangle = -\epsilon < 0$. On the other hand,

$$\delta(\xi_\epsilon, \rho) = \frac{1}{2}\epsilon\||\varphi\rangle\langle\varphi|\|_{\text{tr}} = \frac{1}{2}\epsilon < \epsilon. \quad (1.27)$$

It follows that ρ belongs to the boundary [1]. □

1.4 DECOMPOSITION INTO PURE STATES

We emphasized before that decompositions of density operators are not unique. To illustrate this we make an Example [2].

Example 1.4.1. Consider the state

$$\rho = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|. \quad (1.28)$$

One possible interpretation of this is the ensemble of states $\{|0\rangle, \frac{3}{4}; |1\rangle, \frac{1}{4}\}$. Define then

$$|a\rangle = \sqrt{\frac{3}{4}}|0\rangle + \sqrt{\frac{1}{4}}|1\rangle \text{ and } |b\rangle = \sqrt{\frac{3}{4}}|0\rangle - \sqrt{\frac{1}{4}}|1\rangle. \quad (1.29)$$

Computing yields

$$\frac{1}{2}|a\rangle\langle a| + \frac{1}{2}|b\rangle\langle b| = \rho. \quad (1.30)$$

So we could also think of this state as the ensemble $\{|a\rangle, \frac{1}{2}; |b\rangle, \frac{1}{2}\}$.

Two different ensembles can give the same quantum state, meaning that the decomposition into pure states is not unique. To decide whether two ensembles of states give the same density operator we can use

Theorem 1.4. *Two ensembles $\{|\psi_i\rangle, p_i\}$ and $\{|\phi_j\rangle, q_j\}$ represent the same state*

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_j q_j |\phi_j\rangle\langle\phi_j| \quad (1.31)$$

if and only if

$$\sqrt{p_i}|\psi_i\rangle = \sum_j u_{ij}\sqrt{q_j}|\phi_j\rangle \text{ where } U = (u_{ij}) \text{ is unitary.} \quad (1.32)$$

Remark. If the two sets do not have the same length (w.l.o.g. $1 \leq i \leq n$, $1 \leq j \leq m$ and $m < n$) we fill the list $\{|\phi_j\rangle, q_j\}$ with vectors $|\phi_k\rangle = 0$ for $m < k \leq n$ in order to get a $n \times n$ matrix for U .

Proof. The proof is very technical. It can be found for example in [2]. \square

1.5 BLOCH REPRESENTATION

For finite dimensional systems $\mathcal{S}(\mathcal{H})$ can be represented in a very neat way. As we mentioned earlier, in the finite dimensional case our state space is a subset of the space of all hermitian operators on \mathcal{H} : $\mathcal{S}(\mathcal{H}) \subset \mathcal{T}_s(\mathcal{H})$. We introduce the Hilbert-Schmidt scalar product

$$\langle A|B\rangle := \langle A|B\rangle_{H-S} = \text{tr}(A^*B) \quad (1.33)$$

1.5 Bloch Representation

on $\mathcal{T}_s(\mathcal{H})$. Note that $\mathcal{T}_s(\mathcal{H})$ is a real vector space².

We first have a look at the illustrative two dimensional case.

Example 1.5.1. An operator $\omega \in \mathcal{T}_s(\mathbb{C}^2)$ can always be written as

$$\omega = \begin{pmatrix} a & c + id \\ c - id & b \end{pmatrix} \text{ where } a, b, c, d \in \mathbb{R}. \quad (1.34)$$

We conclude that the dimension of $\mathcal{T}_s(\mathbb{C}^2)$ is $\dim_{\mathbb{R}}(\mathcal{T}_s(\mathbb{C}^2)) = 2^2 = 4$. If ω is normalized we can write:

$$\begin{aligned} \omega &= \frac{1}{2} \begin{pmatrix} (1+z) & (x-iy) \\ (x+iy) & (1-z) \end{pmatrix} \\ &= \frac{1}{2} \left[\mathbb{1} + x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] = \frac{1}{2} [\mathbb{1} +] \end{aligned}$$

test $\vec{t}\sigma$

$$\rho \geq 0 \Leftrightarrow \|\vec{r}\| \leq 1. \quad (1.35)$$

In two dimensions the state space can be represented by the 1-ball in \mathbb{R}^3 which is called the **Bloch Sphere**. From the results above we conclude that only pure states are on the boundary because if $\|\vec{r}\| = 1$ then one eigenvalue of ρ is one and the other is zero (Proposition 1.3).

The generalization of this result for Hilbert spaces of dimension $d > 2$ is still very helpful but not as easy to perform as in the two-dimensional case. First we have to ask ourselves: What is the reason for taking $\{\sigma_0 := \mathbb{1}, \sigma_1, \sigma_2, \sigma_3\}$ as a basis? It is known that the Pauli matrices fulfil $\text{tr}(\sigma_j \sigma_k) = 2\delta_{jk}$. So we are dealing with an orthogonal basis with respect to the Hilbert-Schmidt scalar product. It is easy to show that the dimension of $\mathcal{T}_s(\mathcal{H})$ is in general $\dim_{\mathbb{R}}(\mathcal{T}_s(\mathcal{H})) = d^2$. Suppose we find a basis $\{E_j\}_{j=0}^{d^2-1}$ such that $E_0 = \mathbb{1}$ and E_1, \dots, E_{d^2-1} are orthogonal with $\langle E_j | E_k \rangle = d\delta_{jk}$. The orthogonality of the E_j yields that $\text{tr}(E_j) = d\delta_{j0}$. Therefore all basis vectors except the unity matrix must be traceless. Knowing this we can give

Definition 1.5.1. Given a basis $\{E_j\}_{j=0}^{d^2-1}$ with the above properties we can represent every $\rho \in \mathcal{S}(\mathcal{H})$ as

$$\rho = \frac{1}{d} \left(\mathbb{1} + \vec{r} \cdot \vec{E} \right), \quad (1.36)$$

²A hermitian operator multiplied by i becomes anti-hermitian.

where $\vec{r} \in \mathbb{R}^{d^2-1}$ and $\vec{E} = (E_1, \dots, E_{d^2-1})$. This is the general **Bloch Representation**.

Remark. $\text{tr}(E_j) = d\delta_{j0}$ and therefore trivially: $\text{tr}(\rho) = 1$.

Remark. As in Fourier analysis: $r_i = \text{tr}(\rho E_i)$ for $i = 1, \dots, d^2 - 1$.

Now that it is clear that the normalization is already given by construction the only remaining question is: What are the demands on \vec{r} to make ρ positive? Unfortunately the answer is somewhat complicated and cannot be given in general. A possible approach to narrow down the values \vec{r} can obtain is using Proposition 1.2. Exploiting the properties of the basis $\{E_j\}_{j=0}^{d^2-1}$ we find

$$\mathcal{P}(\rho) = \frac{1}{d} (1 + \|\vec{r}\|^2) \stackrel{!}{\leq} 1. \quad (1.37)$$

This shows that the state space is contained in the $\sqrt{d-1}$ -ball in \mathbb{R}^{d^2-1} . But does it coincide with the ball?

The answer is no. To see this we make an

Example 1.5.2. Let $\rho = \frac{1}{d} (\mathbb{1} + \vec{r} \cdot \vec{E})$ be a pure state, $d > 2$. Then $\rho' := \frac{1}{d} (\mathbb{1} - \vec{r} \cdot \vec{E})$ is not in $\mathcal{S}(\mathcal{H})$.

The antipodal of a pure state is not a state anymore for $d > 2$.

Proof. Let $\rho = |\phi\rangle\langle\phi|$. Then:

$$1 = \langle\phi|\rho|\phi\rangle = \left\langle\phi\left|\frac{1}{d} (\mathbb{1} + \vec{r} \cdot \vec{E})\right|\phi\right\rangle = \frac{1}{d} + \frac{1}{d} \langle\phi|\vec{r} \cdot \vec{E}|\phi\rangle \quad (1.38)$$

i.e. $\langle\phi|\vec{r} \cdot \vec{E}|\phi\rangle = d - 1$.

With that:

$$\langle\phi|\rho'|\phi\rangle = \frac{1}{d} - \frac{1}{d} \langle\phi|\vec{r} \cdot \vec{E}|\phi\rangle = \frac{1}{d} - \frac{1}{d}(d - 1) = \frac{2-d}{d} < 0 \text{ for } d > 2. \quad (1.39)$$

This means that ρ' is not positive and therefore is no state. \square

Describing the geometry of the state space in general goes beyond the scope of this report. The important point to remember is that the two-dimensional case is exceptional in many respects.

1.6 CONCLUSION

Density operators are more general implementations of quantum states than wave functions in many respects. They allow to include missing knowledge and to focus on subsystems by tracing out the environment. The latter is done by taking the partial trace over the environment tr_{env} of the density operator describing the complete system.

The set of density operators, also called the state space, is convex. This turned out to be a helpful property to describe its structure. Defining pure states as extremal points of the state space we found that a pure state is always a one-dimensional projector.

Using the equivalence $\rho \text{ pure} \Leftrightarrow \text{tr}(\rho^2) = 1$, we are provided with a measure of mixedness: $\mathcal{P}(\rho) = \text{tr}(\rho^2)$. The unique maximally mixed state for finite dimensional systems was determined to be $\frac{1}{d}$, where d is the dimension of the corresponding Hilbert space.

It is an important fact that mixed states have no unique decomposition into pure states. In fact there are infinitely many possibilities to do so. Thus, the interpretation of a mixed state as a statistical ensemble is left open to the person dealing with it.

Finally the Bloch Representation was introduced. For $\mathcal{H} = \mathbb{C}^2$ the state space can be represented as the 1-ball in \mathbb{R}^3 . For higher dimensional systems this is not true anymore. The structure gets much more complicated and cannot be described easily in general. An illustrating example for the complexity was given in Example 1.5.2.

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CHAPTER 2

TIME EVOLUTION OF DENSITY OPERATORS

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This paper is treating the time evolution of density matrices for open and isolated systems. The discussion of isolated systems covers the properties of unitary time evolution and the derivation of the Liouville von Neumann theorem.

In the discussion of open systems the properties of non-unitary evolution are discussed by introducing the framework of quantum channels and the consequences of Stinespring Dilation Theorem.

2.1 INTRODUCTION

The formalism of density operators lets us describe a quantum system more generally than with quantum states. The density operators describe a distribution of wave functions for particles inside a system. In the first chapter, the properties of the set of density operators were discussed. In this chapter, we are going to discuss the time evolution of density operators and the behaviour of density operators under unitary and non-unitary transformations. The discussion of isolated systems will find the *Liouville- von Neumann equation* which is somewhat the analogue of *Schrödingers equation* for density operators. In the discussion of open systems the mathematical properties of quantum channels will be addressed, which are defined by the following properties: a quantum channel is a trace preserving, completely positive, linear maps between density operators. We will further discuss the effects of such maps on a quantum system.

2.2 Time evolution of isolated systems

2.1.1 NOTATION

First we will introduce some notation which will be used throughout the paper.

\mathcal{H} are Hilbert spaces

$\psi \in \mathcal{H}$ are state vectors

$\mathcal{S}(\mathcal{H})$ is the space of quantum states on \mathcal{H}

$\rho \in \mathcal{S}(\mathcal{H})$ are density operators, i.e $\text{tr}\rho = 1, \rho \geq 0$

$\mathcal{L}(\mathcal{H})$ is the space of operators acting on \mathcal{H}

2.2 TIME EVOLUTION OF ISOLATED SYSTEMS

A closed or isolated system is a system which does not interact with its surroundings. The behaviour of a closed system is described entirely by its Hamilton operator H and the induced Schrödinger equation. To find the time evolution of density operators is by starting with our knowledge of the time evolution of state vectors according to Schrödinger Equation and we will translate it into the density operator space $\mathcal{S}(\mathcal{H})$

2.2.1 TIME EVOLUTION OF STATE VECTORS

The time evolution of state vectors is governed by the Schrödinger equation.

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \quad (2.1)$$

where $|\psi(t)\rangle \in \mathcal{H}$ is a state vector and $H \in \mathcal{L}(\mathcal{H})$ is the Hamilton operator. Now for later purposes we need to define the *time evolution operator* which describes the transformation from the initial state $|\psi(t_0)\rangle$ into the state vector $|\psi(t)\rangle$ at a later point in time t .

Definition 2.1. The time evolution operator $U(t, t_0)$ is defined by

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle \quad (2.2)$$

To calculate this *time evolution operator* we will need the *exponential function for operators* which is defined analogous to the exponential function for numbers.

Definition 2.2. The exponential function in operator space is defined as

$$\exp[A] = \sum_{n=0}^{\infty} \frac{1}{n!} A^n \quad (2.3)$$

for $A \in \mathcal{L}(\mathcal{H})$

We now calculate the time evolution operator by inserting the definition into Schrödinger's equation.

Proposition 2.1. *In case of a time-independent Hamiltonian, $U(t, t_0)$ is given by*

$$U(t, t_0) = \exp \left[-\frac{i}{\hbar} H(t - t_0) \right] \quad (2.4)$$

Proof. To prove this proposition we insert the definition of $U(t, t_0)$ into Schrödinger Equation (2.1)

$$i\hbar \frac{d}{dt} U(t, t_0) |\psi(t_0)\rangle = H U(t, t_0) |\psi(t_0)\rangle$$

Since this holds for all $|\psi\rangle \in \mathcal{H}$ we obtain

$$i\hbar \frac{d}{dt} U(t, t_0) = H U(t, t_0)$$

It is easy to see that the solution to this differential equation is given by

$$U(t, t_0) = \exp \left[-\frac{i}{\hbar} H(t - t_0) \right]$$

□

Since the time evolution operator is dependent on the time interval we will set t_0 to 0 and $t \rightarrow t - t_0$ and we will further use the notation $U_t := U(t, 0)$.

The time evolution operators satisfy the properties of a *1-parametric group*.

Definition 2.3. A 1-parametric group is a continuous group homomorphism $\Phi : \mathbb{R} \rightarrow G$ with the properties

$$\Phi(t)\Phi(s) = \Phi(t + s) \quad \forall t, s \in \mathbb{R} \quad (2.5)$$

Proposition 2.2. *The time evolution operators form a 1-parametric group*

Proof. This is proved by putting the operators into the definition.

$$U_s U_t = \exp \left[-\frac{i}{\hbar} H(s) \right] \exp \left[-\frac{i}{\hbar} H(t) \right] = \exp \left[-\frac{i}{\hbar} H(s + t) \right] = U_{s+t} \quad (2.6)$$

□

It is easy to see that $U_t = \exp \left[-\frac{i}{\hbar} H(t) \right]$ is unitary and $U_0 = I$ is the group identity.

Using all the properties discussed in this section, we are ready to translate the time evolution operator into the space of density operators.

2.2 Time evolution of isolated systems

2.2.2 TIME EVOLUTION OF DENSITY OPERATORS

To discuss the time evolution of *density operators* we start by describing the time evolution of pure states, because the density operator of a pure state at a given time t is defined as $\rho = |\psi(t)\rangle \langle \psi(t)|$.

We know how the state vectors evolve in time and just applying this to the definition we get

$$\rho(t) = |\psi(t)\rangle \langle \psi(t)| = U_t |\psi(t_0)\rangle \langle \psi(t_0)| U_t^\dagger = U_t \rho(t_0) U_t^\dagger$$

For further use we will call this transformation σ_{U_t} .

Definition 2.4. The time-evolution of the density matrix of a pure state is given by the map σ_{U_t}

$$\begin{aligned} \sigma_{U_t} : \mathcal{S}(\mathcal{H}) &\rightarrow \mathcal{S}(\mathcal{H}) \\ \sigma_{U_t} : \rho(t_0) &\mapsto U_t \rho(t_0) U_t^\dagger = \rho(t) \end{aligned}$$

We have seen in the last section that the time evolution operator form a *1-parametric group*. These group properties have are still true for density matrices.

Proposition 2.3. σ_{U_t} still satisfies the one-parametric group relations, thus

$$\sigma_{U_s} \circ \sigma_{U_t} = \sigma_{U_{t+s}} \tag{2.7}$$

$$\sigma_{U_0} = I \tag{2.8}$$

Proof. To proof this we use the properties of U_t from the proposition 2.2

$$\sigma_{U_s} \circ \sigma_{U_t}(\rho(t_0)) = U_s U_t \rho(t_0) U_t^\dagger U_s^\dagger = \sigma_{U_{s+t}}(\rho(t_0))$$

and

$$\sigma_{U_{(t_0,t_0)}}(\rho(t_0)) = I \rho(t_0) I = \rho(t_0) \Rightarrow \sigma_{U_{(t_0,t_0)}} = I$$

□

Density operators give a more complete description of a quantum system because they describe not only pure states, but also mixed states. The general density operator is defined by the formula

$$\rho = \sum_{\mu} p_{\mu} |\psi_{\mu}\rangle \langle \psi_{\mu}|$$

Each of the state vectors $|\psi_{\mu}\rangle$ evolves according to the *time evolution operator*, thus the density operator is described by

$$\rho(t) = \sum_{\mu} p_{\mu} U_t |\psi_{\mu}(t_0)\rangle \langle \psi_{\mu}(t_0)| U_t^{\dagger} = U_t \left(\sum_{\mu} p_{\mu} |\psi_{\mu}(t_0)\rangle \langle \psi_{\mu}(t_0)| \right) U_t^{\dagger} = \sigma_{U_t}(\rho(t_0))$$

In the third step we assumed linearity of U_t which is obviously true for $U_t = \exp \left[-\frac{i}{\hbar} H t \right]$.

Using this extension onto mixed states we observe that the mixture of states evolves into the mixture of the evolved states, which corresponds to the intuitive result that if we observe each particle in a system we would find the total state to be the same as if we would observe the evolution of the entire system. As we have seen σ_{U_t} describes the unitary transformation of a state into the evolved state.

But these transformations tell only have the story, because we are not only interested in the transformation, but we want to find out what the time dynamics are like. The equation governing the dynamics is called the *Liouville-von Neumann equation*, which can be seen as the analogue of Schrödinger equation for density operators.

Liouville von Neumann theorem. Let $\rho(t) \in \mathcal{S}(\mathcal{H})$ be an arbitrary density operator, $\sigma_{U_t} : \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H})$ the unitary time evolution described by the time-independent Hamiltonian $H \in \mathcal{L}(\mathcal{H})$. Then the dynamics of the time evolution are governed by the Liouville-von Neumann equation.

$$\frac{d}{dt} \rho(t) = -\frac{i}{\hbar} [H, \rho(t)] \quad (2.9)$$

Proof. To proof the theorem we need to take the derivation of $\rho(t)$.

$$\frac{d\rho(t)}{dt} = \lim_{dt \rightarrow 0} \frac{1}{dt} [\rho(t+dt) - \rho(t)]$$

With $\rho(t+dt) = \exp \left[-\frac{i}{\hbar} H dt \right] \rho(t) \exp \left[\frac{i}{\hbar} H dt \right]$ we get

$$\frac{d\rho(t)}{dt} = \lim_{dt \rightarrow 0} \frac{\rho(t+dt) - \rho(t)}{dt} = \lim_{dt \rightarrow 0} \frac{1}{dt} \left[\left(I - \frac{i}{\hbar} H dt + \dots \right) \rho(t) \left(I + \frac{i}{\hbar} H dt + \dots \right) - \rho(t) \right]$$

All higher order terms will vanish when dt goes to zero, so the only terms left over are

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar} H \rho(t) + \frac{i}{\hbar} \rho(t) H = -\frac{i}{\hbar} [H, \rho(t)]$$

□

2.3 Evolution of open systems

Remarks: This theorem was worked out by John von Neumann, Liouville died years before quantum mechanics came around. It is called the Liouville von Neumann theorem because of the similar form to Liouville's theorem of classical mechanics which states

$$\frac{\partial \rho}{\partial t} = -\{\rho, H\}$$

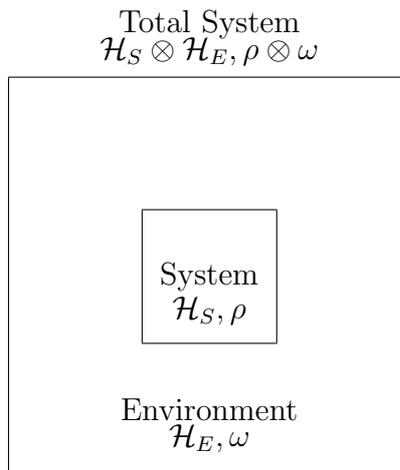
Where H is the classical Hamilton function, ρ is the density function and $\{\cdot, \cdot\}$ are the Poisson brackets.

2.3 EVOLUTION OF OPEN SYSTEMS

2.3.1 TIME EVOLUTION OF SIMPLE OPEN SYSTEMS

Assume we have a lab system described by the Hilbert space \mathcal{H}_S . In section 2 we have seen how a state vector in this system evolves in time if we keep it isolated. But real physical systems are never isolated, and a system \mathcal{H}_S with interacting with an environment \mathcal{H}_E is called an open system. (For example a heat bath interacting with a particle). The total Hilbert space of system and environment is found by tensoring both Hilbert spaces, $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. The Hamiltonian of such an open system can be separated $H = H_S + H_E + H_I$ where H_S describes the behaviour of the system, H_E describes the environment and H_I describes the interaction between system and environment.

Now assume we prepared the state of the system to be ρ and the state of the environment is described by ω . Then the initial total system can be seen in the following figure.



Now the system starts interacting with the environment and we measure the state of the system again at a given time t .

The density operator of the system \mathcal{H}_S is now given by the reduced density operator of the total System at the time t .

$$\rho(t) = \text{tr}_E \left[U_t(\rho(t_0) \otimes \omega) U_t^\dagger \right] \quad (2.10)$$

EXAMPLE: SWAP GATE As an example we construct a swap gate for a two qubit system. The interaction Hamiltonian H_{swap} has the properties

$$H_{swap} |\psi\rangle_S \otimes |\phi\rangle_E \rightarrow |\phi\rangle_S \otimes |\psi\rangle_E.$$

For a two qubit system this Hamiltonian called the *Heisenberg Exchange Hamiltonian* and it is easy to show that it is self-adjoint and unitary, i.e $H_{swap}^\dagger = H_{swap}$ and $H_{swap}^2 = I$.

The unitary time evolution operator U_t is given by

$$U_t = \exp [iH_{swap}t] = \cos(t)I + i \sin(t)H_{swap}$$

This can be seen using the operator exponential (2.2) and $H_{swap}^2 = I$.

Putting this into (2.10) we get.

$$\begin{aligned} \rho &= \text{tr}_E [\exp[-iH_{swap}t](\rho \otimes \omega) \exp[iH_{swap}t]] \\ &= \text{tr}_E [\cos t I - i \sin t H_{swap}(\rho_S \otimes \omega)(\cos t I + i \sin t H_{swap})] \\ &= \text{tr}_E [\cos^2 t(\rho \otimes \omega) + \sin^2 t H_{swap}(\rho \otimes \omega) H_{swap} \\ &\quad \underbrace{-i \sin t \cos t H_{swap}(\rho \otimes \omega) + i \sin t \cos t(\rho \otimes \omega) H_{swap}}_{=0}] \\ &= \text{tr}_E [\cos^2 t(\rho \otimes \omega) + \sin^2 t H_{swap}(\rho \otimes \omega) H_{swap}] \end{aligned}$$

We can see in this equation that the system performs an oscillation between it's initial state and the environment state. If we now choose the environment to be in state $\omega = \frac{1}{2}\mathbb{1}$ and we switch off the interaction at $t = \frac{\pi}{2}$ this leads to

$$\rho = \text{tr}_E \left[H_{swap}(\rho \otimes \frac{1}{2}\mathbb{1}) H_{swap} \right] = \frac{1}{2}\mathbb{1} \quad (2.11)$$

This means that independent of the initial state the final state of the system will be the maximum mixed state $\rho_S = \frac{1}{2}\mathbb{1}$. This transformation is obviously not unitary because pure states are transformed into complete mixtures.

2.3.2 INTRODUCTION TO QUANTUM CHANNELS

Let $\rho \in \mathcal{S}(\mathcal{H}_S)$ be the density operator of the open system, $\omega \in \mathcal{S}(\mathcal{H}_E)$ be the density operator of the environment and $U_t \in \mathcal{L}(\mathcal{H})$ the time evolution operator.

2.3 Evolution of open systems

We have seen in section 2.3.1 that the open system transforms in time according to

$$\rho(t) = \text{tr}_E \left[U_t \rho(t_0) U_t^\dagger \right] \quad (2.12)$$

As seen in the Swapgate example this transformation is not unitary in general. In this section these sorts of transformations will be treated more rigorously, for a general unitary transformation $U \in \mathcal{L}(\mathcal{H}_S \otimes \mathcal{H}_E)$. A general transformation is visualized in the left diagram of figure 2.1. It describes a unitary interaction between system and environment, changing the state of the system ρ as well as the state of the environment ω . Assume we perform such a transformation, then we are most of the time not interested what happens in the environment but we want to know how the state of the system changes. Thus, mathematically speaking, we are looking for a transformation \mathcal{E} which transforms ρ to its final state ρ' . This transformation \mathcal{E} is called a *channel*. This nomenclature can be



Figure 2.1: Unitary evolution of $\mathcal{H}_S \otimes \mathcal{H}_E$ (left), non-unitary quantum channel $\mathcal{H}_S \rightarrow \mathcal{H}'_S$ (right)

motivated by the following picture:

We send a prepared qubit from point A to point B, for example an electron through a conducting wire, and we can only measure its state at point A and point B. In classical communications the transmission medium, in this case the wire, is called a channel. In our case the electron's state is given by a density operator ρ and the channel \mathcal{E} describes the changes of the state while it was being transmitted through the wire. For example the electron might collide with the lattice or other electrons which might lead to a change (error) in its state. The example of a noisy channel can be seen in example 2.3.5, but to understand it we first need to gain a mathematical understanding of channels.

2.3.3 MATHEMATICAL PROPERTIES OF CHANNELS

As we have seen a channel \mathcal{E} is a transformation between two quantum states. This means it is a map

$$\begin{aligned}\mathcal{E} &: \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H}') \\ \mathcal{E} &: \rho \rightarrow \rho'\end{aligned}\tag{2.13}$$

To discuss the properties of the following definitions are needed.

Definition 2.5. A map $\mathcal{E} : \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H}')$ is called positive if it maps positive operators to positive operators.

Definition 2.6. A map \mathcal{E} is called completely positive if $I_B \otimes \mathcal{E} : \mathcal{S}(\mathcal{H}_B \otimes \mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H}_B \otimes \mathcal{H}')$ is positive for all possible extensions \mathcal{H}_B of \mathcal{H} .

Definition 2.7. A mapping $\mathcal{E} : \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H}')$ is called trace preserving if $\text{tr}[\rho] = \text{tr}[\mathcal{E}(\rho)] = \text{tr}[\rho']$

Since density operators are positive operators, we need a mapping between two density operators to be positive. In physical systems, channels are always surrounded by an environment, thus we not only want to require positivity, but complete positivity. An example of a map which is positive but not completely positive is the partial transpose, which can be seen at the bottom of this page. Since density operators have unit trace the following equation must hold $\text{tr}[\rho] = \text{tr}[\mathcal{E}(\rho)] = 1$. To ensure this we require every channel to be trace preserving. The last requirement we want to make is linearity, this is because we want to preserve the indistinguishability of convex decompositions. Meaning, that if we have two convex decompositions we want to them to evolve into the same density operator.

$$\begin{aligned}\rho &= \lambda\rho_1 + (\lambda - 1)\rho_2 = \mu\rho'_1 + (\mu - 1)\rho'_2 && (\lambda, \mu \in [0, 1]) \\ \mathcal{E}(\rho) &= \lambda\mathcal{E}(\rho_1) + (\lambda - 1)\mathcal{E}(\rho_2) = \mu\mathcal{E}(\rho'_1) + (\mu - 1)\mathcal{E}(\rho'_2)\end{aligned}$$

A map with these three properties is called a channel.

Definition 2.8. A mapping $\mathcal{E} : \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H}')$ is called a channel, if \mathcal{E} is trace preserving, completely positive and linear.

The following example will show why we positivity is not sufficient.

2.3 Evolution of open systems

EXAMPLE: PARTIAL TRANSPOSE We take the map: $\mathcal{E} : \rho \rightarrow \rho^T$. It is obviously trace preserving, positive and linear. But it is not completely positive. For example we take a two qubit System in the state $|\psi\rangle = \frac{1}{\sqrt{2}}[|00\rangle + |11\rangle]$

The density matrix is given by $\omega = \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 11|)$

Or in matrix form:

$$\omega = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

Now we use the partial transpose $(I \otimes \mathcal{E})(\omega)$ This gives us

$$\omega^\Gamma = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

ω^Γ has the eigenvalues $\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\}$, which means it is not positive and thus no valid density operator. This means that $\rho \rightarrow \rho^T$ is not extendible to open systems and thus it is no channel.

2.3.4 STINESPRING DILATION THEOREM

Let us now make an important link back to the equation of an open system in (2.12). We could of course prove directly that this map is trace preserving, linear and completely positive (which it is), but we want to use a more abstract formulation by Stinespring which will have some useful consequences.

Stinespring dilation theorem. For every channel (i.e. completely positive, trace preserving map) $\mathcal{E} : \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H}')$ there exists a Hilbert space \mathcal{H}_E , a pure state ξ and a unitary operator $U : \mathcal{H} \otimes \mathcal{H}_E \rightarrow \mathcal{H}' \otimes \mathcal{H}'_E$ such that

$$\mathcal{E}(\rho) = \text{tr}_E [U(\rho \otimes \xi)U^\dagger] \quad \forall \rho \in \mathcal{S}(\mathcal{H}) \quad (2.14)$$

We call a triplet (\mathcal{H}_E, U, ξ) a dilation.

Proof. Stinespring's actual theorem goes much further than the version used here, for a nice version of the proof I recommend to read [4] p. 201-202. \square

A visualization of a Stinespring dilation can be seen in figure 2.2, in which we found a combination of an auxiliary Hilbert space with an initial pure state ξ and a unitary transformation U to describe the behaviour of the quantum channel \mathcal{E} .

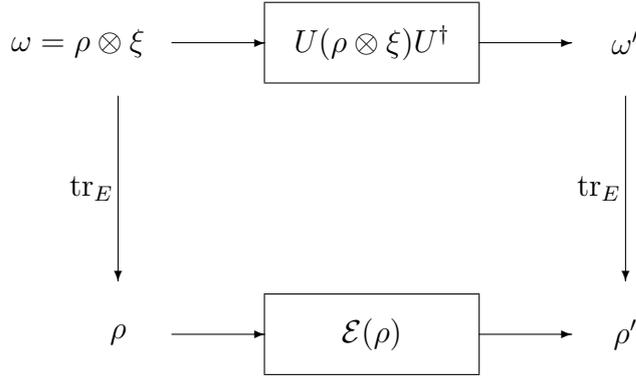


Figure 2.2: Diagram of a quantum channel \mathcal{E} of the System ρ with unitary operator U and environment state ξ

Such dilations are not unique, in fact there are multiple possible dilations for each channel. By allowing us to describe a channel by finding unitary transformations of state vectors of the system and a arbitrarily chosen environment, Stinespring Dilations are very to describe channels, because in most cases such unitary transformations are much easier to find than the expression for \mathcal{E} .

2.3.5 OPERATOR-SUM REPRESENTATION

A direct consequence of the Stinespring Dilation theorem is that each channel \mathcal{E} can be expressed using a countable set of bounded operators $\{A_\mu\}_\mu$. This is called the *Kraus representation theorem*. The operators A_μ are called the *Kraus operators*.

Kraus representation theorem. A mapping $\mathcal{E} : \mathcal{S}(\mathcal{H}) \rightarrow \mathcal{S}(\mathcal{H}')$ is a channel if and only if there exist countable set of bounded operators A_μ such that

$$\mathcal{E}(\rho) = \sum_{\mu} A_{\mu} \rho A_{\mu}^{\dagger} \quad (2.15)$$

and

$$\sum_{\mu} A_{\mu}^{\dagger} A_{\mu} = I$$

Proof. To proof this we assume we found a dilation (\mathcal{H}_E, U, ξ) for our channel, where $\xi = |0\rangle_E \langle 0| \in \mathcal{S}(\mathcal{H}_E)$ is the pure state of the environment and $U : \mathcal{H}_S \otimes \mathcal{H}_E \rightarrow \mathcal{H}'_S \otimes \mathcal{H}'_E$ is a unitary operator. The channel of the subsystem is found by tracing out the environment.

$$\rho' = \mathcal{E}(\rho) = \text{tr}_E [U(\rho_S \otimes \xi)U^{\dagger}]$$

2.3 Evolution of open systems

Now we rewrite the equation

$$\begin{aligned}
\text{tr}_E [U(\rho_S \otimes \xi)U^\dagger] &= \text{tr}_E [U(\rho_S \otimes |0\rangle_E \langle 0|)U^\dagger] \\
&= \sum_{\mu} \langle \mu | U(\rho_S \otimes |0\rangle_E \langle 0|)U^\dagger | \mu \rangle_E \\
&= \sum_{\mu} \langle \mu | U \left(\sum_i |\psi_i\rangle_S \langle \psi_i| \otimes |0\rangle_E \langle 0| \right) U^\dagger | \mu \rangle_E \\
&= \sum_{\mu} \langle \mu | U | 0 \rangle_E \left(\sum_i |\psi_i\rangle_S \langle \psi_i| \right) \langle 0 | U^\dagger | \mu \rangle_E \\
&= \sum_{\mu} \underbrace{\langle \mu | U | 0 \rangle_E}_{A_{\mu}} \rho_S \underbrace{\langle 0 | U^\dagger | \mu \rangle_E}_{A_{\mu}^\dagger} = \sum_{\mu} A_{\mu} \rho_S A_{\mu}^\dagger
\end{aligned}$$

To prove that $\sum_{\mu} A_{\mu}^\dagger A_{\mu} = I$ we start by defining the unitary operation.

$$\begin{aligned}
U : \mathcal{H} \otimes \mathcal{H}_E &\rightarrow \mathcal{H}' \otimes \mathcal{H}'_E \\
U : |\psi\rangle \otimes |0\rangle &\rightarrow |\Psi\rangle
\end{aligned}$$

where $|\psi\rangle \otimes |0\rangle \in \mathcal{H} \otimes \mathcal{H}_E$ is a orthonormal basis vector, and $|\Psi\rangle \in \mathcal{H}' \otimes \mathcal{H}'_E$

$$|\Psi\rangle = U |\psi\rangle \otimes |0\rangle = \sum_{\mu} A_{\mu} |\psi\rangle_S \otimes |\mu\rangle_E$$

Since U is unitary, we have that

$$\langle \Psi | \Psi \rangle = \langle 0 | \otimes \langle \psi | U^\dagger U | \psi \rangle \otimes | 0 \rangle = \langle \psi | \psi \rangle \langle 0 | 0 \rangle = 1$$

Using the Kraus operators we get

$$\begin{aligned}
\langle \Psi | \Psi \rangle &= \sum_{\mu} \langle \mu |_E \otimes \langle \psi |_S A_{\mu}^\dagger A_{\mu} | \psi \rangle_S \otimes | \mu \rangle_E \\
&= \sum_{\mu} \langle \psi | A_{\mu}^\dagger A_{\mu} | \psi \rangle_S \underbrace{\langle \mu | \mu \rangle_E}_{=1} = \sum_{\mu} \langle \psi | A_{\mu}^\dagger A_{\mu} | \psi \rangle_S \\
&= \langle \psi | \sum_{\mu} A_{\mu}^\dagger A_{\mu} | \psi \rangle = 1 \quad \forall |\psi\rangle \in \mathcal{H} \\
&\implies \sum_{\mu} A_{\mu}^\dagger A_{\mu} = I
\end{aligned}$$

□

A consequence of the non-uniqueness of dilations is that multiple dilations lead to multiple sets of Kraus operators: This means that there are multiple sets of

Kraus operators for each channel. More specific, each dilation leads its own set of operators as can be seen easily in the proof of the *Kraus representation theorem*. However, different sets of Kraus operators are not independent. Two sets of operators which define the same channel are connected by a *partial isometry*.

Definition 2.9. A map $\phi : \mathcal{L}_A(\mathcal{H}) \rightarrow \mathcal{L}_B(\mathcal{H})$ where $\mathcal{L}_A(\mathcal{H}), \mathcal{L}_B(\mathcal{H}) \subset \mathcal{L}(\mathcal{H})$ is called a partial isometry if

$$\phi \circ \phi^\dagger \circ \phi = \phi$$

Corollary. If two sets of Kraus Operators $\mathcal{L}_A(\mathcal{H}), \mathcal{L}_B(\mathcal{H}) \subset \mathcal{L}(\mathcal{H})$ define the same channel

$$\sum_j A_j \rho A_j^\dagger = \sum_k B_k \rho B_k^\dagger \quad A_j \in \mathcal{L}_A(\mathcal{H}), B_k \in \mathcal{L}_B(\mathcal{H}) \quad (2.16)$$

then

$$A_j = \sum_k B_k T_{jk}$$

And $\sum_k T_{jk}$ is a partial isometry, i.e. $\sum_j T_{jk} T_{jk}^\dagger = I$

Proof. First we have to prove, that partial isometry is equivalent to $\sum_j T_{jk} T_{jk}^\dagger = I$.

We define

$$\phi(B_1, \dots, B_n) := (\phi_1(B_1, \dots, B_n), \dots, \phi_m(B_1, \dots, B_n))$$

with

$$\phi_j(B_1, \dots, B_n) := \sum_k B_k T_{jk} \text{ and } \phi_k^\dagger(A_1, \dots, A_m) = \sum_j A_j T_{jk}^\dagger$$

where $n = \dim(\mathcal{L}_A(\mathcal{H}))$ and $m = \dim(\mathcal{L}_B(\mathcal{H}))$.

If ϕ is a partial isometry the following equation must hold

$$\phi \circ \phi^\dagger \circ \phi(B_1, \dots, B_n) = \phi(B_1, \dots, B_n)$$

Thus putting in the definition of ϕ we get for the j' -th component.

$$\begin{aligned} (\phi \circ \phi^\dagger \circ \phi(B_1, \dots, B_n))_{j'} &= \sum_{k'} \left(\sum_j \left(\sum_k B_k T_{jk} \right) T_{jk'}^\dagger \right) T_{j'k'} \\ &= \sum_{k'} \sum_k (B_k \underbrace{\sum_j T_{jk} T_{jk'}^\dagger}_{=\delta_{kk'}}) T_{j'k'} \\ &\stackrel{!}{=} \sum_{k'} B_{k'} T_{j'k'} = \phi(B_1, \dots, B_n)_{j'} \end{aligned}$$

2.3 Evolution of open systems

This proves that $\sum_j T_{jk} T_{j'k'}^\dagger = I$ and we will use this to prove the corollary.

$$\sum_j A_j \rho A_j^\dagger = \sum_j \sum_{k,k'} B_k T_{jk} \rho T_{j'k'}^\dagger B_{k'}^\dagger = \sum_j \sum_{k,k'} B_k T_{jk} T_{j'k'}^\dagger \rho B_{k'}^\dagger$$

This means that from (2.16) we follow that

$$\begin{aligned} \sum_{k,k'} B_k \underbrace{\sum_j T_{jk} T_{j'k'}^\dagger}_{=\delta_{kk'} I} \rho B_{k'}^\dagger &\stackrel{!}{=} \sum_k B_k \rho B_k^\dagger \\ \iff \sum_j T_{jk} T_{j'k}^\dagger &= I \end{aligned}$$

Thus, $\sum_k T_{jk}$ is a partial isometry. \square

To see the principle of dilations and Kraus operators we look at the following example.

EXAMPLE: DEPOLARIZING CHANNEL. In this example we send a qubit with initial state $|\psi\rangle$ through a channel. The channel is very noisy and with a high possibility the qubit's state will be changed when it comes out of the channel. If this happened we say that a error occurred.

The possible states of the qubit after it went through the channel are $|\psi\rangle$ (no error occurred), $\sigma_1 |\psi\rangle$ (bit flip), $\sigma_2 |\psi\rangle$ (phase flip), $\sigma_3 |\psi\rangle$ (phase flip & bit flip), where σ_i are the Pauli matrices and describe rotations in spin space. Each of these cases occurs with probability of 25 %.

We now want to find the channel $\mathcal{E}(\rho)$ which describes the transformation of a arbitrary qubit state ρ .

The dilation we choose is the combination (\mathcal{H}_E, U, ξ) where U is the transformation we see below, the pure state ξ is given by $|0\rangle\langle 0|_E$ and \mathcal{H}_E is a four dimensional Hilbert space with orthonormal basis $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$

The unitary transformation is given by

$$U : |\psi\rangle_S \otimes |0\rangle_E \rightarrow \frac{1}{2} |\psi\rangle_S \otimes |0\rangle_E + \frac{1}{2} [\sigma_3 |\psi\rangle_S \otimes |1\rangle_E + \sigma_2 |\psi\rangle_S \otimes |2\rangle_E + \sigma_3 |\psi\rangle_S \otimes |3\rangle_E]$$

With $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = 1$ it can easily be checked that this transformation is in fact unitary.

The Kraus operators are found with in the following way

$$A_\mu = \langle \mu | U | 0 \rangle_E$$

and we get a set of Kraus operators

$$A_0 = \frac{1}{2}I; \quad A_1 = \frac{1}{2}\sigma_1; \quad A_2 = \frac{1}{2}\sigma_2; \quad A_3 = \frac{1}{2}\sigma_1$$

With the identity $\sigma_i^\dagger \sigma_i = \sigma_i^2 = 1$, it is easy to see that $\sum_{\mu} A_{\mu}^{\dagger} A_{\mu} = 1$

The channel \mathcal{E} can now be found using the equation from Kraus representation theorem.

$$\mathcal{E}(\rho) = \sum_{\mu} A_{\mu} \rho A_{\mu}^{\dagger} = \frac{1}{4} (\rho + \sigma_1 \rho \sigma_1 + \sigma_2 \rho \sigma_2 + \sigma_3 \rho \sigma_3) = \frac{1}{2} \mathbb{1}$$

Thus, each state is transformed into the maximum mixed state. This is the same result we get from the swap gate we constructed in section 2.3.5. This means that we found two different dilations which describe the same channel. This is an example that shows that dilations are in fact not unique, and that different dilations lead to a different Kraus representations. This example also shows that open systems can lead to decoherence of quantum objects, because any superposition of spin states will be broken when the qubit leaves the channel and the qubit will be in either one of the states, $|\downarrow\rangle$ or $|\uparrow\rangle$.

2.4 SUMMARY

The density matrix formalism is the most complete description of a quantum system, it generalizes the state vector formalism described by Schrödinger equation. Using the knowledge from Schrödinger equation we derived the time evolution of density matrices. We found that density matrices of isolated evolve under unitary evolution and that the time dynamics are given by the Liouville von Neumann equation. The discussion of open systems, thus systems interacting with a environment, lead us to the concept of quantum channels. An overview of this can be seen in the following table.

As we have seen in isolated systems the state transformation behaves unitary.

	state vectors	isolated systems	open systems
State transformation	unitary U	unitary maps σ_U	channels \mathcal{E}
Dynamics	Schrödinger eq.	L. von Neumann	(master eq.)

This means that the evolution is reversible. For open systems we have seen that it is possible that a pure state is mapped onto a mixed state. This non-unitary behaviour is non-reversible.

2.4 Summary

However, this non-reversibility can lead to interesting effects like decoherence like we have seen in the example of the depolarizing channel.

All in all the density operator formalism and its time evolution provides a number of interesting concepts, which will be discussed further in the course of this proseminar.

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CHAPTER 3

QUANTUM MARGINAL PROBLEM: SPECIFIC RESULTS

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Quantum marginal problems deal with the existence of a joint multipartite state from a given set of reduced states. As an example, we show that in a three-qubit system, the pure states are uniquely determined by its bipartite margins. We furthermore discuss the “polygon inequalities” that determine whether a collection of single-qubit states are compatible with a joint pure n -qubit state.

3.1 INTRODUCTION

Given a set of density operators, can these be regarded as margins of a state on a larger joint system? Or conversely, if we are given a composite system, what form would its reduced density operators have?

Quantum marginal problems examine the condition of existence of a joint state arising from a given set of density operators, or alternatively try to determine the form of the reduced density operators from a given joint multipartite state. Contrary to probability theory, the margins of a pure state in the quantum world are not always pure, and this can render the problem nontrivial.

In this chapter, we shall first consider briefly the definition of a margin and the difference between a classical margin and a quantum margin, as well as the notion of entanglement. We will then have a look at some of the quantum marginal problems, namely the Schmidt decomposition and the three-qubit-system case

3.2 Some Definitions and Notions

with the two-particle margins of which we are going to see the proof-sketch, and finally, the n-qubit-system case with the one-particle margins which will make us acquainted with the polygon inequalities.

3.2 SOME DEFINITIONS AND NOTIONS

3.2.1 MARGIN

Let us consider a bipartite system composed by two Hilbert spaces, i.e. $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. Given two linear operator bases $\{L_A^i\}$, $\{L_B^j\}$ in \mathcal{H}_A , \mathcal{H}_B respectively, the density operator of the bipartite system can be expressed in the operator-basis $L_A^i \otimes L_B^j$:

$$\rho_{AB} = \sum_{i,j} c_{ij} L_A^i \otimes L_B^j. \quad (3.1)$$

The margin A of the composite system AB is defined to be the reduced density operator ρ_A that is defined as:

$$\rho_A := \sum_{i,j} c_{ij} L_B^j \text{Tr}(L_A^i) =: \text{tr}_B(\rho_{AB}), \quad (3.2)$$

where we trace out the system in which we are not interested. Similarly, the margin B is defined as:

$$\rho_B := \sum_{i,j} c_{ij} \text{Tr}(L_A^i) L_B^j =: \text{tr}_A(\rho_{AB}). \quad (3.3)$$

We can extend these definitions to an n -party state and its m -party reduced states ($m < n$). Let this n -party state be in the Hilbert space $\mathcal{H} = \bigotimes_{i \in I} \mathcal{H}_i = \mathcal{H}_J \otimes \mathcal{H}_{\bar{J}}$, where $I = \{1, 2, \dots, n\}$ is an index set with a subset J and its complement set \bar{J} ($J \subset I$, $\bar{J} = I \setminus J$). Then margin ρ_J is simply the reduced density operator ρ_J :

$$\rho_J = \text{tr}_{\bar{J}}(\rho_I). \quad (3.4)$$

3.2.2 CLASSICAL MARGIN VS QUANTUM MARGIN

This concept of margin exists also in probability theory if we consider the probability distribution as a “state” [1]. In other words, for a given probability density $p_I(x_I) := p(x_1, x_2, \dots, x_n)$ in \mathbb{R}^I , the margin p_J is given by

$$p_J(x_J) = \int_{\mathbb{R}^{\bar{J}}} p_I(x_I) dx_{\bar{J}}. \quad (3.5)$$

As we can see, the analogy between the definition of a classical margin and that of a quantum margin is obvious in the sense that one considers only the wanted subsystem from the whole system.

In the classical case, a pure state corresponds to the perfect knowledge of the variables, i.e. every probability is either 0 or 1 [2]. Furthermore, this deterministic character is preserved also in its one-variable margins: the one-variable marginal distributions of a pure joint distribution are also pure. This implies that this assertion is a two-way statement, namely that a multi-variable state is pure **if and only if** its univariant (\equiv one-party) margins are pure.

But in the quantum case, this statement does not hold anymore. A set of pure univariant margins gives arise to a pure joint multipartite state, but **the univariant margins of a given pure multipartite state are not always pure**. The following example illustrates this result. Let us consider the Bell state $|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$ composed of two qubits (labelled A and B). The density operator $\rho = |\Phi^+\rangle\langle\Phi^+|$ of this Bell state is clearly a pure state. But computing the reduced density operator ρ_A , we can observe that it is a mixed state:

$$\rho_A = \text{tr}_B(\rho) \tag{3.6}$$

$$= \text{tr}_B \left(\left(\frac{|00\rangle + |11\rangle}{\sqrt{2}} \right) \left(\frac{\langle 00| + \langle 11|}{\sqrt{2}} \right) \right) \tag{3.7}$$

$$= \frac{\text{tr}_B(|00\rangle\langle 00|) + \text{tr}_B(|11\rangle\langle 00|) + \text{tr}_B(|00\rangle\langle 11|) + \text{tr}_B(|11\rangle\langle 11|)}{2} \tag{3.8}$$

$$= \frac{|0\rangle\langle 0| \langle 0|0\rangle + |1\rangle\langle 0| \langle 1|0\rangle + |0\rangle\langle 1| \langle 0|1\rangle + |1\rangle\langle 1| \langle 1|1\rangle}{2} \tag{3.9}$$

$$= \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2}. \tag{3.10}$$

We can check that it is indeed a mixed state by computing $\text{tr}(\rho_A^2)$ and verifying that it is smaller than 1: $\text{tr}(\rho_A^2) = \frac{1}{2} < 1$.

3.2.3 SEPARABILITY AND ENTANGLEMENT

SEPARABILITY OF A PURE STATE

Given a pure state $|\psi\rangle$ of a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$ with the orthonormal basis of each system $|a_i\rangle$ and $|b_i\rangle$, we can expand $|\psi\rangle$ in the following general way:

$$|\psi\rangle = \sum_{i,j} c_{ij} |a_i\rangle \otimes |b_j\rangle, \tag{3.11}$$

3.3 Quantum Marginal Problems

where $c_{ij} \in \mathbb{C}$ are coefficients. If $c_{ij} = c_i^A \times c_j^B$, then $|\psi\rangle$ can be written as a tensor product of two pure states:

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \quad (3.12)$$

This is what we call a **product state**.

This definition can be extended to a multicomponent system. A pure state of a n-party system is in a product state if and only if:

$$|\psi\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle. \quad (3.13)$$

SEPARABILITY OF A MIXED STATE

For a mixed state ρ_{AB} in a bipartite system $\mathcal{H}_A \otimes \mathcal{H}_B$, the general expansion is the equation (3.1). If this can be rewritten as

$$\rho_{AB} = \sum_k p_k \rho_A^k \otimes \rho_B^k, \quad (3.14)$$

with ρ_A^k and ρ_B^k being mixed states of the respective subsystems and $\sum_k p_k = 1$, then ρ_{AB} is called a **separable state**. If ρ_{AB} cannot be written in this form (3.14), then it is an **entangled state**.

The particular case of a separable state

$$\rho_{AB} = \rho_A \otimes \rho_B \quad (3.15)$$

is called a **product state**. It is worth mentioning here that in a pure state case, a state is in a product state if and only if it is separable.

In a n-party multicomponent system, a mixed state is **fully separable** if and only if

$$\rho_{AB} = \sum_k p_k \rho_1^k \otimes \cdots \otimes \rho_n^k \quad (3.16)$$

with ρ_A^k and ρ_B^k being mixed states of the respective subsystems and $\sum_k p_k = 1$.

3.3 QUANTUM MARGINAL PROBLEMS

With the definitions and concepts we encountered in the previous section, we can now start looking at three particularly interesting quantum marginal problems and at its results.

3.3.1 THE SCHMIDT DECOMPOSITION

STATEMENT

Probably one of the most famous results of the quantum marginal problems, the Schmidt decomposition, demonstrates how tightly the two univariant margins of a bipartite system are related.

Assume that we are given a pure state $|\psi\rangle$ in a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$, with $\dim\mathcal{H}_A = n$, $\dim\mathcal{H}_B = m$, and $n > m$ without loss of generality. Then it follows that

\exists orthonormal set $\{|u_1\rangle, \dots, |u_n\rangle\}$ for system A and $\{|v_1\rangle, \dots, |v_m\rangle\}$ for system B such that

$$\boxed{|\psi\rangle = \sum_i^m \lambda_i |u_i\rangle \otimes |v_i\rangle} \quad (3.17)$$

with $\lambda_i \geq 0$ and $\sum_i \lambda_i^2 = 1$.

This is the so-called **Schmidt decomposition**. One can observe that it is not a trivial decomposition, since the general decomposition in the composite basis contains every possible combination of basis elements $|u_i\rangle$ and $|v_j\rangle$ ($1 \leq i \leq n$ and $1 \leq j \leq m$). It follows straightforwardly from equation (3.17) that the reduced density operators ρ_A and ρ_B are isospectral, i.e. they have the same non-zero eigenvalues:

$$\rho_A = \sum_{i=1}^m \lambda_i^2 |u_i\rangle\langle u_i| \quad (3.18a)$$

$$\rho_B = \sum_{i=1}^m \lambda_i^2 |v_i\rangle\langle v_i|. \quad (3.18b)$$

PROOF-SKETCH

The proof of the Schmidt decomposition can be more or less easily done with the so-called **singular value decomposition** [3].

For simplicity, let us consider the case where the dimension of the Hilbert space is the same for both systems, i.e. $n = m$. Then the singular value decomposition states that a square matrix A can be decomposed to $A = U D V$ where U, V , are unitary matrices and where D is a diagonal matrix with non-negative entries.

3.3 Quantum Marginal Problems

Let us now write $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ in the orthonormal basis $|j\rangle$ of the system A and in the orthonormal basis $|k\rangle$ of the system B:

$$|\psi\rangle = \sum_{j,k} a_{jk} |j\rangle |k\rangle.$$

Since the coefficients a_{jk} can be written in a matrix, we can apply the singular value decomposition, and we obtain:

$$\begin{aligned} |\psi\rangle &= \sum_{j,k} a_{jk} |j\rangle |k\rangle \\ &= \sum_{l,j,k} u_{jl} d_l v_{lk} |j\rangle |k\rangle. \end{aligned}$$

Defining two new states and a value, $|l_A\rangle := \sum_j u_{jl} |j\rangle$, $|l_B\rangle := \sum_k v_{lk} |k\rangle$, $\lambda_l := d_l$, we have:

$$\begin{aligned} |\psi\rangle &= \sum_{l,j,k} u_{jl} d_l v_{lk} |j\rangle |k\rangle \\ &= \sum_l \lambda_l |l_A\rangle |l_B\rangle. \end{aligned} \tag{3.19}$$

The last equation (3.19) is precisely the statement of the Schmidt decomposition, equation (3.17).

We can also use a similar proof for the case $n \neq m$: the matrix A in the singular value decomposition $A = U D V$ would be then a $m \times n$ matrix, D an $m \times n$ diagonal rectangular matrix, $U \in \mathcal{U}^{n \times n}$, and $V \in \mathcal{U}^{m \times m}$ where \mathcal{U} is the set of unitary matrices.

□

3.3.2 THE PURE THREE-QUBIT STATE AND ITS TWO-PARTICLE MARGINS

In this subsection, we consider pure three-qubit states and their bivariant (\equiv two-party) marginal states, which is the subject of the publication [4].

For almost every pure three-qubit state, say ρ_{ABC} , it turns out that its two-party marginal states ρ_{AB} , ρ_{BC} , ρ_{AC} do not contain more information than ρ_{ABC} (see “mutual information” in the chapter written by Felix Bischof). In other words,

almost every pure three-qubit state can be completely determined by its bivariant margins.

In what follows we shall prove this assertion. However, let us first point out that simple consistency conditions may not be enough to guarantee that a collection of density operators are compatible with a global state.

NECESSARY CONDITIONS

Not every arbitrary set of density operators can be margins of a global joint state. For instance, it is necessary for the reduced density operators to obey the consistency conditions:

$$\mathrm{Tr}_Q(\rho_{P \cup Q}) = \mathrm{Tr}_R(\rho_{P \cup R}), \quad (3.20)$$

where P , Q , R are any subsets such that P and Q are disjoint, and P and R are disjoint.

For instance, the univariant reduced density operator ρ_A arising from the bipartite reduced density operator ρ_{AB} has to be the same as the ρ_A arising from ρ_{AC} .

However, this condition is not a sufficient condition: one must verify that the set of states satisfying this consistency condition really corresponds to a legitimate three-party state. Consider the following two-qubit states ρ_{AB} , ρ_{BC} , and ρ_{AC} defined in the following way:

$$\begin{aligned} \rho_{AB} = \rho_{BC} = \rho_{AC} &= |\alpha\rangle\langle\alpha| \quad \text{with} \\ |\alpha\rangle &= \frac{1}{\sqrt{2}} (|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle), \end{aligned} \quad (3.21)$$

i.e. the pairs are all singlets. The one-particle reduced states of these two-qubit states satisfy the consistency condition above, equation (3.20). But these states cannot give rise to a legitimate three-party state, since one system cannot be maximally entangled with two other systems simultaneously [4].

PURE STATES OF THE THREE-QUBIT SYSTEMS

One important ingredient of the proof is that all pure states of a three-qubit system are equivalent under local unitary transformations to the following family of states :

$$|\eta\rangle = a|000\rangle + b|001\rangle + c|010\rangle + d|100\rangle + e|111\rangle, \quad (3.22)$$

each digit within the kets referring to qubit A, B, and C [5], [6].

3.3 Quantum Marginal Problems

IDEA OF THE PROOF

In order to prove that almost every pure three-qubit state can be uniquely determined by its bipartite margins, we show that the above state $|\eta\rangle$, equation (3.22), is the only state consistent with its bivariant reduced states, except when $b = c = d = 0$. The first step is to define a new three-qubit density operator ω whose two-party margins are the same as those of the state $|\eta\rangle$, which can be a priori pure or mixed (i.e. ω is a general three-qubit density operator). If we show that this ω must be in the form η using the arguments of the subsection 3.3.2 (page 39), we therefore show that $|\eta\rangle$ is indeed the only state - whether pure or mixed - consistent with its two-party reduced states.

Purifying ω with an environment that we call E , we obtain a pure state $|\psi\rangle$ on a larger system (A,B,C, and E), and

$$\omega = \text{tr}_E |\psi\rangle \langle \psi|. \quad (3.23)$$

Since ω must have the same two-party reduced states as $|\eta\rangle$, we first get one constraint on the form of $|\psi\rangle$ from the reduced state ρ_{AB} of $|\eta\rangle$, equation (3.22) :

$$\rho_{AB} = |\phi_0\rangle \langle \phi_0| + |\phi_1\rangle \langle \phi_1|, \quad (3.24)$$

where

$$|\phi_0\rangle = a|00\rangle + c|01\rangle + d|10\rangle \quad (3.25)$$

$$|\phi_1\rangle = b|00\rangle + e|11\rangle. \quad (3.26)$$

With this constraint from ρ_{AB} of $|\eta\rangle$, $|\psi\rangle$ must then have the form

$$|\psi\rangle = |\phi_0\rangle |E_0\rangle + |\phi_1\rangle |E_1\rangle, \quad (3.27)$$

where $|\phi_0\rangle, |\phi_1\rangle$ are in the Hilbert space corresponding to the qubit A and B, and $|E_0\rangle, |E_1\rangle$ are in the Hilbert space of qubit C and the environment E. Here, we point out that $|E_0\rangle$ and $|E_1\rangle$ are orthonormal.

Expanding $|E_0\rangle, |E_1\rangle$ with the states of C and the states of E in the following way,

$$|E_0\rangle = |0\rangle |e_{00}\rangle + |1\rangle |e_{01}\rangle \quad \text{and} \quad |E_1\rangle = |0\rangle |e_{10}\rangle + |1\rangle |e_{11}\rangle, \quad (3.28)$$

we can rewrite $|\psi\rangle$:

	$ \eta\rangle$	$ \psi\rangle$
$\langle 11 \rho_{BC} 11\rangle$	$ e ^2$	$ c ^2\langle e_{01} e_{01}\rangle + e ^2\langle e_{11} e_{11}\rangle$
$\langle 11 \rho_{AC} 11\rangle$	$ e ^2$	$ e ^2\langle e_{11} e_{11}\rangle + d ^2\langle e_{01} e_{01}\rangle$
$\langle 01 \rho_{BC} 10\rangle$	bc^*	$bc^*\langle e_{00} e_{11}\rangle$

Table 3.1: Further constraints on the form of $|\psi\rangle$ from the two-particle reduced density operators of $|\eta\rangle$

$$\begin{aligned}
 |\psi\rangle &= (a|00\rangle + c|01\rangle + d|10\rangle)(|0\rangle|e_{00}\rangle + |1\rangle|e_{01}\rangle) \\
 &\quad + (b|00\rangle + e|11\rangle)(|0\rangle|e_{10}\rangle + |1\rangle|e_{11}\rangle).
 \end{aligned} \tag{3.29}$$

We now use other constraints from the other bipartite reduced states of $|\eta\rangle$. In particular, we compute the elements $\langle 11|\rho_{BC}|11\rangle$, $\langle 11|\rho_{AC}|11\rangle$, $\langle 01|\rho_{BC}|10\rangle$ calculated from $|\eta\rangle$ and $|\psi\rangle$, and we require that the results must be the same whether it is from $|\eta\rangle$ or $|\psi\rangle$ (cf. Table 3.1).

Requiring the elements of the first column in Table 3.1 to be equal to the elements of the second column, and using the orthonormality of $|E_0\rangle$ and $|E_1\rangle$, we obtain the following results:

$$\begin{aligned}
 \implies |e_{01}\rangle &= 0 \ \& \ \langle e_{11}|e_{11}\rangle = 1 \\
 \implies |e_{10}\rangle &= 0 \ \& \ \langle e_{00}|e_{00}\rangle = 1, \\
 |e_{00}\rangle &= |e_{11}\rangle,
 \end{aligned}$$

for $b, c, d \neq 0$. Plugging this back into the expansion $|\psi\rangle$, equation (3.29), we obtain

$$|\psi\rangle = (a|000\rangle + b|001\rangle + c|010\rangle + d|100\rangle + e|111\rangle)|e_{00}\rangle \tag{3.30}$$

$$= |\eta\rangle|e_{00}\rangle. \tag{3.31}$$

We can see that this equation (3.31) contains already $|\eta\rangle$. Tracing out the environment E from equation (3.31), it follows that $\omega = |\eta\rangle\langle\eta|$. This leads to the conclusion that $|\eta\rangle$ - which is the generic form of all the pure states - is uniquely determined by its two-particle reduced states, which is the statement we wanted to prove.

3.4 Conclusion

EXCEPTIONS

The above generic property that almost all the pure states of a three-qubit system are completely characterized by its bipartite reduced states, does not apply to pure states that are equivalent to the the following form under local unitary transformations:

$$\alpha|000\rangle + \beta|111\rangle, \quad (3.32)$$

namely, when $b = c = d = 0$ in $|\eta\rangle$. For instance, the two distinct states $\alpha|000\rangle + \beta|111\rangle$ and $\alpha|000\rangle + e^{i\theta}\beta|111\rangle$ have the same two-particle reduced states although they are two different states.

3.3.3 POLYGON INEQUALITIES

Is it possible to find a pure n-qubit state from given n one-qubit reduced states? This non-trivial question was solved in the [2] which shows that the necessary and sufficient condition for the existence of this pure n-qubit state is the so-called **polygon inequalities**.

The polygon inequalities are a set of inequalities

$$\lambda_k \leq \lambda_1 + \cdots + \lambda_{k-1} + \lambda_{k+1} + \cdots + \lambda_n, \quad (3.33)$$

where λ_k is the smaller eigenvalue of the qubit k , i.e. $\lambda_k \leq \frac{1}{2}$. In other words, the smaller eigenvalue of each qubit must be smaller than the sum of the smaller eigenvalues of all the other qubits. These inequalities completely characterize the possible sets of eigenvalues, hence the possible one-particle reduced states of a pure n-qubit state.

3.4 CONCLUSION

A quantum marginal problem, which deals with the existence of a joint multipartite state from a given set of marginal states, is in general a complicated problem. Many considerations have to be taken into account, such as the pureness of the states, the consistency conditions as well as the compatibility of the reduced states with the whole multipartite state. In a three-qubit system, it turns out that almost all pure states of this system can be uniquely determined by its bipartite reduced states. Furthermore, a given set of one-party qubit states can give rise to a pure multipartite state in a larger joint system if and only if their smaller eigenvalues satisfy the polygon inequalities. These cases are only specific

examples of the quantum marginal problem. Many similar problems have been treated in the literature, and many others have yet to be examined.

3.4 Conclusion

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CHAPTER 4

QUANTUM MARGINAL PROBLEM: COMPUTATIONAL COMPLEXITY

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This report introduces the basics of classical and quantum computational complexity. The complexity classes P , NP and QMA are introduced and discussed. Finally the fact that, the quantum marginal problem is a QMA -complete problem, is discussed.

4.1 INTRODUCTION

The classification of problems into different classes of computation complexity is an important field in computer science. But also physicists can learn things from the complexity theory. In this report we want to give a introduction into computational complexity, first for classical computations and then for quantum computing. The aim is then to classify the complexity of the consistency problem, by physicists also known as the quantum marginal problem.

4.2 CLASSICAL COMPUTATIONAL COMPLEXITY

In this first section we introduce the most important definitions for classical computation. This short summary follows chapter 1 and 2 in the book of Kitaev, Shen and Vyalı [1].

There are three reasons why I want to start with classical computation and not directly with quantum computation. First of all classical computation is simpler

4.2 Classical Computational Complexity

to understand. Then there are many analogies between classical and quantum computation and finally we'll need some parts of classical computation to be able work in the field of quantum computation.

To get a measure for the complexity of a given problem, we need a theoretical machine for which we can write a program (algorithm) that solves the problem. For this purpose computational scientists invented the *Turing machine*.

Definition 4.2.1 (Turing machine). A *Turing machine* consist of the following components:

- a finite set S called the *alphabet*;
- a distinguished element $\sqcup \in S$ (blank symbol);
- a subset $A \subset S$, $\sqcup \notin A$, called the *internal alphabet*;
- a finite set Q whose elements are called *states* of the TM;
- an *initial state* $q_0 \in Q$;
- a *transition function*:

$$\delta : Q \times S \rightarrow Q \times S \times \{-1, 0, 1\}. \quad (4.1)$$

A Turing machine needs hardware to work on. This hardware consists of a *tape* which is divided into *cells*. The cells are labeled with integer numbers from zero to infinity, this means that the hardware goes to infinity to the right side (see diagram below). There's also a head that marks the current position the machine is working on.

Position of the head				∇	
Cells	s_0	s_1	\dots	s_p	\dots
Cell number	0	1	\dots	p	\dots

At the beginning the input string of length n (if any) is written in the first n cells, the rest of the cells is filled with the blank symbol \sqcup . The position of the head p is set to 0 and the Turing machine is in the state q_0 .

Once started the Turing machine performs the following procedure:

- it reads the symbol s_p ;
- it computes the transition function $\delta(q, s_p) = (q', s', \Delta p)$;
- it writes the symbol s' into cell p ;

- the head is moved by Δp ;
- the state is set to q' .

The machine repeats this until either the head is out of range ($p \leq -1$) or the transition function is not defined for the present configuration. Once it has stopped, the machine outputs, beginning from the left, the symbols until it reaches a symbol not belonging to A .

Example 4.2.1 (Swap of the first two bits). A simple example for a Turing machine can be given for the function that takes an input string of length $n \geq 2$ and swaps the content of the first two bits. Set $A = \mathbb{B}$ and $S = A \cup \{_ \}$. The transition function is then defined as:

$$\delta(q_0, 0) = (r_0, 0, +1)$$

$$\delta(q_0, 1) = (r_1, 1, +1)$$

$$\delta(r_0, 0) = (l_0, 0, -1)$$

$$\delta(r_0, 1) = (l_1, 0, -1)$$

$$\delta(r_1, 0) = (l_0, 1, -1)$$

$$\delta(r_1, 1) = (l_1, 1, -1)$$

$$\delta(l_0, 0/1) = (q_f, 0, -1)$$

$$\delta(l_1, 0/1) = (q_f, 1, -1).$$

The states q_0, r_0, r_1, l_0, l_1 and q_f are all elements of Q . The machine does the following:

- First we memorize the content of the first cell by setting the state to r_0 or r_1 respectively for $s_0 = 0$ or $s_0 = 1$.
- We move one cell to the right.
- We write the memorized content of the first cell into the second cell and memorize the content of the second cell by setting the state to l_0 or l_1 .
- We move one cell to the left.
- We write the memorized content of cell two into the first cell and move one step to the left.

4.2 Classical Computational Complexity

- Actually it doesn't matter what state we chose (here q_f) in the last step, because the machine stops anyway after this step since it's out of range.

To measure the required “time” for a computation, we can define the *Turing machine time*.

Definition 4.2.2 (Turing machine time). The *Turing machine time* $T(n)$ is the maximal number of steps a Turing machine needs to compute an input of length n .

We'll only focus on a certain kind of problems. We consider problems that have exactly two possible outcomes: “TRUE” and “FALSE”, or “YES” and “NO”. Mathematically those functions are called *predicates*.

Definition 4.2.3 (Predicate). A *predicate* is a function $F : \mathbb{B}^* \rightarrow \mathbb{B}$, where \mathbb{B} denotes the set $\{0, 1\}$. The set A^* is the set of all strings over the alphabet A .

By now we have a general measure for the “time” a function needs to be computed. (Remark: We associate a Turing machine with a function F , if it computes the correct value $F(x)$ for every possible input string x .) The aim is to classify the complexity of a function/problem, so we need a criterion. A possible and intuitive criterion could be the following.

Definition 4.2.4 (Polynomial growth). A function $f(n)$ is of *polynomial growth* if $f(n) \leq cn^d$, for fixed c and d . Notation: $f(n) = \text{poly}(n)$.

So we come to our first complexity class, if we apply this criterion to the Turing machine time.

Definition 4.2.5 (Decidable in polynomial time). A predicate $F : \mathbb{B}^* \rightarrow \mathbb{B}$ is *decidable in polynomial time* if there exists a Turing machine that computes it in time $T(n) = \text{poly}(n)$, where n is the length of the input.

The class of all functions computable in polynomial time is denoted by P .

This class is very famous and all functions in P are also called *efficiently computable*. Some examples for problems in P are addition of two numbers, calculating the greatest common divisor of two integer numbers or the problem of deciding if a number is prime (shown in 2002).

A class of problems that are “harder” to solve is the class NP . This class we'll generalize to quantum computers in the second part.

Definition 4.2.6 (The class NP). A predicate $F : \mathbb{B}^* \rightarrow \mathbb{B}$ belongs to the class NP (non-deterministic polynomial) if there is a (partially defined) function $R \in P$ in two variables such that

$$\begin{aligned} F(x) = 1 & \implies \exists y : (|y| < q(|x|) \text{ and } (R(x, y) = 1)) \\ F(x) = 0 & \implies \forall y : (|y| < q(|x|) \implies (R(x, y) = 0)), \end{aligned}$$

where q is a polynomial and $|x|$ denotes the length of the string x .

Remark 4.2.1. In words, this kind of problem can be described by:

*For a given string x , is there a string y such that $R(x, y) = 1$?
If the answer is “YES” output 1,
if the answer is “NO” output 0.*

The string y is also called *proof*. The idea is that if we have given a proof we can easily verify that the output of F is 1, but it can be arbitrarily complicated how to find such a proof.

Remark 4.2.2. The class is called *non-deterministic polynomial* because an alternative definition uses non-deterministic Turing machines. This is a machine that can produce different outputs for a given input string (i.e. it has different computational paths for one given input string).

An intuitive example for a problem in NP is the SAT-problem.

Problem 1 (SAT-Problem). Given a conditional expression consisting of “AND”, “OR” and “NOT”, is there a vector $\mathbf{x} \in \mathbb{B}^n$ that fulfills the conditional expression?

SAT stands for *satisfiable*.

4.3 QUANTUM COMPUTATIONAL COMPLEXITY

This section gives an introduction to basic quantum computation and introduces one important class of quantum computational complexity. Most definitions are taken from [1].

4.3.1 QUANTUM CIRCUITS

Let $\mathcal{B} = \text{span}_{\mathbb{C}}\{|0\rangle, |1\rangle\}$ be the space of a 1-qubit system (e.g. the spin of an electron: up and down). The two basis vectors $|0\rangle$ and $|1\rangle$ are assumed to be orthogonal. The system of n qubits can be described by $\mathcal{L} = \mathcal{B} \otimes \cdots \otimes \mathcal{B} = \mathcal{B}^{\otimes n}$. Let U be an unitary operator on an r -qubit system $\mathcal{B}^{\otimes r}$. Thus we can write $U = \sum_m X_{m,1} \otimes \cdots \otimes X_{m,r}$, where the $X_{m,t}$ are unitary operators acting on one single qubit. We want to define the operation of U on a larger system $\mathcal{B}^{\otimes n}$ ($n > r$). We label the qubits we want U to operate on with p_i , $i = 1, 2, \dots, r$.

$$U[p_1, \dots, p_r] := \sum_m X_{m,1}[p_1] \cdots X_{m,r}[p_r], \quad (4.2)$$

4.3 Quantum Computational Complexity

with $X_{m,s}[p_s] := I_{\mathcal{B}^{\otimes(p_s-1)}} \otimes X_{m,s} \otimes I_{\mathcal{B}^{\otimes(n-p_s)}}$.

Instead of defining a "Quantum Turing machine" we use the formulation via circuits. A circuit can be imagined as a series of unitary operators which act on a n -qubit system one after the other. Such circuits can be physically realized. The mathematical description is the following:

Definition 4.3.1 (Quantum circuit). Let \mathcal{A} be a fixed set of unitary operators (\mathcal{A} is called *basis* and its elements (*quantum gates*)). A *quantum circuit over the basis \mathcal{A}* is a sequence $U_1[A_1], \dots, U_L[A_L]$, $U_1, \dots, U_L \in \mathcal{A}$. The A_i denote (ordered) sets of qubits.

The *operator realized by the circuit* is $U = U_L[A_L] \cdots U_1[A_1]$. The number L is called the *size* of the circuit.

Remark 4.3.1. Often the quantum circuit itself is denoted by U . So if we talk of a quantum circuit U , we actually mean a quantum circuit that realizes the operator U .

Remark 4.3.2. We're going to use *descriptions* of quantum circuits. This can be seen as a list of the gates the circuit applies in the right order. The list can be encoded (for example in binary code). We can now define a function $Z(x)$ that maps a input string x to a description of a quantum circuit. Remark that for different input strings x and y the descriptions $Z(x)$ and $Z(y)$ can be totally different (even if they have the same length).

This also implies that the dimension of the operator U realized by the quantum circuit depends on the input x .

4.3.2 BASIS FOR QUANTUM CIRCUITS

A problem occurs here. Since there are uncountably many unitary operators there's no finite basis for them that would allow us to produce every unitary operator we can imagine. This is a problem since this won't allow us to build a physical quantum computer (We cannot construct a physical device with infinitely many gates).

Remark 4.3.3. There is an infinite basis consisting only of operators acting on one or two qubits that allows us to realize every unitary operator.

One way to solve the problem above is to allow inexact operators.

Definition 4.3.2 (Approximation of operators). The operator \tilde{U} *approximates the operator U with precision δ* if

$$\| \tilde{U} - U \| \leq \delta, \tag{4.3}$$

with the operator norm

$$\| X \| = \sup_{|\xi\rangle \neq 0} \frac{\| X|\xi\rangle \|}{\| \xi \|}. \quad (4.4)$$

Theorem 4.3.1. *Any unitary operator U on a fixed number of qubits can be realized with precision δ by a $\text{poly}(\log(\frac{1}{\delta}))$ -size quantum circuit over the standard basis (see next definition).*

There is a polynomial Turing machine that constructs this circuit on the description of U .

This theorem is very important and allows us to build physical computer that perform quantum circuits with high precision.

The standard basis mentioned in the theorem is given by:

Definition 4.3.3 (Standard basis). The basis $\mathcal{Q} = \{H, K, K^{-1}, \Lambda(\sigma^x), \Lambda^2(\sigma^x)\}$, where

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad K = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

and

$$\Lambda^k(U)(|x_1, \dots, x_k\rangle \otimes |\xi\rangle) = \begin{cases} |x_1, \dots, x_k\rangle \otimes |\xi\rangle & x_1 \cdots x_k = 0 \\ |x_1, \dots, x_k\rangle \otimes U|\xi\rangle & x_1 \cdots x_k = 1 \end{cases}$$

is called *standard*. (σ^x denotes the first Pauli matrix)

Now let's go back to the computation of classical functions. We want to compute predicates.

A quantum computer is able compute with quantum states. To a quantum circuit we input a vector $|x\rangle$ and it outputs a vector of the same dimension $|F(x), g\rangle$. The g stands for garbage and it's there to match the dimensions of in- and output (the input has dimension n , the output has dimension 1). A simple image of what we want:

$$x \rightarrow |x\rangle \xrightarrow{\text{circuit } U} |F(x), g\rangle \rightarrow F(x)$$

Since we can construct operators only with a certain precision our output can be a superposition of different states. So every time we measure our outcome can be (totally) different. But we saw that the realized operator is near to the wanted operator, so the output will often be correct. We need a criterion for the "quality" of a quantum circuit:

4.3 Quantum Computational Complexity

Definition 4.3.4. A quantum circuit U computes the predicate $F : \mathbb{B}^* \rightarrow \mathbb{B}$ if for any input x we have

$$\sum_g |\langle F(x), g|U|x\rangle|^2 \geq 1 - \epsilon \quad (4.5)$$

for a $\epsilon < \frac{1}{2}$.

In words: The quantum circuit computes the correct result with probability $1 - \epsilon$.

Remark 4.3.4. We sum over all g because we only care what's the content of the first qubit.

Remark 4.3.5. One can repeat this computation k times and then chose the result that occurs the most as the final result. One can then show that the error, that this final result is wrong, is given by $p_{\text{error}} < (2\sqrt{\epsilon(1-\epsilon)})^k$, $2\sqrt{\epsilon(1-\epsilon)} < 1$. This fact is called *amplification of probabilities*.

So if we want $p_{\text{error}} = \exp(-\text{poly}(n))$ it follows that $k = \text{poly}(n)$.

Remark 4.3.6. The definition can be generalized to density matrices the following way:

$$\sum_g |\langle F(x), g|U|x\rangle|^2 \longrightarrow \text{tr} (\Pi^{|F(x)\rangle} U \rho U^\dagger) \quad (4.6)$$

where ρ is the input density matrix and $\Pi^{|F(x)\rangle}$ is the orthogonal projector on the subspace $\mathbb{C}(|F(x)\rangle) \otimes \mathcal{B}^{\otimes(n-1)}$.

4.3.3 THE CLASSES BQP AND QMA

For the completeness I give the definition of the quantum analogon to the class P. This class won't be important in the rest of the report.

Definition 4.3.5 (Quantum algorithm and BQP). A *quantum algorithm* for the computation of a function $F : \mathbb{B}^* \rightarrow \mathbb{B}^*$ is a classical algorithm (i.e. Turing machine) that computes a function of the form $x \mapsto Z(x)$, where $Z(x)$ is a description of a quantum circuit U which computes $F(x)$ on empty input.

The function F is said to belong to the class BQP if there is a quantum algorithm that computes F in time $\text{poly}(n)$.

Remark 4.3.7. With “computes $F(x)$ on empty input” we mean that the quantum circuit U fulfills the condition given in equation 4.5, but instead of $|x\rangle$ we have $|0^N\rangle$, where N is the dimension of the quantum circuit U .

For us QMA will be the complexity class of interest, which is very similar to the NP class. First we need the analogon of the verifying function $R(x, y)$ that we saw in the definition of the class NP.

Definition 4.3.6 (Quantum verifier). A *quantum verifier* V_x is a quantum circuit specified by a description $Z(x)$.

A quantum verifier is called *poly-time* if the function $x \mapsto Z(x)$ is in P.

Definition 4.3.7 (QMA/BQNP). A predicate F is in QMA (or BQNP) if there exists a poly-time quantum verifier V_x and a polynomial p such that

$$\begin{aligned} F(x) = 1 &\implies \exists \text{ quantum state } \rho \text{ on } p(|x|) \text{ qubits : } \text{tr}(\Pi^{|1\rangle} V_x \rho V_x^\dagger) \geq \frac{2}{3} \\ F(x) = 0 &\implies \forall \text{ quantum state } \rho \text{ on } p(|x|) \text{ qubits : } \text{tr}(\Pi^{|1\rangle} V_x \rho V_x^\dagger) \leq \frac{1}{3}, \end{aligned}$$

where $\Pi^{|1\rangle}$ is an orthogonal projector on the subspace $\mathbb{C}(|1\rangle) \otimes \mathcal{B}^{\otimes(N_x-1)}$.

This definition is taken from [2].

Remark 4.3.8. As for the NP class the state ρ is called a *proof*. The expression $\text{tr}(\Pi^{|1\rangle} V_x \rho V_x^\dagger)$ is the probability that the first output qubit equals to $|1\rangle$.

Remark 4.3.9. The values $\frac{2}{3}$ and $\frac{1}{3}$ are conventionally chosen. By repeating the computation and using the amplification of probabilities we can achieve better probabilities. Important: They have to be chosen **constant** and cannot be chosen dependent of n .

Remark 4.3.10. There's a nice story to keep in mind, which allows to get a simpler view on this kind of problems. QMA is shorthand for Quantum-Merlin-Arthur. Merlin plays the part of the all-powerfull wizard that knows everything and is, of course, able to solve QMA-problems. One day King Arthur asks Merlin to help him with a QMA-problem and Merlin directly delivers him a proof ρ . Arthur is not that foolish and he doesn't trust Merlin at all ("He's too intelligent to be loyal"). So Arthur checks if the proof fulfills the quantum verifier. There are now two things that can happen. If there exists a correct proof, Merlin is able to convince Arthur of the correctness of his proof with probability $\frac{2}{3}$. If there doesn't exist a correct proof, Merlin cannot succeed in convincing Arthur that he found a correct proof with probability higher than $\frac{1}{3}$.

Finally we need a last important property. This property is connected to the *reduction* of problems.

Definition 4.3.8 (Karp reducibility). A predicate F_1 is *reducible* to a predicate F_2 if there exists a function $f \in \text{P}$ such that $F_1(x) = F_2(f(x))$ for any input string x .

4.4 Consistency Problem

This leads to the definition of complete problems.

Definition 4.3.9 (Completeness). A predicate $F \in \text{NP/QMA}$ is *NP/QMA-complete* if any predicate in NP/QMA is reducible to it.

The nice thing of reducibility can be expressed with the following lemma.

Lemma 4.3.2. *Let F_1 be reducible to F_2 . Then*

- $F_2 \in P \Rightarrow F_1 \in P$
- $F_2 \in \text{NP} \Rightarrow F_1 \in \text{NP}$
- $F_2 \in \text{QMA} \Rightarrow F_1 \in \text{QMA}$

This means for example: If we can show that a NP-complete problem is in P (or is reducible to a problem in P, which is same as this lemma states) we instantly know that we can reduce every problem in NP to a problem in P and so it would follow that $\text{NP} = \text{P}$.

4.4 CONSISTENCY PROBLEM

4.4.1 FORMULATION OF THE PROBLEM

The formal physical quantum marginal problem, here called the consistency problem, is given by:

Problem 2 (Consistency problem). Consider a system of n qubits. We are given a collection of local density matrices ρ_1, \dots, ρ_m , where each ρ_i acts on a subset of qubits $C_i \subseteq \{1, \dots, n\}$. Each matrix entry is specified with $\text{poly}(n)$ bits of precision. Also, $m \leq \text{poly}(n)$, and each subset C_i has size $|C_i| \leq k$, for some constant k .

In addition, we are given a real number β (specified with $\text{poly}(n)$ bits of precision) such that $\beta \geq \frac{1}{\text{poly}(n)}$.

The problem is to distinguish between the following cases:

- There exists an n -qubit state σ such that, for all i , $\| \text{tr}_{\{1, \dots, n\} - C_i}(\sigma) - \rho_i \|_1 = 0$. In this case, output “YES”. ($F(x) = 1$)
- For all n -qubit states σ , there exists some i such that, $\| \text{tr}_{\{1, \dots, n\} - C_i}(\sigma) - \rho_i \|_1 \geq \beta$. In this case, output “NO”. ($F(x) = 0$)

Remark 4.4.1. We are given a marginal distribution and we want to find a density matrix σ for the whole system that fulfills the given marginal distribution. If there exists such a σ we say that the marginal distribution is *consistent* and output a “YES”. If not we say that the marginal distribution is *not consistent* and we output a “NO”.

Theorem 4.4.1 (Main theorem). *The Consistency problem for $k \leq 2$ is QMA-complete.*

4.4.2 SKETCH OF THE PROOF [3]

Two things have to be shown. The first thing is that the consistency problem itself is in QMA. This can be done by explicitly construct a quantum verifier V for this problem. The paper by Y.-K. Liu uses the class QMA+, see [2], to construct such a verifier. QMA+ is an alternative definition of the class QMA. (In [2] you can find the proof that $\text{QMA} = \text{QMA+}$.)

The second part of the proof is to show that every problem in QMA is reducible to the consistency problem. Figure 4.1 shows a simple diagram of the idea how this can be done.

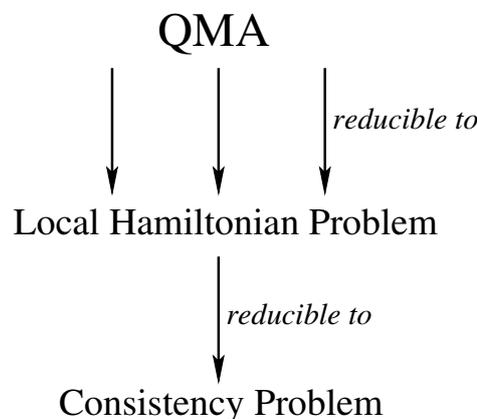


Figure 4.1: Any problem in QMA is reducible to the Local Hamiltonian problem. If we can show, that the Local Hamiltonian problem is reducible to the Consistency problem we immediately now that every problem in QMA is reducible to the Consistency problem.

There’s a famous QMA-complete problem called the *Local Hamiltonian problem*. It’s sometimes said to be the quantum analogon to the SAT-problem. The formal definition is the following:

4.5 Conclusion

Problem 3 (Local Hamiltonian problem). Consider a system of n qubits. We are given a Hamiltonian $H = H_1 + \dots + H_m$, where each H_i acts on a subset of qubits $C_i \subseteq \{1, \dots, n\}$. The H_i are Hermitian matrices, with eigenvalues in $[0, 1]$, and each matrix entry is specified with $\text{poly}(n)$ bits of precision. Also, $m \leq \text{poly}(n)$, and $|C_i| \leq k$ for some constant k .

In addition, we are given two real numbers a and b (specified with $\text{poly}(n)$ bits of precision) such that $b - a \leq \frac{1}{\text{poly}(n)}$.

- If H has an eigenvalue that is $\leq a$, output “YES”. ($F(x) = 1$)
- If all the eigenvalues of H are $\geq b$, output “NO”. ($F(x) = 0$)

It has been shown that the Local Hamiltonian problem is QMA-complete for $k = 5$ [1, 4], $k = 3$ [5] and $k = 2$ [6]. So the idea of the proof is to reduce the Local Hamiltonian problem to the Consistency problem.

4.5 CONCLUSION

QMA-complete problems are believed not to be efficiently solvable on quantum computers. So for us this means that the quantum marginal/consistency problem is a really complicated problem. It's the same dilemma as for the NP and P classes. If anyone would find an algorithm that solves a NP-complete problem in polynomial time we would have a polynomial algorithm for every problem in NP (which would be very astonishing). On the other hand it hasn't been shown yet that for any NP-complete problem there's no polynomial algorithm.

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CHAPTER 5

ENTROPY INEQUALITIES

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This chapter is dedicated to introducing and discussing the notion of entropy as defined in Classical and Quantum Information Theory. In the classical case, we will see that entropy corresponds to the information content of a system. Also, an intuitive connection to thermodynamical entropy will be shown. For the quantum mechanical entropy, our main goal will be understanding which entropies are allowed on composite systems. We will find two inequalities which govern entropy on composite systems, strong subadditivity and weak monotonicity. The question that will be discussed, then, is whether or not those two inequalities completely describe entropy on composite systems.

5.1 SHANNON ENTROPY

5.1.1 ENTROPY IN INFORMATION THEORY

An important problem in information theory is compressing the information inherent in a system to its minimally needed size. To treat this problem, consider a list of random variables $\{X\}$ which assume values $x_i, i \in 1, \dots, n$ with probabilities $p_i = \Pr[X = x_i]$. This could be, for example, a text where the different characters of the alphabet appear seemingly randomly, according to how often they are used in the English language. When representing this text in a binary form, we would like to have a shorter representation for the more abundant letters (like ‘e’) while we don’t mind giving rare letters like ‘z’ a longer binary representation. In this

5.1 Shannon entropy

way, we need less bits to store the same information than by just representing all the letters with an equal number of bits.

There is, however, an exact bound to how good we can compress the information inherent in a list of random variables: No matter how sophisticated our algorithm is, we need at least

$$H(X) = - \sum_{i=1}^n p_i \log(p_i) \quad (5.1)$$

bits per random variable (where \log is the logarithm to base 2 and $0 \log 0 := 0$). This quantity is called the **Shannon entropy**. Since it is always possible to get arbitrarily close to that value, the Shannon entropy is a good way of measuring information (in bits). In fact, one can even consider entropy and information as being the same thing.

5.1.2 EQUIVALENT FORMULATIONS

As we have just seen, entropy is the information (measured in bits) of a random variable. Equivalently, we can think about it as the gain of information when adding a variable, i.e. performing a measurement.

Also, the information gained by measuring a system's state must be the same as the uncertainty about that state before measuring it. If we know perfectly what state a system is in, then measuring it will not give us any information. On the other hand, measuring a state system with fully unknown state (i.e. we are uncertain about the state) gives us information about the nature of the state.

We now have three equivalent ways of thinking about entropy: It can be thought of as the minimal number of bits it takes to store a random variable, the information gained by measuring a system's state or the uncertainty about a state before measuring it.

5.1.3 RELATION TO THERMODYNAMICAL ENTROPY

How does this correspond to the entropy we know from thermodynamics? Let us consider a system of bosons which may assume energies $E_i, i \in \mathbb{N}_0$ (see Fig. 5.1). From thermodynamics, we know that the system can be described as follows at absolute zero temperature:

“All bosons occupy the ground state.”

Also, the (thermodynamical) entropy must be zero. At finite temperature, however, the entropy is positive, and the system may be described as follows:

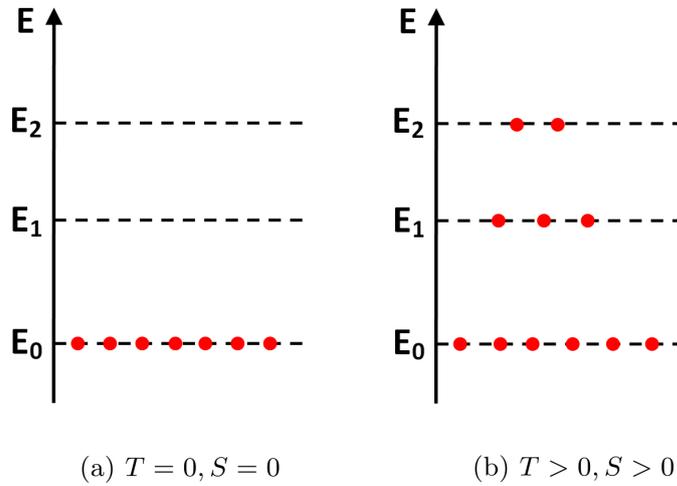


Figure 5.1: System of bosons that may assume discrete energy levels

*“6 bosons occupy the ground state,
 3 bosons occupy the state E_1
 2 bosons occupy the state E_2 ...”*

Obviously, describing the more chaotic system at finite temperature takes much more information. Hence, it makes intuitive sense to identify the Shannon entropy with what we know from thermodynamics. In fact, a detailed analysis shows that the entropy from thermodynamics and the Shannon entropy are the same up to a constant factor. Note however that the reasoning described above is not a strict formalism and that there might be some pitfalls in trying to apply it to a general problem.

5.2 VON NEUMANN ENTROPY

5.2.1 DEFINITION

The quantum mechanical analogous to the Shannon entropy is the **von Neumann entropy**. We shall define the von Neumann entropy and another useful quantity called mutual information:

Definition 5.1. Let ρ be a density operator. Then the **von Neumann entropy** of the system described by ρ is given by

$$S(\rho) = -\text{tr}(\rho \log \rho) \quad (5.2)$$

5.2 von Neumann Entropy

If the eigenvalues λ_x of ρ are known, this can be rewritten as

$$S(\rho) = - \sum_x \lambda_x \log \lambda_x \quad (5.3)$$

where $0 \log 0 := 0$ as before.

Notation. When considering composite systems (e.g. AB consisting of A and B), the entropy of the different subsystems is often indexed as follows:

$$S(A) := S(\rho_A) \quad S(A, B) := S(\rho_{AB})$$

Definition 5.2. The **mutual information** of two systems A and B is given by

$$S(A : B) := S(A) + S(B) - S(A, B) \quad (5.4)$$

Mutual information describes the information shared by two systems. Returning to our example from 5.1.1, if Alice owns “The Lord of the Rings” and “Harry Potter” and Bob has “The Hobbit” and “The Lord of the Rings” in his bookshelf, then “The Lord of the Rings” is the mutual information of Alice and Bob.

5.2.2 BASIC PROPERTIES

A short selection of properties of the von Neumann entropy is shown in the following theorem:

Theorem 5.1. Basic properties of the von Neumann entropy

- a) The von Neumann entropy is non-negative: $S(\rho) \geq 0$. It is zero if and only if the state ρ is pure.
- b) Let d be the dimension of the Hilbert space. Then $S(\rho) \leq \log d$.
- c) Suppose a composite system is in a pure state. Then $S(A) = S(B)$

Proof.

- a) ρ is a positive operator with $\text{tr } \rho = 1$. Hence, the eigenvalues λ_x of ρ fulfil $\lambda_x \geq 0$ and $\sum_x \lambda_x = 1$ and thus $\forall x : 0 \leq \lambda_x \leq 1$. For the entropy, we get:

$$S(\rho) = - \sum_x \underbrace{\lambda_x}_{\geq 0} \underbrace{\log \lambda_x}_{\leq 0} \geq 0$$

- b) see 5.2.3
- c) From the Schmidt decomposition we know that ρ_A and ρ_B have the same eigenvalues. With equation 5.3, it follows that $S(A) = S(B)$

□

5.2.3 RELATIVE ENTROPY

An extremely useful tool for showing properties of the von Neumann entropy is the **relative entropy** of two density operators ρ and σ given by

$$S(\rho\|\sigma) := \text{tr}(\rho \log \rho) - \text{tr}(\rho \log \sigma) \quad (5.5)$$

The relative entropy is non-negative, a result known as *Klein's inequality*:

Theorem 5.2. Klein's inequality

The relative entropy is non-negative,

$$S(\rho\|\sigma) \geq 0 \quad (5.6)$$

with equality if and only if $\rho = \sigma$.

Proof. (from [1])

Since ρ and σ are positive operators, there are (by the spectral decomposition theorem) orthonormal decompositions $\rho = \sum_i p_i |i\rangle\langle i|$ and $\sigma = \sum_j q_j |j\rangle\langle j|$. We can rewrite the relative entropy as

$$S(\rho\|\sigma) = \sum_i p_i \log p_i - \sum_i \langle i|\rho \log \sigma|i\rangle$$

by writing the trace in the basis $\{|i\rangle\}_i$.

Into this equation, we substitute $\langle i|\rho = p_i|i\rangle$ and

$$\langle i|\log \sigma|i\rangle = \langle i|\left(\sum_j \log(q_j)|j\rangle\langle j|\right)|i\rangle = \sum_j \log(q_j)P_{ij},$$

where $P_{ij} := \langle i|j\rangle\langle j|i\rangle$ to get

$$S(\rho\|\sigma) = \sum_i p_i \left(\log p_i - \sum_j P_{ij} \log q_j \right)$$

P_{ij} satisfies $P_{ij} \geq 0$, $\sum_i P_{ij} = 1$ and $\sum_j P_{ij} = 1$. Using the fact that \log is a strictly concave function, we get $\sum_j P_{ij} \log q_j \geq \log r_i$ where $r_i := \sum_j P_{ij} q_j$, with equality if and only if there is a j_0 such that $P_{ij} = \delta_{ij_0}$. Note also that $\sum_i r_i = 1$. Hence we get

$$S(\rho\|\sigma) \geq \sum_i p_i \log \frac{p_i}{r_i}$$

5.3 Entropy of composite systems

with equality if and only if P_{ij} describes a permutation matrix (i.e. the eigenstates are the same up to permutation). Noting that $\ln 2 \log x = \ln x \leq x - 1$ (with equality if and only if $x = 1$) and $\log \frac{1}{x} = -\log x$, we get

$$\begin{aligned} S(\rho\|\sigma) &\geq \frac{1}{\ln 2} \sum_i p_i \left(1 - \frac{r_i}{p_i}\right) \\ &= \frac{1}{\ln 2} \sum_i (p_i - r_i) \\ &= \frac{1}{\ln 2} (1 - 1) = 0 \end{aligned}$$

with equality if and only if $r_i = p_i$, i.e. the eigenvalues are the same. In combination with the result above, this shows that equality occurs if and only if $\rho = \sigma$. \square

APPLICATION OF KLEIN'S INEQUALITY

With Klein's inequality, we can show b) from Theorem 5.1 ($S(\rho) \leq \log d$):

First we note that for $\sigma = I/d$, $S(\sigma) = -\text{tr}(\sigma \log \sigma) = -\frac{\log(\frac{1}{d})}{d} \underbrace{\text{tr} I}_{=d} = \log d$,

i.e. σ saturates the inequality.

For a general density operator ρ , we know from Klein's inequality that $S(\rho\|I/d) \geq 0$. Since

$$S(\rho\|I/d) = \text{tr}(\rho \log \rho) - \text{tr} \rho \log I/d = -S(\rho) + \log d \underbrace{\text{tr} \rho}_{=1}$$

we get $-S(\rho) + \log d \geq 0 \Leftrightarrow S(\rho) \leq \log d$.

5.3 ENTROPY OF COMPOSITE SYSTEMS

5.3.1 STRONG SUBADDITIVITY AND WEAK MONOTONICITY

The entropy of composite systems can have properties that do not occur in the classical case. For example, consider a state ρ_A with non-zero entropy $S(A) > 0$. We know that we can find a system B purifying A, i.e. ρ_{AB} is in a pure state. But then $S(A, B) = 0$ must hold.

Trying to explain this with our intuition about information fails, because there appears to be more information in a subsystem of AB than in the whole system. This strange behaviour leads us to the question what rules govern entropy on composite systems. In other words:

What entropies are allowed on composite systems?

The main results concerning this question are known as strong subadditivity (SSA) and weak monotonicity (WM).

Theorem 5.3. (SSA) and (WM)

Let A, B, C be a trio of quantum systems. Then the following inequalities hold:

$$\begin{aligned} S(A, B, C) + S(B) &\leq S(A, B) + S(B, C) && \text{(SSA)} \\ S(A) + S(B) &\leq S(A, C) + S(B, C) && \text{(WM)} \end{aligned}$$

For a proof of this theorem, see [1].

In fact, the two inequalities are equivalent. The proof of their equivalence makes use of the fact that we can always find a purifying system R s.t. ABC is in a pure state:

Proof.

i) $WM \implies SSA$

Applying (WM) on the triplet R, B, C gives us

$$S(R) + S(B) \leq S(R, C) + S(B, C)$$

from Schmidt decomposition, we know that $S(A, B, C) = S(R)$ and $S(A, B) = S(R, C)$ and therefore

$$S(A, B, C) + S(B) \leq S(A, B) + S(B, C)$$

which is (SSA).

ii) $SSA \implies WM$

Applying (SSA) on the triplet R, B, C and $S(A) = S(C, B, R)$ and $S(B, R) = S(A, C)$ (from Schmidt decomposition), we get:

$$\underline{S(A) + S(B)} = S(R, B, C) + S(B) \leq S(B, C) + S(B, R) = \underline{S(A, C) + S(B, C)}$$

□

5.3 Entropy of composite systems

5.3.2 GEOMETRICAL INTERPRETATION

To get an intuition about what (SSA) and (WM) imply in a general n -part quantum system Ω , we represent a given state by using all the entropies on non-zero subsystems of Ω . Since there are $2^n - 1$ such subsystems, this gives us a vector in $\mathbb{R}^{2^n - 1}$ called the *allocation of entropy*.

Definition 5.3. Let $\Omega = \Omega_1 \times \Omega_2 \times \dots \times \Omega_n$ be a n -part quantum system. For $I \subseteq N := 1, \dots, n$, denote by Ω_I the subsystem given by $\Omega_I = \prod_{i \in I} \Omega_i$. The **allocation of entropy** of a state ρ on Ω is then given by

$$\{S(\Omega_I)\}_{I \subseteq N} \equiv \{S(\rho_{\Omega_I})\}_{I \subseteq N} \quad (5.7)$$

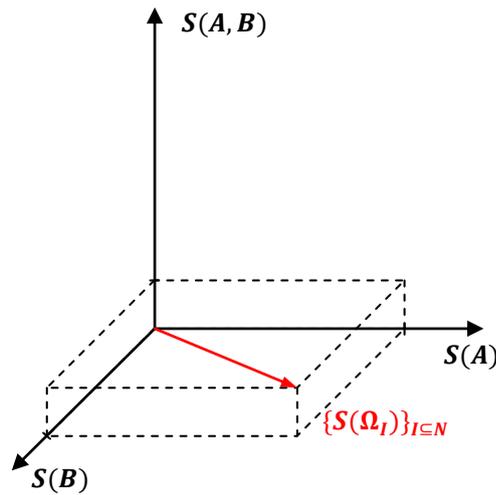


Figure 5.2: Example of an allocation of entropy for a two-part quantum system

Since we are interested in what states are physically possible, we would like to know the shape of the set $\mathcal{A}_n := \{\{S(\Omega_I)\}_{I \subseteq N}\}_{\Omega \text{ n-part q.s.}}$ of allocations of entropy on an *arbitrary* n -part quantum system allowed by the rules of quantum mechanics.

In particular, we would like to know whether (SSA) and (WM) are all the inequalities we need, i.e. if $\mathcal{B}_n := \{\mathbf{x} \in \mathbb{R}^{2^n - 1} : \mathbf{x} \text{ satisfies (SSA) and (WM)}\}$ is the same as \mathcal{A}_n .

CONVEX CONES

A first result concerning the question whether \mathcal{A}_n and \mathcal{B}_n are the same is the fact that \mathcal{B}_n and the closure of \mathcal{A}_n , denoted by $\overline{\mathcal{A}_n}$, are both *convex cones*.

Definition 5.4. Let G be a set of point in \mathbb{R}^k . G is called a **convex cone** if

$$\text{CC 1 } \forall \mathbf{x} \in G \text{ and } \forall \lambda \in \mathbb{R}, \lambda \geq 0 : \lambda \mathbf{x} \in G$$

$$\text{CC 2 } \forall \mathbf{x}, \mathbf{y} \in G \text{ and } \forall \lambda \in \mathbb{R}, 0 \leq \lambda \leq 1 : \lambda \mathbf{x} + (1 - \lambda)\mathbf{y} \in G$$

From (CC 1), we know that if a point \mathbf{x} is in a convex cone, then so is the ray (with origin at 0) passing through that point. (CC 2) on the other hand tells us that if two points are in a convex cone, then so is the line connecting the points. Therefore, one can think of a convex set by imagining a convex set on a (hyper-)plane in \mathbb{R}^k . The cone is then given by all the points lying on rays passing through that set.

Note that, in order for (CC 1) to be fulfilled, it is important that Ω can be an arbitrary n -part quantum system because the entropy in any given system is always bounded by $\log d$, where d is the dimension of the corresponding Hilbert space.

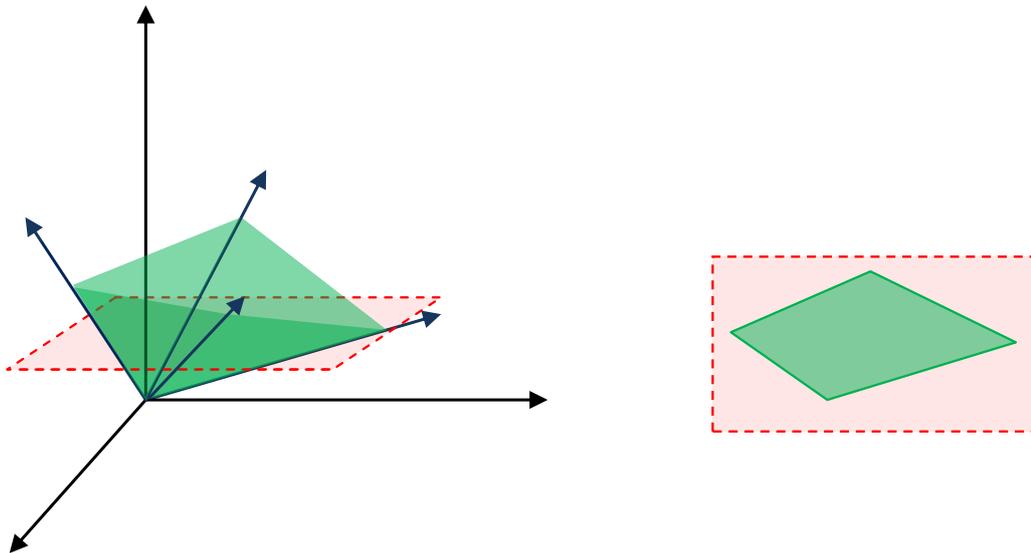


Figure 5.3: A polyhedral convex cone in \mathbb{R}^3 . The set given by intersecting it with a plane (right) must be convex. It is called polyhedral because that set is a polygon.

5.3 Entropy of composite systems

RELATION BETWEEN $\overline{\mathcal{A}}_n$ AND \mathcal{B}_n

Since we now know that $\overline{\mathcal{A}}_n$ and \mathcal{B}_n are both convex cones, we will first consider the question whether $\overline{\mathcal{A}}_n = \mathcal{B}_n$. The answer to this question depends on the dimensionality of the system:

For $n \leq 3$, it can be shown that the $\overline{\mathcal{A}}_n$ and \mathcal{B}_n are actually equal. Since \mathcal{A}_n is the image of the set of density operators under S, this means that the allowed allocations of entropy lie dense in the set described by (SSA) and (WM).

However, there is no proof for the same result for $n \geq 4$. In fact, it is believed that $\overline{\mathcal{A}}_n$ is actually a strict subset of \mathcal{B}_n in that case. The reason for this speculation is that in the classical analogous, the same is true, i.e. $\overline{\mathcal{A}}_n^{class.} = \mathcal{B}_n^{class.}$ for $n \leq 3$ but $\overline{\mathcal{A}}_n^{class.} \subsetneq \mathcal{B}_n^{class.}$ for $n \geq 4$.

5.3.3 CONSTRAINED INEQUALITIES

The attempt to prove that $\overline{\mathcal{A}}_n \subsetneq \mathcal{B}_n$ for $n \geq 4$ has led to the development of *constrained inequalities*. These inequalities do not hold in a general case, but only when a given condition is fulfilled.

QUADRIPARTITE QUANTUM SYSTEMS

Let us consider a four - part quantum system. Although a more generalized result can be found for n-part quantum systems, its essentials are captured by this example.

Theorem 5.4. *Constrained inequality for a quadripartite quantum system*

Let A, B, C, D be a four - part quantum system. Suppose the triplets ABC , CAB and ADB saturate the strong subadditivity, i.e.

$$\begin{aligned} S(A, B, C) + S(B) &= S(A, B) + S(B, C) \\ S(A, B, C) + S(A) &= S(A, B) + S(A, C) \\ S(A, B, D) + S(D) &= S(A, D) + S(B, D) \end{aligned}$$

Then the following inequality holds:

$$S(C : D) \geq S(C : A, B) \tag{5.8}$$

which can be rewritten as

$$S(A, B, C) + S(D) \geq S(C, D) + S(A, B) \tag{5.9}$$

For a proof of this theorem, see [2].

It is worth noting that the condition that strong subadditivity must be saturated means that we are talking about the surface of the convex cone defined by (SSA) and (WM).

INDEPENDENCE OF INEQUALITIES

It is not immediately clear that the constrained inequality from above is actually something new and not a complicated way of rewriting (SSA) or (WM). To show that this is not the case, we need a notion of independence of inequalities.

Definition 5.5. An inequality (B) is **independent of (A)** if there is a vector $\mathbf{x} \in \mathbb{R}^{2^n-1}$ which satisfies (A) but not (B).

This definition does not take into account that the vectors have to represent physical states. For example, for (SSA) and (WM), which we have shown to be equivalent, we can show that (SSA) is independent of (WM)

Proposition 5.5. *Strong subadditivity is independent of weak monotonicity.*

Proof. Suppose we have an n-part quantum system Ω . Consider a vector for which the entropy on the total system is the only non-zero entropy, i.e.

$$S(\Omega_I) = \begin{cases} 1, & \text{if } I = N \\ 0, & \text{else} \end{cases}$$

Dividing the n-part quantum systems into three non-zero parts A,B,C, we get $S(A, B, C) = 1$ and $S(B) = S(A, B) = S(B, C) = 0$, hence (SSA) is not fulfilled. For this allocation of entropy, $\Omega_I \subset \Omega_J \Rightarrow S(\Omega_I) \leq S(\Omega_J)$. Hence, for any tripartite subsystem A,B,C, we get $S(A) \leq S(A, C)$ and $S(B) \leq S(B, C)$, which shows that (WM) is fulfilled. \square

The tricky part in this proof is that (WM) actually has to be fulfilled on any tripartite subsystem of Ω . For example, if Ω is itself tripartite system A,B,C, then (WM) has to be fulfilled for $\tilde{A} = (A, B)$; $\tilde{B} = \emptyset$; $\tilde{C} = C$ as well.

With the same type of argument, it can be shown that the constrained inequality is independent of (SSA) and (WM).

5.3 Entropy of composite systems

CONCLUSION

The fact that the constrained inequalities are independent means that the reason they hold is not because the inequality is redundant, but it is a physical reason. Also, this implies that not all points in \mathcal{B}_4 satisfy the constrained inequality. However, it does not imply that $\overline{\mathcal{A}_n} \subsetneq \mathcal{B}_n$ because of the constraints given:

As pointed out before, the constrained inequality only affects the surface of the cone \mathcal{B}_n . There might therefore still be points in \mathcal{A}_n arbitrarily close to the surface and \mathcal{A}_n might still be dense in \mathcal{B}_n .

Also, this does not imply that $\mathcal{A}_n \subsetneq \overline{\mathcal{A}_n}$ because it is not clear whether the points in \mathcal{B}_n affected by the inequality actually lie in $\overline{\mathcal{A}_n}$. What we have shown, then, is that $\mathcal{A}_n \subsetneq \mathcal{B}_n$ for $n \geq 4$.

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CHAPTER 6

ENTANGLEMENT OF RANDOM STATES

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We give a basic introduction into the importance of entangled states for many-particle quantum physics in general and quantum information theory in particular. First, the main definitions are given and basic properties of entangled states explained. Then, entanglement measures, which serve to quantify the amount of entanglement in states, are introduced and discussed. In the end, special emphasis will be put on the analysis of entanglement of random states in high dimensional bipartite systems, following the first part of [1].

6.1 INTRODUCTION

According to one of the postulates of quantum mechanics, the Hilbert space of a system composed of two subsystems is given by the tensor product of the Hilbert spaces of the subsystems. In classical mechanics however, the total configuration space is the cartesian product of the individual configuration spaces. One of the fundamental differences of these two postulates is that in the quantum world there exist so called entangled states which cannot be written as a product of states of the subsystems. In the classical world this is always possible. This difference gives rise to pure quantum effects without classical analogue; entangled states allow to perform non-classical tasks such as quantum dense coding and quantum teleportation.

In the first part of this chapter we discuss the definition of entangled states and its relation to entropy. Then, entanglement measures will be introduced which serve

6.2 Entanglement

as an indicator how entangled a state is. After a historic motivation of certain entanglement measures, we will discuss the axiomatic approach which defines entanglement measures by two basic axioms. Based on these axioms we will be able to write down several classes of entanglement measures which will then be compared and classified via their additional properties. The last and main part of this chapter will deal with entanglement of random states in high-dimensional bipartite systems. We will see that there exist large subspaces in which all pure states are close to maximally entangled. Therefore, (near-maximally) entangled states play a major role in quantum mechanics.

6.2 ENTANGLEMENT

6.2.1 DEFINITION

We will start by defining what not-entangled states are. Suppose two finite dimensional Hilbert spaces $\mathcal{H}_A, \mathcal{H}_B$ are given. If we choose two orthonormal bases $\{|i\rangle_A \in \mathcal{H}_A\}, \{|j\rangle_B \in \mathcal{H}_B\}$, a generic element of the product space $\mathcal{H}_A \otimes \mathcal{H}_B$ can be expressed as $|\psi\rangle_{AB} = \sum_{i,j} c_{ij} |i\rangle_A \otimes |j\rangle_B$. We call this state separable if and only if one can find a decomposition $c_{ij} = c_i c_j$ of the complex coefficients into product form for all pairs (i, j) . This, in turn, implies that $|\psi\rangle_{AB}$ can be written in product form $|\psi\rangle_{AB} = \left(\sum_i c_i |i\rangle_A\right) \otimes \left(\sum_j c_j |j\rangle_B\right)$. States for which such a decomposition does not exist are called entangled. This means that for these states it is not possible to assign a single state vector to any subsystem.

Example. For $\dim \mathcal{H}_A = \dim \mathcal{H}_B = 2$, $\mathcal{H}_A \otimes \mathcal{H}_B$ is spanned by the four Bell-state entangled basis

$$|\psi^\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle|1\rangle \pm |1\rangle|0\rangle) \quad (6.1)$$

$$|\phi^\pm\rangle = \frac{1}{\sqrt{2}} (|0\rangle|0\rangle \pm |1\rangle|1\rangle). \quad (6.2)$$

We show as an example that $|\phi^+\rangle$ is entangled. We have that $c_{10} = c_{01} = 0$, which either implies (if we assume a decomposition to exist) that $c_0 = 0$ or $c_1 = 0$ (or both). Each of the three possibilities contradicts however that $c_{00} = c_{11} = 1/\sqrt{2}$ and therefore $|\phi^+\rangle$ must be entangled. The other cases work similarly.

To extend the above definition to mixed states, one can also define separability and entanglement in the language of density matrices. A generic density matrix ρ_{AB} acting on $\mathcal{H}_A \otimes \mathcal{H}_B$ is called separable if and only if it can be written as a

convex combination of product states, i.e.

$$\rho_{AB} = \sum_k p_k \rho_A^k \otimes \rho_B^k, \quad (6.3)$$

where the p_k form a probability distribution and each $\rho_{A/B}^k$ acts on A or B , respectively. Again, a density matrix is called entangled if it is not separable in the light of the above definition. The language of density matrices provides the advantage that, in contrast to states, we are able to assign a density matrix to any subsystem, namely the reduced density matrix of that subsystem. But for entangled density matrices (which from now on shall also be called states) something peculiar happens. If we start, say, with the pure entangled state $\rho = |\psi^-\rangle\langle\psi^-|$ its reduced density matrix on A or B $\rho_{A,B} = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ is mixed. This means that although we have maximal knowledge about the total state (because its pure), the states of the subsystems are unknown. This property is exclusive for entangled states; one can show that a bipartite pure state is entangled if and only if all reduced states are mixed.

6.2.2 ENTANGLEMENT AND ENTROPY

In order to relate to the previous chapter and to reformulate some of the statements of the previous section, it is instructive to discuss the relation between entanglement and entropy. The von Neumann entropy of a density matrix ρ is given by $S(\rho) = -\text{Tr}(\rho \log_2 \rho)$. If ρ acts on a finite dimensional Hilbert space and has eigenvalues $\lambda_1, \dots, \lambda_n$, the Shannon entropy is recovered; by using the spectral decomposition $\rho = \sum_i \lambda_i |i\rangle\langle i|$, $S(\rho)$ can be computed with respect to the eigenbasis $\{|i\rangle\}$, leading to $S(\rho) = -\sum_i \lambda_i \log_2 \lambda_i$. Pure states have trivial decomposition $\lambda_i = \delta_{ij}$ and therefore entropy equal to zero (convention: $0 \log 0 = 0$). In particular, this applies to $\rho = |\psi^-\rangle\langle\psi^-|$, i.e. $S(\rho) = 0$. However, for the reduced density matrix $\rho_A = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ we have $S(\rho_A) = -2 \cdot \frac{1}{2} \log_2 \frac{1}{2} = 1 > 0$. This behaviour arises because ρ is pure, whereas its reduced state ρ_A is maximally mixed; a property which is unique to entangled states. Therefore, this behaviour is a pure quantum effect which cannot happen in the classical world. It has been proved that separable states, similarly to classical states, satisfy

$$S(\rho_{AB}) \geq S(\rho_A), \quad S(\rho_{AB}) \geq S(\rho_B). \quad (6.4)$$

For pure states these inequalities are violated if and only if the state is entangled, since in this case all reduced states are mixed and have therefore entropy greater than zero. This property and the above discussion motivate that $E(\rho_{AB}) = S(\rho_A)$

6.3 Entanglement measures

(entropy of subsystem) might be a good measure in order to quantify entanglement. In fact, this function will turn out to be the most useful entanglement measure for pure states in order to discuss entanglement of random states at the end of this chapter.

6.3 ENTANGLEMENT MEASURES

According to the above definition of entanglement, a generic state is either entangled or not. However, among the entangled states some are more entangled than others and it turns out to be useful to quantify the notion of entanglement by entanglement measures. These are functions which map the space of states into the real numbers such that the output tells us how entangled a state is. For instance, in the case of the above example, an entanglement measure can be consistently defined by how many Bell states can be extracted from the state in the limit of infinite copies of itself. This section provides an overview over various of such entanglement measures and their (defining) properties.

6.3.1 QUANTUM TELEPORTATION

The initial idea to quantify entanglement was connected with its usefulness in terms of communication. In order to understand the connection between entangled states and communication, an interlude about quantum teleportation is needed. Furthermore, the appearing notions will be of importance for the rest of this chapter.

Suppose Alice wants to send an unknown quantum bit $|\psi\rangle_C = \alpha|0\rangle_C + \beta|1\rangle_C$ to Bob. By the following method she is able to do so at the price of erasing the state at her side. They have at disposal a classical communication channel and one pair of entangled qubits i.e. they share a maximally entangled state e.g.

$$|\phi^+\rangle_{AB} = \frac{1}{\sqrt{2}} (|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B). \quad (6.5)$$

The total initial state is given by the tensor product of the two states

$$|\phi^+\rangle_{AB} \otimes |\psi\rangle_C, \quad (6.6)$$

which can be rewritten as a linear combination of the Bell basis on the system AC , yielding

$$|\phi^+\rangle_{AB} \otimes |\psi\rangle_C = \frac{1}{\sqrt{2}} (|0\rangle_A|0\rangle_B + |1\rangle_A|1\rangle_B) (\alpha|0\rangle_C + \beta|1\rangle_C) \quad (6.7)$$

$$= \frac{1}{2} [|\phi^+\rangle_{AC} (\alpha|0\rangle_B + \beta|1\rangle_B) + |\phi^-\rangle_{AC} (\alpha|0\rangle_B - \beta|1\rangle_B) \quad (6.8)$$

$$+ |\psi^+\rangle_{AC} (\beta|0\rangle_B + \alpha|1\rangle_B) + |\psi^-\rangle_{AC} (\beta|0\rangle_B - \alpha|1\rangle_B)]. \quad (6.9)$$

If Alice now measures her system AC , the total state collapses into eigenstates of the measurement result, in this case into one of the four Bell states times a certain qubit with equal probability. The resulting state on Bob's side is very similar to the original qubit $|\psi\rangle_C = \alpha|0\rangle_C + \beta|1\rangle_C$ which Alice wanted to send him. In fact, the four possible states are related to $|\psi\rangle_C$ by unitary representations, in this case rotations. To get the desired qubit, Bob has to apply the corresponding inverse rotation to his state, for which he needs to know Alice measurement result. For this reason, Alice sends her result to Bob in binary form using the classical communication channel. The four possibilities are

- a) $|\phi^+\rangle_{AC} \otimes (\alpha|0\rangle_B + \beta|1\rangle_B) \xrightarrow{\text{to Bob}} 00$
- b) $|\phi^-\rangle_{AC} \otimes (\alpha|0\rangle_B - \beta|1\rangle_B) \xrightarrow{\text{to Bob}} 01$
- c) $|\psi^+\rangle_{AC} \otimes (\beta|0\rangle_B + \alpha|1\rangle_B) \xrightarrow{\text{to Bob}} 10$
- d) $|\psi^-\rangle_{AC} \otimes (\beta|0\rangle_B - \alpha|1\rangle_B) \xrightarrow{\text{to Bob}} 11.$

According to the received bits, Bob performs unitary operations on his qubit to get the desired state, e.g. if he receives 11, he can obtain $|\psi\rangle_C$ from his state by applying $U = -i\sigma_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ to it. In this way, Alice is able to send her qubit to Bob at the price of simultaneously erasing it at her side. This is because she ends up with one of the four Bell states and no information about the initial qubit is left with her. Therefore the procedure, although only information and no matter is transferred, is a teleportation rather than duplication of the initial qubit. In this way, the no cloning principle is respected. In summary, two qubits in one of the Bell states (which are also called ebit) together with local operations (either on Alice's or Bob's side) and classical communication i.e. LOCC operations allow for the teleportation of one qubit.

It is crucial for the whole process to use one of the Bell states, which will later turn out to be *maximally* entangled states, rather than generic entangled states. Non-maximally entangled states do not allow for faithful communication. However, in the limit of infinite copies of an entangled state, faithful communication might me

6.4 Axiomatic approach

achieved at some rate. This rate is exactly the output value of the entanglement measure *Distillable entanglement*

$$E_D(\rho_{AB}) = \sup \left\{ \frac{m}{n} : \lim_{n \rightarrow \infty} \left(\inf_{\Lambda \text{ LOCC}} \|\Lambda(\rho_{AB}^{\otimes n}) - (\Phi_2^+)^{\otimes m_n}\|_1 \right) = 0 \right\}. \quad (6.10)$$

The input is a generic bipartite state ρ_{AB} . The output tells how many ebits can be extracted from n copies of ρ_{AB} per copy by LOCC operations in the limit $n \rightarrow \infty$. Because of the teleportation process, this is equal to the number of qubits per copy one is able to teleport with this state i.e. its *usefulness for communication*. Evidently, $E_D = 0$ for separable states and $E_D = 1$ for Bell states.

Another measure, dual to E_D , is *Entanglement cost*. It counts the number of ebits per copy which are needed in order to create $\rho_{AB}^{\otimes n}$ by LOCC operations. Again, by the teleportation procedure, the output is equal to the number of qubits one has to teleport in order to create the state. Its precise definition is

$$E_C(\rho_{AB}) = \inf \left\{ \frac{m}{n} : \lim_{n \rightarrow \infty} \left(\inf_{\Lambda \text{ LOCC}} \|\rho_{AB}^{\otimes n} - \Lambda((\Phi_2^+)^{\otimes m_n})\|_1 \right) = 0 \right\}. \quad (6.11)$$

It can be shown that generally $E_D \leq E_C$ i.e. more qubits are needed to build up a state than can be extracted from it. Furthermore equality $E_D = E_C$ holds on pure states.

6.4 AXIOMATIC APPROACH

The above measures describe entanglement in terms of certain tasks (optimisation of protocols). A more general approach consists of postulating a set of axioms which are fulfilled by the above measures, but allow any function to be a measure, provided it satisfies the axioms. The most important axiom is

- **Axiom 1 (Monotonicity under LOCC):**

\forall LOCC operations Λ , an entanglement measure $E(\rho)$ has to satisfy

$$E(\Lambda(\rho)) \leq E(\rho),$$

i.e. entanglement can only decrease under LOCC. This postulate has two immediate consequences which one would expect from an entanglement measure and therefore motivate the axiom. First, a measure $E(\rho)$ satisfying axiom 1 is constant on separable states. This is because every separable state can be mapped to any other by LOCC operations. Since the LOCC set is closed under inversion we get equality. Even more, $E(\rho)$ must be minimal on separable states, since any separable state can be obtained by LOCC from any other state. Since by

definition separable states are not entangled, it is natural to set this constant to zero. This is however not a consequence of axiom 1 and must therefore be required as an additional axiom.

- **Axiom 2 (Minimal entanglement):**

An entanglement measure $E(\rho)$ has to satisfy

$$E(\rho_{sep}) = 0.$$

Note, that both axioms impose E to be a non-negative function.

In addition to minimal entanglement, imposed by both axioms, it can be shown that there exists maximal entanglement in bipartite systems. More precisely, in a finite dimensional bipartite system $\mathcal{H} = \mathbb{C}^d \otimes \mathbb{C}^{d'}$ ($d = d'$ for simplicity) the following holds: $\forall |\psi\rangle \in \mathcal{H} \exists \Lambda LOCC$ such that $|\psi\rangle = \Lambda(|\phi_d^+\rangle)$ with $|\phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_i |i\rangle_A |i\rangle_B$, i.e. one can get any state by applying the appropriate LOCC operation to $|\phi_d^+\rangle$ (the d -dimensional generalisation of $|\phi^+\rangle$). Since entanglement can only decrease under LOCC, $|\phi_d^+\rangle$ has to be maximally entangled. This property is not exclusive to $|\phi_d^+\rangle$. In fact, it can be shown that all maximal entangled states can be obtained from $|\phi_d^+\rangle$ via unitary transformations $|\psi_{max}\rangle = U_A \otimes U_B |\phi_d^+\rangle$. Since unitary transformations are a subspace of LOCC transformations, every state can be obtained by any maximally entangled state by applying LOCC.

Entanglement measures often satisfy a stronger condition than axiom 1, namely they do not increase on average i.e.

$$\sum_i p_i E(\sigma_i) \leq E(\rho), \quad \text{with } \rho \xrightarrow{LOCC} \sum_i p_i \sigma_i. \quad (6.12)$$

Later on, stronger monotonicity (6.12) will be needed in order to classify all bipartite entanglement measures.

6.4.1 ADDITIONAL POSSIBLE POSTULATES

The above axioms are the only ones necessarily required from entanglement measures. However, there are other properties which can be useful and are natural in some context. Examples include

1. *Normalisation.* In bipartite systems, a natural postulate in order to compare entanglement measures is normalisation on maximally entangled states. For instance, one could require

$$E(\phi_d^+) = \log d,$$

6.4 Axiomatic approach

a property which is fulfilled by E_D and E_C . For multipartite systems, there is generally no such natural condition due to the non-existence of maximally entangled states.

2. *Asymptotic continuity.* In the asymptotic limit of infinite copies of one state, it turns out to be useful to require the following form of continuity. Suppose ρ_n, σ_n act on \mathcal{H}_n with dimension d_n , then asymptotic continuity requires

$$\text{if } \|\rho_n - \sigma_n\|_1 \rightarrow 0 \quad \Rightarrow \quad \frac{|E(\rho_n) - E(\sigma_n)|}{\log d_n} \rightarrow 0.$$

Note, that for finite dimensional Hilbert spaces asymptotic continuity is equivalent to regular continuity, but gets modified for $n \rightarrow \infty$. Later on, asymptotic continuity will be needed to obtain a unique measure of entanglement for pure states.

3. *Convexity.* Most of the known entanglement measures are convex, i.e. satisfy for $t \in [0, 1]$

$$E(t\rho + (1-t)\sigma) \leq tE(\rho) + (1-t)E(\sigma).$$

6.4.2 CLASSES OF ENTANGLEMENT MEASURES

As examples for functions build up to satisfy both entanglement axioms, we will show two classes of entanglement measures, containing two of the most important measures. More examples can be found in [2].

Entanglement measures based on distance

A class of entanglement measures are based on the natural intuition, that the closer the state is to the set of separable states, the less entangled it is. A more general approach consists of minimising distance to a generic set \mathcal{S} which is closed under LOCC operations. Let \mathcal{D} be a metric on $\mathcal{S}(\mathcal{H})$. Then

$$E_{\mathcal{D}, \mathcal{S}}(\rho) = \inf_{\sigma \in \mathcal{S}} \mathcal{D}(\rho, \sigma)$$

satisfies axiom 1 if \mathcal{D} is monotonous under all operations T , i.e. $\mathcal{D}(\rho, \sigma) \geq \mathcal{D}(T(\rho), T(\sigma))$. If \mathcal{S} is chosen to be the set of separable states, axiom 2 is also satisfied. The most important measure in this class is *relative entropy of entanglement*

$$E_R = \inf_{\sigma \in \text{SEP}} \text{Tr} \rho (\log \rho - \log \sigma).$$

Convex roof measures

Here, one starts with a strong monotonous entanglement measure $E|_{\text{pure}}$ defined on pure states. It is then extended to mixed states by convex roof

$$E(\rho) = \inf \sum_i p_i E(\psi_i), \quad \sum_i p_i = 1, \quad p_i \geq 0,$$

where the infimum is taken over all ensembles $\{p_i, \psi_i\}$ for which $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. The infimum is reached on a particular ensemble which is called optimal. It has been shown that convex roof measures satisfy stronger monotonicity and axiom 2, if one starts with a strong monotonous entanglement measure on pure states as required above. Furthermore, one can check that $E(\rho)$ is convex. The most important measure in this class is *entanglement of formation* E_F , being the convex roof extension of entropy of subsystem

$$E(\rho_{AB})|_{\text{pure}} = S(\rho_A).$$

This construction has the advantage that statements solely proven for pure states can sometimes easily be extended to mixed states. Because of this reason and the fact that one can make strong statements about entropy in high dimensional bipartite systems, we will use E_F as entanglement measure for the remainder of this chapter.

There are various other (classes of) entanglement measures with useful properties in specific contexts, lots of which are described in [2].

6.4.3 ALL MEASURES FOR PURE BIPARTITE STATES

Now, that we have seen examples of entanglement measures and discussed useful additional properties, it is natural to wonder whether these entanglement measures, looking very different at first sight, can be written in a unified way. This is related to the construction of new measures and to the question whether one can build up measures from functions which properties are easier verifiable than monotonicity. In fact, these question can be answered in the case of pure bipartite states. Let $E(\rho_{AB})$ be a strong monotonous entanglement measure. Then E can be written on pure states as

$$E(\rho_{AB})|_{\text{pure}} = f(\rho_A), \quad \text{for some } f \text{ satisfying}$$

- (i) $f(\lambda_1, \dots, \lambda_k, 0, \dots, 0)$ symmetric, expansible
- (ii) f is concave in ρ .

6.5 Entanglement of random states

Expansibility means, that one can forget about the zero eigenvalues, i.e.

$f(\lambda_1, \dots, \lambda_k, 0, \dots, 0) = f(\lambda_1, \dots, \lambda_k)$. In this way, all possible entanglement measures for pure states are characterised. Conversely, if one starts with $E(\rho_{AB}) = f(\rho_A)$, where f satisfies (i) and (ii), one can construct an entanglement measure by convex roof extension. Therefore, we see that entanglement of formation E_F with $f = S$, satisfying (i) and (ii), has a natural form in this context.

6.4.4 ASYMPTOTIC CASE, UNIQUENESS

Although all entanglement measures for pure states can be characterised in a unified way, they might have very different behaviour. For instance, one can show that entanglement measures generally impose different orderings, i.e. for two measures E, E' there can exist states ρ, σ with $E(\rho) \geq E(\sigma)$, but $E'(\rho) < E'(\sigma)$. Since in the rest of this chapter we will work with a very specific entanglement measure E_F , it is natural to ask whether the proven properties can be transferred to other measures. Therefore, it is good to know that for measures with certain properties, including E_F , there is a *unique* entanglement measure and we can work with E_F without loss of too much generality.

In the asymptotic limit, where one considers the limiting case of infinite copies of one system, entanglement measures have to be regularised in order to be well defined. The regularisation of any function f is defined as

$$f^\infty(\rho) = \lim_{n \rightarrow \infty} \frac{1}{n} f(\rho^{\otimes n}), \quad (6.13)$$

if the limit exists. Regularised entanglement measures have the nice property that they are proportional to the number of copies of a state, i.e. $E^\infty(\rho^{\otimes n}) = nE^\infty(\rho)$. It turns out, that if a function E is regularisable, monotonous under LOCC, asymptotically continuous and satisfies $E(\psi_d^+) = \log d$, then we have

$$E_D \leq E^\infty \leq E_C. \quad (6.14)$$

Because of $E_D = E_C$ on pure states, this in particular implies that all measures with the above properties are the same on pure states. In this sense, one can say that for pure states regularisation of any entanglement measure is equal to entropy of subsystem $S(\rho_A)$, i.e. we have a unique entanglement measure.

6.5 ENTANGLEMENT OF RANDOM STATES

Up to now, we have discussed the basic notion of entanglement and how one can consistently define functions which measure the amount of entanglement in

a state. However, it is natural to wonder whether entangled states play an important part in nature and how much entanglement one can typically expect. We shall see, that surprisingly in bipartite systems, if the dimension is chosen large enough, nearly all states are near-maximally entangled. To be more precise, randomly drawn states are extremely likely to have near-maximal entanglement, in fact, so likely that, with high probability, a random subspace of dimension close to the total dimension contains only near-maximally entangled states. This will turn out to be a consequence of the "concentration of measure" phenomenon, meaning that with large probability, certain parameters of randomly chosen states are close to their expectation.

Notation. First, we will collect the conventions and general assumptions used throughout the following part. The Hilbert space of the high dimensional bipartite system under consideration will be denoted by $\mathcal{H} = A \otimes B$, where A and B have dimension $d_A \leq d_B$, respectively. Density matrices on \mathcal{H} will be denoted by φ and can be, unless otherwise stated, mixed or pure. Pure states $\varphi = |\varphi\rangle\langle\varphi|$ will be associated with the ket $|\varphi\rangle$. The expectation value of a random variable X will be denoted by $\mathbb{E}X$. Finally, we will use entanglement of formation as entanglement measure, i.e.

$$E(\varphi) = E_F(\varphi) = \min_{\varphi = \sum_i p_i |\varphi^i\rangle\langle\varphi^i|} \sum_i p_i S(\varphi_A^i),$$

which on pure states is simply entropy of subsystem

$$E_F(|\varphi\rangle) = S(\varphi_A). \quad (6.15)$$

Since we will often mention near-maximal entanglement, we will now calculate the maximal possible entanglement in the system. We know, that $|\phi_{d_A}^+\rangle = \frac{1}{\sqrt{d_A}} \sum_i |i\rangle|i\rangle$ is a maximally entangled state. By calculating the matrix representation of its orthogonal projector $\phi_{d_A}^+ = |\phi_{d_A}^+\rangle\langle\phi_{d_A}^+|$ with respect to the basis $|i\rangle|j\rangle$ and taking the partial trace, one ends up with $(\phi_{d_A}^+)_A \hat{=} \frac{1}{d_A} \mathbb{1}$. Therefore, we see that $(\phi_{d_A}^+)_A$ has d_A times the eigenvalue $1/d_A$ and can calculate its entropy by using the formula from part 1.2.2. The maximal entanglement in our system is hence $S(\frac{1}{d_A} \mathbb{1}) = \log d_A$.

6.5.1 RANDOM STATES AND SUBSPACES

The statements, that we will proof in the following, are based on the assumption that states are drawn uniformly at random from the large bipartite system $\mathcal{H} = A \otimes B$. The fact, that for pure states there is a unique "uniform" distribution that is unitarily invariant allows us to define a precise prescription of what

6.5 Entanglement of random states

we mean by "random state". It is induced by the Haar measure on the unitary group, which is a generalisation of the Lebesgue measure to locally compact topological groups.

Definition 1 (random state)

A random pure state φ is any random variable distributed according to the unique unitarily invariant probability measure on the pure states $\mathcal{P}(\mathcal{H})$ of \mathcal{H} . We formally express this by writing $\varphi \in_R \mathcal{P}(\mathcal{H})$.

Furthermore, we will also need to draw subspaces of a certain dimension uniformly at random, which can be defined similarly.

Definition 2 (random subspace)

A random subspace S of dimension s is any random variable distributed according to the unitarily invariant measure on the s -dimensional subspaces of \mathcal{H} , denoted by $\mathcal{G}_s(\mathcal{H})$. We express this using the notation $S \in_R \mathcal{G}_s(\mathcal{H})$.

An analogous definition for mixed states is not possible, since unitary invariance in this case does not uniquely specify a probability measure. Instead, one can use the unitarily invariant measure on pure states to induce a probability measure on mixed states by partial tracing, see [1].

With the above definitions, one is able to demonstrate that the expectation value of entanglement $\mathbb{E}S(\varphi_A)$ in our system is bounded below in the following way.

Lemma 1 (Near-maximal expectation value of entanglement)

Let $|\varphi\rangle \in_R \mathcal{P}(A \otimes B)$ be chosen uniformly at random. For $d_A \leq d_B$, we have

$$\mathbb{E}S(\varphi_A) > \log d_A - \frac{1}{2}\beta, \quad \beta = \frac{1}{\ln 2} \frac{d_A}{d_B}.$$

Because of $d_A \leq d_B$, the function $\beta(d_A, d_B)$ does not grow for $d_A \rightarrow \infty$ and is at most of the order of magnitude 10^0 . Therefore, for d_A large enough, the term proportional to β is negligible and the expectation value of entanglement is only slightly less than the maximal possible value $\log d_A$.

6.5.2 CONCENTRATION OF MEASURE

Every "slowly varying" function on the unit sphere \mathbb{S}^k , interpreted as a random variable induced by the sphere's uniform measure, will take values close to the *average* except for a set of volume exponentially small in k . This is the basic statement of Levy's Lemma, which rigorously formalises the above. It describes a phenomenon of concentration of function values for functions on \mathbb{S}^k , if the

dimension is chosen large enough. Since normalised states ("kets") are elements of the unit sphere of a certain dimension, Levy's Lemma can be applied to functions acting on physical states. In fact, applied to the special case of entanglement measure, it will turn out to be the crucial theorem in order to prove all following statements.

To put it more formally, we observe that the unit sphere is isomorphic to the set of normalised pure states $\mathbb{S}^k \simeq \mathcal{P}(A \otimes B)$ if their dimensions agree. Since $A \otimes B$ has $2d_A d_B$ real dimensions and the normalisation condition removes one real degree of freedom, we have to require $k = 2d_A d_B - 1$. We then are able to apply Levy's Lemma, which reads as

Lemma 2 (Levy's Lemma)

Let $f: \mathbb{S}^k \rightarrow \mathbb{R}$ be a function with Lipschitz constant $\eta = \max|\nabla f(X)|$. Let $X \in_R \mathbb{S}^k$ be chosen uniformly at random. For $\alpha \geq 0$, we have

$$\Pr \{|f(X) - \mathbb{E}f| \geq \alpha\} \leq 2 \exp(-C_1(k+1)\alpha^2/\eta^2),$$

with an absolute real constant $C_1 > 0$, which may be chosen as $C_1 = (9\pi^3 \ln 2)^{-1}$.

This means, that the probability that f deviates from its expectation value more than by α is upper bounded by the term on the right side. If f is slowly varying, i.e. η^2 grows slower with d_A than k , and α is fixed, the right expression approaches zero if d_A and thus k is chosen large enough. Therefore, under the above conditions, it is very likely that f is close to its expectation if d_A is large enough.

We are going to apply Levy's Lemma to entanglement E of a random state $|\varphi\rangle \in_R A \otimes B$, i.e. we fix $f(|\varphi\rangle) = S(\varphi_A)$. In order to ensure that f is slowly varying, it is possible to show that the Lipschitz constant η of $S(\varphi_A)$ is upper bounded by $\sqrt{8} \log d_A$, if $d_A \geq 3$. The combination of both Lemmas then immediately implies the first theorem; Lemma 1 states that the expectation value of entanglement $S(\varphi_A)$ is near-maximal. Lemma 2 states that it is very likely that $S(\varphi_A)$ does not deviate very much from its expectation value. We can therefore conclude

Theorem 1 (Concentration of entropy)

Let $|\varphi\rangle \in_R \mathcal{P}(A \otimes B)$ be a random state on $A \otimes B$, with $d_B \geq d_A \geq 3$. Then

$$\Pr \{S(\varphi_A) < \log d_A - \alpha - \beta\} \leq \exp\left(-\frac{(d_A d_B - 1)C_2 \alpha^2}{(\log d_A)^2}\right),$$

where $\beta(d_A, d_B)$ is the same as in Lemma 1 and $C_2 = (8\pi^2 \ln 2)^{-1}$.

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Because of $(d_A d_B > d_A^2)/(\log d_A)^2 \rightarrow \infty$ for $d_A \rightarrow \infty$, the expression on the right is negligible for fixed α , if d_A is large. Since $\log d_A \gg \beta$ for $d_A \rightarrow \infty$ and α can be chosen small, we conclude: with very high probability, a random pure state is almost maximally entangled, if d_A is large enough.

6.5.3 MAXIMALLY ENTANGLED SUBSPACES

The goal of this section is to put together the insights from the previous section to make an even "stronger" statement than Theorem 1; we show that a randomly chosen large subspace of $\mathcal{P}(A \otimes B)$ with appropriate dimension, will with high probability contain only near-maximally entangled states. A further necessary tool in order to prove the theorem is a specifically constructed "small" net in state space.

Lemma 3 (Existence of small nets)

For $0 < \epsilon < 1$ and $\dim \mathcal{H} = d$ there exists a subset of pure states $\mathcal{N} \subset \mathcal{H}$ with $|\mathcal{N}| \leq (5/\epsilon)^{2d}$ such that:

$\forall |\varphi\rangle \in \mathcal{H} \exists |\tilde{\varphi}\rangle \in \mathcal{N}$ with $\| |\varphi\rangle - |\tilde{\varphi}\rangle \|_2 \leq \epsilon/2$ and $\|\varphi - \tilde{\varphi}\|_1 \leq \epsilon$. (We call such a set an ϵ -net.)

This means, that the ϵ -net is constructed in such a way, that for any pure state in our system we are able to find an element of the net which is at most ϵ "away", i.e. is contained in the ball of radius ϵ around the state. Now, we are able to formulate and prove the main theorem.

Theorem 2 (Entangled subspaces)

Consider quantum systems A, B with dimensions $d_B \geq d_A \geq 3$. Let $0 < \alpha < \log d_A$. Then, there exists a subspace $S \subset A \otimes B$ of dimension

$$s = \left\lfloor d_A d_B \frac{\Gamma \alpha^{2.5}}{(\log d_A)^{2.5}} \right\rfloor$$

such that all $|\varphi\rangle \in S$ have entanglement at least

$$E(\varphi) = S(\varphi_A) \geq \log d_A - \alpha - \beta,$$

with β as in Lemma 1 and an absolute constant $\Gamma = 1/1753$. The probability that a random subspace of dimension s will not have this property, i.e. there is at least one state with less entanglement, is bounded above by

$$\left(\frac{15 \log d_A}{\alpha} \right)^{2s} \exp \left(- \frac{(d_A d_B - 1) \alpha^2}{32 \pi^2 \ln 2 (\log d_A)^2} \right)$$

Proof: Let $S \subset_R A \otimes B$ be a random subspace of $\mathcal{P}(A \otimes B)$ of dimension s . Let \mathcal{N}_S be an ϵ -net on S , where we choose ϵ to be $\epsilon = \alpha/(\sqrt{8} \log d_A)$. Given $|\varphi\rangle \in S$, we can find $|\tilde{\varphi}\rangle \in \mathcal{N}_S$ such that $\| |\varphi\rangle - |\tilde{\varphi}\rangle \|_2 \leq \epsilon/2$. We then estimate the difference in entanglement of $|\varphi\rangle$ and $|\tilde{\varphi}\rangle$

$$|S(\varphi_A) - S(\tilde{\varphi}_A)| \leq \frac{\epsilon}{2} \cdot \eta \leq \frac{\alpha}{2\sqrt{8} \log d_A} \cdot \sqrt{8} \log d_A = \frac{\alpha}{2}, \quad (6.16)$$

where in the second inequality we used the Lipschitz estimate for $S(\varphi_A)$ from before, as well as the explicit choice of ϵ . By using Theorem 1, we are now able to estimate

$$\begin{aligned} \Pr \left\{ \inf_{|\varphi\rangle \in S} S(\varphi_A) < \log d_A - \alpha - \beta \right\} &\leq \Pr \left\{ \min_{|\tilde{\varphi}\rangle \in \mathcal{N}_S} S(\tilde{\varphi}_A) < \log d_A - \frac{\alpha}{2} - \beta \right\} \\ &\leq |\mathcal{N}_S| \Pr \left\{ S(\varphi_A) < \log d_A - \frac{\alpha}{2} - \beta \right\} \\ &\leq \left(\frac{15 \log d_A}{\alpha} \right)^{2s} \exp \left(-\frac{(d_A d_B - 1)\alpha^2}{32\pi^2 \ln 2 (\log d_A)^2} \right). \end{aligned}$$

In the first line, we went from a generic pure state to the closest element of the net, thereby changing the upper bound by using (1.16). Since the net is a finite set, the infimum becomes a minimum. In the second line, we did a basic estimate following from the axioms of probability theory, to show that the probability that the least entangled states has entanglement less than $\log d_A - \alpha/2 - \beta$ is upper bounded by the size of the net times the probability that a randomly chosen state has entanglement less than $\log d_A - \alpha/2 - \beta$. In the third line, we inserted the size of the net according to Lemma 3 and used Theorem 1 to estimate the probability factor. Our previous analysis of the large d_A -behaviour of the right factor of the final bound is valid here as well. Additionally, we see that in the limit $d_A \rightarrow \infty$, the right factor goes faster to zero than the left factor to infinity and therefore the whole expression to zero. Hence, we conclude that the probability to find an element of S with entanglement less than $\log d_A - \alpha/2 - \beta$ becomes negligible if we choose d_A large enough. Note, on the other hand, that the dimension s of the subspace is in the large d_A -limit comparable to the total dimension $d_A d_B$, i.e. random subspaces with the previous property can be considered large. In summary, we can conclude that for high-dimensional bipartite systems random subspaces of appropriate (large) dimension are very likely to contain only near-maximally entangled pure states. Because of the convex roof construction of our entanglement measure E_F , a similar statement follows for generic mixed states as a corollary, see [1].

6.6 CONCLUSION

We have seen, that the transition from classical configuration space to quantum Hilbert space gives rise to a new class of states in the description of composite systems. These entangled states are the source of non-classical phenomenon and a requirement for performing non-classical tasks such as quantum teleportation. Furthermore, we discussed measures which quantify the amount of entanglement in a state; we have seen, what properties are required from these measures, which properties are desirable in certain contexts and answered questions of unified description and uniqueness. At last, we have seen that the concentration of measure phenomenon in high dimensional bipartite systems has the implication that random physical states are extremely likely to have near-maximal entanglement. Therefore, entangled states play a major role in the description of quantum systems.

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CHAPTER 7

TRANSPORTING INFORMATION BY DESTROYING CORRELATIONS

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7.1 INTRODUCTION

The aim of this work is to illustrate communication over noisy channels. The focus of the first part will be on classical communication theory, whereas in the following part attention will be spent to explain quantum communication. This will be done making use of one important property of quantum mechanics, which allows to find, given any reduced density matrix, a pure state on a larger Hilbert space compatible with it. Basically, to do this, the so-called purification theory will be applied to quantum communication. This will eventually allow the reader to understand the meaning of transporting information by destroying correlations.

7.2 CLASSICAL COMMUNICATION OVER NOISY CHANNELS

The transfer of information is in reality always related to a certain degree of noise. For example, almost everybody has encountered in his daily life some troubles in communicating with someone on the opposite side of a telephone line. In the specific case, it is due to some kind of interference occurring along the connection line. This kind of interference, better known as "noise", is basically present to different extents in every information processing system. As a result, to cope

7.2 Classical communication over noisy channels

with this problem, several error-correcting codes have been developed to allow a reliable communication and computation in spite of the presence of severe noise. Given a particular noisy communication channel \mathcal{N} an interesting question is how much information can be transmitted reliably through that channel. Figure 7.1 depicts the scheme of a typical classical communication channel. In our example, let's assume that Alice wants to send the message m from a message set $[M] = \{1, \dots, M\}$ to her friend Bob. In this model, an encoder \mathcal{E} will create for each m a binary sequence of n bits $x^n = (x_1, \dots, x_n)$, which will pass through a noisy channel, denoted in the figure as \mathcal{N} . Finally a decoder \mathcal{D} will be required to decode the codeword $y^n = (y_1, \dots, y_n)$ that corresponds to the output of the channel and to create the message \hat{m} that will be received by Bob. In this case, the communication will be successful if Bob's message is the same as Alice's message, suggesting that the encoder/decoder pair was able to transmit the information through the noisy channel.

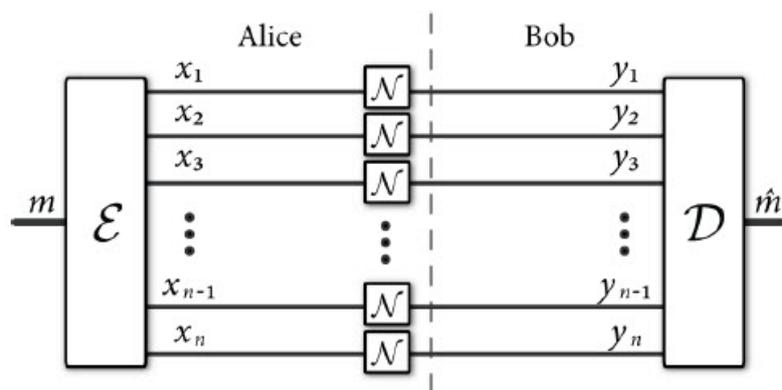


Figure 7.1: The classical channel code

To obtain a successful decoder/encoder pair, a larger number of bits needs to be produced than one would need if there would be no noise in the system. Let's go back to Alice and Bob's situation. In this case, the message set has M elements. The smallest binary representation of this set would be $\lceil \log_2(M) \rceil$. However, the encoder will create a binary string with n elements that are more than $\lceil \log_2(M) \rceil$ bits to allow the decoder to filter out the noise. At this point, to define the performance of communication scheme, it is necessary to introduce the so-called rate, which relates the message bits $\log_2(M)$ with the n bits created by the decoder. This is defined as

$$\text{Rate } R = \frac{\text{number of message bits}}{\text{number of channel uses}} = \frac{\log_2(M)}{n}$$

Let's assume that for a channel there are 12 different uses to transmit 6 bits of information (a message set with 64 elements) using an appropriate encoder/decoder pair. In this case the code will have a rate of $R = \frac{6}{12} = \frac{1}{2}$. One fundamental problem in information theory is the determination of the maximum rate for reliable communication through n uses of the channel. The maximum rate is defined as the capacity of the channel. For classical noisy communication channels the capacity of the channel can be inferred by using the so-called Shannon's noisy channel coding theorem. To better understand the application of this theorem, some preliminary concepts will be presented in the next paragraphs.

7.2.1 SHANNON ENTROPY

The Shannon entropy theorem is fundamental to define the amount of information in an object. Therefore it can be seen as the basis of all concepts developed in quantum information theory.

MATHEMATICAL DEFINITION

$$H(X) = - \sum_{i=1}^n p(x_i) \log_2 p(x_i)$$

where X is a random variable (a source), which takes possible value $\{x_1, \dots, x_n\}$ with probability $\{p(x_1), \dots, p(x_n)\}$. As can be seen from this equation, the Shannon entropy is nothing else than the information content of X or, in other words, a measure of the lack of information about X.

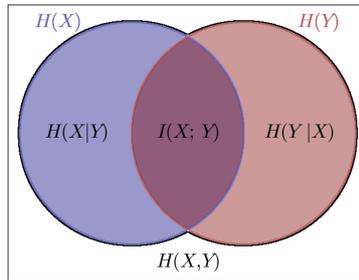


Figure 7.2: Different entropies for two random variables X and Y.

7.2 Classical communication over noisy channels

EXAMPLES

- n possible values sharing all the same probability $p(x_i) = \frac{1}{n}$:

$$H(X) = - \sum_{i=1}^n \frac{1}{n} \log_2 \frac{1}{n} = \log_2 n$$

- for a binary variable with two values: 1 with probability p and 0 with probability $1-p$. The binary entropy function $H(p)$ is

$$H(p) = -p \log_2 p - (1-p) \log_2 (1-p)$$

- Conditional entropy $H(X|Y)$ is defined by

$$H(X|Y) = - \sum_y p(y) \sum_x p(x|y) \log_2 p(x|y) = - \sum_y \sum_x p(x,y) \log_2 p(x|y)$$

where $p(y)p(x|y) = p(x,y)$. It is a measure of what Y is not saying about X . The relation $H(X|Y) = H(X,Y) - H(Y)$ holds (can be seen graphically in figure 7.2), where $H(X,Y)$ is the information content of X and Y .

- Mutual Information is a measure of how much X and Y contain information about each other and is defined by

$$I(X : Y) = - \sum_x \sum_y p(x,y) \log_2 p(x : y)$$

where $p(x : y) = \frac{p(x)p(y)}{p(x,y)}$ is the mutual probability.

7.2.2 CLASSICAL CAPACITY OF A NOISY CHANNEL

The Shannon's noisy channel coding theorem describes the capacity of a memoryless channel. This theorem owes his name to the mathematician Claude Shannon, who has developed it in 1948 by using techniques that were not common at that time. The "capacity" of a channel can be seen as the maximal possible amount of data that can be sent through that channel, while "memoryless" means that the channel acts in the exact same way for every use, i.e. the uses of each channel are completely independent. For this reason, it is typical to draw in the communication scheme n equal channels instead of n uses of the same channel. Figure 3 illustrates the basic idea behind the Shannon's noisy channel coding theorem. Going back to Alice and Bob's example, in the first stage one of 2^{nR} possible messages M is produced by Alice and is encoded using a map

$$\mathcal{E} : \{1, \dots, 2^{nR}\} \longrightarrow \mathcal{X}^n$$

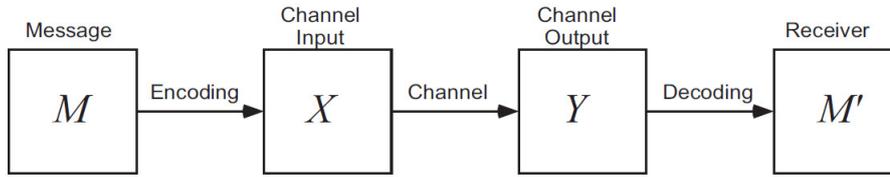


Figure 7.3: The noisy coding problem for classical messages. The channel changes the binary signal X to Y with a certain probability.

which assigns to each of Alice's possible messages an input. This is then sent through n uses of the channel to Bob, who decodes the channel output using a map

$$\mathcal{D} : \mathcal{Y}^n \longrightarrow \{1, \dots, 2^{nR}\}$$

which assigns a message to each string for each possible output from the channel. In principle all messages may have different probabilities to be changed through the communication line. For a given encoding and decoding pair, the error probability is defined as

$$Pr_e(\mathcal{E}_n, \mathcal{D}_n) = \max_{m \in \mathcal{M}} Pr(m \neq \hat{m})$$

where \hat{m} is the message at the output.

A rate R is said to be achievable if there is such a sequence of encoding/decoding pairs $(\mathcal{E}_n, \mathcal{D}_n)$ so that $Pr_e(\mathcal{E}_n, \mathcal{D}_n) \longrightarrow 0$ as $n \longrightarrow \infty$. The **capacity** $C(\mathcal{N})$ of a given noisy channel \mathcal{N} is defined to be the supremum over all achievable rates for the channel.

$$C(\mathcal{N}) = \sup\{R | R \text{ achievable}\}$$

SHANNON NOISY CHANNEL CODING THEOREM

For a noisy channel \mathcal{N} the capacity is given by

$$C(\mathcal{N}) = \max_{p(x)} I(X : Y)$$

where the maximum is taken over all input distributions $p(x)$ for X , for one use of the channel. Y is the corresponding induced random variable at the output of the channel.

From the above description, it is well apparent that the Shannon's noisy channel coding theorem dramatically simplifies the calculation of capacity, reducing it to a simple and well-defined optimization problem that can be solved exactly in many cases.

7.2 Classical communication over noisy channels

CLASSICAL BIT-FLIP CHANNEL

In this section the bit-flip channel will be considered in the classical and quantum mechanical context. This is a rather simple case, which is nevertheless very useful to illustrate the basic concept of a noisy channel coding. The bit-flip channel is a noisy communication channel for a single bit of information, whose main function lies in flipping the bit being transmitted with probability $p > 0$, while the bit is transmitted without error with probability $1 - p$. The effect of this channel is shown in figure 7.4.

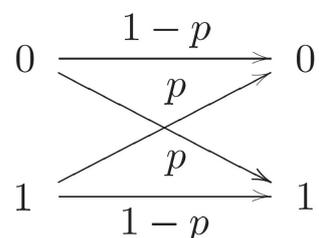


Figure 7.4: The effect of noise for a single bit

Using error-correcting codes it is possible to transmit information through this channel.

Let's now assume that every input bit of the channel has a fixed probability distribution of q for 0 and $1 - q$ for 1 and that every message from the message set gets from the encoder \mathcal{E} a codeword $x^n = (x_1, \dots, x_n)$. It is assumed that the codeword $(0, \dots, 0) = c_0$ will be sent through the bit-flip channel. The channel will then flip np bits of the codeword c_0 resulting in a new codeword that contains with high probability np ones and $(1-p)n$ zeros (under the assumption of large n). As can be seen from Figure 5, the most probable output messages will necessarily lie on the surface of a sphere with radius np , called the Hamming sphere.

Thus, the elements of the message set can be graphically represented as a Hamming sphere containing $2^{nH(p)}$ elements (Figure 6). Recalling the definition of the rate it is therefore possible to write $M = 2^{nR}$, which implies - according to theorem of typical sequences - that the space where all spheres lie is about the size of $2^{nH(Y)}$.

Requiring no or just a small overlap between the Hamming spheres, will result in the condition:

$$M2^{nH(p)} < 2^{nH(Y)}$$

which can be reformulated to

$$R < H(Y) - H(p)$$

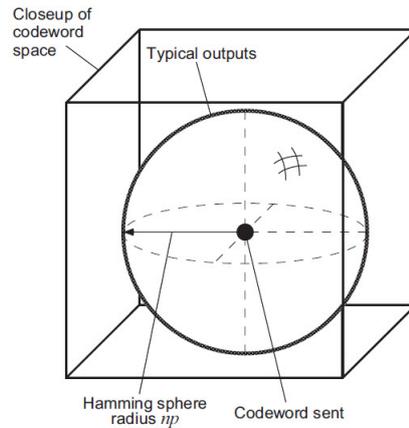


Figure 7.5: Hamming sphere

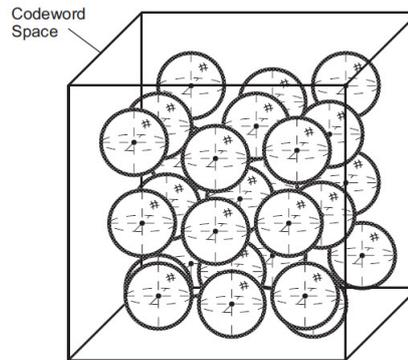


Figure 7.6: Hamming spheres in the typical output space

$H(p)$ is related with the flipping probability of the channel and is typically specified by the error probability p of the channel. Since the capacity of the channel is given by the highest achievable rate, the right-hand part of the equation should be as large as possible, leading to a higher value for R . As the Shannon entropy $H(Y)$ for the random variable Y depends from the *a priori* distribution $(q, 1 - q)$, it is fundamental to find a value for q so that $H(Y)$ is maximal. A simple calculation shows that this is achieved by using the uniform *a priori* distribution corresponding to $q = \frac{1}{2}$, for which $H(Y) = 1$. This means that it is possible to achieve the rate R for any R less than $1 - H(p)$. However, for any R higher than $1 - H(p)$, the Hamming spheres start to overlap too much making impossible - no matter how the codewords were chosen - the determination of codeword that was sent. Thus

$$1 - H(p) =: C(\mathcal{N})$$

7.3 The purified quantum theory

is the capacity of the bit-flip channel. In the case the Hamming spheres do not overlap, it is rather easy to decode the output of the channel. In our example, Bob will simply check whether the output is in one of the Hamming spheres and, if so, output the corresponding codeword. Otherwise the message will be discharged and Alice has to resend the message.

By applying the Shannon's noisy channel coding theorem for the bit-flip channel it is now possible to show that the same expression for the capacity of the channel will be obtained.

According to the Shannon's noisy channel coding theorem the capacity is given over the maximum of all mutual entropies $I(X : Y)$, therefore

$$I(X : Y) = H(Y) - H(Y|X) = H(Y) - \sum_x p(x)H(Y|X = x)$$

But for each x , $H(Y|X = x) = H(p)$ so

$$I(X : Y) = H(Y) - H(p)$$

which is maximized by choosing $q = \frac{1}{2}$, so $H(Y) = 1$ and therefore the capacity is

$$C(\mathcal{N}) = 1 - H(p)$$

as already shown before. For further information on classical and quantum Shannon Theory see [1].

7.3 THE PURIFIED QUANTUM THEORY

In the following part the focus will move from the classical to the quantum information theory. To better understand this, it is necessary to introduce some basic tools that will be used along the chapter. Let's start first with the purification of a system. The lack of information about a set of quantum states can be seen as resulting from entanglement with another system, which is inaccessible. Making use of this inaccessible system it is possible to purify the set of quantum states leading to a pure state in a bigger system.

The Bell state $|\Phi^+ \rangle^{AR}$, which is known to be a maximally entangled state, can be used as an example. This state is a pure state on the joint system of Alice A and a reference system R, but the local state in Alice system is the maximally mixed state $\Pi^A = \frac{I}{2}$. Purification can be interpreted by thinking that Alice state Π^A arises from the entanglement of her system with the reference system R. (See also [2])

7.3.1 PURIFICATION THEOREM

Suppose a density operator ρ^A on a system A is given, which is arising from the ensemble $\{p_X(x), |x \rangle\}$. As mentioned above, connected to Alice's system there is a reference system R (Figure 7). A purification of ρ^A is a pure bipartite state $|\psi \rangle^{RA}$ with the property that the reduced state on system A is equal to

$$\rho^A = Tr_R\{|\psi \rangle \langle \psi|^{RA}\}$$

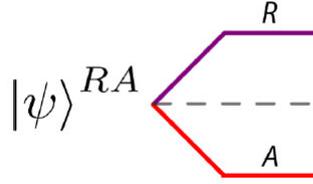


Figure 7.7: The pure state $|\psi \rangle^{RA}$ is the purification of the state ρ_A

It is important to note that for any density operator a purification on a joint system with the reference system R will exist. One possible realisation of a purification could be, for example

$$|\psi \rangle^{RA} = \sum_x \sqrt{p_X(x)} |x \rangle^R |x \rangle^A$$

where the set $\{|x \rangle^R\}_x$ of vectors are some set of orthonormal vectors for the reference system R.

7.3.2 THEOREM OF UNITARY EQUIVALENCE OF PURIFICATIONS

Let $\mathcal{H}(A)$ and $\mathcal{H}(E)$ be Hilbert spaces and suppose that $|\phi \rangle, |\psi \rangle \in \mathcal{H}(A) \otimes \mathcal{H}(E)$ satisfies

$$Tr_E(|\phi \rangle \langle \phi|^{AE}) = Tr_E(|\psi \rangle \langle \psi|^{AE})$$

Then there exists a unitary operator U such that $|\psi \rangle^{AE} = (1_A \otimes U)|\phi \rangle^{AE}$. This operator $(1_A \otimes U)$ leaves the states in $\mathcal{H}(A)$ unchanged and changes only the states in the environment $\mathcal{H}(E)$.

7.3.3 ISOMETRIC EXTENSION OF A GENERAL NOISY QUANTUM CHANNEL

Until now it has been shown how to purify a density matrix. A similar idea will be applied to purify noisy channels. Let $\mathcal{N}^{A \rightarrow B}$ denote a noisy quantum

7.3 The purified quantum theory

channel, where this notation implies the quantum system A as an input and the quantum system B as an output. The purification of this channel is called isometric extension denoted by $U_{\mathcal{N}}^{A \rightarrow BE}$, where an additional environment system E comes into play (Figure 8).

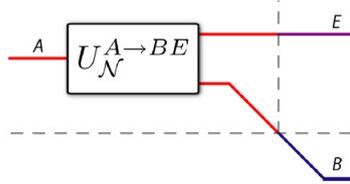


Figure 7.8: Isometric extension of a channel $\mathcal{N}^{A \rightarrow B}$

By ignoring the additional environment E, the noisy channel $\mathcal{N}^{A \rightarrow B}$ will result. An isometry will therefore possess the following two properties:

- By tracing out the environment system, it produces the evolution of the noisy quantum channel $\mathcal{N}^{A \rightarrow B}$:

$$\text{Tr}_E\{U_{\mathcal{N}}^{A \rightarrow BE}(\rho)\} = \mathcal{N}^{A \rightarrow B}(\rho)$$

where ρ is any density operator input to the channel $\mathcal{N}^{A \rightarrow B}$

- It is analogous to a rectangular matrix that behaves somehow like a unitary operator with the two properties:

$$U_{\mathcal{N}}^\dagger U_{\mathcal{N}} = I^A$$

$$U_{\mathcal{N}} U_{\mathcal{N}}^\dagger = \Pi^{BE}$$

ISOMETRIC EXTENSION OF A BIT-FLIP CHANNEL

The bit-flip channel works in a similar way to the bit-flip channel in classical communication theory. Basically, the channel flips a qubit with a probability of p and leaves it unchanged with the corresponding probability $(1 - p)$. The matrix representation of this operation is given by the Pauli matrix:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

When a qubit system A in the state $|\psi\rangle$ is used as an input for this type of channel, the ensemble corresponding to the state at the output has the form:

$$\{\{1 - p, |\psi\rangle\}, \{p, X|\psi\rangle\}\}$$

and the density operator of the resulting state is

$$\rho_A = (1 - p)|\psi\rangle\langle\psi| + pX|\psi\rangle\langle\psi|X^\dagger$$

One possible representation of the purification of ρ_A is:

$$\sqrt{1-p}|\psi\rangle^A |0\rangle^E + \sqrt{p}X|\psi\rangle^A |1\rangle^E$$

The above map is an isometric extension of the bit-flip channel, that can be rewritten as

$$U^{A \rightarrow AE} : |\psi\rangle^A \longrightarrow \sqrt{1-p}|\psi\rangle^A |0\rangle^E + \sqrt{p}X|\psi\rangle^A |1\rangle^E$$

An isometry is very similar to a unitary operator with the sole difference that it maps states on one input system to states on a joint system. The matrix representation of the bit flip isometry is given by:

$$U^{A \rightarrow AE} = \begin{bmatrix} \sqrt{1-p} & 0 \\ 0 & \sqrt{p} \\ 0 & \sqrt{1-p} \\ \sqrt{p} & 0 \end{bmatrix}$$

For $p \neq 0$, i.e. when noise is present in the channel, there is entanglement of the input system with the environment E. By tracing out the environment E, it is possible to obtain the noisy evolution of the input system and, similarly, tracing out Bob's system, to obtain the information reaching the environment E. This will be the topic of the next subsection.

COMPLEMENTARY CHANNEL

Coming back to the the example of Alice and Bob, some quantum information can be transferred from Alice's system to the environment E. As already pointed out before, it is possible to get the output of environment from the quantum channel simply by tracing out every system except the environment itself. The map from the sender to the environment is defined as a complementary channel. Tracing out A from the isometric extension of the bit-flip channel, one could compute that the environment receives the following density operator

$$\begin{aligned} & Tr_A \{ (\sqrt{1-p}|\psi\rangle^A |0\rangle^E + \sqrt{p}X|\psi\rangle^A |1\rangle^E) (\sqrt{1-p}\langle\psi|^A \langle 0|^E + \sqrt{p}X^\dagger \langle\psi|^A \langle 1|^E) \} \\ & = \dots = (1-p)|0\rangle\langle 0|^E + \sqrt{p(1-p)}2Re(\alpha^*\beta)(|1\rangle\langle 0|^E + |0\rangle\langle 1|^E) + p|1\rangle\langle 1|^E \end{aligned}$$

7.4 Quantum information theory

assuming that the qubit has the form $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$.

If the noise parameter assume the two extreme values of $p = 0$ or $p = 1$, the environment receive no quantum information at all about the state $|\psi\rangle$ transmitted down the channel, because the state in E does not contain the probability amplitudes α or β . As a result, the channel is fully devoid of noise, which means that the channel does not leak quantum information to the environment. On the other hand, when $0 < p < 1$, the environment receives some probability amplitudes α or β , which can be interpreted as "stealing" information from A. Interestingly, when $p = \frac{1}{2}$, the environment gets most information about the state $|\psi\rangle$, because $\sqrt{p(1-p)}$ reaches a maximum.

7.4 QUANTUM INFORMATION THEORY

7.4.1 QUANTUM ENTROPY

The basic concepts of quantum information theory have been initially developed by von Neumann in the early 20th century, when he introduced the concept of entropy, later called Neumann entropy in his honour, which is defined as

$$H(X)_\rho = -Tr(\rho_x \log_2(\rho_x))$$

X is the quantum source that produces pure states $|\Psi_1\rangle, \dots, |\Psi_m\rangle$ with probability p_1, \dots, p_m , whereas ρ_x is the density matrix of that source. The Neumann entropy represents the degree of uncertainty contained in ρ_x . When $|\Psi_1\rangle, \dots, |\Psi_m\rangle$ are mutually orthogonal, then ρ is diagonal and the Shannon entropy is equal to the Neumann entropy. Generally the density matrix is not diagonal and the quantum entropy is smaller than the classical one. Assumed a pure state, then the density matrix has only off-diagonal elements and the Neumann entropy is therefore 0.

7.4.2 COHERENT INFORMATION OF A QUANTUM CHANNEL

Generally a noisy channel manipulates the pure state at the input and changes its correlation to the reference system. To quantify the ability of a quantum channel to preserve correlation, it is necessary to make use of the coherent information of a noisy channel.

In the example of Alice and Bob, the sender purifies the state to $\phi^{AA'}$ and inputs the A' system to a quantum channel $\mathcal{N}^{A' \rightarrow B}$. This transmission leads to a noisy state ρ^{AB} at the output where

$$\rho^{AB} = \mathcal{N}^{A' \rightarrow B}(\phi^{AA'})$$

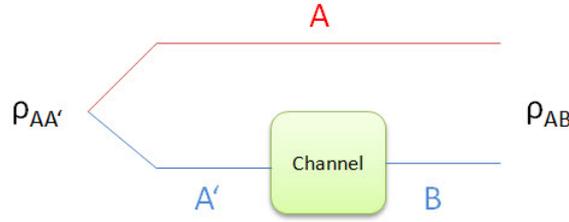


Figure 7.9: Scheme illustrates the coherent information

The coherent information of the state ρ^{AB} is given by

$$I(A > B)_\rho = H(B)_\rho - H(AB)_\rho$$

The coherent information $Q(\mathcal{N})$ of a quantum channel is the maximum of the coherent information over all input states

$$Q(\mathcal{N}) = \max_{\Phi^{AA'}} I(A > B)_\sigma$$

The coherent information can be shown to be a good lower bound on the rate at which Alice transmit quantum information to Bob and, in some special cases, it is even the capacity of a quantum channel.

7.4.3 THE QUANTUM CAPACITY THEOREM

The quantum capacity can be interpreted in a similar way to the classical capacity, since it is impossible to transmit more qubits per channel use than the capacity of the channel allows. The capacity of a quantum channel $\mathcal{N}^{A \rightarrow B}$ is the supremum over all achievable rates for quantum communication

$$\sup\{Q | Q \text{ achievable}\} = C(\mathcal{N})$$

where Q is the coherent information which is a lower bound for the rate.

It is fundamental to remember that so far the corresponding of the Shannon's coding theorem in classical communication does not exist in quantum communication, which would allow to compute the capacity of every possible channel in a straightforward way. However, it is possible to compute the capacity in some special cases. The general treatment of the quantum capacity goes however far beyond the scope of the present project.

In analogy to classical communication theory, the rate Q of this scheme is equal to the number of qubits transmitted per channel use

$$Q = \frac{1}{n} \log d_{A_1} + \delta$$

where d_{A_1} is the dimension of the space A_1 and δ is an arbitrarily small positive number.

7.4.5 THE NO-CLONING THEOREM

The no-cloning theorem has some of the most profound consequences in quantum theory, despite of its simplicity. Basically, it states that it is impossible to build a universal copier of quantum states.

In the classical view, one could do a copy of the original message and compare the output of the decoder with the copy of the original message. The no-cloning theorem does not allow this procedure. The only way to evaluate whether a message has been changed during the transmission, would be to rely on a reference system, which is entangled with the initial message. Notably, comparing both density matrices is the wrong approach to prove that the message at the decoder is the same as the original message, because the density matrix contains only probability distributions of the ensemble and different states can share the same density matrix. In other words, the density matrix is not unique and comparing both density matrices is not a sufficient condition for having equal states.

7.5 REALISATION OF QUANTUM COMMUNICATION USING THE DECOUPLING THEOREM

The previous section has clearly pointed out that there is a need to correlate the message states with a reference system R in order to transmit qubits. Again, this will be done using the purification theory. The pure state $|\phi_{MR}\rangle$ is the purification of ρ_M .

Similarly, an isometric extension of channels is performed to to purify channels. The resulting environment states from these purified n channels are given by the space $E^{\otimes n}$.

The information that is not needed at the decoder will be stored in E_D , which is the purification of the decoder. The final representation of such a communication model is depicted in figure 7.11.

To create the communication protocol the following procedure must be followed. First of all, the states in (1) have to be by construction in the state $\phi_{R\hat{M}} \otimes$

7.5 Realisation of quantum communication using the decoupling theorem

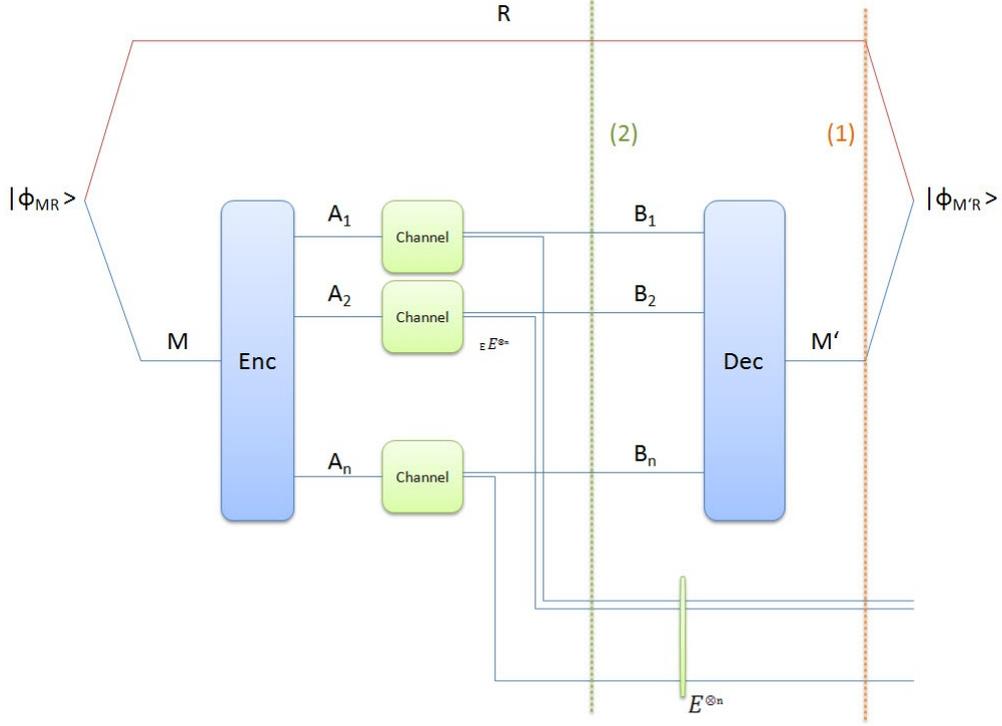


Figure 7.11: Communication scheme

$\psi_{E_D E^{\otimes n}}$, because it is necessary that the message state at the output is in a product state with the different environments. However, this implies that R is decorrelated to $E^{\otimes n}$. As a result, the reference system R and the environment of the channels are not allowed to be entangled together. Moreover, both the reference system R and the environment are purifications and therefore the state in (1) is a purification of R and $E^{\otimes n}$. For the states in (2) let us assume a general pure state with the mathematical representation $\varphi_{R B^{\otimes n} E^{\otimes n}}$. Now the decoder has no possibilities to act neither on the reference system R nor on the environment. Since in (1) R and $E^{\otimes n}$ are purifications and the decoder cannot influence both states, they have to be purifications in (2) as well.

Having now purifications of R and $E^{\otimes n}$ in (1) and (2), it would be helpful to use the theorem of unitary equivalence of purifications. This theorem states that it is possible to obtain a map from the states in (2) to the states in (1). This mapping can be written mathematically as

$$(1_R \otimes 1_E^{\otimes n} \otimes U)$$

One can interpret U as the mapping of the decoder \mathcal{D} . This is the decoder for this problem.

The problem to find an appropriate communication protocol has been reduced to simply require that $E^{\otimes n}$ and R are decorrelated in (2). To do this, the decoupling theorem can be successfully applied.

7.5.1 DECOUPLING THEOREM

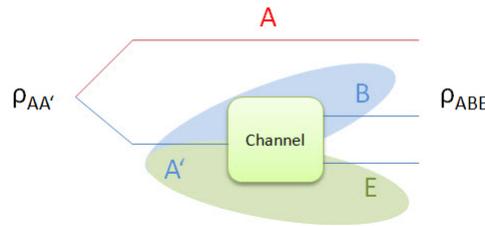


Figure 7.12: This figure shows the channel used in the decoupling theorem

Let $W_{M \rightarrow A^{\otimes n}}$ be a partial isometry and the channel be an isometric extension $U_{\tau}^{A \rightarrow EB}$ shown in figure 7.12. The blue and green areas represent the mapping $\mathcal{N}_{A \rightarrow B}$ and $\tau_{A \rightarrow E}$, respectively. The output of each channel is

$$|w \rangle_{A'EB} = (U_{\tau} \otimes 1_{A'})|\phi \rangle_{AA'}$$

where A and A' are systems of equal dimension.

Then, for every $\delta > 0$ there is an n_0 so that for all $n \geq n_0$ there is a map W

$$\|\tau^{\otimes n}(W\rho_{MR'}W^{\dagger}) - w_E^{\otimes n} \otimes \rho_R\|_1 \leq \sqrt{d_M 2^{-n(I(A' > B)_w - \delta)}}$$

The complete proof of the theorem can be found on [3]. The encoder will be represented mathematically by W , which means that it transforms $\rho_{MR'}$ to $W\rho_{MR'}(W)^{\dagger}$ corresponding to an evolution of a density matrix.

The equation above will imply that as long as the right-hand side of the equation is small enough, R and $E^{\otimes n}$ are in a product state $w_E^{\otimes n} \otimes \rho_R$, i.e. they are decoupled. From what has been presented before, it is now clear that for a decoupled R and $E^{\otimes n}$ there will be a decoder for Bob.

Let's have a closer look to the right-hand side of the equation and let $\log_2 d_M = m$ be the size of the message in number of qubits. The expression $2^{m-n(I(A' > B)_w - \delta)}$ makes clear that, as long as

$$m \leq nI(A' > B)_w$$

the left-hand side of the equation is smaller and therefore the decoder will exist. As a result, one could see $I(A' > B)_w$ as an achievable rate for the channel

7.6 Conclusion

because a protocol to send $I(A' > B)_w$ qubits per use of the channel has been successfully constructed.

7.6 CONCLUSION

During this project, it has been shown that, in the classical world, the Shannon's theorem reflects an upper bound for the achievable rate. In quantum communication theory there is no counterpart for this theorem available at the moment. Thus, the highest achievable rate must be necessarily found by constructing a communication protocol. This has been extensively shown "at work" by using the decoupling theorem. One could interpret this finding as a way to transmit information by destroying correlations between R and $E^{\otimes n}$. Finally, it has been demonstrated that

$$I(A' > B)_w$$

is an achievable rate for the communication protocol drawn in figure 7.11. If a counterpart for the Shannon's theorem in the quantum world will be found in the future is still an open question.

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CHAPTER 8

THERMAL EQUILIBRIUM VIA ENTANGLEMENT

TILEMAN CONRING
SUPERVISOR: JOHAN AABERG

In this chapter we consider an approach to explain thermal equilibrium. In this approach we take a “big” universe in a pure quantum state, and look at a small subsystem. We prove that a randomly chosen global state with high probability is close to an equilibrium state on the small subsystem.

8.1 INTRODUCTION

A crucial question in standard statistical mechanics is about the role of entropy and probabilities, which can both be interpreted as some kind of ignorance. In quantum mechanics a subsystem can be totally mixed even though the total state of the universe is pure. This observation has been the starting point for several approaches to explain thermal equilibrium states. In the following I am going to present an approach taken by Sandru Popescu, Anthony Short and Andreas Winter in the papers [1], [2] and [3]. A different approach can be studied in [4] and [5].

Firstly I will introduce some basic results of standard statistical mechanics written with density matrices. This will help to see similarities between the standard and the quantum mechanical approach later. This will lead to three principles, which conclude in a theorem. We prove this theorem in the main part of this chapter, and conclude with some remarks.

8.2 CONNECTION BETWEEN STANDARD STATISTICAL MECHANICS AND QUANTUM MECHANICS

In standard statistical mechanics a commonly used picture is that of a small system connected to a big reservoir. Usually the following three assumptions are made:

- the states are a priori equally probable
- the interactions between the system and the environment are small
- the environment has an appropriate spacing of the energy levels

Using these assumptions the well known ensembles are derived. It is also possible, as shown in the last chapter of the “Theorie der Waerme” script [6] to write these ensembles with density matrices. To see some similarities later, I will briefly give a repetition of these results. Let $|m\rangle$ be a orthonormal basis of dimension d_m and denote the inverse temperature with $\beta = \frac{1}{k_b T}$. The microcanonical ensemble with constant number of particles, constant volume and constant energy, which can be interpreted as an ensemble of isolated systems, can be expressed as follows

$$\Omega_S^{\mu c} = \frac{\sum_m |m\rangle \langle m|}{d_m} = \frac{\mathbb{1}}{d_m}. \quad (8.1)$$

The canonical ensemble is an ensemble of systems connected to a large heat reservoir, so that it has a well defined temperature and is in equilibrium with the heat bath. This can be written in the following way:

$$\Omega_S^c = \frac{\sum_m e^{-\beta E_m} |m\rangle \langle m|}{\sum_n e^{-\beta E_n}} = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})}. \quad (8.2)$$

In standard statistical mechanics a crucial question is about the role of probabilities and entropy, which can both be interpreted as some kind of ignorance. Now think of the universe being in a pure quantum state $|\phi\rangle$. This means that there is no lack of knowledge and thus the entropy must be zero.

In the following we take a commonly used approach and only take a look at a small part, called the “system”. As mentioned in the talk about entanglement by Felix Bischof, when there is entanglement between the system and the environment, locally the entropy is greater than zero. Here we use entropy as a measure of entanglement.

The aim of this chapter is to show that thermal equilibrium, here used equivalently to canonical state, is a generic property of pure states of the universe.

We will work on a Hilbert space \mathcal{H}_R with dimension d_R , which is a subspace of $\mathcal{H}_U = \subseteq \mathcal{H}_S \otimes \mathcal{H}_E$ with respective dimensions d_U, d_S , and d_E . The Hilbert space \mathcal{H}_R is a subspace determined by arbitrary global constraints (e.g. the total energy is constant). One assumption in standard statistical mechanics is that there are equal a priori probabilities for each state. Following from that, the universe is in an equiprobable state $\mathcal{E}_R = \frac{\mathbb{1}_R}{d_R}$ with respect to the arbitrary global constraint R . A visualisation of the allowed states is given in figure 8.1. This state is the maximally mixed state on subspace \mathcal{H}_R and therefore also the state with maximum entropy. To derive from this state the canonical state of the system, corresponding to the restriction R , we have to trace out the environment: $\Omega_S = Tr_E \mathcal{E}_R$. It is important to note that this must not necessarily coincide the usual thermal canonical state.

As mentioned earlier, the universe is in a pure state $|\phi\rangle$, which is chosen randomly according to the uniform Haar measure. Out of this pure state would result a reduced state of the system $\rho_S = Tr_E |\phi\rangle \langle \phi|$. The aim is now to show that for almost every pure state of the universe (where there is no lack of knowledge) the system behaves as if the universe was actually in the equiprobable mixed state \mathcal{E}_R (which represents a subjective lack of knowledge about its state). This is equivalent to

$$\rho_S \approx \Omega_S . \tag{8.3}$$

This results in three principles, which we later will redefine by a theorem and prove.

General Canonical Principle. *Given a sufficiently small subsystem of the universe, almost every pure state of the universe is such that the subsystem is approximately in the canonical state Ω_S .*

If we now take into account what we know about the canonical state of the system, we could reformulate the general canonical principle in the following way:

Principle of Apparently Equal a priori Probability. *For almost every pure state of the universe, the state of a sufficiently small subsystem is approximately the same as if the universe were in the equiprobable state \mathcal{E}_R . In other words, almost every pure state of the universe is locally (i.e. on the system) indistinguishable from \mathcal{E}_R .*

As the theorem is quite abstract, the following third principle is useful to give some intuition for results of the theorem, which we are going to prove.

8.3 Thermal equilibrium via Entanglement

Thermal Canonical Principle. *Given that the total energy of the universe is approximately E , interactions between the system and the rest of the universe are weak, and that the energy spectrum of the universe is sufficiently dense and uniform, almost every pure state of the universe is such that the state of the system alone is approximately equal to the thermal canonical state $e^{-\beta H_S}$, with temperature T (corresponding to the energy E).*

8.3 THERMAL EQUILIBRIUM VIA ENTANGLEMENT

Theorem 1. *For a randomly chosen state according to the uniform Haar measure $|\phi\rangle \in \mathcal{H}_R \subseteq \mathcal{H}_S \otimes \mathcal{H}_E$ and arbitrary $\epsilon > 0$, the distance between the reduced density matrix of the system $\rho_S = \text{Tr}|\phi\rangle\langle\phi|$ and the canonical state $\Omega_S = \text{Tr}\mathcal{E}_R$ is given probabilistically by*

$$\text{Prob}[\|\rho_S - \Omega_S\|_1 \geq \eta] \leq \eta', \quad (8.4)$$

where

$$\eta = \epsilon + \sqrt{\frac{d_S}{d_E^{\text{eff}}}}, \quad (8.5)$$

$$\eta' = 2 \exp(-C d_R \epsilon^2). \quad (8.6)$$

In these expressions, C is a positive constant (given by $C = (18\pi^3)^{-1}$), d_S and d_R are the dimensions of \mathcal{H}_S and \mathcal{H}_R respectively, and d_E^{eff} is a measure of the effective size of the environment, given by

$$d_E^{\text{eff}} = \frac{1}{\text{Tr}\Omega_E^2} \geq \frac{d_R}{d_S}, \quad (8.7)$$

where $\Omega_E = \text{Tr}_s \mathcal{E}_R$. Both η and η' will be small quantities, and thus the state will be close to the canonical state with high probability, whenever $d_E^{\text{eff}} \gg d_S$ (i.e. the effective dimension of the environment is much larger than that of the system) and $d_R \epsilon^2 \gg 1 \gg \epsilon$. This latter condition can be ensured when $d_R \gg 1$ (i.e. the total accessible space is large), by choosing $\epsilon = d_R^{-1/3}$.

This is the mathematical formulation of the three principles mentioned in section 8.2 which states that thermal equilibrium is achieved for almost all states. Before we turn to the proof, I would like to point out two interesting properties of this theorem:

- it has an exponentially small bound on the relative volume of the exceptional state, which means that it is a rare event to find the system in a state far from the canonical state

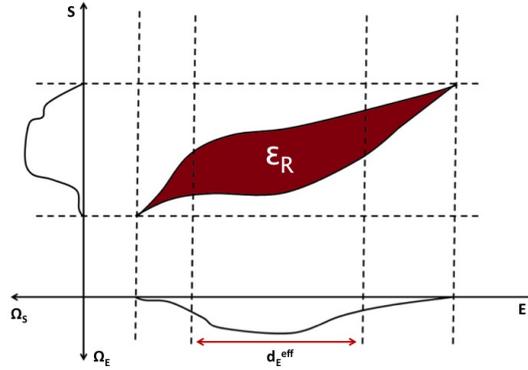


Figure 8.1: A schematic picture of the state space with the environment on the horizontal axis and the system on the vertical axis. The shaded region \mathcal{E}_R represents the allowed states of the universe and the functions along the axes represent the number of configurations in \mathcal{E}_R consistent with a given configuration of E or S.

- the exponential of the probabilistic bound scales $\propto d_R$ and the deviation ϵ scales $\propto \frac{d_S}{d_E^{\text{eff}}}$

In the theorem an effective dimension of the environment d_E^{eff} is used. Picture 8.1 provides some intuition in this regard. Basically it can be interpreted as just looking at the more probable states.

Before coming to the proof of theorem 1 two more technicalities need to be introduced.

8.3.1 DISTANCE MEASURES

In the proof two different norms are used as a measure of distance. The first is the trace norm

$$\|M\|_1 = \text{Tr}|M| = \text{Tr}\sqrt{M^\dagger M} = \sup_{\|O\| \leq 1} \text{Tr}(MO). \quad (8.8)$$

As it is easier to manipulate, also the Hilber-Schmidt norm will be used, which is defined as follows:

$$\|M\|_2 = \sqrt{\text{Tr}(M^\dagger M)}. \quad (8.9)$$

There exists also a useful relation between these two norms, stated in the following lemma.

Lemma 1. For any $n \times n$ matrix M , $\|M\|_1 \leq \sqrt{n} \|M\|_2$.

8.3 Thermal equilibrium via Entanglement

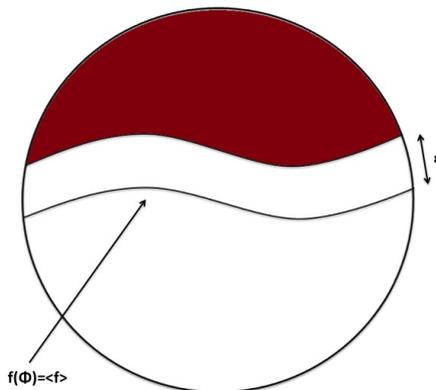


Figure 8.2: A visualisation of the statement of Levy's Lemma for $d = 2$. In this case the surface of a sphere is just a normal sphere and the shaded region corresponds to the region where the function is more than ϵ greater than the mean. This area reduces exponentially with growing dimension.

8.3.2 LEVY'S LEMMA

As the main part of the proof will be the application of Levy's Lemma, this paragraph provides a short introduction. The basic statement of Levy's Lemma is that for a randomly chosen point according to the Haar measure on a hypersphere with high dimension and not too rapidly varying function $f(\phi)$ then $f(\phi) \approx \langle f \rangle$ with high probability. Here the $\langle \cdot \rangle$ denotes the ensemble average according to the Haar measure. This lemma is kind of a generalisation of the law of large numbers for functions. Some more details about it can be found in chapter three of [7] and a proof is demonstrated in [8]. A graphical demonstration is shown in figure 8.2.

Levy's Lemma 1. *Given a function $f : \mathbb{S}^d \rightarrow \mathbb{R}$ defined on the d -dimensional hypersphere \mathbb{S}^d , and a point $\phi \in \mathbb{S}^d$ chosen uniformly at random according to the Haar measure,*

$$\text{Prob}[|f(\phi) - \langle f \rangle| \geq \epsilon] \leq \exp\left(\frac{-2C(d+1)\epsilon^2}{\eta^2}\right), \quad (8.10)$$

where η is the Lipschitz constant of f , given by $\eta = \sup|\nabla f|$, and C is a positive constant (which can be taken to be $C = (18\pi^3)^{-1}$).

We will now turn to the proof of Theorem 1. There are different ways of proving this theorem. One quite technical way is by applying Levy's Lemma directly to the trace norm $\|\rho_S - \Omega_S\|_1$. The second way, which I think is more intuitive and

descriptive, is by applying Levy's Lemma to the expectation values. The idea behind this proof is that if the expectation values of all observables on two states are close to each other, then the states themselves must be close.

We now consider the expectation values of a complete set of observables and choose an arbitrary O_S on S with the only condition that it must be bounded. Our aim is to show that the difference between all these observables on the reduced state ρ_S and the canonical state Ω_S is small. The reduced state is the state obtained by tracing out the environment of the according to the Haar measure randomly chosen state $|\phi\rangle$.

Proof. We let f in (8.10) be $f(\phi) = Tr(O_S \rho_S)$. It is quite easy to show that for any finite operator on \mathcal{H}_R holds

$$\eta \leq 2 \|O_S\| . \quad (8.11)$$

Due to normalisation we loose one dimension and can choose in formula (8.10)

$$d = 2d_R - 1 . \quad (8.12)$$

Plugging these things into formula (8.10), it becomes:

$$Prob [|Tr(O_S \rho_S) - \langle Tr(O_S \rho_S) \rangle| \geq \epsilon] \leq 2exp \left(\frac{-Cd_R \epsilon^2}{\|O_S\|^2} \right) . \quad (8.13)$$

Due to the linearity of the trace we can take the average over all states inside the trace

$$\langle Tr(O_S \rho_S) \rangle = Tr(O_S \langle \rho_S \rangle) . \quad (8.14)$$

In a next step we compute the Haar measure, which results in the totally mixed state

$$\int_{\mathcal{H}_R} |\phi\rangle \langle \phi| d\phi = \frac{\mathbb{1}}{d_R} . \quad (8.15)$$

By tracing out the environment in equation (8.15) we see that the average over all states for ρ_S is the canonical state Ω_S

$$\langle \rho_S \rangle = Tr_E \left(\frac{\mathbb{1}}{d_R} \right) = \Omega_S . \quad (8.16)$$

Plugging the result (8.16) back into equation (8.14) we have

$$\langle Tr(O_S \rho_S) \rangle = Tr(O_S \Omega_S) . \quad (8.17)$$

8.3 Thermal equilibrium via Entanglement

Using these results and choosing $\epsilon = d_R^{-\frac{1}{3}}$ equation (8.13) becomes:

$$Prob \left[|Tr(O_S \rho_S) - Tr(O_S \Omega_S)| \geq d_R^{-\frac{1}{3}} \right] \leq 2exp \left(-\frac{C d_R^{\frac{1}{3}}}{\|O_S\|^2} \right). \quad (8.18)$$

As the last equation shows, for $d_R \gg 1$ the expectation values will be close to each other and following from that a randomly chosen state will be close to the canonical state with high probability.

But as the expectation values for all the operators must be close to each other, we now consider a complete basis of d_S^2 unitary operators U_S^x , where $x \in \{0, 1, \dots, d_S^2 - 1\}$. They form a complete orthogonal operator basis for \mathcal{H}_S by satisfying

$$Tr(U_S^{x\dagger} U_S^y) = d_S \delta_{xy}. \quad (8.19)$$

Due to unitarity they also fulfill $\|U_S^x\| = 1$. We now choose $O_S = U_S^x$. Equation (8.18) becomes

$$Prob \left[|Tr(U_S^x \rho_S) - Tr(U_S^x \Omega_S)| \geq d_R^{-\frac{1}{3}} \right] \leq 2exp \left(-C d_R^{\frac{1}{3}} \right) \quad \forall x. \quad (8.20)$$

This equation could be rearranged if we now just look at one of the d_S^2 choices of the unitary operators U_S^x

$$Prob \left[\exists x : |Tr(U_S^x \rho_S) - Tr(U_S^x \Omega_S)| \geq d_R^{-\frac{1}{3}} \right] \leq 2d_S^2 exp \left(-C d_R^{\frac{1}{3}} \right). \quad (8.21)$$

In the last part of the proof, we are deriving a probabilistic bound on $\|\rho_S - \Omega_S\|_1$. As U_S^x is a complete basis, both states could be expanded

$$\rho_S = \frac{1}{d_S} \sum_x Tr(U_S^{x\dagger} \rho_S) U_S^x = \frac{1}{d_S} \sum_x Tr(U_S^x \rho_S)^* U_S^x \quad (8.22)$$

$$= \frac{1}{d_S} \sum_x C_x(\rho_S) U_S^x, \quad (8.23)$$

$$\Omega_S = \frac{1}{d_S} \sum_x Tr(U_S^{x\dagger} \Omega_S) U_S^x = \frac{1}{d_S} \sum_x Tr(U_S^x \Omega_S)^* U_S^x \quad (8.24)$$

$$= \frac{1}{d_S} \sum_x C_x(\Omega_S) U_S^x. \quad (8.25)$$

Using these two results in equation (8.20) leads to

$$Prob [\exists x : |C_x(\rho_S) - C_x(\Omega_S)| \geq \epsilon] \leq 2 d_S^2 exp(-C d_R \epsilon^2). \quad (8.26)$$

We now would like to derive an upper bound for the distance between the two expansion coefficients. Therefore we require $|C_x(\rho_S) - C_x(\Omega_S)| < \epsilon \quad \forall x$. As

mentioned in section 8.3.1 the Hilbert-Schmidt norm is more easy to manipulate and so we will now make use of it.

$$\|\rho_S - \Omega_S\|_2^2 = \left\| \frac{1}{d_S} \sum_x (C_x(\rho_S) - C_x(\Omega_S)) U_S^x \right\|_2^2 \quad (8.27)$$

$$= \frac{1}{d_S^2} \text{Tr} \left(\sum_x (C_x(\rho_S) - C_x(\Omega_S))^2 (U_S^{x\dagger} U_S^x) \right) \quad (8.28)$$

$$= \frac{1}{d_S} \sum_x (C_x(\rho_S) - C_x(\Omega_S))^2 \leq d_S \epsilon^2 . \quad (8.29)$$

Using here the relation between the trace norm and the Hilbert Schmidt norm explained in Lemma 1 we get:

$$\|\rho_S - \Omega_S\|_1 \leq \sqrt{d_S} \|\rho_S - \Omega_S\|_2 \leq d_S \epsilon . \quad (8.30)$$

Taking equation (8.26) and plugging this upper bound in, which is valid for all x , we obtain

$$\text{Prob} [\|\rho_S - \Omega_S\|_1 \geq d_S \epsilon] \leq 2d_S^2 \exp(-Cd_R \epsilon^2) . \quad (8.31)$$

We now would like to have $d_S \epsilon$ small and the exponent $Cd_R \epsilon^2$ big in order of the bound to be small. Therefore we choose $\epsilon = \left(\frac{d_S}{d_R}\right)^{\frac{1}{3}}$ and define $\beta = \left(\frac{d_R}{d_S^2}\right)^{\frac{1}{3}}$. With these abbreviations equation (8.31) looks like:

$$\text{Prob} \left[\|\rho_S - \Omega_S\|_1 \geq \frac{1}{\beta} \right] \leq 2d_S^2 \exp(-C\beta) . \quad (8.32)$$

The difference between the two states in (8.32) is going to be small with high probability whenever the dimensions fulfill:

$$\beta \gg \log_2(d_S) \gg 1 , \quad (8.33)$$

$$d_R \gg d_S^2 . \quad (8.34)$$

□

The constraints on the dimensions in equation (8.33) and (8.34) look quite similar to the ones from Theorem 1 but are slightly weaker. The reason for this difference is found in the way we made the proof. The stronger bounds originate by directly applying Levy's Lemma to the distance between the two states, and not the expectation values.

There are ways to make the theorem even stronger as shown in [1]. They suggest the following improvements. If you for example take a closer look at d_E^{eff} it is clear that it may be too small due to large eigenvalues of Ω_E . These could be eliminated by projecting onto a typical subspace. Another improvement could be made by thinking about \mathcal{H}_S and asking the question if the system occupies it completely. Both of these improvements would give rise to stronger bounds.

8.4 CONCLUSION

The main result of this chapter has been a theorem, which shows that the reduced state on a small subsystem of a randomly chosen global pure state, is close to the canonical state with high probability. This tells us that the averages used in standard statistical mechanics are not necessary. We could obtain the same state of the system by taking the approach of the Principle of apparently equal a priori probabilities. This states that almost every pure state of the universe is locally indistinguishable from the canonical state. In the theorem we have assumed that the global pure state is restricted to a subspace \mathcal{H}_R , corresponding to some restriction R . The nature of this restriction is left completely open, and generalises the assumption of constant total energy in standard statistical mechanics.

Perhaps you are left wondering why my topic was called thermal equilibrium via entanglement, while I never really said anything about entanglement. Building on the theory of previous chapters, entropy can be seen as a measure of entanglement. The upper bound of the entropy was obtained by the equiprobable state or in other words the totally mixed state \mathcal{E}_R . The following short calculation where we denote by λ_i the i -th eigenvalue of the density matrix and use the von-Neumann entropy shows this property.

$$S(\rho) = -Tr(\rho_S \log_2(\rho_S)) \quad (8.35)$$

$$= -\sum_i \lambda_i \log_2(\lambda_i) \quad (8.36)$$

$$= \log_2(d_S) . \quad (8.37)$$

As shown, the maximal entropy is proportional to the logarithm of the dimension of the system. This explains the choice of name of this chapter.

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CHAPTER 9

APPROACHING THERMAL EQUILIBRIUM

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How a system reaches thermal equilibrium and under which circumstances this will happen is still today an open question. Despite considerable progress can not derive this from basic dynamical laws. First we address on the problem of equilibration. We show, that a large system always equilibrate if we use the concept of realistic observables, say that the Hamiltonian has a generic character and throw away degrees of freedom. Next we show, that a system which is coupled to a much large bath will equilibrate even if we do not use the concept of realistic observables. If we have additionally the weak coupling condition, the energy distribution in a small interval and an exponentially density of states we have thermalization.

9.1 INTRODUCTION

Note added: This talk is based on the following references [1, 2, 3, 4, 5, 6].

Imagine a hot cup of coffee and a cold beer at room temperature. What happens? It is clear that the hot cup of coffee cools down and the cold beer gets warmer. We all know this from our observations in nature and this is called reaching thermal equilibrium.

From macroscopic point of view we know that a coffee, which reached thermal equilibrium, does not suddenly get hotter.

9.1 Introduction

But how can we explain this phenomenon from a microscopic point of view, from the basic dynamical laws of nature such as Newton's or Schrödinger's equation.

That the coffee in thermal equilibrium not suddenly gets hotter is not obvious. For example in quantum mechanics I can have a state, which evolves with time, and the evolution backwards is also valid.

For example by replacing t by $-t$ the time evolution backwards does not violate quantum mechanics. But if the coffee suddenly gets hotter, so in other words the time evolution backwards, this would violate the thermodynamic laws, because the Entropy would get smaller.

We need a rough definition of thermalization and equilibration to continue. Equilibration means that the ensemble approaches a stationary long time behavior. Thermalization means that the ensemble exhibits a sharply peaked energy distribution. Thermalization is characterized by equilibration, Initial state independence and the Boltzmann form of the equilibrium state, also called the Gibbs state.

Today it is still an open question to theoretically explain the phenomenon equilibration and thermalization. The main idea is to make some restrictions to observables and to the Hamiltonian and throw away degrees of freedom. Throwing away degrees of freedom means for example that we do not distinguish two states when on a microscopic level we can see differences between two states, even if on a macroscopic point of view and with observables we cannot distinguish those two states. And with this we can explain those phenomena.

9.2 EQUILIBRATION FOR AN ISOLATED SYSTEM

9.2.1 GENERAL FRAMEWORK

Consider an isolated system, which incorporates all relevant parts of the environment such as thermal baths, reservoirs and so on. We say that the system is macroscopic large and has a finite number of particles. So we have $1 \ll f < \infty$, where f are the degrees of freedom.

So we write the Hamiltonian

$$H = \sum_n E_n |n\rangle\langle n|, \quad (9.1)$$

where $|n\rangle$ are the eigenvecrots of the corresponding eigenvalues E_n . According to standard quantum mechanics, the state of the system is at any time t given by a density operator $\rho(t)$.

The time evolution can be written as $\rho(t) = U_t \rho(0) U_t^\dagger$ with the unitary propagator

$$U_t = e^{-\frac{iHt}{\hbar}} = \sum_n e^{-\frac{iE_n t}{\hbar}} |n\rangle\langle n|. \quad (9.2)$$

The matrix element can be easy found by $\rho_{mn} = \langle m | \rho(t) | n \rangle$. This leads to the following important result:

$$\rho(t) = \sum_{mn} \rho_{mn}(0) e^{-\frac{i(E_m - E_n)t}{\hbar}} |m\rangle\langle n| \quad (9.3)$$

We also introduce level population as

$$p_n = Tr\{|n\rangle\langle n| \rho(t)\} = \rho(t) = \rho_{nn}(0). \quad (9.4)$$

In other words we can say p_n is the expectation value of the observable $|n\rangle\langle n|$. Similarly to p_n , we define the ensemble aberaged occupation probability of an energy eigenvalue E_n as

$$p_{E_n} = Tr\{P_{E_n} \rho(t)\} = \sum_{E_m=E_n} \rho_{mm}(t) = \sum_{E_m=E_n} p_n, \quad (9.5)$$

where P_{E_n} is the projector to the corresponding energy subspace.

The normalization condition says us that

$$1 = Tr \rho(t) = \sum_n \rho_{nn}(t) = \sum_n p_n = \sum_{E_n} P_{E_n}. \quad (9.6)$$

9.2 Equilibration for an isolated system

We introduce here the sub-Hilbert space $\mathcal{H}_+ \subset \mathcal{H}$ spanned by those vectors for which we have a finite probability to occur. This leads to the definition

$$\mathcal{H}_+ = \text{span}\{|n\rangle \mid p_{E_n > 0}\}. \quad (9.7)$$

We say that P_+ is the projector into this subspace. And from now on we use the $\rho_+(t) = P_+\rho(t)P_+$

Now, an observable is always represented by hermitian operators. The expectation value is $\langle A \rangle (t) = \text{Tr}\{\rho(t)A\} = \text{Tr}\{\rho(t)A_+\}$ according to the sub-Hilbert space, where $A_+ = P_+AP_+$ is the projection of A onto \mathcal{H}_+ . So we see that just the sub-Hilbert space matters and from now on we replace \mathcal{H} , A and $\rho(t)$ by \mathcal{H}_+ , A_+ and $\rho_+(t)$.

9.2.2 THE PROBLEM OF EQUILIBRATION

Imagine we have an observable $A = \hat{A} + \hat{A}^+$, where $\hat{A} = |0\rangle\langle 1|$. We see that this is an observable, because it is hermitian. Now we calculate with (3) the expectation value of this observable

$$\langle A \rangle (t) = \text{Tr}\{\rho(t)A\} = 2\rho_{0,1}(0) \cos\left(\frac{E_1 - E_0 t}{\hbar}\right) \quad (9.8)$$

and we see that this would never equilibrate. The ensemble exhibits permanent oscillations.

So we can conclude from this, that we need at least a restricted class of observables, which we call realistic observables. Additionally we see that the formula above depends also on the initial conditions. So we will also look for realistic initial conditions.

9.2.3 REALISTIC OBSERVABLES

A realistic observable A must represent an experimental device with a finite range of possible outcomes of a measurement. So we define the range

$$\Delta_A = \max_{\mathcal{H}} \langle \Psi|A|\Psi \rangle - \min_{\mathcal{H}} \langle \Psi|A|\Psi \rangle. \quad (9.9)$$

We say δA is the resolution limit and defines the precision that we can measure. Within δA we cannot see the differences. All measurements known to the present yield $\frac{\Delta_A}{\delta A} \leq 10^{20}$.

So we know now what realistic observables are and now we define

$$\Delta'_A = \max_{\mathcal{H}_+} \langle \Psi|A|\Psi \rangle - \min_{\mathcal{H}_+} \langle \Psi|A|\Psi \rangle, \quad (9.10)$$

where we replaced \mathcal{H} by \mathcal{H}_+ . Remember that \mathcal{H}_+ throws away the states, which have no probability to occur. So we have $\Delta'_A \leq \Delta_A$.

Now consider an observable of the form

$$B(\vec{b}) = \sum_n n_n |n\rangle\langle n|, \quad (9.11)$$

with arbitrary real coefficients $\vec{b} = (b_0, b_1, \dots)$. We see this observable is stationary. We consider now any observable of the form $A - B(\vec{b})$. So we discount the stationary part, because the stationary part always equilibrates. So we don't care about it. We then end up with

$$\Delta''_A = \min_{\vec{b}} \left\{ \max_{\mathcal{H}_+} \langle \Psi | A - B(\vec{b}) | \Psi \rangle - \min_{\mathcal{H}_+} \langle \Psi | A - B(\vec{b}) | \Psi \rangle \right\}. \quad (9.12)$$

And this leads to $\Delta''_A \leq \Delta'_A \leq \Delta_A$ and thus

$$\frac{\Delta''_A}{\delta A} \leq 10^{20}. \quad (9.13)$$

9.2.4 REALISTIC INITIAL CONDITIONS

Consider $p_n = \rho_{nn}(0)$, where ρ_{nn} is the initial condition. Now we do not know how p_n exactly looks like. For this we say that we can write the concomitant ensemble averaged level populations in the form $p_n = h(E_n) + \delta p_n$, where $h(E_n)$ is a smooth function and δp_n is the fluctuation.

To get an idea of exotic order of the magnitude of p_n , consider a macroscopic system with f degrees of freedom. We get roughly $10^{(10^{23})}$ energy levels per Joule. Even if we have a very small energy interval, we still have very many energy levels in this interval. So the energy levels are very dense. Even if the energy levels are populated extremely unequally, we still expect that

$$\max_n p_n = 10^{-O(f)}. \quad (9.14)$$

This should be clear, if we use the normalization condition (6) and say that the fluctuations are small.

We take it for granted, that the multiples of the degenerate energies are not exactly large, very much smaller than $10^{-O(f)}$. So we can make the rough estimate

$$\max_{E_n} p_{E_n} = 10^{-O(f)}. \quad (9.15)$$

9.2 Equilibration for an isolated system

9.2.5 GENERIC HAMILTONIANS

The true Hamiltonian of a given system is usually not known in detail. We assume that our Hamiltonian has a generic. So we say that the energy differences are never exactly equal. Formally:

$$\begin{aligned} &\text{If } E_j \neq E_k \text{ and } E_m \neq E_n \\ &\text{and } E_j - E_k = E_n - E_m \\ &\text{This implies that } E_j = E_m \text{ and } E_k = E_n \end{aligned}$$

We call this the non-resonance condition or the non-degenerate energy gap condition.

9.2.6 EQUILIBRATION FOR AN ISOLATED SYSTEM

We define

$$\rho_{eq} = \overline{\rho(t)} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \rho(t) dt. \quad (9.16)$$

and thus

$$\rho_{eq} = \sum_n \rho_{nn}(0) |n\rangle \langle n| = \sum_n p_n |n\rangle \langle n| \quad (9.17)$$

So we see, that the equilibrium state depends on the initial condition.

Consider the mean square deviation

$$\sigma_A^2 = \overline{[\langle A \rangle(t) - \langle A \rangle]^2}. \quad (9.18)$$

In some further steps, which you can find in the paper "Canonical thermalization" of P. Reimann, we finally obtain

$$\sigma_A^2 = (\Delta_A'')^2 \max_n p_{E_n}. \quad (9.19)$$

In this proof we used the fact, that the Hamiltonian is generic.

Next we involve Chebychevs inequality

$$Prob(|x - \mu| > \kappa) < \left(\frac{\sigma}{\kappa}\right)^2, \quad (9.20)$$

where x is a random variable μ the average and $\kappa > 0$.

With this we get

$$Prob(|Tr\{\rho(t)A\} - Tr\{\rho_{eq}A\}| \geq \delta A) \leq \left(\frac{\sigma_A}{\delta A}\right)^2. \quad (9.21)$$

So the difference of $Tr\{\rho(t)A\}$ and $Tr\{\rho_{eq}A\}$ is below the resolution limit δA for any realistic observable. If we put in equation (19) and then use (13) and (15) we get

$$Prob(|Tr\{\rho(t)A\} - Tr\{\rho_{eq}A\}| \geq \delta A) \leq (10^{20})^2 10^{-O(f)}. \quad (9.22)$$

With this we can say that the system looks exactly as if it were in the steady state ensemble ρ_{eq} for the overwhelming majority of time, because $(10^{20})^2 10^{-O(f)}$ is so small, that we can neglect it.

This deviation is based on the exact quantum mechanical time evolution without any modification or approximation. The full quantum mechanical time-inversion invariance is still contained in our result.

9.3 EQUILIBRATION FOR AN SYSTEM IN CONTACT WITH A LARGE BATH

We want to show in this section that a system, which is in contact with a large enough bath, equilibrates. This is contained in the previous section but now we do not use the concept of realistic observables.

9.3.1 SETUP AND DEFINITIONS

Consider a large quantum system in a Hilbert space \mathcal{H} , which can be decomposed in a subsystem and a bath $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$. We assume that the corresponding dimensions are finite. To mention is that we did not make special properties to the both systems. We assume also that our Hamiltonian is generic like in the previous section.

Denote by $|\Psi(t)\rangle$ the global pure state of the system (bath and subsystem) at time t . We can thus write the density matrix $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ and we obtain the reduced density matrix by tracing over B or S:

$$\rho_S(t) = Tr_B \rho(t) \quad (9.23)$$

and

$$\rho_B(t) = Tr_S \rho(t). \quad (9.24)$$

We define the time-averaged state

$$\omega = \overline{\rho(t)} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \rho(t) dt \quad (9.25)$$

and similarly we define ω_S and ω_B .

9.3 Equilibration for an system in contact with a large bath

The effective dimension of state ρ is defined as

$$d^{eff}(\rho) = \frac{1}{Tr(\rho^2)}. \quad (9.26)$$

This tells us how many pure states contribute to the mixture.

Finally we define the distance between two density matrices by a strong and very natural distance, namely the trace-distance

$$\mathcal{D}(\rho_1, \rho_2) = \frac{1}{2}Tr(\sqrt{(\rho_1 - \rho_2)^2}). \quad (9.27)$$

This characterizes how hard it is to distinguish two states experimentally.

9.3.2 EQUILIBRATION

A central result of this section will be:

Every pure state of a large quantum system that is composed of a large number of energy eigenstates and which evolves under any arbitrary Hamiltonian (with non-degenerate energy gaps) is such that every small subsystem will equilibrate.

A large number of energy eigenstates means that we have a lot of change during the time evolution.

For this we first want to show, that whenever the state of the bath goes through many distinct states, any small subsystems reaches equilibrium.

Evolving through many distinct states is mathematically encapsulated by the effective dimension of the time-averaged state.

Suppose

$$|\Psi(t)\rangle = \sum_n c_n e^{-\frac{iE_n t}{\hbar}} |n\rangle, \quad (9.28)$$

where

$$\sum_n c_n^2 = 1. \quad (9.29)$$

With (3) and (25) we finally obtain

$$d^{eff}(\omega) = \frac{1}{Tr(\omega^2)} = \frac{1}{\sum_n |c_n|^4}. \quad (9.30)$$

So we see, the more distinct energy eigenstates we have, the bigger is $d^{eff}(\omega)$.

Now we come to our first Theorem:

Theorem 1 Consider any state $|\Psi(t)\rangle \in \mathcal{H}$ evolving under a Hamiltonian with non-degenerate energy gaps. Then the average distance between $\rho_S(t)$ and its time-average ω_S is bounded by

$$\overline{\mathcal{D}(\rho_S(t), \omega_S)} \leq \sqrt{\frac{d_S}{d^{eff}(\omega_B)}} \leq \sqrt{\frac{d_S^2}{d^{eff}(\omega)}} \quad (9.31)$$

The proof of this Theorem can be found in the paper "Quantum mechanical evolution towards thermal equilibrium" from N.Linden.

Our subsystem will equilibrate when $d^{eff}(\omega)$ is much larger than two copies of the subsystem.

This result about equilibration is completely general. We did not assume anything special about the interaction, neither have we assumed any special properties of the bath. Theorem 1 depends only on the dimension of the subsystem and on the effective dimension of ω and not on what that particular subsystem is or how we partitioned our total system.

In some few words we put a bound on the fluctuation state of the subsystem around the time-average.

Now we just have to show that $d^{eff}(\omega)$ is a big number and this causes the bound in Theorem 1 to be much sharper. For this we consider a restricted Hilbert space $\mathcal{H}_R \subset \mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$ with dimension d_R . A restriction could for example be that the energy is conserved.

9.4 Thermalization

Now we come to our second Theorem:

Theorem 2

(i) The average effective dimension $\langle d^{eff}(\omega) \rangle_{\Psi}$, where the average is computed over uniformly random pure states $|\Psi\rangle \in \mathcal{H}_R$ is

$$\langle d^{eff}(\omega) \rangle_{\Psi} \geq \frac{d_R}{2} \quad (9.32)$$

(ii) For a random state $|\Psi\rangle \in \mathcal{H}_R$, the probability that $d^{eff}(\omega)$ is larger than $\frac{d_R}{4}$ is exponentially small

$$Pr_{\Psi}\{d^{eff}(\omega) < \frac{d_R}{4}\} \leq 2e^{-c\sqrt{d_R}} \quad (9.33)$$

The proof of this Theorem can be found in the paper "Quantum mechanical evolution towards thermal equilibrium" from N.Linden.

So we see, that $d^{eff}(\omega)$ is a really big number for a macroscopic system and it scales with the dimension d_R . In other words we showed that the subsystem will equilibrate if $d_R \gg d_S$, for almost all initial states of the bath or subsystem.

9.4 THERMALIZATION

Imagine again that we are in a system which can be decomposed $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$, like in the previous section, where S is the subsystem and B is the bath. We have the Hamiltonian $H = H_0 + V$ where $H_0 = H_S + H_B$ and V is the coupling between both.

We know from before that Thermalization is characterized by:

- (i) Equilibration
- (ii) Initial state independence
- (iii) the Boltzmann form of the equilibrium state

The Boltzmann form of the equilibrium state $\rho = \frac{1}{Z} e^{\frac{-H_S}{k_B T}}$ is also called Gibbs state sometimes.

In the previous section we explained equilibration. So we fulfilled the first point. For the initial state independence we need an energy distribution, which is in a small interval $[E, E + \Delta]$ and vanishes otherwise. Additionally we need the weak coupling approximation $\|V\|_{\infty} \ll k_B T < \Delta$.

To fulfill the last point we need additionally the case with an exponential density of states and thus we will get to equilibration towards a Gibbs state.

9.5 CONCLUSION

The problem of equilibration can be explained by using the concept of realistic observables and generic Hamiltonian and by throwing away degrees of freedom. In our consideration we showed that equilibration can be explained for a large system or for system which is connected to a much larger bath. So we can explain why the hot cup of coffee equilibrates in room temperature. The reason is that the hot cup of coffee is coupled to a much larger environment. To explain thermalization we need some more restrictions like to have a small energy interval, weak coupling and exponential density of states. The main problem of explaining the problem of equilibration and thermalization is, that we could not until now derive those phenomena from the basic dynamical laws such as Newtons or Schrodingers equation.

9.5 Conclusion

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CHAPTER 10

JAYNES' PRINCIPLE

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The maximum entropy (or Jaynes') principle is introduced as a principle of statistical inference, which is least biased with respect to available information. Based on this principle, a generalized form of statistical mechanics is established, that does not rely on assumptions on the physical nature of a system other than its accessible quantum states. In quantum statistical mechanics the density matrix has the meaning of a generalized probability distribution, and can be inferred by maximum entropy in the same way. Finally, it is discussed how irreversible phenomena in a macroscopic closed system can be identified with information loss from the point of view subjective statistical mechanics.

10.1 INTRODUCTION TO STATISTICAL INFERENCE

10.1.1 INTERPRETATION OF PROBABILITY

Probability theory is a rigorous field of mathematics. However, application to real systems always demands an interpretation of what probabilities represent. This is important when making predictions about physical behaviour based on experimental data.

The most intuitive way to imagine probabilities is to regard them as frequency ratios. Rolling a die a thousand times and counting the numbers for each side to appear gives an impression of whether it is biased or not. This *objective* school

10.1 Introduction to Statistical Inference

of thought is thus based on the notion that probabilities are experimentally verifiable. They are deemed intrinsic properties of a system.

On the other hand we might consider a deterministic machine that obeys to some mechanism unknown to us. Then the probability that it produces some outcome is rather a statement of our ignorance about its true dynamics. Thus from a *subjective* point of view probabilities represent a state of knowledge of the observer. Setting up a probability distribution in the subjective sense requires getting informed about what we really know¹.

Both of these concepts are necessary in statistical mechanics, neither can cover all problems that are encountered[1]. A connection between them is established in that objective experimental results are often taken as the information available for a subjective treatment. Statistical inference, the process of estimating a probability distribution from empirical data, can rely on either one. The two inference models presented here, Bayesian updating and the maximum entropy method, are both of the subjective kind.

10.1.2 BAYESIAN INFERENCE

The method of Bayesian inference employs a mechanism of *updating* prior probabilities by experimental data to give posterior probabilities. This is based on Bayes theorem[2]

$$P[A|B] = \frac{P[B|A] P[A]}{P[B]}, \quad (10.1)$$

which relates the conditional probability of an event A given the event B , $P[A|B]$, to its counterpart B given A . To make use of this in statistical inference consider an event space $\Omega = \{\omega_1, \dots, \omega_K\}$ and the space $\mathcal{P}(\Omega)$ of all probability distributions on Ω . Let X be a random variable on Ω . In N independent measurements of X , $x_i = X(\omega_i)$ is obtained n_i times ($i = 1, \dots, K$, $\sum_i n_i = N$). Denote by $\mathbf{n} = (n_1, \dots, n_K)$ the frequency vector of events $\{X = x_i\}$ and $\mathbf{p} = (p_1, \dots, p_K)$ the corresponding probability vector. Bayes theorem now provides a framework to describe the likelihood that some probability distribution \mathbf{p} is realized posterior to the measurement \mathbf{n}

$$\pi[\mathbf{p}|\mathbf{n}] = \frac{P[\mathbf{n}|\mathbf{p}] \pi[\mathbf{p}]}{P[\mathbf{n}]}. \quad (10.2)$$

¹This rather philosophical statement resembles the famous words of Socrates, “I know that I know nothing”.

Here $\pi[\mathbf{p}]$ is the *prior* probability that the true distribution is \mathbf{p} and $\pi[\mathbf{p}|\mathbf{n}]$ is the *posterior or updated* probability that it is still \mathbf{p} . $P[\mathbf{n}|\mathbf{p}]$ must be calculated with some model which is often a multinomial distribution

$$P[\mathbf{n}|\mathbf{p}] = \frac{N!}{\prod_{i=1}^K n_i!} \prod_{i=1}^K p_i^{n_i} .$$

$P[\mathbf{n}]$ is calculated from the law of total probability

$$P[\mathbf{n}] = \sum_{\mathbf{q} \in \mathcal{P}(\Omega)} P[\mathbf{n}|\mathbf{q}] \pi[\mathbf{q}] .$$

Finally a prediction about the probability of the event $\{X = x_i\}$ in the $N + 1^{\text{th}}$ step can be made:

$$P[x_i|\mathbf{n}] = \sum_{\mathbf{p} \in \mathcal{P}(\Omega)} p_i \pi[\mathbf{p}|\mathbf{n}] . \quad (10.3)$$

If the frequencies of the single events n_i are not known, but only the average value $\bar{X} = \sum_i \frac{n_i}{N} x_i$, the model has to be slightly adapted:

$$P[x_i|\bar{X} = x] = \frac{\sum_{\{\mathbf{n}|\bar{X}=x\}} p_i P[x_i|\mathbf{n}] P[\mathbf{n}]}{P[\bar{X} = x]} . \quad (10.4)$$

It has not been answered yet, what the prior probability $\pi[\mathbf{p}]$ should be. Clearly, in a case when no information is given, it should be a uniform distribution over the entire probability space. In fact, Bayesian updating can be seen as an iterative process. At the beginning, no information is given. Then, measurements are performed that yield data sets \mathbf{n} on the basis of which the prior probability can be updated to the corresponding posterior. If there is yet another source of information, the process can be repeated with the previous posterior as new prior.

10.1.3 MAXIMUM ENTROPY

As Shannon [3] pointed out, the entropy of a probability distribution $S(\mathbf{p}) = -\sum_i p_i \ln p_i$ is the unique measure of its uncertainty that satisfies the properties positivity, concavity and subadditivity. In the usual problem of statistical inference, the probability distribution of a random variable is to be estimated from partial knowledge. Thus our motivation in finding the distribution which maximizes the associated entropy is to take account of our restricted knowledge. The maximum entropy distribution is expected to be least biased.

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Suppose now we have access to experimental data about some function $f(X)$ where X is a random variable as in the Bayesian case. This means we know the average value $\overline{f(X)}$. The maximum entropy probability distribution of X can now be calculated by means of Lagrange multipliers. The constraints are

$$\overline{f(X)} = \langle f(X) \rangle = \sum_i p_i f(x_i), \quad \text{and} \quad (10.5)$$

$$1 = \sum_i p_i. \quad (10.6)$$

Thus the maximizing condition is

$$0 = \delta \left(- \sum_i p_i \ln p_i - \alpha \left(\sum_i p_i - 1 \right) - \beta \left(\sum_i p_i f(x_i) \right) \right). \quad (10.7)$$

which leads to²

$$\begin{aligned} \hat{p}_i(\beta) &= Z(\beta)^{-1} e^{-\beta f(x_i)}, \\ Z(\beta) &= \sum_i e^{-\beta f(x_i)}, \\ \hat{S}(\langle f(X) \rangle) &= \ln Z(\beta) + \beta \langle f(X) \rangle. \end{aligned} \quad (10.8)$$

The quantity Z is called the *partition function* and contains all the information about the system available to us. It is the central property in this formalism. Note that the entropy is a function of $\langle f(X) \rangle \equiv \langle f \rangle$ only. The Lagrange multiplier β is determined from

$$\langle f \rangle = - \frac{\partial \ln Z(\beta)}{\partial \beta}.$$

This condition also specifies that S and $\ln Z$ are linked by a Legendre transformation. An equivalent constituting equation for β is thus

$$\beta = \frac{\partial \hat{S}(\langle f \rangle)}{\partial \langle f \rangle}.$$

If f is a function of an additional parameter ξ we can calculate the expected value of the derivative

$$\left\langle \frac{\partial f}{\partial \xi} \right\rangle = - \frac{\partial \ln Z}{\partial \xi}.$$

²The extremal quantities are denoted by a $\hat{\cdot}$.

In the case that there are multiple quantities f_r available to experiments, the results are easily generalized:

$$\begin{aligned}\hat{p}_i(\boldsymbol{\beta}) &= Z(\boldsymbol{\beta})^{-1} \exp\left(-\sum_r \beta_r f_r(x_i)\right), \\ Z(\boldsymbol{\beta}) &= \sum_i \exp\left(-\sum_r \beta_r f_r(x_i)\right), \\ \hat{S} &= \ln Z + \sum_r \beta_r \langle f_r \rangle.\end{aligned}\tag{10.9}$$

We can further calculate the covariances

$$\text{Cov}(\langle f_r \rangle, \langle f_s \rangle) = \frac{\partial^2 \ln Z}{\partial \beta_r \partial \beta_s}.$$

Finally, consider a small perturbation of the system affecting both the functions f_r as well as their observed average values $\overline{f_r}$ independently of each other. In the MEP picture, the infinitesimal change in entropy is

$$\begin{aligned}\delta S &= \delta \ln Z + \sum_r \delta(\beta_r \langle f_r \rangle) \\ &= \sum_r \left(\frac{\partial \ln Z}{\partial \beta_r} \delta \beta_r - \beta_r \langle \delta f_r \rangle \right) + \left(\langle f_r \rangle \delta \beta_r + \beta_r \delta \langle f_r \rangle \right) \\ &= \sum_r \beta_r \left(\delta \langle f_r \rangle - \langle \delta f_r \rangle \right).\end{aligned}\tag{10.10}$$

In contrast to the Bayesian approach, it is apparent that the Maximum Entropy method delivers closed form analytical expressions for the estimated probabilities. The associated rules for computation are based on the partition function as central quantity, whose derivatives yield information about the properties of the studied system.

10.1.4 CRITIQUE

Both methods establish a closed formalism for the inference of a probability distribution based on partial information. It is worth noting, that the Bayesian approach is sensitive to the size of the data sample N . On the contrary, the maximum entropy method starts with equating the average with the expectation value and thus loses this sensitivity. From this observation it would be a condition of consistency if both methods gave the same results in the large N limit. However this is not always the case.

10.1 Introduction to Statistical Inference

Assume, e.g., a die, that shows an average of 3.5 after N tosses [2, 4]. If N is large one would expect to have an unloaded die, i.e. $p_i = 1/6$ for all i . This is exactly the result obtained from the MEP. Bayesian updating, however, starting with a uniform prior, yields a probability distribution that is symmetric around 3.5 – i.e. $p_1 = p_6, p_2 = p_5, p_3 = p_4$ – yet slightly biased towards 3 and 4. The bias only grows in the large N limit. Mathematically both results are justified as they reproduce the experimental result. However it reveals a conceptual difference between them. The MEP is completely unbiased, whereas Bayes puts extra weight to outcomes that lie closer to the observed average. It is a general feature of MEP that it cannot produce any peaked probability distributions since $e^{-\beta f_i}$ is monotonic in f_i .

Finally, it is worth examining the structure of the MEP. The idea behind maximizing entropy is to create a probability distribution which is “maximally non-committal with respect to given information” [1]. One first observation is that the probability distribution, as well as the partition function from eq. 10.9 factor out into a product over the various constraints:

$$\begin{aligned}\hat{p}_i(\boldsymbol{\beta}) &= \prod_r Z_r(\beta_r)^{-1} \exp(-\beta_r f_r(x_i)) = \prod_r \hat{p}_{i,r}(\beta_r) , \\ Z(\boldsymbol{\beta}) &= \prod_r \sum_i \exp(-\beta_r f_r(x_i)) = \prod_r Z_r(\beta_r) .\end{aligned}$$

This means that MEP automatically imposes an independence assumption on the various constraints. In practice this is not a big problem as most quantities are indeed independent [4]. However including experimental data from interdependent quantities has less information content and therefore less predictive capacity. MEP would thus lead to stronger assumptions than really allowed. This feature is changed in the treatment of quantum probability.

Another core element of MEP is the *constraint rule*. In the beginning, the constraint rule was established by equating the empirical average with the expectation value $\bar{f} = \langle f \rangle$. This is a voluntary step of discarding information about the sample size. Still, the sample average is an unbiased and consistent estimator for the expected value and thus a reasonable choice³. Another objection is one could as well choose the harmonic mean instead of the arithmetic mean and get different results. However this is a decision that depends on the type of experiment one performs, whether one measures $\overline{f(X)}$ or the inverse quantity $\overline{f(X)^{-1}}$.

³Meaning $\langle \bar{X} - \langle X \rangle \rangle = 0$ (unbiased), and $\lim_{N \rightarrow \infty} P[|\bar{X} - \langle X \rangle| > \varepsilon] = 0 \quad \forall \varepsilon > 0$ (consistent).

The constraint rule also establishes a bridge between event-based Bayesian updating and probability-based MEP [2]. The Bayes method is designed to estimate the posterior probability $\pi[x_i|A]$ of an event $\{X = x_i\}$ after observation of an event $A \subset \Omega^N$ (i.e. $A = \{\bar{X} = x\}$). Jaynes' principle on the other hand uses information about the probability distribution itself, i.e. a constraint $\langle X \rangle = x$. Now the bridge is to express a such constraint in terms of observed events, like the previous $\langle X \rangle = \bar{X} = x$.

Still, MEP does not include any possibility for updating an existing probability distribution. This could be implemented by means of the relative entropy

$$S(P|Q) = - \sum_i p_i (\ln p_i - \ln q_i) = S(P) - \langle -\ln Q \rangle .$$

where Q, P represent the probability distributions defined by the q_i, p_i . The relative entropy is a measure for the distinguishability between Q and P . Q could be interpreted as the prior and P as the posterior probability. $\langle -\ln Q \rangle$ is the prior uncertainty. It can be shown [2], that maximizing $S(P|Q)$ with respect to the constraint that a given observed event A has probability 1, i.e. $P[A] = 1$, directly gives the Bayesian posterior $P[x_i|A]$. Thus in this context of maximum relative entropy, Jaynes' principle is a generalization of Bayesian inference.

10.2 GENERALIZED STATISTICAL MECHANICS

10.2.1 MOTIVATION

It is now at the time to turn over to statistical mechanics and see how the maximum entropy principle can be applied to lead to a more general theory. For this purpose consider an arbitrary macroscopic system.

A *microstate* is a quantum state of the studied system. A *macrostate* is the set of all microstates that are macroscopically equivalent, i.e. they produce the same macroscopic behavior. Take as an example a lattice of N indistinguishable spins. Then configurations with the same number K of "spin ups" might be considered macroscopically equivalent, as they give rise to the same . Microscopically, however, every such macrostate is degenerate by a factor given by the number of permutations of spins $\binom{N}{K}$. In principle this can be generalized to the multiplicity of a macrostate, specified by the occupancy vector $\mathbf{n} = (n_1, \dots, n_k)$ of microstates labelled $1, \dots, k$,

$$W(\mathbf{n}) = \frac{\mathcal{N}!}{\prod_{i=1}^k n_i!} = \binom{\mathcal{N}}{n_1, \dots, n_k},$$

10.2 Generalized Statistical Mechanics

where $\sum_{i=1}^k n_i = \mathcal{N}$ is the total number of microstates. Following Boltzmann's definition of the entropy of a macrostate defined by the occupancy \mathbf{n}

$$S(\mathbf{n}) = -\frac{k_B}{\mathcal{N}} \ln W(\mathbf{n}),$$

one obtains in the limit of a system of infinite degrees of freedom and by use of Stirling's formula

$$\begin{aligned} S(\mathbf{n}) &= -k_B \frac{\ln \mathcal{N}! - \sum_i \ln n_i!}{\mathcal{N}} \\ &\stackrel{\mathcal{N} \rightarrow \infty}{\sim} -k_B \sum_i \frac{n_i}{\mathcal{N}} \ln \frac{n_i}{\mathcal{N}}. \end{aligned}$$

Here the assumption has been made that the n_i grow large with \mathcal{N} as well, asymptotically with a proportionality constant $p_i = \lim_{\mathcal{N} \rightarrow \infty} \frac{n_i}{\mathcal{N}}$ which can be interpreted as the probability of the system to be in microstate i . Thus the Shannon entropy is retrieved from the Boltzmann entropy in the limit of a system of infinite degrees of freedom. However, this link between information theory and thermodynamics is not compulsive as it is not clear whether the Boltzmann entropy itself is a correct expression for thermodynamic entropy.

The standard task of statistical mechanics really is to infer the probability distribution over all microstates that results in the macroscopically observed behavior. Conventional statistical mechanics imposes some assumptions, such as equal a priori probabilities or ergodicity, which in fact cannot be easily justified for real physical systems. More fundamental is the notion of *macroscopic uniformity*: For macroscopic systems to show reproduceable behavior it is necessary that their probability distribution over macrostates are strongly peaked around one specific macrostate. From that point of view the physical behavior is dominated by the most probable macrostate (with maximal multiplicity), which is in this case equivalent to choosing the maximum entropy distribution over all microstates.

The generalization by the MEP lies in making entropy the fundamental concept. This way one obtains the broadest possible distribution over microstates compatible with initial, i.e. average energy. Jaynes interprets this as an ergodic property [1]: “[The MEP] assigns positive weight to every situation that is not absolutely excluded by the given information.” In contrast to the previous line of reasoning assumptions about the real distribution over macrostates is not needed any more to make appropriate predictions. Instead, the MEP distribution, honestly reflecting the present state of knowledge about the system, is the most adequate choice from a subjective point of view. Thus statistical mechanics is treated as a theory of statistical inference.

10.2.2 MICROCANONICAL, CANONICAL AND GRAND CANONICAL ENSEMBLE

The central quantity of a physical system is its energy. Suppose a given system is known to be in a quantum state of energy E . This is the only information available in the *microcanonical ensemble*. We can translate this to a constraint on the probability distribution of the system: Only those states have nonzero probability which have energy E , or equivalently $1 = \sum_{\{i|E_i=E\}} p_i$. Using this within the MEP we obtain a uniform distribution on all degenerate microstates with energy E . This is precisely the statement of the notion of *equal a priori probabilities*.

A less severe constraint is to fix the average energy of a system, i.e. $\bar{E} = \langle E \rangle = \sum_i p_i E_i$. Applying the MEP to this *canonical ensemble* leads to

$$\hat{p}_i = Z^{-1} e^{-\beta E_i}, \quad (10.11)$$

$$Z = \sum_i e^{-\beta E_i}, \quad (10.12)$$

$$\hat{S} = \ln Z + \beta \langle E \rangle. \quad (10.13)$$

β is the inverse temperature⁴ $1/T$ as obtained from an analog of eq. (10.1.3), $F = -k_B \beta^{-1} \ln Z$ is the free energy. Eq. (10.13) states $F = \langle E \rangle - TS$. By taking its total differential it follows

$$\begin{aligned} d\hat{S} &= d \ln Z + \langle E \rangle d\beta + \beta d\langle E \rangle \\ &= -\langle E \rangle d\beta + (d \ln Z)_\beta + \langle E \rangle d\beta + \beta d\langle E \rangle \\ \Rightarrow d\langle E \rangle &= T d\hat{S} - k_B T (d \ln Z)_\beta. \end{aligned}$$

The first term accounts for an energy change due to exchange of entropy which is heat in the thermodynamic sense. Considering that the partition function may depend on additional parameters via the E_i , i.e. volume, external fields, etc., the second term can be identified with isothermal work done by the system. This statement thus strongly resembles the *first law of thermodynamics*. In addition eq. (10.10) can be interpreted in this way. The quantities $\delta Q_r = \delta \langle f_r \rangle - \langle \delta f_r \rangle$ have the meaning of a sort of generalized heat with their Lagrange multipliers β_r corresponding to generalized temperatures.

Finally, information about the number of particles N in the system might be available, too. Note that together with the additional constraint $\bar{N} = \sum_{i,N} p_{i,N} N$ there is a change in the energy level structure. The energies depend on N , too,

⁴in units of $k_B \text{Joule}^{-1}$

10.2 Generalized Statistical Mechanics

and there is no such factorization as seen in the beginning. The probability distribution of the *grand canonical ensemble* is

$$\begin{aligned}\hat{p}_{i,N} &= Z(\beta, \gamma)^{-1} e^{-\beta E_{i,N} - \gamma N} , \\ Z(\beta, \gamma) &= \sum_{i,N} e^{-\beta E_{i,N} - \gamma N} = \sum_N e^{-\gamma N} Z^{(N)}(\beta) .\end{aligned}$$

where $Z^{(N)}(\beta) = \sum_i e^{-\beta E_{i,N}}$ is the canonical partition function of an N particle system, $\gamma = -\beta\mu$ with μ being the chemical potential[1]. Here, we can draw an analogy to the free energy of the canonical ensemble and define the grand potential $f(\beta, \mu) = -\beta^{-1} \ln Z(\beta, \mu)$. Since the derivatives of the partition function allow in principle to calculate any physical property of the system, the free energy and the grand potential are the naturally arising thermodynamic potentials.

10.2.3 EXTENSION TO THE DENSITY MATRIX FORMALISM

In the quantum case, observables are represented by self-adjoint operators and the state of a system is fully described by a density matrix ρ . Expectation values are calculated via

$$\langle A \rangle = \text{tr}(\rho A) .$$

The von Neumann entropy is

$$S(\rho) = -\text{tr}(\rho \ln \rho) . \quad (10.14)$$

The von Neumann entropy generalizes the Shannon entropy because the density matrix ρ is hermitian and thus diagonalizable with eigenvalues λ_i with orthonormal eigenvectors ψ_i . An alternative version of eq. (10.14) is thus

$$S(\rho) = - \sum_i \lambda_i \ln \lambda_i . \quad (10.15)$$

Since its eigenvalues satisfy the normalization condition $\sum_i \lambda_i = 1$, the spectrum of a density matrix can be interpreted as a probability measure. The λ_i 's are the probabilities of the system to be in the pure state $|\psi_i\rangle\langle\psi_i|$.

Some important properties of the von Neumann entropy are [5]:

- (1) *positivity*: $S(\rho) \geq 0$ and $S(\rho) = 0$ iff ρ is pure.
- (2) *concavity*: $S(\sum_i \lambda_i \rho_i) \geq \sum_i \lambda_i S(\rho_i)$.
- (3) *unitary invariance*: $S(U\rho U^\dagger) = S(\rho) \forall U$ unitary.
- (4) *subadditivity*: Let the Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and for a density matrix ρ on \mathcal{H} denote $\rho' = \rho_A \otimes \rho_B$, with reduced density matrices $\rho_{A,B}$. Then $S(\rho) \leq S(\rho') = S(\rho_A) + S(\rho_B)$ with equality iff $\rho = \rho'$.

Most interestingly, unitary invariance implies that the von Neumann entropy of a closed Hamiltonian system is constant in time. Microscopically all physical processes have time inversion symmetry, i.e. they are reversible. This seems to stand in contradiction with macroscopically irreversible phenomena in closed systems [5, 6]. An approach to solve this conflict is presented in section 10.3.

Maximum entropy inference of the density matrix of a quantum system proceeds in the same way as in the classical case. Suppose the average values of some observables F_i have been measured. Then the maximization condition writes

$$\begin{aligned} 0 &= \delta \left(S(\rho) - \alpha(\text{tr}(\rho) - 1) - \sum_i \beta_i(\text{tr}(\rho F_i) - \overline{F_i}) \right) \\ &= \delta \left(\text{tr} \left(\rho \left(-\ln \rho - \alpha \text{id} - \sum_i \beta_i F_i \right) \right) + \alpha + \sum_i \lambda_i F_i \right). \end{aligned}$$

This leads to the MEP states [6]

$$\begin{aligned} \hat{\rho} &= Z^{-1} \exp\left(-\sum_i \beta_i F_i\right), \\ Z &= \text{tr}\left(\exp\left(-\sum_i \beta_i F_i\right)\right), \\ \hat{S} &= \ln Z + \sum_i \lambda_i \langle F_i \rangle. \end{aligned}$$

in complete analogy to the result (10.9). All previous equations can be adapted from the previous discussion with the important difference is that the F_i are operators and need not commute in principle. An example are the quadratures of a quantum mechanic oscillator or field mode. Correspondingly, their quantum nature forces them to obey certain uncertainty relations. Thus even if we are equipped with information about their expectation values, measurement imprecision will always have quantum noise as a lower bound. This uncertainty is then transferred to the inferred density matrix. In fact, quantum measurement itself is linked with an entropy change, too[7].

10.2 Generalized Statistical Mechanics

10.2.4 COUPLED SYSTEMS – BATHS

Consider a composite system $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ with operators

$$\begin{aligned} H &= H_1 \otimes 1 \otimes 1 + 1 \otimes H_2 \otimes 1 , \\ G &= G_1 \otimes 1 \otimes 1 + 1 \otimes 1 \otimes G_3 , \\ F &= F_1 \otimes 1 \otimes 1 . \end{aligned} \tag{10.16}$$

Note that this choice of operators does not contain any coupling terms of the form, e.g. $H_{12} = V_1 \otimes V_2 \otimes 1$. The systems can thus be regarded independent, an approximation valid in the case when couplings are small compared to the existing energy level spacings. In the following the abbreviation $1 \otimes A \equiv A$ is made for all operators on the right-hand-side of eq. (10.16). The partition function for a system with known expectation values of the above observables is

$$\begin{aligned} Z(\beta, \gamma, \lambda) &= \text{tr} \exp(-\beta H - \gamma G - \lambda F) \\ &= \text{tr} \exp\left(-(\beta H_1 + \gamma G_1 + \lambda F_1) - \beta H_2 - \gamma G_3\right) \\ &= \text{tr} \exp(-\beta H_1 - \gamma G_1 - \lambda F_1) \cdot \text{tr} \exp(-\beta H_2) \cdot \text{tr} \exp(-\gamma G_3) \\ &= Z_1(\beta, \gamma, \lambda) \cdot Z_2(\beta) \cdot Z_3(\gamma) . \end{aligned}$$

It factors out into contributions from either system. Likewise the density matrix writes

$$\begin{aligned} \rho(\beta, \gamma, \lambda) &= Z^{-1} \exp(-\beta H - \gamma G - \lambda F) \\ &= \frac{\exp(-\beta H_1 - \gamma G_1 - \lambda F_1)}{Z_1(\beta, \gamma, \lambda)} \otimes \frac{\exp(-\beta H_2)}{Z_2(\beta)} \otimes \frac{\exp(-\gamma G_3)}{Z_3(\gamma)} \\ &= \rho_1(\beta, \gamma, \lambda) \otimes \rho_2(\beta) \otimes \rho_3(\gamma) . \end{aligned}$$

It is now apparent that the parameters β and γ are simultaneous properties of systems 1 and 2, respectively 1 and 3. They are equilibrium properties which can be fully determined by measuring the conjugate observable in either of the corresponding subsystems.

For example, H might be the Hamiltonian of the total system and β the inverse temperature. Then β satisfies both of the equations

$$\langle H_1 \rangle = \frac{\partial \ln Z_1}{\partial \beta} , \tag{10.17}$$

$$\langle H_2 \rangle = \frac{\partial \ln Z_2}{\partial \beta} . \tag{10.18}$$

One can think of \mathcal{H}_1 as the main system of interest and \mathcal{H}_2 as an energy bath, a *thermometer*. Then after calibrating temperature to the energy spectrum of

\mathcal{H}_2 in virtue of (10.18) full information about the average energy of \mathcal{H}_1 can be obtained from measuring β in \mathcal{H}_2 . Information is transferred between the two systems without interference [6]. The same is valid for the relation between systems 1 and 3. It is thus possible to imagine a system coupled to several baths operating as measurement devices for certain properties of the original system.

10.3 IRREVERSIBILITY THROUGH INFORMATION LOSS

As already mentioned, the unitary time evolution of a closed quantum mechanical system directly imposes that its von Neumann entropy be constant in time. However this principle of microscopic reversibility is not valid any more for a macroscopic system. In this section, this apparent contradiction shall be lifted by adopting a *subjective* point of view. The idea is to treat irreversibility not as an intrinsic property of a physical system, but as a property of an observer with incomplete knowledge of its true state[6]. Increase in entropy is, in this picture, identified with information loss.

Two primary mechanisms that discard information are voluntary. Suppose that we are interested merely in one particular observable F and its expectation value. Then it is convenient to work in the eigenbasis of F :

$$\langle F \rangle = \text{tr}(\rho F) = \sum_i \rho_{ii} f_i,$$

where the f_i are the eigenvalues of F . A suitable approximation to ρ would thus be to make the replacement $\rho_{kl} \mapsto \rho'_{kl} = \delta_{kl} \rho_{ll}$ in the eigenbasis of F . $\langle F \rangle$ is not changed by this so-called *removal of coherences*[6]. However this simplification comes at the cost of any other observable that does not commute with F . In terms of entropy it is valid that $S(\rho) \leq S(\rho')$ which follows from the concavity of S .

In another circumstance a composite system $\mathcal{H} = \bigotimes_{k=1}^n \mathcal{H}_k$ might be treated, with the principal observable writing as a sum over single subsystem terms: $F = \sum_k F_k$, where F_k acts on \mathcal{H}_k only. In this case

$$\langle F \rangle = \text{tr}(\rho F) = \sum_k \text{tr}(\rho F_k) = \sum_k \text{tr}(\rho_k F_k) = \text{tr}\left((\rho_1 \otimes \dots \otimes \rho_n) F\right),$$

with reduced density matrices $\rho_k = \text{tr}_{\neq k} \rho$. The partial trace $\text{tr}_{\neq k}$ leaves only \mathcal{H}_k untouched. Provided we are only interested in $\langle F \rangle$ it would be equivalent to treat $\rho' = \rho_1 \otimes \dots \otimes \rho_n$ instead of ρ . This simplifies the calculation without cutting back on precision in $\langle F \rangle$. Again, this process of *removing correlations*[6] gives rise to

10.3 Irreversibility through Information Loss

an increase in entropy due to its subadditivity.

We now want to have a look at the case of a system whose hamiltonian does not commute with the observable we are interested in. An example would be a system of N identical spins with the magnetization in z-direction being measured: $S^z = \sum_i \sigma_i^z$. The Hamiltonian may have the general Ising form

$$\begin{aligned} \mathcal{H} &= -\sum_i \mathbf{h}_i \cdot \boldsymbol{\sigma}_i - \sum_{i<j} J_{ij}^x \sigma_i^x \sigma_j^x + J_{ij}^y \sigma_i^y \sigma_j^y + J_{ij}^z \sigma_i^z \sigma_j^z \\ &= \underbrace{\sum_i \mathcal{H}_i}_{\mathcal{H}_0} + \underbrace{\sum_{i<j} \mathcal{V}_{ij}}_{\mathcal{V}} . \end{aligned}$$

In the second line, abbreviations for the one particle hamiltonians \mathcal{H}_i and two particle interactions \mathcal{V}_{ij} are introduced. Note that $[S^z, \mathcal{V}] \neq 0$ in general. Thus even for a magnetic field applied in z-direction, for which the single particle hamiltonians contain σ_i^z only, \mathcal{H} and S^z do not commute. In virtue of *removal of correlations* one could make a product ansatz $\rho' = \rho_1 \otimes \dots \otimes \rho_N$ for the initial state with⁵.

$$\rho_i = \frac{e^{-\beta \mathcal{H}_i}}{\text{tr}(e^{-\beta \mathcal{H}_i})} . \quad (10.19)$$

Assuming weak coupling, a perturbational treatment of \mathcal{V} may be chosen in the interaction representation[8]⁶ with. This does not affect ρ' as it commutes with \mathcal{H}_0 . However a time evolution with the interaction propagator

$$\tilde{U}'(t) = \mathcal{T} \exp \left(-\frac{i}{\hbar} \int_0^t U_0^\dagger(t') \mathcal{V} U_0(t') dt' \right)$$

creates some nonzero correlations again. These are not intended as it does not correspond to our state of knowledge. Only information about S^z is of interest. From that point of view any such correlation is not only useless to our goal, but also injects false information about the true state of the system[6]. Another *removal of correlations* could balance that which in turn leads to an increase in entropy. Repeated iteratively, an irreversible process is created based fully on information loss.

⁵This is a very rough estimate and could be refined by including a nearest neighbour mean-field approximation. However this only adds a constant vector to \mathbf{h}_i and is thus not relevant here. Moreover an additional term $-\gamma \sigma_i^z$ could be implemented to account for information about S^z

⁶The interaction representation induces the transformations $\tilde{A} = U_0^\dagger A U_0$ for any operator A (including the density matrix) with the propagator $U_0(t) = \exp(-i\mathcal{H}_0 t/\hbar)$

In principle, a generalization of the above example is a quantum markov chain that loses information in each step. Jaynes[6] proposed an “information game” in which density matrices of a perturbed system are passed between different observers. Since the nature of the perturbation remains unknown during the process each iteration accumulates new uncertainty about the true state of the system. Another example for sources of information loss would be a stochastic perturbation to a system that is distributed like $\sum_{\alpha} p_{\alpha} V_{\alpha}$ with probabilities p_{α} . Finally, a non-selective measurement on a quantum statistical ensemble induces random projections π_i on the eigenspaces of the observable:

$$\rho \mapsto \rho' = \sum_i \pi_i \rho \pi_i .$$

This has been shown to lead to an decrease in relative entropy [7] between two different pre-measurement states, meaning that they become harder to distinguish from each other. Moreover there is an entropy increase in the measurement apparatus that outweighs the entropy decrease in the system.

10.4 CONCLUSION

The MEP has been successfully applied to problems of statistical inference when only partial information is given. Motivated by the interpretation of entropy as a measure of uncertainty a probability distribution inferred by the MEP is designed to merely use given information and not more. However it appears delicate how to formulate available information as a constraint to the sought for distribution. Still, a great advantage of applying the MEP to statistical mechanics has shown to provide the entire formalism without arbitrary assumptions on the physical nature of an ensemble. This kind of “subjective statistical mechanics” [6] treats physical systems from an information theoretic point of view.

The question which density matrix to choose to represent a physical system is strongly related to what answers we expect it to give. If a Stern-Gerlach type of experiment is considered, the complete density matrix including all correlations between single spins would certainly be required to predict the outcome of any possible experiment. However the reduced density matrix of a single spin is sufficient to set up an experimentally verifiable probability distribution for a given situation. Considering the typically small amount of available information it would even be inappropriate to use the full density matrix. The MEP has proven a powerful tool to infer density matrices for such reduced problems and model interactions with baths.

Finally, regarding statistical physics as an inference problem also turned out

10.4 Conclusion

to suggest how irreversible macroscopic behavior can arise from microscopic reversibility. The idea that information about large systems is constantly liable to being lost is a subjective notion that includes the observer of a system as an equally important variable. Still, this entire formalism relies on the assumption that entropy in a quantum system adopts the von Neumann form. In general it is not clear what the real expression for thermodynamic entropy is. Altogether it is vital to keep in mind that the MEP is primarily a statistical rather than a physical theory and as such has a more abstract significance.

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CHAPTER 11

NMR QUANTUM COMPUTING

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This chapter gives a short introduction into the idea of nuclear magnetic resonance (NMR) quantum computation and some of the major problems are discussed. After the introduction to the basic tools of NMR quantum computation, a closer look at so-called pseudo-pure states is taken. Also the question how to deal with an ensemble readout is treated during this Chapter.

11.1 INTRODUCTION

11.1.1 MOTIVATION

Why are we interested in realizing a quantum computer? Today we need more and more computer resources to solve computational problems and many of them are not solvable at all on a classical computer, at least not in reasonable time. This is because of the huge amount of resources that would be needed to solve them and not because they are in principle insolvable. Quantum computers would allow new algorithms which provide a reasonable speed-up over several classical algorithms and thus allow to solve some of the yet unsolvable problems.

In general we need two-level systems to realize quantum bits and also a possibility to manipulate and readout the quantum states. Thus the difficulty is, that we need a quantum computer which is well isolated so that it keeps its quantum properties, but is also accessible for manipulation and readout.

A single nuclear spin is basically ideal for the representation of a qubit, but as it has nearly no coupling to the environment it is hard to readout the orientation of

11.1 Introduction

the single nuclei. Thus the basic idea is to take molecules, where the Fermi contact interactions provide strong natural couplings, but it is very difficult to cool and trap a single molecule. That is why the idea came up to use nuclear magnetic resonance (NMR) to directly manipulate and detect the nuclear spin states using electromagnetic waves. Another advantage of this idea is, that NMR is a widely used and well known technique, e.g. in chemistry for NMR spectroscopy or in medicine for magnetic resonance imaging. Despite some challenges one has to deal with, the first quantum computer was realized in 2001 using nuclear magnetic resonance to realize Shor's quantum factoring algorithm [1].

The challenges one still has to deal with are on the one hand, that NMR is typically applied to physical systems in thermal equilibrium at room temperature, which basically means that the initial state of the spins is nearly completely random, and on the other hand, one has to deal with a large number of molecules ($> 10^8$) to produce a measurable induction signal [2]. This leads to the following two questions: How can quantum computation be performed with a system in a high entropy mixed state instead of a pure state? And can the average output of an ensemble of quantum computers be meaningful? In this Chapter we will introduce the basic techniques for dealing with NMR quantum computers and answer these questions.

11.1.2 EXPERIMENTAL SETUP

The spectrometer consists of a large superconducting magnet to produce a strong magnetic field B_0 in \hat{z} -direction, which is trimmed to be uniform. In the transverse plane there are radio-frequency (RF) coils which allow to apply small oscillating magnetic fields along \hat{x} - and \hat{y} -directions. The same coils are also used to pick up the RF signal of the precessing nuclei. For controlling the RF coils and readout of the induced signal some RF technique is needed, which will not be specified here. The general setup can be seen in Figure 11.1 and Ref. [2].

Another important part is represented by molecules which are typically dissolved in a solvent to reduce the concentration such that inter-molecular interactions become negligible. A typical molecule contains a number n of protons with spin $\frac{1}{2}$ or other possible nuclei with spin $\frac{1}{2}$, e.g. ^{13}C or ^{19}F . The frequencies of identical nuclei can differ by a few kHz upto hundreds of kHz due to the chemical shift. The chemical shift is denoted by σ and describes the fact that there are differences in the local magnetic field because of chemical environment shielding effects inside the molecule. For example in the Trichloroethylene molecule in Figure 11.2 the two carbon nuclei have different frequencies because of the different environment.

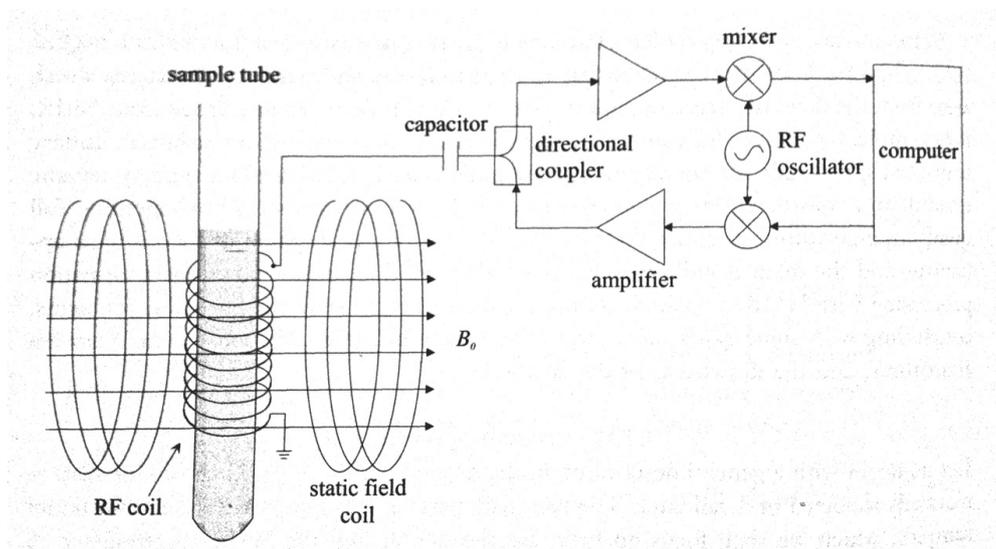


Figure 11.1: General setup taken from Ref. [2].

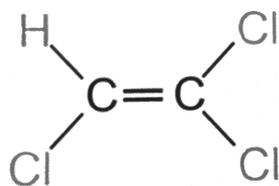


Figure 11.2: Trichloroethylene molecule with three qubit:, one proton and two carbon nuclei (taken from Ref. [2]).

11.1 Introduction

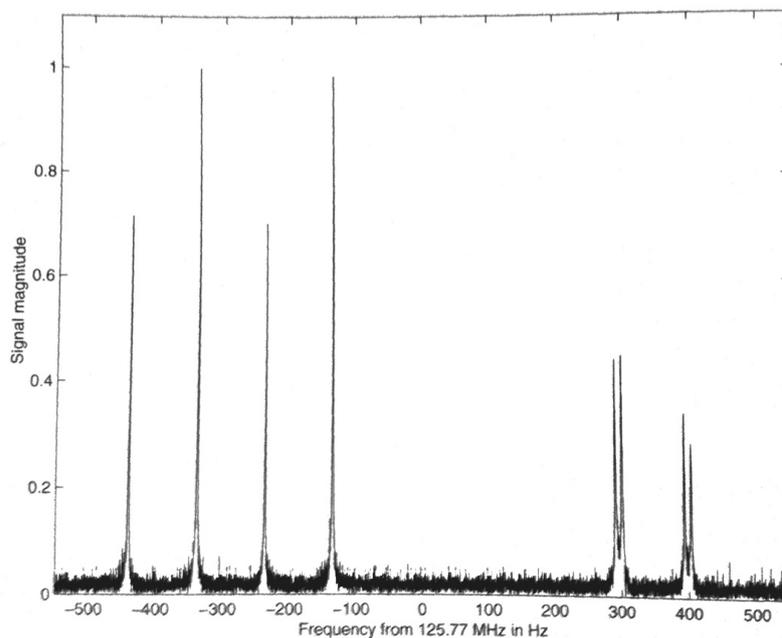


Figure 11.3: The carbon frequency spectrum of Trichloroethylene. The left four lines belong to the carbon nuclei next to the proton and the right four lines to the second carbon nuclei. The four lines are due to couplings to the proton and the other carbon, that is also why the four lines on the right are closely spaced, because the coupling to the proton is less strong (taken from Ref. [2]).

To sum up, in typical experiments, one waits several minutes until the nuclei are settled at thermal equilibrium and then apply the RF pulses to effect the desired transformations. Afterwards a sensitive pre-amplifier measures the final state of the spin, which is basically given by the free induction decay signal. A Fourier transform of this signal gives then the frequency spectrum. An example for this is given in figure 11.3 which also illustrates the effect of the chemical shift.

11.2 THE HAMILTONIAN

This section treats only the easiest one and two dimensional cases, as the multidimensional versions can be derived in an analogous way. First we will derive the Hamiltonian for a single spin system and then go on with the Hamiltonians for the different couplings that are present in molecules.

11.2.1 SINGLE SPIN HAMILTONIAN

As we are only interested in the magnetic interaction of a classical electromagnetic field with the two-state spin we neglect the kinetic term and the Hamiltonian is given by:

$$\mathcal{H} = -\boldsymbol{\mu} \cdot \mathbf{B} = -\gamma \hbar \mathbf{I} \cdot \mathbf{B} \quad (11.1)$$

where γ is the gyromagnetic ratio and \mathbf{I} the angular momentum operator of the nuclear spin:

$$\mathbf{I} = \begin{pmatrix} I_x \\ I_y \\ I_z \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} \quad (11.2)$$

We choose now the strong uniform and static magnetic field B_0 to be oriented along the \hat{z} -direction and the small, oscillating magnetic fields B_1 with frequency ω and phase ϕ to be applied along the \hat{x} - and \hat{y} -directions. A typical applied field is therefore given by

$$\mathbf{B} = B_0 \hat{z} + B_1 [\hat{x} \cos(\omega t + \phi) - \hat{y} \sin(\omega t + \phi)] \quad (11.3)$$

So we get

$$\mathcal{H} = -\gamma \hbar [B_0 I_z + B_1 I_x \cos(\omega t + \phi) - B_1 I_y \sin(\omega t + \phi)] \quad (11.4)$$

We now define the Larmor frequency

$$\omega_0 = \gamma B_0 \quad (11.5)$$

and analogously

$$\omega_1 = \gamma B_1 \quad (11.6)$$

So the Hamiltonian is now

$$\mathcal{H} = -\frac{\hbar\omega_0}{2} \sigma_z - \frac{\hbar\omega_1}{2} [\sigma_x \cos(\omega t + \phi) - \sigma_y \sin(\omega t + \phi)] \quad (11.7)$$

For a form that is nicer to handle we look at the situation in the frame which is rotating with the frequency ω :

$$|\varphi(t)\rangle = e^{-i\omega t \sigma_z / 2} |\chi(t)\rangle \quad (11.8)$$

11.2 The Hamiltonian

Substituting this into the Schrödinger equation

$$i\hbar\partial_t|\chi(t)\rangle = \mathcal{H}|\chi(t)\rangle \quad (11.9)$$

, we obtain

$$-\hbar\frac{\omega\sigma_z}{2}e^{i\omega t\sigma_z/2}|\varphi(t)\rangle + i\hbar e^{i\omega t\sigma_z/2}\partial_t|\varphi(t)\rangle = \mathcal{H}e^{i\omega t\sigma_z/2}|\varphi(t)\rangle \quad (11.10)$$

and finally

$$i\hbar\partial_t|\varphi(t)\rangle = \left[e^{-i\omega t\sigma_z/2}\mathcal{H}e^{i\omega t\sigma_z/2} + \hbar\frac{\omega\sigma_z}{2} \right] |\varphi(t)\rangle \quad (11.11)$$

Where we used the property

$$e^{-i\omega t\sigma_z/2}\sigma_z e^{i\omega t\sigma_z/2} = \sigma_z \quad (11.12)$$

. One can also show that

$$e^{i\omega t\sigma_z/2}\sigma_x e^{-i\omega t\sigma_z/2} = \sigma_x \cos \omega t - \sigma_y \sin \omega t \quad (11.13)$$

So if we calculate $e^{-i\omega t\sigma_z/2}\mathcal{H}e^{i\omega t\sigma_z/2}$ from Equation 11.11 we get

$$\begin{aligned} & e^{-i\omega t\sigma_z/2}\mathcal{H}e^{i\omega t\sigma_z/2} \\ &= e^{-i\omega t\sigma_z/2} \left(-\frac{\hbar\sigma_z}{2}\omega_0 - \frac{\hbar\omega_1}{2}(\sigma_x \cos(\omega t + \phi) - \sigma_y \sin(\omega t + \phi)) \right) e^{i\omega t\sigma_z/2} \\ &= -\frac{\hbar\sigma_z}{2}\omega_0 - \frac{\hbar\omega_1}{2}e^{-i\omega t\sigma_z/2}e^{i(\omega t + \phi)\sigma_z/2}\sigma_x e^{-i(\omega t + \phi)\sigma_z/2}e^{i\omega t\sigma_z/2} \\ &= -\frac{\hbar\sigma_z}{2}\omega_0 - \frac{\hbar\omega_1}{2}e^{i\phi\sigma_z/2}\sigma_x e^{-i\phi\sigma_z/2} \\ &= -\frac{\hbar\sigma_z}{2}\omega_0 - \frac{\hbar\omega_1}{2}(\sigma_x \cos \phi - \sigma_y \sin \phi) \end{aligned} \quad (11.14)$$

Thus the Hamiltonian in the rotating frame reads

$$\mathcal{H} = -\frac{\hbar\sigma_z}{2}(\omega_0 - \omega) - \frac{\hbar\omega_1}{2}(\sigma_x \cos \phi - \sigma_y \sin \phi) \quad (11.15)$$

One can see that the effect of $B_1(= \frac{\omega_1}{\gamma})$ on the spin is rather small if ω is far away from ω_0 . But if $\omega \approx \omega_0$ the field $B_0(= \frac{\omega_0}{\gamma})$ contributes nearly nothing and even a small B_1 field has a rather big influence on the spin, that is why this technique is called nuclear magnetic "resonance".

11.2.2 HAMILTONIAN OF COUPLED SPINS

In the system we are usually interested in, we have more than one spin. We consider a nuclear spin of 1/2. The spins interact through two dominant mechanisms:

- direct dipolar coupling
- indirect through-bond electron mediated mechanisms

DIRECT DIPOLAR COUPLING From classical electrodynamics it is known that the field of a magnetic dipole is given by

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi r^5} [3(\boldsymbol{\mu} \cdot \mathbf{r})\mathbf{r} - (\mathbf{r} \cdot \mathbf{r})\boldsymbol{\mu}] \quad (11.16)$$

If we introduce a second dipole at \mathbf{r}_{12} that couples to this field, we get the interaction energy and thus the interaction Hamiltonian:

$$\mathcal{H}_{12}^D = -\mathbf{B}(\mathbf{r}_{12}) \cdot \boldsymbol{\mu}_2 = \frac{\mu_0 \gamma_1 \gamma_2 \hbar^2}{4\pi r_{12}^3} \left[\mathbf{I}_1 \cdot \mathbf{I}_2 - \frac{3}{r_{12}^2} (\mathbf{I}_1 \cdot \mathbf{r}_{12})(\mathbf{I}_2 \cdot \mathbf{r}_{12}) \right] \quad (11.17)$$

If ω_0 is large (which means B_0 is large) and $|\omega_0^1 - \omega_0^2|$ is much larger than the coupling strength, the spins are aligned in the \hat{z} -direction and the Hamiltonian can be approximated by

$$\mathcal{H}_{12}^D = \frac{\mu_0 \gamma_1 \gamma_2 \hbar^2}{4\pi r_{12}^3} I_z^1 I_z^2 [1 - 3 \cos^2 \theta_{12}] \quad (11.18)$$

In a liquid with low viscosity the dipolar interactions are averaged out, it can easily be shown that $\int_0^\pi (1 - 3 \cos^2 \theta) \sin \theta d\theta = 0$ and thus the spherical average over \mathcal{H}_{12}^D goes to zero. For a system with N spins it follows directly that the Hamiltonian is given by

$$\mathcal{H}^D = \frac{\mu_0 \hbar^2}{4\pi} \frac{1}{2} \sum_{i=1}^N \sum_{k=1}^N \left[\frac{\gamma_i \gamma_k \mathbf{I}_i \cdot \mathbf{I}_k}{r_{ik}^3} - \frac{3(\gamma_i \mathbf{I}_i \cdot \mathbf{r}_{ik})(\gamma_k \mathbf{I}_k \cdot \mathbf{r}_{ik})}{r_{ik}^5} \right] \quad (11.19)$$

THROUGH-BOND INTERACTIONS / J-COUPLING These indirect interactions describe the fact, that the nuclei are coupled due to electrons that are shared in the chemical bond. The coupling is also known as J -coupling or scalar-coupling. In general the Hamiltonian for the scalar coupling between two spins is given by

$$\mathcal{H}_{12}^J = 2\pi \mathbf{I}_1 \cdot J \cdot \mathbf{S}_2 \quad (11.20)$$

Where J in general is a tensor. A first sensible approximation is to assume a scalar coupling constant which then leads to the expression

$$\mathcal{H}_{12}^J = 2\pi J_{12} \mathbf{I}_1 \cdot \mathbf{S} = 2\pi \hbar J_{12} \mathbf{I}_1 \cdot \mathbf{I}_2 \quad (11.21)$$

If we again consider that $|\omega_0^1 - \omega_0^2| \gg 2\pi J_{12}$ the Hamiltonian is approximately given by

$$\mathcal{H}_{12}^J \approx 2\pi \hbar J_{12} I_z^1 I_z^2 \quad (11.22)$$

Again we can easily switch to an N spin system

$$\mathcal{H}^J = \hbar \pi \sum_{i=1}^N \sum_{k=1}^N J_{ik} I_z^i I_z^k \quad (11.23)$$

11.3 Quantum gates

11.2.3 DENSITY OPERATOR

As already mentioned NMR differs a lot from other methods of quantum computation, as it is consisting of an ensemble of systems and the measurement is an ensemble average. Since the system is not prepared in a special ground state, the initial state is given by the thermal equilibrium state

$$\rho = \frac{e^{-\beta\mathcal{H}}}{\mathcal{Z}} \quad (11.24)$$

, where $\mathcal{Z} = \text{tr}(e^{-\beta\mathcal{H}})$ is the usual partition function normalization, which ensures that $\text{tr}(\rho) = 1$. As the experiment is normally set up at room temperature, we have for modest fields $\mathcal{H}\beta \approx 10^{-4}$ and the high temperature approximation is appropriate:

$$\rho \approx \frac{1 - \beta\mathcal{H}}{\text{tr}(1 - \beta\mathcal{H})} = 2^{-n} [1 - \beta\mathcal{H}] \quad (11.25)$$

Note that we have used that the Hamiltonian is traceless due to the fact, that the Pauli matrices are traceless. Let us consider the following two examples.

The density operator for a single spin at thermal equilibrium is simply

$$\rho \approx \frac{1}{2} - \frac{\hbar\omega_0}{4k_B T} \sigma_z = \frac{1}{2} - \frac{\hbar\omega_0}{4k_B T} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (11.26)$$

If we assume a 2 spin system with $4\omega_A \approx \omega_B$ we get

$$\rho \approx \frac{1}{4} - \frac{\beta}{4} (\mathcal{H}_A \otimes 1 + 1 \otimes \mathcal{H}_B) = \frac{1}{4} - \frac{\hbar\omega_B}{8k_B T} \begin{bmatrix} 5 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & -3 & 0 \\ 0 & 0 & 0 & -5 \end{bmatrix} \quad (11.27)$$

11.3 QUANTUM GATES

It was shown that any unitary transformation U acting on N qubits can be composed of CNOT gates and single qubit rotations. That is the reason why we limit the discussion to the implementation of these two gates, which are represented by the matrices

$$U_{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad R_{\hat{n}}(\theta) = e^{-i\frac{\theta\hat{n}\cdot\sigma}{2}} \quad (11.28)$$

Where R denotes the rotation of an angle θ about the axis \hat{n} .

11.3.1 ROTATIONS

Analogue to the rotation operator $R_{\hat{n}}(\theta) = e^{-i\frac{\theta}{\hbar}\hat{n}\cdot\mathbf{L}}$ we define for the spin rotation

$$R_{\hat{n}}(\theta) = e^{-i\frac{\theta}{\hbar}\hat{n}\cdot\mathbf{S}} = e^{-i\frac{\theta}{2}\hat{n}\cdot\boldsymbol{\sigma}} \quad (11.29)$$

The rotation operators about the \hat{x} , \hat{y} , and \hat{z} axes are then given by the expressions:

$$R_x(\theta) = e^{-i\frac{\theta\sigma_x}{2}} \quad (11.30)$$

$$R_y(\theta) = e^{-i\frac{\theta\sigma_y}{2}} \quad (11.31)$$

$$R_z(\theta) = e^{-i\frac{\theta\sigma_z}{2}} \quad (11.32)$$

11.3.2 CNOT-GATE

In the following we want to look at the case of a two qubit system. Let us consider only the coupling Hamiltonian \mathcal{H}_J , which is reasonable since we can tune two oscillators exactly to the rotating frequencies of the nuclei and thus in the rotating frame of the oscillators we only have to deal with

$$\mathcal{H}_J = 2\pi\hbar J I_z^1 I_z^2 \quad (11.33)$$

So the evolution of the spin is given by

$$U_J(t) = e^{-i\mathcal{H}_J t/\hbar} = e^{-i2\pi J I_z^1 I_z^2 t} = \begin{bmatrix} e^{-i\frac{\pi J t}{2}} & 0 & 0 & 0 \\ 0 & e^{i\frac{\pi J t}{2}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\pi J t}{2}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\pi J t}{2}} \end{bmatrix} \quad (11.34)$$

We choose a free evolution period of time $t = \frac{1}{2J}$ due to J-coupling, which gives us

$$U_J\left(\frac{1}{2J}\right) = \begin{bmatrix} e^{-i\frac{\pi}{4}} & 0 & 0 & 0 \\ 0 & e^{i\frac{\pi}{4}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\pi}{4}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\pi}{4}} \end{bmatrix} \quad (11.35)$$

Combined with some single qubit rotations and an irrelevant global phase we get the CNOT gate

$$U_{CNOT} = e^{i\frac{\pi}{4}} R_{z1}\left(\frac{\pi}{2}\right) R_{z2}\left(-\frac{\pi}{2}\right) R_{x2}\left(\frac{\pi}{2}\right) U_J\left(\frac{1}{2J}\right) R_{y2}\left(\frac{\pi}{2}\right) \quad (11.36)$$

11.3 Quantum gates

This can be seen from the matrix representation of the rotations

$$R_{y2}\left(\frac{\pi}{2}\right) = 1 \otimes e^{-i\frac{\pi\sigma_y}{4}} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \quad (11.37)$$

$$R_{x2}\left(\frac{\pi}{2}\right) = 1 \otimes e^{-i\frac{\pi\sigma_x}{4}} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \quad (11.38)$$

$$R_{z2}\left(-\frac{\pi}{2}\right) = 1 \otimes e^{i\frac{\pi\sigma_z}{4}} = \begin{bmatrix} e^{i\frac{\pi}{4}} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\pi}{4}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\pi}{4}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\pi}{4}} \end{bmatrix} \quad (11.39)$$

$$R_{z1}\left(\frac{\pi}{2}\right) = e^{-i\frac{\pi\sigma_z}{4}} \otimes 1 = \begin{bmatrix} e^{-i\frac{\pi}{4}} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\pi}{4}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\pi}{4}} & 0 \\ 0 & 0 & 0 & e^{i\frac{\pi}{4}} \end{bmatrix} \quad (11.40)$$

Finally by simply matrix multiplication we get

$$U_{CNOT} = \begin{bmatrix} \frac{1}{2}(1 - e^{i\frac{\pi}{2}i}) & -\frac{1}{2}(1 + e^{i\frac{\pi}{2}i}) & 0 & 0 \\ \frac{1}{2}(1 - e^{-i\frac{\pi}{2}i}) & \frac{1}{2}(1 + e^{-i\frac{\pi}{2}i}) & 0 & 0 \\ 0 & 0 & \frac{1}{2}(e^{i\pi} - e^{i\frac{\pi}{2}i}) & -\frac{1}{2}(e^{i\pi} + e^{i\frac{\pi}{2}i}) \\ 0 & 0 & \frac{1}{2}(1 - e^{i\frac{\pi}{2}i}) & \frac{1}{2}(1 + e^{i\frac{\pi}{2}i}) \end{bmatrix} \\ = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad (11.41)$$

11.3.3 REFOCUSING

We saw that if we apply a RF field at a proper frequency the Hamiltonian is basically given by \mathcal{H}_{RF} , the time evolution is approximately given by

$$e^{-i\frac{\mathcal{H}t}{\hbar}} \approx e^{-i\frac{\mathcal{H}_{RF}t}{\hbar}} \quad (11.42)$$

This allows to perform single qubit operations with excellent fidelity. We define the 90° rotation about the \hat{x} -axis on spin 1 as

$$R_{x1} = e^{-i\frac{\pi\sigma_{x1}}{4}} \quad (11.43)$$

and similarly for spin 2. Then we find that the 180° rotation R_{x1}^2 has the special property that

$$R_{x1}^2 e^{-ia\sigma_{z1}t} R_{x1}^2 = -e^{ia\sigma_{z1}t} \quad (11.44)$$

With a being a constant or an operator which is not acting on the z_1 -component. This equation can again be proven by simply matrix multiplication. The matrix representations of the rotations are given by:

$$R_{x1}^2 = e^{-i\frac{\pi\sigma_x}{2}} \otimes 1 = - \begin{bmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix} \quad (11.45)$$

$$e^{-ia\sigma_{z1}t} = e^{-ia\sigma_z t} \otimes 1 = \begin{bmatrix} e^{-iat} & 0 & 0 & 0 \\ 0 & e^{-iat} & 0 & 0 \\ 0 & 0 & e^{iat} & 0 \\ 0 & 0 & 0 & e^{iat} \end{bmatrix} \quad (11.46)$$

So by simple multiplication we get

$$R_{x1}^2 e^{-ia\sigma_{z1}t} R_{x1}^2 = - \begin{bmatrix} e^{iat} & 0 & 0 & 0 \\ 0 & e^{iat} & 0 & 0 \\ 0 & 0 & e^{-iat} & 0 \\ 0 & 0 & 0 & e^{-iat} \end{bmatrix} = -e^{ia\sigma_{z1}t} \quad (11.47)$$

Which proves Equation 11.44. Because this transformation reverses the time evolution, except for an irrelevant global phase, in a way that spins that started together at some point of the Bloch sphere come back to the same point, this is known as refocusing. And thus the 180° pulses are called refocusing pulses. Note that as long as it contains no operator acting on spin 1, a can be a operator as well as a constant. That means if we apply refocusing pulses to spin 1 and spin 2 we can remove the coupled time evolution of spins. Refocusing even allows to remove all time evolution entirely.

11.4 PSEUDO-PURE STATES

As seen so far, we are able to realize any unitary transformation on a spin system using RF pulses. This and the fact that it is possible with high precision, is one of the most attractive aspects of NRM quantum computing. But we are still left with the question, how we can deal with the initial state, which is normally a thermal equilibrium state and thus has a high entropy. In this section so-called

11.4 Pseudo-pure states

pseudo-pure states (or also effective pure states) are introduced to show how to deal with this problem. Therefore different methods are introduced, starting with temporal averaging.

11.4.1 TEMPORAL AVERAGING

The temporal averaging method uses several experiments with different preparation steps and the final answer is given by the average over the measurements. The advantages of this method are that it can be implemented at any temperature; there is no need for ancillary qubits and it is not necessary to distinguish subensembles of quantum computers. As our sample is normally at room temperature, the following discussion is limited to the high-temperature methods. There are three high-temperature methods:

- exhaustive averaging
- labeled flip and swap
- randomized flip and swap

The flip and swap methods rely on the inversion symmetry of high-temperature thermal states of non-interacting particles. Where the labeled flip and swap uses a limited form of ancillary qubits, whereas the randomized flip and swap works without ancillary qubits, but may need some more experiments. In the following the first method, exhaustive averaging, is discussed in detail, as it is the most demonstrative method and shows the key principles of temporal averaging.

EXHAUSTIVE AVERAGING This method is in general based on two important facts: Quantum operations are linear and the measured observables are traceless for NMR quantum computation. Assume a two qubit example at room-temperature; this is generally given by:

$$\rho_0 = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & d \end{bmatrix}, \quad a + b + c + d = 1 \quad (11.48)$$

If our goal is to perform some computation U on $|00\rangle\langle 00|$, the other states, namely $|01\rangle\langle 01|$, $|10\rangle\langle 10|$, $|11\rangle\langle 11|$, constitute noise and we have to get rid of them. The idea is now to set up different experiments where we permute the entries of ρ

that represent the states we want to get rid of. In our general example we use circuits P_1 and P_2 to permute the entries b, c, d

$$\rho_1 = P_1 \rho_0 P_1^\dagger = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & c & 0 & 0 \\ 0 & 0 & d & 0 \\ 0 & 0 & 0 & b \end{bmatrix} \quad (11.49)$$

$$\rho_2 = P_2 \rho_0 P_2^\dagger = P_1^\dagger \rho_0 P_1 = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & d & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & c \end{bmatrix} \quad (11.50)$$

This means we have to deal with three experiments, which can be carried out at different times. Now we take the average over the three resulting density matrices, which gives us the following expression for $\bar{\rho}$, where P_0 is simply the identity:

$$\begin{aligned} \bar{\rho} &= \frac{1}{3} \sum_{k=0}^2 P_k \rho_0 P_k^\dagger = \frac{1}{3} \begin{bmatrix} 3a & 0 & 0 & 0 \\ 0 & b+c+d & 0 & 0 \\ 0 & 0 & b+c+d & 0 \\ 0 & 0 & 0 & b+c+d \end{bmatrix} \\ &= \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & \frac{1-a}{3} & 0 & 0 \\ 0 & 0 & \frac{1-a}{3} & 0 \\ 0 & 0 & 0 & \frac{1-a}{3} \end{bmatrix} \end{aligned} \quad (11.51)$$

Here, we have used the fact that $a+b+c+d=1$. Now we can split this in to two matrices, where one looks like a pure state and the other one is just a multiple of the identity.

$$\bar{\rho} = \frac{4a-1}{3} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \frac{1-a}{3} \mathbf{1} \quad (11.52)$$

As mentioned before, in NMR the observables M fulfil $\text{tr}(M) = 0$, so that we get for a measurement after performing some unitary transformation U :

$$\text{tr}(U \bar{\rho} U^\dagger M) = \frac{4a-1}{3} \text{tr}(U |00\rangle\langle 00| U^\dagger M) + \frac{1-a}{3} \underbrace{\text{tr}(M)}_{=0} \quad (11.53)$$

Although we are dealing with a high entropy mixed state we are able to construct a pseudo-pure state and thus are able to perform computations on our systems.

11.4 Pseudo-pure states

This method works for any initial state that is diagonal in the computational basis state, but for a n qubit system we need to cyclically permute the non-ground state in $2^n - 1$ ways [3]. This means the number of required experiments grows exponentially and thus, it is only reasonable to implement this method for a small number of qubits.

11.4.2 LOGICAL LABELING

Logical labeling is based on similar considerations, but does not require multiple experiments to be performed. The fundamental idea is to identify equally populated states that naturally exist in a thermal ensemble and use unitary transformations to group together these entries of the density matrix and thus form a uniform background against which a differently populated single pure state can be distinguished. Then we use some other spins to label this group and produce a state where we have a few spins in a pure states (qubit spins) which conditioned on the state of the other spins (ancillary spins). Afterwards one freezes the time evolution of the ancillary spins using refocusing techniques so that there is no need to deal with the dynamics of the ancillary spins [4]. For a better understanding I give an example of a three spin state. Let us consider the density matrix of an arbitrary initial three spin state:

$$\rho = \delta \mathbf{1} + \alpha \text{diag}(6, 2, 2, -2, 2, -2, -2, -6) \quad (11.54)$$

Where $\delta \mathbf{1}$ denotes an unobservable background population and $\alpha \ll \delta$. Now we use a unitary transformation P to permute the entries and group them together:

$$\rho' = P\rho P^\dagger = \delta \mathbf{1} + \alpha \text{diag}(6, -2, -2, -2, -6, 2, 2, 2) \quad (11.55)$$

, where the upper block of this matrix represents a pseudo pure state:

$$\begin{bmatrix} 6 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix} = 8 |00\rangle\langle 00| - 2 \mathbf{1} \quad (11.56)$$

With the help of the label (ancillary spins) we can isolate the signal of the subspace of states in order to get the results of a computation performed on the pure state $|00\rangle\langle 00|$.

11.4.3 SPATIAL LABELING

For the sake of completeness the general idea of spatial labeling is also mentioned. Basically spatial labeling describes a method where exhaustive averaging is done

simultaneously, which means, that we partition the ensemble of quantum computers into a number of subensembles and apply different unitary operator to each of them. Experimentally this can be done, by applying gradient magnetic fields which vary systematically over a single sample.

11.5 MEASUREMENT

The free induction decay is measured, which contains the computational result (the precession frequency) and readout the response (amplitude and phase). Mathematically the induced voltage is given by

$$V(t) = V_0 \operatorname{tr} \left[e^{-i\frac{\mathcal{H}}{\hbar}t} \rho e^{i\frac{\mathcal{H}}{\hbar}t} (i\sigma_x^k + \sigma_y^k) \right] \quad (11.57)$$

The voltage $V(t)$ is induced in the RF coils by the rotating magnetization of the sample. Finally the Fourier transform gives the frequency spectrum as shown in Figure 11.3. Still there is the question if the ensemble readout can lead a meaningful result, since the average of random variables does not necessarily give any relevant information. To get an idea we take a closer look at an example: the quantum factoring algorithm. Generally it produces a random rational number $\frac{c}{r}$, where c is a random unknown integer and r is the desired result. One performs first a projective measurement to obtain $\frac{c}{r}$ and then a classical fraction algorithm to obtain c with high probability. Then the result is checked by inserting it. But since c is nearly uniform distributed, the average value $\langle \frac{c}{r} \rangle$ contains no meaningful information. To solve this we append any required classical post-processing step to the quantum computation, which is always possible since a quantum computer subsumes classical computation. In our example we ask each individual quantum computer (molecule) to perform a continued fraction algorithm. The result is then checked on each quantum computer and only those who succeed return an output. Thus, the average over the ensemble gives us $\langle r \rangle$. A similar procedure is possible for every quantum algorithm.

11.6 DRAWBACKS

The big advantages of NMR are that the required techniques are already well known and widely used and that the experiments can be done at room temperature. This is the reason why it was the first realized quantum computer. But beside that there are still a lot of drawbacks to the idea of NMR quantum computing, which is the reason, why we are still not able to realize a large quantum computer using NMR. One of the drawbacks is the fact that it is difficult to find

11.7 Conclusion

molecules with more than ≈ 10 spins in them, that still have a strong coupling between every pair of them [5]. Also the preparation of pseudo-pure states reduces the signal exponentially in the number of qubits as the probability for one component of the density operator scales exponentially namely proportional to $n2^{-n}$). It was roughly estimated that the absolute limit on what any practical NMR computer can handle remains well below 100 qubits by assuming that the error in an estimated expectation value should be less than 2^{-2n} and require that with a fixed probability at least one molecule samples at least one solution [5]. Concluding this, the big problem is that NMR quantum computers are not arbitrary scalable.

11.7 CONCLUSION

This chapter gave a general overview over the techniques used to realize NMR quantum computation. Especially we have answered the question how we can deal with high entropy mixed states by introducing so called pseudo-pure states. We have seen some fundamental examples of different methods for obtaining such a state. We also discussed how we can get a reasonable result out of an ensemble readout by using classical post-processing steps. And finally we summarized the rough limitations of NMR quantum computing and concluded that it is not arbitrary scalable. Even though many other simple quantum computers were realized using different techniques, NMR gives a nice illustration of the basic techniques for quantum computation and provides a testbed for quantum algorithms.

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CHAPTER 12

THE DENSITY-MATRIX RENORMALIZATION GROUP METHOD

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S. R. White developed a numerical algorithm called Density-Matrix Renormalization Group (DMRG) Method, which was firstly mentioned 1991[1]. This algorithm can be used to efficiently compute the ground state wave function of one dimensional systems. The main idea of DMRG is an efficient truncation of the Hilbert space. The approximation of the ground state is amazingly accurate; for example, the ground-state energy per site of the $S = 1$ isotropic antiferromagnetic Heisenberg chain has been computed up to many digits ($E_0 = -1.401484038970$)[2].

12.1 INTRODUCTION

The DMRG method of S. R. White solves one dimensional problems much better than other algorithms as Quantum Monte-Carlo, which is limited by the negative-sign problem¹, and other less powerful coupled-cluster methods and series expansion techniques.

The Hilbert space of a system increases exponentially with size of the system. For example, a system of L sites with N_{Site} states per site has $(N_{Site})^L$ basis vectors.

¹The negative-sign problem implies that the error bar diverges exponentially with system size and inverse temperature ($\Delta \approx \exp(N/T)$).

12.1 Introduction

Therefore, the corresponding total Hilbert space,

$$\mathcal{H}_{system} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_L \quad (12.1)$$

has the dimension $(N_{Site})^L$, where the Hilbert space of each site \mathcal{H}_i has the dimension N_{Site} .

The main goal of the DMRG method is to reduce the Hilbert space by an efficient truncation, where relevant states are kept and non-relevant states are discarded.

12.1.1 EXAMPLE HAMILTONIANS

A typical problem is to find the ground state of a system with interactions, which is described by a Hamiltonian. These problems are often not exactly solvable. Even for simplified Hamiltonians, which efficiently describe the system, the problems are hard to solve. Here are some examples of well known Hamiltonians:

THE FERMIONIC HUBBARD MODEL

A famous example is the fermionic Hubbard model with on-site repulsion

$$\hat{H}_{Hubbard} = - \sum_{\langle ij \rangle, \sigma} t (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (12.2)$$

The first term describes the (isotropic) hopping of the electrons between nearest neighbors. The expression $\langle ij \rangle$ means that the summation takes terms into account, where i and j are nearest neighbors, and the abbreviation h.c. means the hermitian conjugate of $c_{i\sigma}^\dagger c_{j\sigma}$. The second term describes the (Coulomb) repulsion of electrons on the same site. The basis on each site can be written as $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ and the number of states per site is $N_{Site} = 4$.

In two dimensions the Hubbard model is even harder to solve. Since 20 years, it is an open question, if high-temperature superconductors could be described by the 2 dimensional Hubbard model.

THE HEISENBERG MODEL

Another example is the Heisenberg model given by

$$\hat{H}_{Heisenberg} = \sum_{\langle ij \rangle} \mathbf{J}_i \mathbf{S}_i \mathbf{S}_j \quad (12.3)$$

which is an effective model of the Hubbard model at half-filling and $\frac{U}{t} \gg 1$, with $J = 4\frac{t^2}{U}$. This model describes the spin-interaction of nearest neighbors on a

lattice. For the spin- $S = \frac{1}{2}$ chain, the basis on each site can be written as $|\uparrow\rangle, |\downarrow\rangle$ and the number of states per site is $N_{Site} = 2$ (the spin- $S = 1$ chain has three states per site).

In one dimension, the spin- $S = 1$ Heisenberg model is gapped but the spin- $S = \frac{1}{2}$ model is critical, which implies that it is harder to solve with DMRG (see section 12.5).

12.2 PROCEDURE

There are two variants of the DMRG method, the infinite-system DMRG and the finite-system DMRG. On one hand, the infinite-system DMRG is the technique, in which the system size grows at every step. On the other hand, the system size is fixed in the finite-system DMRG, and it can be used to further improve the precision.

We use the following notation:

Definition 12.1. I denote a system block with S and an environment block with E , as illustrated in Fig.12.1, and further:

- the number of states per site with N_{Site} ,
- the number of states of the system block S with $M^{(S)}$, and
- the number of states of the environment block E with $M^{(E)}$.

12.2.1 INFINITE-SYSTEM DMRG

The infinite-system DMRG algorithm enlarges the system and the corresponding environment at every iteration step.

At system length l , a step consist of the following parts:

0. Initialization (only once) of the Hamiltonian in the basis of size $M^{(S)}$ for the system and $M^{(E)}$ for the environment,
1. Adding one site to each the system and the environment; build the superblock (of dimension $N^{(S)}N^{(E)}$, but this is not performed explicitly for reasons of efficiency) from the new system $S\bullet$ and the environment $\bullet E$;
2. Find the new ground state of the Hamiltonian represented in the superblock (as in Eq. 12.6) by large sparse-matrix diagonalization,

12.2 Procedure

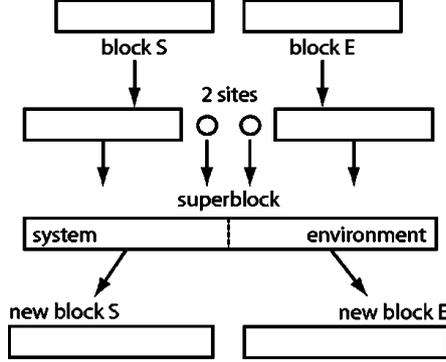


Figure 12.1: The infinite-system DMRG consists mainly of three parts. Firstly, adding one site to the system and to the environment. Secondly, forming the superblock out of the system and the environment with the additional sites. Thirdly, splitting up the superblock into new system and environment. The figure is taken from Ref. [3].

3. Determine the eigenbasis and -values of the reduced density matrix $\hat{\rho}^{(S)}$ and keep the $M^{(S)}$ eigenvectors with the largest eigenvalues,
4. Transform the Hamiltonian in the new basis for the system and environment of dimension $M^{(S)}$ and $M^{(E)}$ respectively.

Here are further details of the individual steps:

INITIALIZATION (STEP 0)

The initialization often takes place at small size (i.e. $(N_{Site})^L \leq M^{(S)}$), such that the Hamiltonian is still in an exact basis.

ADDING ONE SITE AND BUILD THE SUPERBLOCK (STEP 1)

The ground state wave function can be represented in the basis $\{|m, \sigma\rangle\}$ with $m^{(S)}$ and $m^{(E)}$ as the basis states of the system and environment respectively and $\sigma^{(S)}$ and $\sigma^{(E)}$ the basis states of the added site at system and environment respectively. Then, the ground state of the combined superblock can be written as

$$|\psi\rangle = \sum_{m^{(S)}=1}^{M^{(S)}} \sum_{\sigma^{(S)}=1}^{N_{Site}} \sum_{m^{(E)}=1}^{M^{(E)}} \sum_{\sigma^{(E)}=1}^{N_{Site}} \psi_{m^{(S)}\sigma^{(S)}m^{(E)}\sigma^{(E)}} |m^{(S)}, \sigma^{(S)}\rangle |m^{(E)}, \sigma^{(E)}\rangle \quad (12.4)$$

or in the combined basis

$$\boxed{|\psi\rangle = \sum_{i=1}^{N^{(S)}} \sum_{j=1}^{N^{(E)}} \psi_{ij} |i\rangle |j\rangle} \quad (12.5)$$

where $|i\rangle$ is the basis states of the system and $|j\rangle$ is the basis state of the environment including the new sites and dimensions $N^{(S)} = M^{(S)} \cdot N_{Site}$ and $N^{(E)} = M^{(E)} \cdot N_{Site}$.

CALCULATION OF THE NEW GROUND STATE (STEP 2)

The calculation of the ground state is efficiently done by large sparse-matrix diagonalization. The Lanczos method and the Jacobi-Davidson method (for linear eigenvalue problems, see [4]) are algorithms that converge fast to the largest or smallest eigenvalue of the Hamiltonian \hat{H} at high precision. Even the next lower or higher eigenvalues can be determined with slightly more operations. This is the most expensive part of the DMRG method where the number of operations scales with M^4 (where M the dimension of the Hilbert space after the truncation). The number of operations scales with M^3 for next neighbor interacting Hamiltonians because the superblock Hamiltonian decomposes into Hamiltonians acting on the blocks, on the blocks with neighboring sites and on the two single sites [3],

$$\hat{H} = \hat{H}_S + \hat{H}_{S\bullet} + \hat{H}_{\bullet\bullet} + \hat{H}_{\bullet E} + \hat{H}_E. \quad (12.6)$$

BASIS TRUNCATION (STEP 3)

Definition 12.2. The reduced density matrix is defined by

$$\hat{\rho}^{(S)} := \text{Tr}_E \hat{\rho} = \text{Tr}_E |\psi\rangle \langle \psi| \quad (12.7)$$

depending on the ground state wave function $|\psi\rangle$.

This definition means that the reduced density matrix is explicitly

$$\hat{\rho}^{(S)} = \sum_{j''} \langle j'' | \left(\sum_{ij} \psi_{ij}^* |i\rangle |j\rangle \sum_{i'j'} \psi_{i'j'} \langle i' | \langle j' | \right) |j''\rangle \quad (12.8)$$

$$= \sum_{j''} \sum_{ij i'j'} \psi_{ij}^* \psi_{i'j'} |i\rangle \langle i' | \delta_{jj''} \delta_{j'j''} \quad (12.9)$$

$$= \sum_{ii'j} \psi_{ij}^* \psi_{i'j} |i\rangle \langle i' | \quad (12.10)$$

12.2 Procedure

and in diagonalized form

$$\hat{\rho}_S = \sum_{\alpha=1}^{N^{(S)}} w_{\alpha} |\alpha\rangle \langle\alpha|. \quad (12.11)$$

The truncation of the basis of the Hilbert space is performed by taking the eigenvectors $|\alpha\rangle$ with the $M^{(S)}$ largest eigenvalues w_{α} of the reduced density matrix. The original ground state wave function (after adding one site to each the system and the environment) is given by Eq. 12.5. In order to reduce the number of basis states, the wave function is approximated by

$$|\tilde{\psi}\rangle = \sum_{\alpha=1}^{M^{(S)}} \sum_{j=1}^{N^{(E)}} \tilde{\psi}_{\alpha j} |\alpha\rangle |j\rangle \quad (12.12)$$

with $|\alpha\rangle$ a new orthonormal basis with only $M^{(S)} < N^{(S)}$ states

$$|\alpha\rangle := \sum_{i=1}^{N^{(S)}} u_{\alpha i} |i\rangle \quad (12.13)$$

(such that $\langle\alpha|\alpha'\rangle = \delta_{\alpha\alpha'}$). The Eq. 12.13 can be understood as the basis transformation into the truncated space while keeping the $M^{(S)}$ relevant eigenvectors with largest eigenvalues of the reduced density matrix in Eq. 12.11.

Definition 12.3. The expression $\epsilon_{\rho^{(S)}} = 1 - \sum_{\alpha=1}^{M^{(S)}} w_{\alpha} = \sum_{\alpha>M^{(S)}}^{N^{(S)}} w_{\alpha}$ is called the truncated weight.

The Hilbert space of the environment is truncated in a similar way.

12.2.2 FINITE-SYSTEM DMRG

The finite-system DMRG method further improves the precision of the wave function obtained from the infinite-system DMRG at fixed system size.

In order to get the additional two sites, it is possible to enlarge the system by one site and reduce the environment by one site or vice versa. This idea leads to the finite-system DMRG (see Fig. 12.2). The system size is reduced e.g. until the system can be solved exactly with $(N_{Site})^L \leq M^{(S)}$ states as in the initialization. The system or environment of size L are taken from the L -th step in infinite-system DMRG.

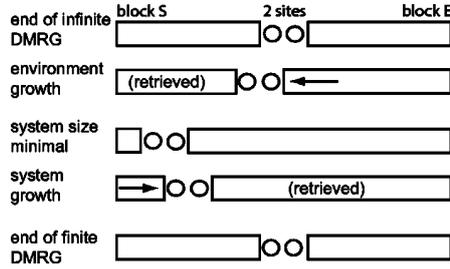


Figure 12.2: The finite-system DMRG works similarly as the infinite-system DMRG, just the part of adding a site is handled differently to keep the total system size (together with the environment) constant. The system block size is shrunk as the environment block is enlarged and after having reached a minimal system size the growth direction is reversed. The figure is taken from Ref. [3].

12.2.3 TYPICAL SIMULATION PARAMETERS

A typical system length is several 100 sites and the number of states to describe such a system is typically between 100 – 10000 states. These values highly dependent on the problem considered.

12.3 ORIGIN

The DMRG algorithm is based on the ideas of the real-space renormalization; especially Wilson’s success in solving the Kondo problem[5] and other impurity problems had large influence on White’s development of the DMRG method. The real-space renormalization-group method in principle reduces the system in every step to a certain a number of basis states.

The renormalization-group method, which was responsible for the success of Wilson, was ineffective for solving Hamiltonians as mentioned in section 12.1.1 (without impurities). In this method, the size of the system A is doubled to a compound system AA as shown in Fig. 12.3 by keeping the M lowest energy eigenstates of H per block.

The particle in a box problem illustrates that this method can fail. The new lowest lying eigenfunction of a compound block AA is not a linear combination of the eigenstates of the single block A as illustrated by Fig. 12.3. Hence, this variant of the real-space renormalization group fails to efficiently represent the ground state of the compound block.

This problem was solved with DMRG, where the density matrix is used to find the important states.

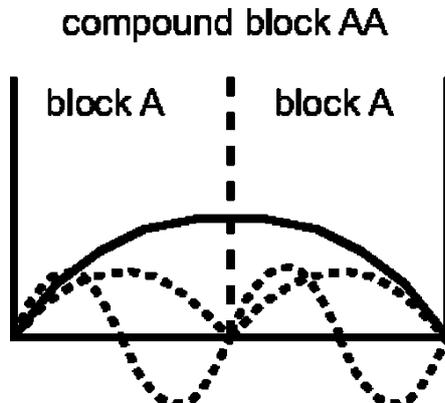


Figure 12.3: The continuous line describes lowest lying eigenfunction of the compound block AA and the dashed lines symbolize the eigenfunctions of the single block A . The figure is taken from Ref. [3].

12.4 KEY IDEA OF DMRG

The key idea of DMRG (as a renormalization group method) is to keep the $M^{(S)}$ eigenstates of the reduced density matrix with largest weights (eigenvalues) w_α . This choice is optimal as shown in the following section.

12.4.1 OPTIMIZING THE WAVE FUNCTION

Proposition 12.1. *The difference $|\psi\rangle - |\tilde{\psi}\rangle$ is minimized in the quadratic norm with respect to the variables $\tilde{\psi}_{\alpha j}$.*

Proof. The wave functions $|\psi\rangle$ and $|\tilde{\psi}\rangle$ are given by Eq. 12.5 and Eq. 12.12 respectively. Assuming real coefficients, we get

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|^2 = |\langle \psi | \psi \rangle| - 2\Re(\langle \tilde{\psi} | \psi \rangle) + |\langle \tilde{\psi} | \tilde{\psi} \rangle| \quad (12.14)$$

$$= 1 - 2 \sum_{\alpha j} \psi_{ij} \tilde{\psi}_{\alpha j} u_{\alpha i} + \sum_{\alpha j} \tilde{\psi}_{\alpha j}^2 \quad (12.15)$$

and taking the derivative

$$\partial_{\tilde{\psi}_{\alpha j}} \| |\psi\rangle - |\tilde{\psi}\rangle \|^2 = \partial_{\tilde{\psi}_{\alpha j}} \left(1 - 2 \sum_{\alpha j} \psi_{ij} \tilde{\psi}_{\alpha j} u_{\alpha i} + \sum_{\alpha j} \tilde{\psi}_{\alpha j}^2 \right) \quad (12.16)$$

$$= -2 \sum_i \psi_{ij} u_{\alpha i} + 2\tilde{\psi}_{\alpha j} \stackrel{!}{=} 0 \quad (12.17)$$

With the solution of Eq. 12.17 $\tilde{\psi}_{\alpha j} = \sum_i \psi_{ij} u_{\alpha i}$, the norm can be rewritten as

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|^2 = 1 - \sum_{\alpha i i'} u_{\alpha i} \underbrace{\sum_j \psi_{ij} \psi_{i'j} u_{\alpha i'}}_{=: \rho_{ii'}^{(S)}} \quad (12.18)$$

The expression $\rho_{ii'}^{(S)}$ is the matrix of the coefficients of the reduced density matrix $\hat{\rho}^{(S)}$. The density matrix is symmetric positive definite implying that all eigenvalues are positive. Therefore, Eq. 12.18 can be minimized by taking the M^S eigenvectors of $\rho_{ii'}^{(S)}$ with the largest eigenvalues w_α for the coefficients $u_{\alpha i}$. With this choice, the norm is minimal,

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|^2 = 1 - \sum_{\alpha=1}^{M^{(S)}} w_\alpha = \epsilon_{\rho^{(S)}} \quad (12.19)$$

where $\epsilon_{\rho^{(S)}}$ is the truncated weight. □

12.4.2 OPTIMIZED EXPECTATION VALUES

The expectation value of a certain operator \hat{P} (observable on some sites), which acts only on the system, is given by

$$\langle \hat{P} \rangle := \langle \psi | \hat{P} | \psi \rangle = \sum_{i'j} \psi_{ij}^* P_{i'j} \psi_{i'j} = \sum_{ii'} \rho_{ii'} P_{ii'} = \text{Tr}(\hat{\rho} \hat{A}) \quad (12.20)$$

for normalized wave functions ψ using the definition of the reduced density matrix 12.2.

The error on the expectation value due to the truncation from $|\psi\rangle$ to $|\tilde{\psi}\rangle$ is bounded by

$$|\langle \hat{P} \rangle_\psi - \langle \hat{P} \rangle_{\tilde{\psi}}| \leq \epsilon_{\rho^{(S)}} \|\hat{P}\|, \quad (12.21)$$

where $\|\hat{P}\| := \max_{\phi \in \mathcal{H}^{(S)}} |\langle \phi | \hat{P} | \phi \rangle|$ is the operator norm of \hat{P} . By minimizing the truncated weight, the error on the expectation value of the operator \hat{P} is minimized too.

12.4.3 OPTIMIZED ENTANGLEMENT

The entanglement entropy of the system is given by

$$S(\hat{\rho}^{(S)}) := -\text{Tr}(\hat{\rho}^{(S)} \log(\hat{\rho}^{(S)})) = -\sum_{\alpha} w_\alpha \log(w_\alpha).^2 \quad (12.22)$$

²If the weight $w_1 = 1$ and all other weights $w_\alpha = 0$, the entanglement entropy is $S = 0$, and the state corresponds to a product state $|\psi\rangle = |\psi^{(S)}\rangle \cdot |\psi^{(E)}\rangle$.

12.4 Key Idea of DMRG

For numbers w in the range of $[0, 1]$, the term $-w \log(w)$ is maximized for w as large as possible. Therefore, taking the largest weights w_α maximize the entanglement entropy.

For example, a maximally entangled state has $w_\alpha = \frac{1}{M^{(S)}}$. Therefore, the number of relevant states scales as $M^{(S)} \approx \exp(S)$ for a given entanglement entropy S .

SCHMITT DECOMPOSITION

With the Schmitt decomposition, the wave function can be written as

$$|\psi\rangle = \sum_i^{N^{(S)}} \sum_j^{N^{(E)}} \psi_{ij} |i\rangle |j\rangle \quad (12.23)$$

$$= \sum_{\alpha=1}^{N^{(S)}} \lambda_\alpha |S_\alpha\rangle |E_\alpha\rangle, \quad (12.24)$$

with the basis transformations

$$|S_\alpha\rangle = \sum_{i=1}^{N^{(S)}} U_{\alpha i} |i\rangle \quad (12.25)$$

$$|E_\alpha\rangle = \sum_{j=1}^{N^{(E)}} V_{\alpha j} |j\rangle. \quad (12.26)$$

The summation over i and j reduces to a sum over $\alpha = 1, \dots, \min(N^{(S)}, N^{(E)})$, where we assume $N^{(S)} < N^{(E)}$ in the following.

The Schmitt decomposition can be obtained from a singular-value decomposition $\psi_{ij} = U\Lambda V^T$, where Λ is a diagonal matrix with λ_α on the diagonal (called Schmitt coefficients). Using this representation of the wave function, it is possible to directly calculate the diagonalized reduced density matrix of the system

$$\hat{\rho}^{(S)} = \text{Tr}_E |\psi\rangle \langle \psi| \quad (12.27)$$

$$= \sum_{\alpha} \langle E_\alpha | |\lambda_\alpha|^2 |S_\alpha\rangle |E_\alpha\rangle \langle S_\alpha| \langle E_\alpha| |E_\alpha\rangle \quad (12.28)$$

$$= \sum_{\alpha} |\lambda_\alpha|^2 |S_\alpha\rangle \langle S_\alpha| \quad (12.29)$$

By comparing Eq. 12.29 with Eq. 12.7, one finds that $|\lambda_\alpha|^2 = w_\alpha$.

The Schmitt coefficients play an essential role for the matrix product state method (see next chapter).

12.5 AREA LAW OF ENTANGLEMENT ENTROPY

In general for a random state, the entanglement entropy scales with the system size of a block A in the system,

$$\boxed{S(A) \propto A} \quad (12.30)$$

where $S(A) = S(\rho^{(A)})$, c.f. Eq. 12.22.

Physical states of local (gapped³) Hamiltonians obey the area law of the entanglement entropy

$$\boxed{S(A) \propto \partial A}. \quad (12.32)$$

This means, that much less states are needed to describe a block. The entanglement entropy is given by Eq. 12.29.

Consider a block A of length l in an one dimensional system. The boundary of this block ∂A is constant, i.e. $S(A) = c'$ using Eq. 12.32 and the number of relevant states is consequently

$$M^{(S)} \approx \exp(S(A)) = \exp(c') = c \quad (12.33)$$

where c, c' are constants.⁴ Thus, with increasing system size the number of states can be kept constant (for sufficiently large systems).

12.6 CONCLUSION

The density matrix plays the key role in the DMRG method. This is in contrast to e.g. Wilson's approach, which fails for many important systems.

With the area law, the reason for the success of DMRG can be better understood. The constant size of the relevant subspace to describe a block of arbitrary length l in an one dimensional system is the reason for the success of DMRG.

³Critical (gapless) systems in one dimension have a logarithmic correction to the area law $S(A) \propto \log(A)$. In this case, the number of relevant states increases polynomially with system size,

$$M^{(S)} = \exp(S(A)) \approx L^p, \quad (12.31)$$

where p is a (small) constant.

⁴For a random state in the Hilbert space, the entanglement entropy is extensive and the number of relevant states grows exponentially

$$M^{(S)} = \exp(S(A)) \approx \exp(L) \quad (12.34)$$

12.6 Conclusion

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CHAPTER 13

MATRIX PRODUCT STATES AND PROJECTED ENTANGLED-PAIR STATES

MAXIMILIAN VOSS

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The study of one-dimensional highly correlated quantum lattice systems has experienced major successes since the development of very efficient simulation algorithms like the density-matrix renormalization group method (DMRG). Initially elaborated in a separate context, matrix product states (MPS) proved to be an interesting class of states for the study of quantum chains. They provide an efficient parametrization of the physical state space and allow for a variational study of the ground state of the system. As a consequence of the area law of entanglement, the DMRG/MPS approach becomes ineffective in higher-dimensional systems. In 2D, a generalization of MPS, the so-called projected entangled-pair states (PEPS), was developed and basically relies on a denser tensor network. PEPS are able to handle efficiently the entanglement related to two-dimensional quantum lattices.

13.1 INTRODUCTION

The description of highly correlated quantum many-body problems on lattices is a very important problem to solve in quantum physics since these systems are found in various contexts, particularly in condensed matter physics. Giving a full analytic description of these systems is nearly impossible and even numerically they remain hard to study, so that exact solutions only exist for very few simple cases.

To tackle the problem, simulation algorithms have proved to be very efficient tools, working where conventional perturbation theory fails. Popular methods include Wilson's renormalization group algorithm or the quantum Monte Carlo method. Yet, the density matrix renormalization group method (DMRG) has imposed itself as the leading algorithm for the computation of one-dimensional quantum lattice models. It benefits from a remarkable precision for typical local and gapped hamiltonians.

Even before the invention of DMRG, matrix product states (MPS) showed interesting properties as a class of quantum states for analytical studies. They were used in a variety of situations before being associated to DMRG as a powerful parametrization of the state space associated to quantum chain models. They allowed to give an accurate local description of a system without losing the essential global quantum non-locality.

We will discuss the structure of an MPS in detail and see how it is used to compute important quantities of these models like the ground state or the ground state energy. From there, we will analyze why the DMRG/MPS method gets ineffective for higher dimensional systems and how we can handle this problem by generalizing the concept as it was done with the development of projected entangled-pair states for two-dimensional quantum lattice models.



Figure 13.1: *An L -site quantum chain*

13.2 MATRIX PRODUCT STATES (MPS)

We want to solve the problem of describing a one-dimensional lattice of L highly correlated quantum particles with d -dimensional local state spaces $\{\sigma_i\}_{i=1,\dots,L}$. The key issue with these systems is that the dimension of the Hilbert space \mathbf{H}

grows exponentially with the number of lattice sites ($\dim \mathbf{H} = d^L$). Finding the ground state in such a huge space seems like an unsolvable task.

The ansatz we make in this situation is that for physical hamiltonians the amount of relevant states we have to consider in our search is not that huge. We affirm that our Hilbert space can be parametrized efficiently so to isolate this subspace and then apply DMRG-like algorithms to answer our fundamental questions about the physics of the system. This efficient parametrization of the state space is given by matrix product states.

In this section we will discuss the basic tools required for the construction of an MPS, and we will thoroughly go through the decomposition of an arbitrary quantum state into an MPS. We will introduce the concept of matrix product operators (MPO) and see what methods exist to optimize our MPS towards the ground state we are looking for.

13.2.1 SINGULAR VALUE DECOMPOSITION

The construction of an MPS is based mostly on a theorem from linear algebra called singular value decomposition (SVD). This theorem is also notably used to derive the Schmidt decomposition of an arbitrary quantum state defined on a bipartite system.

SVD states that for an arbitrary matrix $M \in \mathbb{C}^{N_A \times N_B}$ we have a decomposition of the following form [1]:

$$M = U \cdot S \cdot V^\dagger \tag{13.1}$$

where U , S and V^\dagger have following properties:

- * $U \in \mathbb{C}^{N_A \times \min(N_A, N_B)}$ has orthonormal columns, i.e. $U^\dagger U = \text{id}$.
- * $S \in \mathbb{C}^{\min(N_A, N_B) \times \min(N_A, N_B)}$ is a diagonal matrix with r non-zero entries s_a . The entries s_a are called *singular values* and are positive ($s_a > 0$) and the number $r \leq \min(N_A, N_B)$ is the *Schmidt rank* of M .
- * $V^\dagger \in \mathbb{C}^{\min(N_A, N_B) \times N_B}$ has orthonormal rows, i.e. $V^\dagger V = \text{id}$.

As we already mentioned, SVD is notably used to derive the Schmidt decomposition of an arbitrary quantum state defined on a bipartite system AB . The most general form of such a state writes as:

$$|\psi\rangle = \sum_{i,j} \psi_{ij} |i\rangle_A |j\rangle_B \tag{13.2}$$

13.2 Matrix product states (MPS)

where $\{|i\rangle_A\}$ and $\{|j\rangle_B\}$ denote orthonormal bases for the system parts A and B respectively. If we see the coefficients ψ_{ij} as entries of a matrix Ψ , we can then apply SVD on Ψ and get the following equality:

$$\begin{aligned} |\psi\rangle &= \sum_{i,j} \sum_{a=1}^r U_{ia} S_{aa} V_{aj}^\dagger |i\rangle_A |j\rangle_B \\ &= \sum_{a=1}^r \left(\sum_i U_{ia} |i\rangle_A \right) s_a \left(\sum_j V_{aj}^\dagger |j\rangle_B \right) \\ &= \sum_{a=1}^r s_a |a\rangle_A |a\rangle_B \end{aligned}$$

Thanks to the orthonormality of U and V^\dagger , the new bases $|a\rangle_A$ and $|a\rangle_B$ are also orthonormal and can be extended to orthonormal bases of A and B . The last line of the equation shows directly the Schmidt decomposition of the state $|\psi\rangle$. This is a very useful tool since it allows for instance to read off easily the expression for the reduced density operators for each system part A and B :

$$\begin{aligned} \hat{\rho}_A &= \text{Tr}_B |\psi\rangle\langle\psi| = \sum_{a=1}^r s_a^2 |a\rangle_A \langle a|_A \\ \hat{\rho}_B &= \text{Tr}_A |\psi\rangle\langle\psi| = \sum_{a=1}^r s_a^2 |a\rangle_B \langle a|_B \end{aligned}$$

The previous equations reveal a fact which we will use in the following subsections. In the mixed state defined for example over subsystem A , the pure states with the highest weights in the reduced density matrix, i.e. the states which are the most likely to occur, are the ones related to the largest singular values s_a [2]. This will play an important role when we will define a truncation procedure for the Hilbert space as we build up a numerically manageable MPS.

13.2.2 DECOMPOSITION OF A GENERAL QUANTUM STATE INTO AN MPS

We now want to demonstrate how to actually create an MPS starting from an arbitrary quantum state. We consider again a one-dimensional quantum lattice model with L particles that all admit a d -dimensional local Hilbert space $\{\sigma_i\}_{i=1,\dots,L}$. The most general pure quantum state defined on such a system is given by:

$$|\psi\rangle = \sum_{\sigma_1, \sigma_2, \dots, \sigma_L} c_{\sigma_1 \dots \sigma_L} |\sigma_1 \dots \sigma_L\rangle \quad (13.3)$$

were we have d^L coefficients $c_{\sigma_1 \dots \sigma_L}$ in the sum. There are three main ways of building an MPS. We will discuss just one in detail here. However the other two constructions are very analog and we will present them shortly afterwards. The first type of MPS is called *left-canonical MPS*. The procedure goes as follows: We see the coefficients c as entries of a row vector of dimension $(1 \times d^L)$. We now reshape this vector into a matrix $\Psi_{\sigma_1, (\sigma_2 \dots \sigma_L)}$ of dimension $(d \times d^{L-1})$ where the entries of the matrix are given by:

$$\Psi_{\sigma_1, (\sigma_2 \dots \sigma_L)} = c_{\sigma_1 \dots \sigma_L} \quad (13.4)$$

We now apply SVD on the newly created matrix Ψ . This gives a relation:

$$\begin{aligned} c_{\sigma_1 \dots \sigma_L} = \Psi_{\sigma_1, (\sigma_2 \dots \sigma_L)} &= \sum_{a_1=1}^{r_1} U_{\sigma_1, a_1} S_{a_1, a_1} V_{a_1, (\sigma_2 \dots \sigma_L)}^\dagger \\ &\equiv \sum_{a_1=1}^{r_1} A_{a_1}^{\sigma_1} c_{a_1 \sigma_2 \dots \sigma_L} \end{aligned}$$

where in the last step we have multiplied the matrices S and V^\dagger together and reshaped the resulting matrix into a vector $c_{a_1 \sigma_2 \dots \sigma_L}$. We have also decomposed the matrix U_{σ_1, a_1} into a collection of d row vectors A^{σ_1} with entries $A_{a_1}^{\sigma_1} = U_{\sigma_1, a_1}$. In the next step, we take our new vector $c_{a_1 \sigma_2 \dots \sigma_L}$ of dimension $(1 \times r_1 d^{L-1})$ and reshape it again into a matrix $\Psi_{(a_1 \sigma_2), (\sigma_3 \dots \sigma_L)}$ of dimension $(r_1 d \times d^{L-2})$ with the coefficient relation $\Psi_{(a_1 \sigma_2), (\sigma_3 \dots \sigma_L)} = c_{a_1 \sigma_2 \dots \sigma_L}$. Once again, we apply SVD on $\Psi_{(a_1 \sigma_2), (\sigma_3 \dots \sigma_L)}$:

$$\begin{aligned} c_{\sigma_1 \dots \sigma_L} &= \sum_{a_1=1}^{r_1} A_{a_1}^{\sigma_1} \Psi_{(a_1 \sigma_2), (\sigma_3 \dots \sigma_L)} = \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A_{a_1}^{\sigma_1} U_{(a_2 \sigma_1), a_2} \underbrace{S_{a_2, a_2} V_{a_2, (\sigma_3 \dots \sigma_L)}^\dagger}_{\equiv \Psi_{(a_2 \sigma_3), (\sigma_4 \dots \sigma_L)}} \\ &= \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A_{a_1}^{\sigma_1} A_{a_1, a_2}^{\sigma_2} \Psi_{(a_2 \sigma_3), (\sigma_4 \dots \sigma_L)} \end{aligned}$$

where we have again replaced the matrix U by a collection of d matrices A^{σ_2} with entries $A_{a_1, a_2}^{\sigma_2} = U_{(a_2 \sigma_1), a_2}$. The end of the procedure now follows from applying several additional SVD. This results in a decomposition of the following form:

$$c_{\sigma_1 \dots \sigma_L} = \sum_{a_1, \dots, a_{L-1}} A_{a_1}^{\sigma_1} A_{a_1, a_2}^{\sigma_2} \dots A_{a_{L-1}}^{\sigma_L} = A^{\sigma_1} \dots A^{\sigma_L} \quad (13.5)$$

where in the last step we have have written the coefficient product in the more compact matrix product form. The initial arbitrary quantum state can now be represented *exactly* as a matrix product state:

13.2 Matrix product states (MPS)

$$|\psi\rangle = \sum_{\sigma_1\sigma_2\dots\sigma_L} A^{\sigma_1}A^{\sigma_2}\dots A^{\sigma_L}|\sigma_1\sigma_2\dots\sigma_L\rangle \quad (13.6)$$

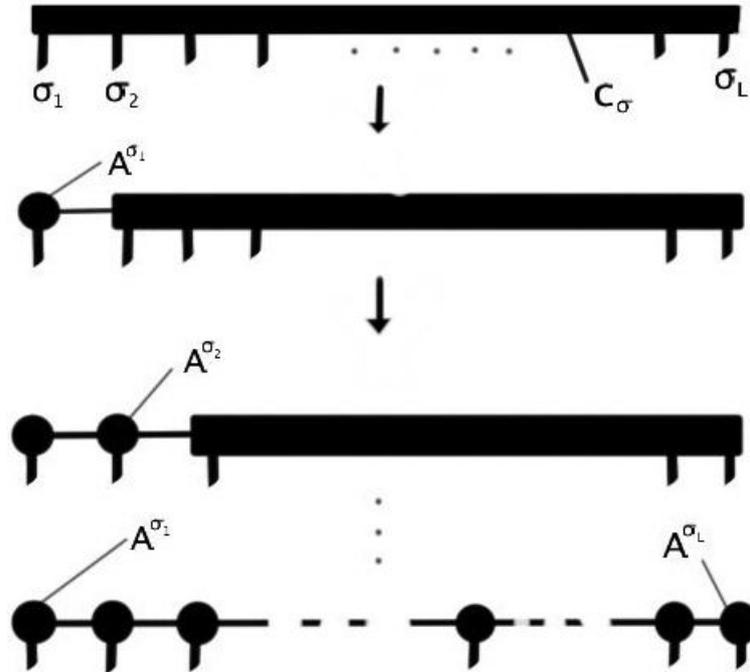


Figure 13.2: *Graphical interpretation of the MPS decomposition. Every step corresponds to one SVD. The last line represents an entirely decomposed MPS.*

As we already mentioned, the MPS decomposition is not unique. We could have for example started our decomposition from the right end of the chain instead of initiating it from the left. This is known as a *right-canonical MPS*. It is technically almost identical to our previous construction. In the first step, we simply reshape our initial state vector $c_{\sigma_1\dots\sigma_L}$ into a matrix Ψ of dimension $(d^{L-1} \times d)$ instead of $(d \times d^{L-1})$. Then, after having applied SVD to Ψ , we isolate the V^\dagger instead of the U matrices and we decompose them into a set of d B matrices in a fully analog way to left-canonical MPS. We will not go further into technical details and simply give the resulting MPS:

$$|\psi\rangle = \sum_{\sigma_1\sigma_2\dots\sigma_L} B^{\sigma_1}B^{\sigma_2}\dots B^{\sigma_L}|\sigma_1\sigma_2\dots\sigma_L\rangle \quad (13.7)$$

The fundamental difference between these two decomposition is related to their orthonormality. Due to the properties of the SVD matrices U and V^\dagger , we have following identities for our A and B matrices:

$$\sum_{\sigma_l} A^{\sigma_l \dagger} A^{\sigma_l} = \text{id} \quad \sum_{\sigma_l} B^{\sigma_l} B^{\sigma_l \dagger} = \text{id} \quad (13.8)$$

Because of these properties, A -matrices are referred to as *left-normalized* whereas the B -matrices are *right-normalized*. This has major consequences on the DMRG approach of our system. If we split our system up so to have a bipartite system which comprises lattice sites 1 to l in subsystem A and sites $l+1$ to L in subsystem B, we want to build an MPS which is orthogonal on both subsystems. Our approach is then to undertake a left-canonical decomposition from sites 1 to l and a right-canonical decomposition from sites L to $l+1$. The final state is called *mixed-canonical MPS* and is written as:

$$|\psi\rangle = \sum_{\sigma_1 \sigma_2 \dots \sigma_L} A^{\sigma_1} \dots A^{\sigma_l} S B^{\sigma_{l+1}} \dots B^{\sigma_L} |\sigma_1 \sigma_2 \dots \sigma_L\rangle \quad (13.9)$$

where S is the diagonal matrix from the SVD. If we now introduce vectors:

$$\begin{aligned} |a_l\rangle_A &= \sum_{\sigma_1 \dots \sigma_l} (A^{\sigma_1} \dots A^{\sigma_l})_{1, a_l} |\sigma_1 \dots \sigma_l\rangle \\ |a_l\rangle_B &= \sum_{\sigma_{l+1} \dots \sigma_L} (B^{\sigma_{l+1}} \dots B^{\sigma_L})_{a_l, 1} |\sigma_{l+1} \dots \sigma_L\rangle \end{aligned}$$

Then our state ψ can be rewritten in the form:

$$|\psi\rangle = \sum_{a_l} s_a |a_l\rangle_A |a_l\rangle_B \quad (13.10)$$

where the coefficients s_a denote the diagonal entries of our singular value matrix S from the mixed-canonical representation. This last form of the state is exactly the Schmidt decomposition of ψ , which fulfills the requirement of providing an orthonormal basis on A and B respectively.

13.2.3 COMPRESSION OF A MATRIX PRODUCT STATE

Let us consider again a mixed-canonical MPS as derived in (1.9):

$$|\psi\rangle = \sum_{\sigma_1 \sigma_2 \dots \sigma_L} A^{\sigma_1} \dots A^{\sigma_l} S B^{\sigma_{l+1}} \dots B^{\sigma_L} |\sigma_1 \sigma_2 \dots \sigma_L\rangle \quad (13.11)$$

If we look at the matrices in our MPS, we see that their respective dimensions still increase exponentially. Counting reveals that the highest-dimensional matrix

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of the decomposition could be of maximum dimension $(d^{L/2} \times d^{L/2-1})$, which cannot be handled numerically. Therefore, to be able to actually do computation with our state, we need to reduce this dimension by somehow diminishing the dimension of the considered state space. This procedure is called *truncation* of the Hilbert space. We give an overview of how this truncation is actually implemented. The trick is to define some *bond dimension* D on our system. The number D basically describes the maximum number of degrees of freedom of a subsystem we allow in our state representation.

Let us now consider we have an MPS describing block A with a bond dimension of D . If we now add a site to the decomposition ($l \rightarrow l + 1$), the total associated state space will also grow by a factor of d . If the new Hilbert space now has a dimension $d_H > D$ we will have to truncate the state space. To do this, we look at our SVD decomposition and retain only the D largest singular value s_a in the matrix S and trace out all other entries so to effectively have a new S matrix of dimensions $(D \times D)$. In the same time, we retain only the D first columns (resp. rows) in the U (V^\dagger) matrix.

The argument which motivates that we only keep the states with the largest singular values is related to the previously discussed fact about the reduced density matrix (RDM). We have seen that the states which have the highest weights in the RDM (i.e those who are the more likely to occur) are exactly those with the largest singular values.

13.2.4 MATRIX PRODUCT OPERATORS

In a complete analog to the discussion about quantum state, we also want to convert operators into a matrix product form so to efficiently operate on MPS. This is achieved by building so-called matrix product operators (MPO). They have the form

$$\hat{O} = \sum_{\sigma_1 \dots \sigma_L, \sigma'_1 \dots \sigma'_L} W^{\sigma_1 \sigma'_1} \dots W^{\sigma_L \sigma'_L} \underbrace{|\sigma_1 \dots \sigma_L\rangle}_{=:|\sigma\rangle} \underbrace{\langle \sigma'_1 \dots \sigma'_L|}_{=:\langle \sigma'|} \quad (13.12)$$

so that we can write coefficients $\langle \sigma | \hat{O} | \sigma' \rangle$ as

$$\langle \sigma | \hat{O} | \sigma' \rangle = W^{\sigma_1 \sigma'_1} W^{\sigma_2 \sigma'_2} \dots W^{\sigma_{L-1} \sigma'_{L-1}} W^{\sigma_L \sigma'_L} \quad (13.13)$$

The $W^{\sigma_i \sigma'_i}$ in the previous equations denote matrices just in the same sense as M^{σ_i} did in an MPS. The difference is now that every matrix is indexed by two coefficients instead of one. The coefficients denote respectively the physical index

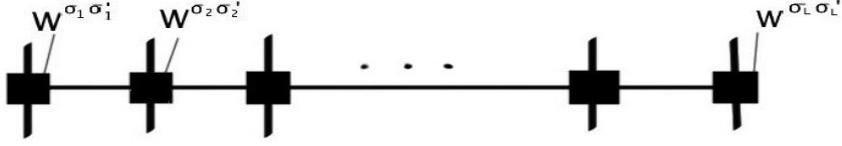


Figure 13.3: Graphical representation of an MPO. Every tensor now has two physical indexes σ_i and σ'_i , respectively denoting the ingoing and the outgoing state sites.

of the ingoing state (σ_i) and the one of the outgoing state (σ'_i).

There are a two important facts concerning MPO. First, any operator can be brought into an MPO form. This is due to following identity:

$$\begin{aligned} \hat{O} &= \sum_{\sigma_1 \dots \sigma_L, \sigma'_1 \dots \sigma'_L} c_{(\sigma_1 \dots \sigma_L), (\sigma'_1 \dots \sigma'_L)} |\sigma_1 \dots \sigma_L\rangle \langle \sigma'_1 \dots \sigma'_L| \\ &= \sum_{\sigma_1 \dots \sigma_L, \sigma'_1 \dots \sigma'_L} c_{(\sigma_1 \sigma'_1) \dots (\sigma_L \sigma'_L)} |\sigma_1 \dots \sigma_L\rangle \langle \sigma'_1 \dots \sigma'_L| \end{aligned}$$

where we can now decompose the last line in the exact same way as we did for MPS, the double index $\sigma_i \sigma'_i$ taking the role of the index σ_i in the MPS. The other important property of MPO is that they leave the form of an MPS invariant. This means that when one applies an MPO \hat{O} on an MPS $|\psi\rangle$ as in

$$\hat{O}|\psi\rangle = |\phi\rangle \tag{13.14}$$

the resulting state $|\phi\rangle$ will be a new MPS with a larger bond dimension.

13.2.5 FINDING GROUND STATES USING MPS

What we did until now was to build an efficient representation for the state vector $|\psi\rangle$ using MPS decomposition. The actual goal of this procedure is to be able to compute ground states of very complex highly correlated systems, given by specific hamiltonians \hat{H} . In order to do this, we want to optimize our MPS $|\psi\rangle$ so to minimize the quantity

$$E = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}. \tag{13.15}$$

which is the energy of the system. There are several optimization methods which are used to minimize this quantity and the most well known are the variational

13.2 Matrix product states (MPS)

searches using renormalization methods like DMRG and imaginary time evolution. We will briefly introduce both of these methods here.

ITERATIVE GROUND STATE SEARCH

The idea of this first method is to extremize the quantity

$$\langle \psi | \hat{H} | \psi \rangle - \lambda \langle \psi | \psi \rangle \quad (13.16)$$

so that, in the end, ψ will converge towards the desired ground state and λ towards the ground state energy. This is far from being a trivial computation. Indeed, since all the matrices in the MPS are variables and as they appear in the form of products, this is a highly non-linear optimization problem. The idea will be to optimize every matrix separately one after the other by solving an eigenvalue problem in order to lower their respective energy contribution. This is done using the DMRG algorithm which comprises a series of sweeping through the system from one site to the other and repeating the optimization procedure until the MPS converges towards the desired ground state.

IMAGINARY TIME EVOLUTION

A second popular method for the computation of ground states is the so-called imaginary time evolution. The idea is to act with the operator $e^{-\beta \hat{H}}$ ($\beta = \frac{1}{k_B T}$) on an initial state ψ so that it (hopefully) converges like

$$e^{-\beta \hat{H}} |\psi\rangle \xrightarrow{\beta \rightarrow \infty} |\psi_0\rangle \quad (13.17)$$

where ψ_0 is the ground state of the system. The problem we encounter here is that we struggle to write the operator $e^{-\beta \hat{H}}$ as an MPO (i.e. as a product of matrices). If we can write the hamiltonian $\hat{H} = \sum_i \hat{h}_i$ as a sum of local operators, a naive approach to this would be to write

$$e^{-\beta \hat{H}} = e^{-\beta \hat{h}_1} e^{-\beta \hat{h}_2} \dots e^{-\beta \hat{h}_{L-1}} + O(\beta^2) \quad (13.18)$$

which contains an error since we did not consider that the \hat{h}_i do not commute. An efficient solution to this issue was found with the development of the *Trotter-Suzuki decomposition*. This decomposition states that if we discretize time $\beta = N\tau$ with $\tau \rightarrow 0$ and $N \rightarrow \infty$, we can make the valid approximation that $\tau[\hat{h}_i, \hat{h}_{i+1}] \approx 0$ holds for small time scales τ . Thereby we approximate

$$e^{-\hat{H}\tau N} = \left(e^{-\tau \hat{H}} \right)^N = \left(e^{-\tau \sum_i \hat{h}_i} \right)^N \approx \left(\prod_i e^{-\tau \hat{h}_i} \right)^N \quad (13.19)$$

and the resulting operator is a product of MPO with which we can operate on our initial MPS. One open question concerns the choice of the initial state ψ . Typically one could rely on an educated guess which would usually converge. Even if the initial state is chosen nearly randomly, it will usually converge if it has a finite overlap with the ground state. However there is no guarantee for this convergence. Yet, both methods introduced here have had considerable success in the past and continue to be widely used for ground state computations.

13.3 PROJECTED-ENTANGLED PAIR STATES (PEPS)

MPS has been very successful in past attempts to efficiently describe one-dimensional lattice systems. However, this efficiency decreases dramatically for higher-dimensional systems. The explanation to this phenomena is closely linked to the area law of entanglement, which gives a relation between the entanglement entropy of a system and its dimensionality. This problem was solved for two-dimensional systems by introducing projected entangled-pair states, which are basically a generalization of MPS for two-dimensional systems.

13.3.1 AREA LAW OF ENTANGLEMENT

Entanglement is the crucial factor that makes quantum systems behave differently from classical systems. When describing such a system, knowing how much entanglement is present in it indicates the amount of resources required to actually be able to represent it. The entanglement entropy can be computed using for example by the von Neumann entropy, given by the formula

$$S(\rho) = -\text{Tr}(\rho \ln \rho) = -\sum_a \lambda_a \log(\lambda_a) \quad (13.20)$$

where ρ has a spectral decomposition as given in section 13.2.1 and $\lambda_a = s_a^2$. If we are in a maximally entangled system with d relevant states, we know that for every state: $\lambda_a = \lambda = 1/d$. Thereby the entropy will have a maximum value:

$$S(\rho) = -\sum_a \lambda_a \log(\lambda_a) = -\sum_{a=1}^d d^{-1} \log(d^{-1}) = \log(d) \quad (13.21)$$

In an *arbitrary n-dimensional quantum system* ($L \times L \times \dots \times L$), the entanglement entropy scales like the volume of the system[3].

$$S \propto L^n \quad (13.22)$$

13.3 Projected-entangled pair states (PEPS)

The area law now states that for an n -dimensional quantum lattice model defined by a local and gapped hamiltonian \hat{H} , the entanglement entropy of a lattice block will actually scale like the size of the boundary of the block.

$$S \propto L^{n-1} \tag{13.23}$$

This has important consequences. For example, for $\mathbf{n} = \mathbf{1}$ the theorem states that for sufficiently long chains, the entanglement entropy and the number of relevant states are constant and do not depend on the number of lattice sites:

$$\log(d) = S \propto L^{n-1} = L^0 \implies d \propto \exp(L^0) \equiv \text{const.} \tag{13.24}$$

For $\mathbf{n} = \mathbf{2}$, the entanglement entropy does not scale like the surface of the spin block but only like the sidelength of the block. Therefore the number of relevant states will scale like:

$$\log(d) = S \propto L^{n-1} = L \implies \boxed{d \propto \exp(L)} \tag{13.25}$$

13.3.2 MPS FOR TWO-DIMENSIONAL SYSTEMS

The main reason why MPS is not efficient in higher dimensions is directly linked to the area law. Indeed, we have seen that for example in 2 dimensions, the entanglement scales like the sidelength of a spin block. If we apply an MPS on a 2D lattice, the tensor network looks like in Figure 13.4.

If we break such a lattice into two blocks in the spirit of DMRG, we see that the whole entanglement of the system is carried by one single tensor (red line in the sketch). Yet, since this tensor has bond dimension D , it will not be able to contain the number of relevant states necessary to describe the lattice efficiently ($d \propto \exp(L)$), particularly as the system grows in size. Since MPS suffered these limitations in two-dimensional computations, a generalization of the method, the so-called projected entangled-pair states, was developed to allow a more efficient parametrization of these systems.

13.3.3 PROJECTED ENTANGLED-PAIR STATES

The idea of PEPS is to modify the MPS structure of the tensor network on the two-dimensional lattice so to ensure that, as the system grows in size, we still have enough degrees of freedom in our decomposition to ensure that the total entanglement of the system can be handled efficiently. We will not go further

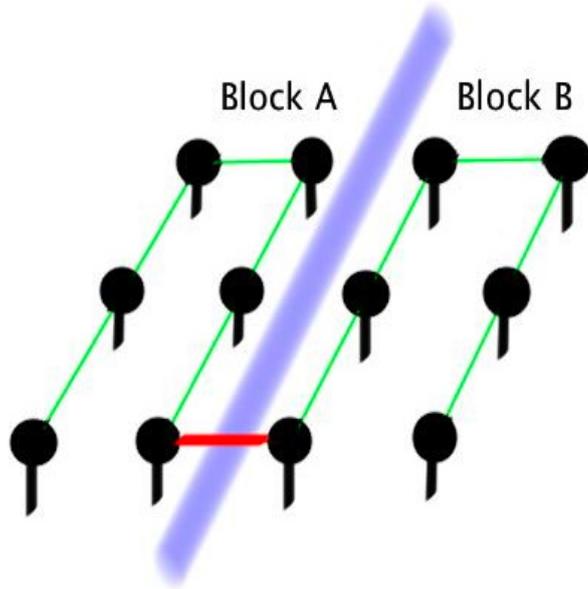


Figure 13.4: An MPS tensor network on a two-dimensional lattice. The green and red lines describe the degrees of freedom linking the respective sites. The red line denotes the tensor connecting blocks A and B.

into technical details, but simply give the graphical representation of the final tensor network in Figure 13.5.

As we can see, every site is connected to its four nearest neighbors via a link representing D degrees of freedom. If we now split the system again into two blocks A and B, the entanglement entropy will again scale proportionally to the sidelength L of the block, according to the area law:

$$S \propto L. \quad (13.26)$$

However, thanks to our new PEPS decomposition, we see that the amount of degrees of freedom between the blocks $D_{connect} = D^L$ scales like the number of relevant states d needed to describe our system. The scaling of d is predicted by the area law, as we have seen in equation 13.25 for two-dimensional systems:

$$d \propto \exp(L) \propto D^L \propto D_{connect} \Rightarrow \boxed{D_{connect} \propto d} \quad (13.27)$$

13.4 CONCLUSION

In a combination with the density matrix renormalization group algorithm, matrix product states play a leading role in the efficient representation of one-

13.4 Conclusion

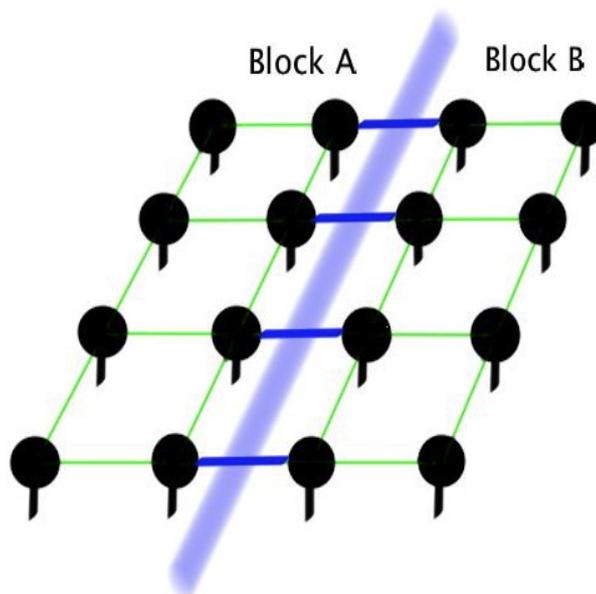


Figure 13.5: *Tensor network on a 2-dimensional lattice according to the PEPS decomposition. All the tensors are connected via D degrees of freedom represented by the green and blue lines. As the system is cut into two subsystems A & B, the amount of available degrees of freedom $D_{connect}$ connecting the blocks scales like D^L (as represented by the number of blue lines), leading to an entanglement entropy $S \propto L$.*

dimensional quantum lattice models. They allow to parametrize the associated state space easily using the decomposition algorithm presented in section 13.2.2. Using matrix product operators, we can apply different optimization methods on an initial MPS to hopefully make it converge towards the ground state of the system. Computing ground states and ground state energies is far from being a trivial achievement for these systems whose Hilbert space grows exponentially with the number of lattice sites.

In two dimensions, we have seen that MPS becomes an ineffective approach, particularly as the considered lattices grow in size. To overcome this issue, we can build a generalization of the method, the projected entangled-pair states, which allows for an efficient representation of two-dimensional lattice models.

The fact that we are able to produce such efficient decomposition is due to the presence of an area law of entanglement for quantum lattice systems defined by a physical hamiltonian. This law states that, for these systems, the entanglement between two subsystems (also called "blocks") will scale like the size of the boundary of the block, as opposed to general quantum systems where the

entanglement would scale like the volume of an analog block. This property allows to build efficient parametrization for complex highly correlated quantum many-body problems on lattices.

13.4 Conclusion

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CHAPTER 14

N-REPRESENTABILITY PROBLEM: PAULI PRINCIPLE AND BEYOND

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The N -representability problem asks about the correlation between a joint state of N fermions and its reduced states, thus can be considered a special case of the quantum marginal problem. Starting with the Pauli principle, a statement about the skew-symmetry of a fermionic wave function, this paper presents a way to find such constraints beyond the Pauli principle for the case of the one point N -representability problem, illustrated by a system of three fermions of rank six. It turns out, that one point N -representability is solvable and can be reduced to a finite set of linear inequalities in terms of the spectra of joint and reduced state.

14.1 INTRODUCTION

In the mid 90s, a problem that was known from 30 years earlier was included in the list of the ten most prominent research challenges in quantum history - the *N -representability problem* [1].

The underlying physical problem stems from calculating energy states for fermionic systems like an atom, with pairwise interaction. It turns out, that the energy of such a system depends only on the two point reduced density matrix (RDM) and the ground state energy in particular is given by

14.2 Quantum Marginal Problem

$$E_0 = \binom{N}{2} \min_{\rho^{(2)}=\text{RDM}} \text{Tr}(H^{(2)}\rho^{(2)}), \quad (14.1)$$

where $H^{(2)}$ is the reduced two particle Hamiltonian and $\rho^{(2)}$ the two particle RDM. Therefore, knowing what conditions the two point RDM should satisfy, would essentially allow the calculation of almost all properties of matter [1].

This is what the quantum marginal problem (QMP) is about and one can therefore think of the N -representability problem as the QMP in the setting of N fermions. It turns out however, that the two point N -representability problem is QMA complete [2] and therefore, discussions about overlapping reduced states are beyond the scope of this paper, for both QMP and N -representability problem.

The following section 1.2 contains a brief review of the quantum marginal problem. Section 1.3 then introduces the one point N -representability problem, the *Pauli principle* and how it constrains the amount of possible states of a system of N fermions and a way to construct a possible basis of antisymmetric wave functions, using *natural spin orbitals*. Section 1.3.4 then goes through one of the very few completely solved cases - the condition on the one-matrix for three-body fermion wavefunction with one-rank equal to six, $\psi \in \wedge^3 \mathcal{H}_6$, following Borland and Dennis [3]. Finally, Section 1.3.5 refers to a paper by Klyachko, who has found a general solution for the one point N -representability problem, which motivates, that the constraints can be expressed through a finite set of linear inequalities in terms of the spectra of joint and reduces state respectively[1].

14.2 QUANTUM MARGINAL PROBLEM

The quantum marginal problem (QMP) is about the relation between a joint state $\Psi \in \mathcal{H}$ and its reduced states $\rho_j, j \in J$. In plain words, this could be stated as follows.

Say one is given a couple of matrices $\rho_A, \rho_B, \rho_C, \dots$, then what are possible joint (mixed) states ρ , such that the set of matrices are actually reduced density matrices of said ρ . So in a sense, the QMP asks about the existence of a mixed state ρ_I of composite system

$$\mathcal{H}_I = \bigotimes_{i \in I} \mathcal{H}_i$$

with given reduced states ρ_J for some $J \subset I$ [1].

One of the most trivial cases is, where there is no constraint at all on ρ . Then

one can simply take the tensor product of all reduced states to get a valid state. But given even little constraints on the upperlying state, say it's supposed to be pure, then the reduced states might be correlated very strongly.

EXAMPLE

Consider a general pure state Ψ of a two component system

$$\Psi = \sum_{i,j} \psi_{ij} \alpha_i \otimes \beta_j \in \mathcal{H}_A \otimes \mathcal{H}_B,$$

where the coefficients ψ_{ij} can be thought of as matrix coefficients, with orthonormal basis α_i, β_j of $\mathcal{H}_A, \mathcal{H}_B$. Then, the reduced density matrices of Ψ are given by

$$\rho_A = \psi^\dagger \psi, \quad \rho_B = \psi \psi^\dagger,$$

which leads to isospectrality

$$\text{Spec} \rho_A = \text{Spec} \rho_B,$$

except additional zeros if $\dim \mathcal{H}_A \neq \dim \mathcal{H}_B$. This implies the so-called *Schmid-decomposition*

$$\Psi = \sum_i \sqrt{\lambda_i} \psi_i^A \otimes \psi_i^B,$$

with ψ_i^A, ψ_i^B being eigenvectors of ρ_A, ρ_B with the same eigenvalue λ_i . This shows, that the reduced states of a bipartite system are strongly correlated.

14.3 N-REPRESENTABILITY PROBLEM

Based on the QMP one could ask himself, what happened if there were further constraints on the joint state ψ . Such a constraint could be given by natural symmetries, e.g. permutation symmetries for identical particles. In the setting of N fermions, the Pauli principle states that the state space is skew symmetric. Using second quantization formalism, the one point RDM is of the form

$$\rho^{(1)} = \langle \psi | a_i^\dagger a_j | \psi \rangle. \tag{14.2}$$

Following chemist notation, we use the normalization $Tr \rho^{(1)} = N$ and $Tr \rho = 1$.

14.3 N -representability problem

14.3.1 THE PAULI PRINCIPLE

There are two ways how to think of the Pauli principle, discovered in 1925 and 1926 respectively[4].

The Pauli exclusion principle states, that no two identical particles could occupy the same quantum space at the same time.

Let $|\psi\rangle^N \in \mathcal{H}^{\otimes N}$ be the state of an N -electron system and ρ_i be the reduced density matrix of the i^{th} electron. The probability of the i^{th} electron to be in state $|\psi\rangle$ is given by $\langle\psi|\rho_i|\psi\rangle$. The electron density matrix ρ of a system of N electrons is defined as $\rho = \sum_i \rho_i$, thus $\langle\psi|\rho|\psi\rangle$ is the number of electrons in the state $|\psi\rangle$. But due to Pauli exclusion principle, this number has to be smaller or equal to 1, which binds the eigenvalues of ρ_i by 1, $0 \leq \lambda_i \leq 1, \lambda_i \in \text{Spec}\rho_i$.

An alternative version was given one year later, which implied the skew symmetry of a fermionic wave function. Consider again a setting of N identical particles. As they are identical, their corresponding wave function $|\psi\rangle^N \in \mathcal{H}^{\otimes N}$ must be invariant under permutation of two particles. Such permutation can be described mathematically by an element of the symmetric group $\pi \in S_N$,

$$\pi|\psi\rangle = e^{i\phi}|\psi\rangle.$$

This gives a one-dimensional representation of the symmetric group S_N , and as there are only two one-dimensional representations of S_N for any N , namely identity and signum, it has to be either one of them. In the end, the identity and symmetric tensors correspond to bosons, whereas latter representation and anti symmetric tensors correspond to fermions [4].

Given these conclusions, the resulting question is:

What is the constraint on the one point reduced density matrix $\rho^{(1)}$ beyond the Pauli principle?

14.3.2 NATURAL SPIN ORBITALS

By knowing that the Pauli principle constrains all possible joint states $|\psi\rangle$ to be anti symmetric, which will be denoted by $|\psi\rangle \in \wedge^N \mathcal{H}_r$, where N is the number of fermions and r the dimension of the Hilbertspace of a single fermion, it would be reasonable to have an anti symmetric basis for $\wedge^N \mathcal{H}_r$, to describe possible joint wave functions.

There is a common way to construct such a basis, using so called *Slater determinants*. For a general r and N , $r \geq N$, the basis vectors are given by

$$|i, j, \dots, p\rangle = \begin{vmatrix} \phi_i(1) & \phi_i(2) & \cdots & \phi_i(N) \\ \phi_j(1) & \phi_j(2) & \cdots & \phi_j(N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_p(1) & \phi_p(2) & \cdots & \phi_p(N) \end{vmatrix}, \quad (14.3)$$

with $\{i, j, \dots, p\} \in \{1, 2, \dots, r\}$, $i \leq j \leq \dots \leq p$, thus any state ψ can be written in terms of these Slater determinants as

$$\psi(1, 2, \dots, N) = \sum_i \sum_j \dots \sum_p a_{ij\dots p} \phi_i(1) \phi_j(2) \dots \phi_p(N). \quad (14.4)$$

The functions ϕ_k are the basis vectors of \mathcal{H}_r and the natural numbers i represent the spin and orbital function of the i^{th} particle.

Eventhough this would essentially be a valid representation of ψ , it's easy to see that the number of Slater determinants needed is given by $\binom{r}{N} = \frac{r!}{N!(r-N)!}$, which grows very fast for increasing r and fixed N . This is a valid argument, as each fermion in an atom potentially lives in an infinite dimensional Hilbertspace. Therefore, the question is, if there is a better choice of basis $\psi_1, \psi_2, \dots, \psi_r$ for the one particle Hilbertspace \mathcal{H}_r , such that some of the coefficients in (14.4) become zero and the answer is - sometimes. These basis vectors are called *natural spin orbitals*.

Given a particular state $\psi \in \mathcal{H}^{\otimes N}$, the *natural spin orbitals* are the eigenfunctions of the one point RDM. By expressing the old basis in terms of these natural spin orbitals might reduce the number of non-zero coefficients and therefore the number of Slater determinants needed to express ψ . Using this method, Borland and Dennis found reductions for the cases where $N = 2$, where the eigenvalues of the one-body reduced matrix occur in degenerate pairs, the case $N = 3$ with $M = 6$ as well as the case where $M = N + 2$ [5].

14.3.3 THE N+2 SPIN-ORBITAL APPROXIMATION TO THE N-BODY ANTISYMMETRIC WAVE FUNCTION

Eventhough the idea of natural spin orbitals is simple, it might still be non intuitive how a reduction in slater determinants could occur, which would also imply further restrictions beyond the Pauli principle. This can be illustrated using the

14.3 N -representability problem

example where $M = N + 2$, following the idea of the same named paper of Bell, Borland and Dennis[5].

A wave function describing a joint state $\Psi \in \wedge^N \mathcal{H}_{N+2}$ can be written either in terms of the Slater determinants as in equation (14.4), or using second quantization formalism, namely

$$|\Psi\rangle = \sum_i \sum_j d_{ij} a_i a_j |N + 2\rangle \quad (14.5)$$

with $|N + 2\rangle$ being an $N + 2$ fermionic state represented by a single slater determinant and $a_i, i \in \{1, 2, \dots, N + 2\}$ the destruction operator of a fermion in state ϕ_i . This can be written as a matrix multiplication

$$|\Psi\rangle = A^T D A |N + 2\rangle, \quad (14.6)$$

where A is the column matrix with entries a_i and D the skew symmetric matrix with coefficients d_{ij} of order $N + 2$.

Because of the skew symmetry of D , one can find a unitary matrix Q , such that

$$D' = Q^T D Q \quad (14.7)$$

is a matrix of block diagonal structure, where the k^{th} block is of the form

$$\begin{pmatrix} 0 & \frac{1}{2}\mu_k \\ -\frac{1}{2}\mu_k & 0 \end{pmatrix}. \quad (14.8)$$

By denoting the column matrix $Q^H A$ by A' , the wave function Ψ is finally of the form

$$|\Psi\rangle = \sum_k \frac{1}{2} \mu_k (a'_{2k-1} a'_{2k} - a'_{2k} a'_{2k-1}) = \sum_k \mu_k a'_{2k-1} a'_{2k} \quad (14.9)$$

using the anti commutation relation for fermions in the last step. Here, the summation of k only runs from 1 to $\frac{1}{2}N + 1$ and therefore, the expected amount of $\binom{N+2}{N} = (N + 1)(N + 2)$ slater determinants is significantly reduced. It is yet to show, that the states $\psi_r = \sum_i q_{ir}^* \phi_i$ just happen to be the natural spin orbitals, thus the one-point reduced density matrix defined in (14.2) is diagonal in terms of this basis ψ . This can be seen by calculating the one-body density matrix in terms of these potential natural spin orbitals

$$B_{rs} = \langle \Psi | a_r'^{\dagger} a_s' | \Psi \rangle, \quad (14.10)$$

which gives

$$B_{rs} = \sum_k \sum_l \mu_k^* \mu_l \langle N + 2 | a_{2k}^\dagger a_{2k-1}^\dagger a_r^\dagger a'_s a'_{2l-1} a'_{2l} | N + 2 \rangle. \quad (14.11)$$

But this expression is only non-zero, if the creation operators recreate the same orbitals destroyed by the destruction operators. This is only possible for $l = k$, thus $r = s$ and therefore, B is diagonal.

So it has been shown, that in this natural spin orbital representation of Ψ , the one point RDM is diagonal and the number of Slater determinants is reduced in this particular case.

Finally, in this representation, the eigenvalues λ_i of the one-point RDM are given by

$$\lambda_i = N! \sum_{k \supset i} |A_k|^2, \quad (14.12)$$

where A_k is the coefficient $A_{ij\dots p}$ from (14.4) and the summation is over all configurations k which include the i^{th} orbital.

14.3.4 THE CONDITIONS ON THE ONE-MATRIX FOR THREE-BODY FERMION WAVEFUNCTIONS WITH ONE-RANK EQUAL TO SIX

When Borland and Dennis wrote their paper on a pure, joint state $\Psi \in \wedge^3 \mathcal{H}_6$ of three fermions, each living in a six-dimensional Hilbertspace in 1971, they justified studying such a special case by the difficulty but importance of the general N -representability problem [3].

Nonetheless, this specific problem can be used to illustrate, how one can now derive the relation between the joint state and the one-point RDM, thus solve the *one representability problem*.

In their paper, Borland and Dennis referred to analytical results by Ruskai and Kingley, proving that in terms of the natural spin orbitals, the only non-zero configurations coefficients were $A_{123}, A_{145}, A_{246}, A_{356}, A_{124}, A_{135}, A_{236}$ and A_{456} , where A_{ijk} denotes the coefficient corresponding to the $|ijk\rangle^{\text{th}}$ Slater determinant as in (14.3). So in this particular case, the number of Slater determinants can be reduced from expected 20, down to a mere 8 basis vectors.

First, consider the case where the wavefunction only consists of the four normalized Slater determinants with coefficients $A_{123}, A_{145}, A_{246}$ and A_{356} , in the process denoted by $\alpha_1, \alpha_2, \alpha_3$ and α_4 .

14.3 N -representability problem

Since we are using natural spin orbital, equation (14.12) must hold, which gives, together with the normalization condition, the following equations:

$$\lambda_1 = |\alpha_1|^2 + |\alpha_2|^2 \quad (14.13)$$

$$\lambda_2 = |\alpha_1|^2 + |\alpha_3|^2 \quad (14.14)$$

$$\lambda_3 = |\alpha_1|^2 + |\alpha_4|^2 \quad (14.15)$$

$$\lambda_4 = |\alpha_2|^2 + |\alpha_3|^2 \quad (14.16)$$

$$\lambda_5 = |\alpha_2|^2 + |\alpha_4|^2 \quad (14.17)$$

$$\lambda_6 = |\alpha_3|^2 + |\alpha_4|^2 \quad (14.18)$$

$$1 = |\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 + |\alpha_4|^2. \quad (14.19)$$

Combining these equations lead to

$$\lambda_1 + \lambda_6 = 1 \quad (14.20)$$

$$\lambda_2 + \lambda_5 = 1 \quad (14.21)$$

$$\lambda_3 + \lambda_4 = 1 \quad (14.22)$$

Without loss of generality, one can assume that the eigenvalues are in decreasing order, $\lambda_i \geq \lambda_{i+1}$. Furthermore, one can solve the first six equations for $|\alpha_i|^2$, leading to the equations

$$2|\alpha_1|^2 = \lambda_1 + \lambda_2 + \lambda_3 - 1 = \lambda_1 + \lambda_2 - \lambda_4 \quad (14.23)$$

$$2|\alpha_2|^2 = \lambda_1 + \lambda_4 + \lambda_5 - 1 = \lambda_1 + \lambda_5 - \lambda_3 \quad (14.24)$$

$$2|\alpha_3|^2 = \lambda_2 + \lambda_4 + \lambda_6 - 1 = \lambda_5 + \lambda_6 - \lambda_5 \quad (14.25)$$

$$2|\alpha_4|^2 = \lambda_3 + \lambda_5 + \lambda_6 - 1 = \lambda_5 + \lambda_6 - \lambda_4 \quad (14.26)$$

where the first three equation are only self consistency conditions with the ordering of the eigenvalues, but the last one is non trivial and contributes another condition.

All together, the eigenvalues for this more specific problem satisfy

$$\lambda_1 + \lambda_6 = 1 \quad (14.27)$$

$$\lambda_2 + \lambda_5 = 1 \quad (14.28)$$

$$\lambda_3 + \lambda_4 = 1 \quad (14.29)$$

$$\lambda_5 + \lambda_6 \geq \lambda_4 \quad (14.30)$$

$$\lambda_i \geq 0 \quad (14.31)$$

with ordering, such that $\lambda_i \geq \lambda_{i+1}$.

However, these conditions have been derived using a wavefunction consisting of only four Slater determinants, thus it is yet to show, that these sufficient conditions are also necessary. It turns out, that by using the same argument, the same conditions can be derived using all eight Slater determinants [3], which proves that the just found conditions are both sufficient and necessary.

So to check a given 6×6 matrix for its three-representability, one would have to find the eigenvalues, and check for the inequalities.

14.3.5 GENERAL RESULTS

The result from the previous sections outlines a way how to derive constraints for a very specific problem. As mentioned above however, the extension onto higher dimensions (higher r values) becomes very difficult as the number of free parameters (i.e. number of Slater determinants) increases very quickly and therefore asks for different approaches.

For the one-point RDM, a general solution is presented by Klyachko [1]

For a mixed state ρ of an N -fermionic system of rank r , the constraints on the one-point RDM are given by the following equalities in terms of the spectra

$$\sum_i a_i \lambda_{\nu(i)} \leq \sum_j (\wedge^N)_j \nu_{\omega(j)}, \quad (14.32)$$

with $\nu \in S_r$ and $\omega \in S_{\binom{r}{N}}$ being permutations and a so called *test spectra*. These *test spectra* satisfy the conditions $a : a_1 \geq a_2 \geq \dots \geq ar, \sum_i a_i = 0$ and could give the intuition, that there is an infinite number of choices for a and therefore infinitely many inequalities. However, it is rather obvious, that there are linear combinations of test spectra, which lead to the same inequalities, thus one can define a finite number of equivalence classes for a .

All together, this formula motivates the observation, that all constraints are linear in terms of the respective spectra of joint and one-point reduced state or likewise, that all the eigenvalues lie within a multidimensional polytope.

14.4 SUMMARY

We have now seen how to derive relations on the spectra of the one body RDM, in particular for the problem where $N = 3, M = 6$. By using natural spin orbitals, there can be a reduction in the number of non-zero coefficients for the Slater determinants. The possibility of such a reduction has been shown explicitly for

14.4 Summary

the case where $M = N + 2$. However, after some research on further settings where $N = 3$, $M = 7$ and $M = N + 3$ with $N = 4$, Borland and Dennis concluded [6], that it seemed unlikely that there existed further cases, where reduction was possible. But even without fewer non-zero coefficients, the discussion above is still valid and Borland and Dennis examined other cases for $N = 3$, $M = 7$; $N = 4$, $M = 7$ and $N = 4$, $M = 8$ and found all sufficient conditions using numerical research, and expect them to be necessary as well.

Criteria for pure N -representability for two particles or two holes are also well understood, but even the case for a system $\wedge^2 \mathcal{H}_5$ leads to a set of 522 independent inequalities. More modern methods are representation theoretical approaches and at the time it is understood, that the eigenvalues lie within a multidimensional polytope. Klyachko seems to have even found a general solution for the mixed one-point representability problem [1]. On the other hand, overlapping systems or two-point representability is still even less understood and was declared to be QMA complete [2].

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CHAPTER 15

N-REPRESENTABILITY PROBLEM: SEMIDEFINITE CONSTRAINTS

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The ground state energy of a many-electron system is determined. The groundstate problem as an exponentially large eigenvalue problem is called FCI. FCI can be solved only for very small systems. There are two traditional approximations of FCI: SDCI and CCSD. These two approximations need only a few seconds to solve the groundstate problem. The groundstate problem is written as a semidefinite programming problem where the full density matrix is needed. The full density matrix is not suitable as a component of an efficient computation method. Therefore we consider reduced density matrices. The groundstate problem written as a semidefinite programming problem with reduced density matrices requires the N-representability. This N-representability condition requires the reconstruction of the large full density matrix. In a SDP-relaxation there have been found conditions for the N-representability which don't require the reconstruction of the full density matrix.

15.1 ELECTRONIC STRUCTURE PROBLEM

Note added: This talk is based on [1] and [2].

15.2 Electronic structure problem as SDP problem

The electronic structure problem is to determine the energies of a many-electron system in a given external potential. In the presentation we consider only the ground state energy. For a N-electron system this ground state energy is the smallest eigenvalue of the Hamiltonian.

Because we have electrons, which are fermions, the N-electron wavefunction has to be totally antisymmetric under the interchange of any pair of electrons.

We can discretize the many-electron space of wave functions by discretizing the single-electron space of wave functions. We take for this single-electron basis functions $\psi_i (i = 1, 2, \dots, r)$ where r is the basis size. Under the discretization we get a discrete Hamiltonian H which can be written as a matrix. The discretized ground state problem is then $H\vec{c} = E_0\vec{c}$ where \vec{c} is the discretized wavefunction and E_0 is the minimum eigenvalue.

The discretized wavefunction \vec{c} has to be antisymmetric. Therefore we can reduce the dimension of the wavefunction to $\frac{r!}{N!(r-N)!}$.

15.1.1 FCI,SDCI,CCSD

This discrete formulation of the electronic structure problem as an exponentially large eigenvalue problem is called full configuration interaction (FCI). It is important to say that FCI can be solved only for very small systems. There are two approximations of FCI, which reduce the basis, they are called SDCI and CCSD.

15.2 ELECTRONIC STRUCTURE PROBLEM AS SDP PROBLEM

The SDP-problem is a subfield of a convex optimization. The semidefinite programming deals with optimization problems of the type

$$\begin{array}{ll} \text{MIN} & (i) \quad \langle C, X \rangle \\ X & \\ \text{subject to} & (ii) \quad \langle A_i, X \rangle \leq b_i \quad i = 1, \dots, m \\ & (iii) \quad X \succeq 0 \end{array}$$

C, X, A are hermitesch matrices. A_i are the rows of A . \langle, \rangle is the inner product.

The minimum eigenvalue E_0 of the discretized electron structure can equivalently computed by the SDP-problem.

$$\begin{array}{ll} \text{MIN} & (i) \quad \langle H, \Gamma^{full} \rangle_{S^n} \\ \Gamma^{full} \in S^n & \end{array}$$

subject to $(ii) \langle \Gamma^{full}, I \rangle_{S^n} = 1$
 $(iii) \Gamma^{full} \succeq 0$

where Γ^{full} = FULL DENSITY MATRIX

S^n = space of all $n \times n$ real symmetric matrices

I = identity matrix

(iii) $A \succeq B$ means that $A - B$ has to be a positive semidefinite symmetric matrix. We know that a density matrix has to be positiv-semidefinit and hermitesch. Therefore $\Gamma^{full} \succeq 0$ must held.

(ii) The inner product in the space S^n is defined as: $\langle A, B \rangle_{S^n} = tr(A^T B) = \sum_{i,j=1} A_{ij} B_{ij}$. This implies that (ii) is equivalent to $tr(\Gamma^{full}) = 1$

(i) Expected value of an observable A is: $\langle \hat{A} \rangle = \frac{tr(\hat{A}\rho)}{tr\rho}$ The expectation value for the Hamiltonian is therefore $\langle H \rangle = \frac{tr(H\Gamma^{full})}{tr(\Gamma^{full})} = tr(H^T \Gamma^{full}) = \langle H \Gamma^{full} \rangle$.

15.2.1 THE FULL DENSITY MATRIX

The full density matrix has the following form $\Gamma^{full} = \Gamma^{full}(i_1, \dots, i_N; i'_1, \dots, i'_N)$. As we see we have two pairs of indices. The indices i_1, \dots, i_N take different values from 1 to r , where r is the basis size. Like the wavefunction Γ^{full} is antisymmetric under the interchange of any set of indices:

$$\Gamma^{full}(i_1, \dots, i_a, \dots, i_b, \dots, i_N; i'_1, \dots, i'_N) = -\Gamma^{full}(i_1, \dots, i_b, \dots, i_a, \dots, i_N; i'_1, \dots, i'_N)$$

The antisymmetrized Γ^{full} is a $\frac{r!}{N!(r-N)!} \times \frac{r!}{N!(r-N)!}$ matrix, where we have taken the factor $\frac{r!}{N!(r-N)!}$ is from before and gives the size of the discretized antisymmetric wavefunction. We see that the size of the full density matrix is exponentially large in r and N . This is not suitable as a component for an effective computation method. To get to an efficient computation we will consider now reduced density matrices.

15.3 ELECTRONIC STRUCTURE PROBLEM AS SDP PROBLEM WITH REDUCED DENSITY MATRICES

15.3.1 P-BODY REDUCED DENSITY MATRIX

First we define the p-body reduced density matrix (RDM) Γ_p . For the definition we have to remind to the partial trace $\rho_A = tr_B \rho_{AB}$. ρ_A is the partial trace of ρ

15.3 Electronic structure problem as SDP problem with reduced density matrices

with respect to the system B. The p-body reduced density matrix is defined as follow:

$$\Gamma_p(i_1, \dots, i_p; i'_1, \dots, i'_p) = \frac{N!}{(N-p)!} \sum_{i_{p+1}, \dots, i_N=1}^r \Gamma^{full}(i_1, \dots, i_p, i_{p+1}, \dots, i_n; i'_1, \dots, i'_p, i_{p+1}, \dots, i_N)$$

The factor $\frac{N!}{(N-p)!}$ is a normalization factor. The p-body reduced density matrix has as the full density matrix the following properties:

- (i) real symmetric
- (ii) positive semidefinite
- (iii) antisymmetric under interchange of any set of indices

It is easy to see that $tr(\Gamma_p) = \langle \Gamma_p, I \rangle = \frac{N!}{(N-p)!}$.

15.3.2 SDP-PROBLEM WITH REDUCED DENSITY MATRICES

Now we assume that the Hamiltonian has only one-body and two-body interaction terms. The Hamiltonian looks therefore as following:

$$H = \sum_{i=1}^N H(i) + \sum_{i<j} H(ij)$$

where $H(i)$ indicates the one-body interaction and $H(ij)$ indicates the two-body interaction. Therefore the energy of a many-electron system depends only on the one-body and two-body reduced density matrix. The normalization leads to $\langle \Gamma_1, I \rangle_{S^n} = N$ and $\langle \Gamma_2, I \rangle_{S^n} = N(N-1)$ and therefore we can write:

$\langle H, \Gamma^{full} \rangle = \langle H_1, \Gamma_1 \rangle + \langle H_2, \Gamma_2 \rangle$ where $H_1 = H(i)$ is the one-body Hamiltonian, $H_2 = H(ij)$ is the two-body Hamiltonian, Γ_1 the one-body reduced density matrix, Γ_2 the two-body reduced density matrix. Now we can formulate the electronic structure problem as an SDP-problem with reduced density matrices.

$$\begin{aligned} \text{MIN} & \quad \langle H, \Gamma_1 \rangle_{S^n} + \langle H, \Gamma_2 \rangle_{S^n} \\ \text{subject to} & \quad \langle \Gamma_1, I \rangle_{S^n} = N \quad \langle \Gamma_2, I \rangle_{S^n} = N(N-1) \\ & \quad \text{and the N-representability: There is a positive semidefinite full density matrix such that } \Gamma_1 \text{ is a one-body RDM} \\ & \quad \text{and } \Gamma_2 \text{ is a 2-body RDM.} \end{aligned}$$

This N-representability condition requires the reconstruction of the large full density matrix. But we want to have necessary and sufficient conditions for the N-representability that don't require the reconstruction of the large matrix Γ^{full} .

15.4 SPECIFIC N-REPRESENTABILITY CONDITIONS

Remind: S^n is the space of all real symmetric $n \times n$ matrices. Because Γ_1 has the form $\Gamma_1(i_1; i'_1)$ and i_1, i'_1 take different values from 1 to r , we get $\Gamma_1 \in S^r$.

Γ_2 has the form $\Gamma_2(i, j; i', j')$. Therefore it depends on two sets of indices. Γ_2 is a $\frac{r!}{2!(r-2)!} * \frac{r!}{2!(r-2)!}$ matrix and therefore $\Gamma_2 \in S^{r(r-1)/2}$

Because $\Gamma_1 \in S^r$ and $\Gamma_2 \in S^{r(r-1)/2}$ the sizes of the variables in the SDP-problem with reduced density matrices depend only on r and not any more on N as the origin SDP-problem.

For the one-body reduced density matrix the remaining necessary and sufficient N-representability conditions are:

$$I \succeq \Gamma_1 \succeq 0$$

This means that Γ_1 should be a positive semidefinite matrix and that the largest eigenvalue of Γ_1 is 1. This comes from a corollary.

For the two-body reduced density matrix a complete family of necessary and sufficient conditions is not known yet. For diagonal two-body reduced density matrices the N-representability problem is well understood. This N-representability problem is equivalent to the characterization of the correlation polytope (Boolean Quadric Polytope). The optimization over the Boolean Quadric Polytope is NP-hard.

15.4.1 SDP-RELAXATION

Because we have only necessary, but not sufficient conditions for the N-representability of two-body reduced density matrices we look for a SDP-relaxation. This means that only a reduced number of conditions for the N-representability of two-body reduced density matrices is checked such that an effective computation is possible. There has been found (here without derivation) following conditions:

$P \succeq 0, Q \succeq 0, G \succeq 0, T_1 \succeq 0, T_2 \succeq 0$ where all these matrices are linear combinations of the entries of Γ_1 and Γ_2 :

$$P \equiv \Gamma_2$$

$$Q(i, j; i', j') \equiv \Gamma_2(i, j; i', j') - \delta(i, i')\Gamma_1(j, j') - \delta(j, j')\Gamma_1(i, i') + \delta(i, j')\Gamma_1(j, i') + \delta(j, i')\Gamma_1(i, j') + \delta(i, i')\delta(j, j') - \delta(i, j')\delta(j, i')$$

The matrices P and Q have the same size as Γ_2 and have the same antisymmetry property. Therefore they belong to $S^{r(r-1)/2}$.

15.5 Numerical results for the RDM method

Figure 15.1: ground state energies

Figure 15.2: time and memory for SDP

$$G(i, j : i', j') = \Gamma_2(i, j'; j, i') + \delta(i, i')\Gamma_1(j', j)$$

In the matrix G there is no antisymmetry, therefore G belongs to S^{r^2} .

$$T_1(i, j, k; i', j', k') = A[i, j, k]A[i', j', k'](\frac{1}{6}\delta(i, i')\delta(j, j')\delta(k, k') - \frac{1}{2}\delta(i, i')\delta(j, j')\Gamma_1(k, k') + \frac{1}{4}\delta(i, i')\Gamma_2(j, k; j', k'))$$

T_1 is fully antisymmetric in both its index triples. Therefore it belongs to $S^{r(r-1)(r-2)/6}$

$$T_2(i, j, k; i', j', k') = A[j, k]A[j', k'](\frac{1}{2}\delta(j, j')\delta(k, k')\Gamma_1(i, i') + \frac{1}{4}\delta(i, i')\Gamma_2(j', k'; j, k) - \delta(j, j')\Gamma_2(i, k'; i', k))$$

$T_2(i, j, k; i', j', k')$ is antisymmetric in (j,k) and in (j',k'). Therefore it belongs to $S^{r^2(r-1)/2}$

15.5 NUMERICAL RESULTS FOR THE RDM METHOD

We compare now in the figure 1 the SDP-method with Hartree-Fock (HF) and the mainstream electronic structure methods CCSD and SDCl. CCSD and SDCl are approximations of FCI.

As a reference we take the Full Configuration Interaction method (FCI).

All energies are given as a difference to the FCI-values.

Since the RDM-method is an SDP-relaxation of the FCI, it always gives a lower bound for the energy. The origin for this is that the reduced conditions for the SDP-method yield a bigger space than the space for the full conditions.

On the other hand SDCl and HF give upper bounds.

The entry "F/C" means: Fail to converge.

We see that the RDM-method with P, Q, T_1, T_2 we have better results than the best traditional electronic structure method CCSD. We see that CCSD sometimes doesn't converge. The RDM-method converges always for the chosen chemical elements.

We see in the figure 2 that the RDM-method is not competitive in time because CCSD provide results in a few seconds.

With the RDM-method it is also possible to calculate the dipole moments. With

P, Q, G the RDM-method is better than HF and with P, Q, T_1, T_2, G we have almost results of FCI.

15.6 CONCLUSION

With the RDM method with all conditions we get better ground state energies than current electronic structure methods. In the examples RDM-method always converge which is not the case for the traditional electronic structure methods. RDM-method can't compete in time compared to other methods. For example with basis size $r=18$ and all conditions the RDM-method needs 12 hours. The traditional electronic method needs only few seconds. There are open questions: search new N-representability conditions such that we have a faster algorithm and to solve very large systems with $r > 26$.

15.6 Conclusion

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CHAPTER 16

FERMIONIC DENSITY FUNCTIONAL THEORY

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This chapter is dedicated to the theoretical foundations of Density Functional Theory. A theory, which was tailored to solve the electronic problem efficiently and which allows to determine the properties of a N-electron system using solely the electronic density.

16.1 INTRODUCTION

Note added: This talk is based on the following references [1, 2, 3, 4, 5].

The Schrödinger equation is certainly one of the most important equations of physics and it improved our understanding of matter drastically. But as every student of physics learns very soon, there are only special cases where an analytic solution of the Schrödinger equation exists. In most cases we have to use approximation methods such as perturbation theory or variational principles to solve a concrete problem.

In 1927, one year after the introduction of the Schrödinger equation and its success in explaining the properties of the hydrogen atom, the Thomas-Fermi model was proposed. It was a first attempt to understand more complex atoms than hydrogen and helium and can be understood as an approximate solution of the quantum N-body problem. However, the Thomas-Fermi model is based on semi-classical considerations and the central object is the electronic density (an observable), not the wave function. This is one of the reasons why this method

16.1 Introduction

is not very accurate and furnishes only the qualitative scaling behavior of the analyzed system. But the most severe problem in the original Thomas-Fermi theory is the non-existence of chemical bindings, which arises from ignoring the Pauli exclusion principle. Different extensions have been proposed to overcome these difficulties, but the method is still not very accurate.

Better results can be obtained by a method, which is based on the Schrödinger equation and which incorporates the Pauli exclusion principle. The Hartree-Fock method with its orbitals and Slater determinants meets these criteria and provides much better results than Thomas-Fermi theory. Because Hartree-Fock theory respects Pauli's principle it can describe chemical bindings and thus molecules, but there are still deviations from experimental data. The deviations arise from the neglected correlation between the electrons. Nevertheless, Hartree-Fock theory has many advantages and it's still used today as starting point for more advanced methods or for first calculations in hybridized models. However, this chapter is not about a descendant of Hartree-Fock method but about a theory on its own: Density Functional Theory (DFT).

P. Hohenberg, W. Kohn and L.J. Sham developed this theory in 1964 / 1965. They went back to the roots and took the best from Thomas-Fermi and Hartree-Fock theory to create a new formalism for the quantum N-body problem. In DFT the electronic density from Thomas-Fermi theory replaces the wave function as fundamental object and is connected to self-consistent equations and determinantal states known from Hartree-Fock theory.

At first thought it may look strange to replace the anti-symmetric spin-wave function of $4N$ variables, which is believed to contain the most information about the system by a quantity of only three variables, which basically tells us something about the distribution of charges. But there are good reasons to look for an alternative to the wave function. Suppose we want to solve the N-body problem for oxygen ($N=8$) by solving the many-particle Schrödinger equation. Then we would have to deal with 24 coordinates (neglecting the spin). Assuming ten entries per coordinate and one byte per entry we end up with 10^{24} bytes. A DVD stores about 10^{10} bytes and thus we would need 10^{14} DVD's to store the information contained in the wave function. Clearly, this is not a practicable way to master the electronic problem. In the following we will develop a new formalism that allows us to solve our problem more efficiently.

16.1.1 INTERLUDE ON FUNCTIONALS

This preparative section is dedicated to the notion of functionals and their derivatives since they play an important role in DFT. Every physicist should be familiar

with functionals and their derivatives since they already appear in Hamilton's principle from classical mechanics. Very often, functionals are regarded as "functions of functions". Because this definition is a bit sloppy, we should have a look at the correct

Definition 16.1. Let V be a \mathbb{K} function space with $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. Denote by $D(F) \subseteq V$ the definition space of F . Then $F: D(F) \rightarrow \mathbb{E} \subseteq \mathbb{K}$ is called a functional.

We will denote functionals as $F[f]$. Note that it follows directly from the definition that a functional depends on the whole function f . Expressions like $F[f(x)]$ do not make sense and have to be avoided since they suggest that the functional depends on the function value $f(x)$ and not on the whole function f . Functionals depending on a parameter x will be denoted as $F[f](x)$.

The action $S[\mathbf{q}]$ from the already mentioned mechanical principle is a basic example of a functional and as every physicist knows, the first variation (first functional derivative) of $S[\mathbf{q}]$ equated to zero leads to the Euler-Lagrange equations. At this point we should repeat the definition of functional derivative.

Definition 16.2. Let V be a \mathbb{K} function space, F a functional, $\lambda \in \mathbb{K}$ and $f, h \in V$. Then

$$\frac{\delta F[f]}{\delta f} := \lim_{\lambda \rightarrow 0} \frac{F[f + \lambda h] - F[f]}{\lambda} \quad (16.1)$$

is called the functional derivative of $F[f]$ (if the right hand side exists $\forall h \in V$).

The idea is the same as for the conventional derivative: Find a linearization in a given point. For functionals this means find a linearization in a given function.

16.1.2 FROM DENSITY MATRICES TO ELECTRONIC DENSITIES

The next important step towards DFT is to define the electronic density and to explore its properties. For the following we introduce the variable $x := (\mathbf{r}, s)$ as helpful abbreviation and define the electronic density n over the one-particle density matrix:

$$n(\mathbf{r}_1) := \sum_{s_1} \rho_1(x_1; x_1) = N \sum_{s_1, \dots, s_N} \int |\psi(x_1, \dots, x_N)|^2 d^3 r_2 \cdots d^3 r_N \quad (16.2)$$

Note that the electronic density does not depend on which variable is left out in the integral and we can drop the index 1 and just write $\mathbf{r}_1 \equiv \mathbf{r}$, $x_1 \equiv x$ and $s_1 \equiv s$. Moreover, the electronic density n is an observable and has easy to proof properties like $n(\mathbf{r}) \geq 0 \forall \mathbf{r} \in \mathbb{R}^3$, $\int n(\mathbf{r}) d^3 r = N$ and there's an operator $\hat{n}(\mathbf{r})$ belonging to the electronic density which has the form $\hat{n}(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{r}_i)$. An

16.2 Basics of Density Functional Theory

other nice property of the electronic density is that it allows us to express the expectation value of a multiplicative operator of the form $\hat{A} = \sum_{i=1}^N \hat{a}(\mathbf{r}_i)$ as

$$\langle \psi | \hat{A} | \psi \rangle = \int a(\mathbf{r}) n(\mathbf{r}) d^3r. \quad (16.3)$$

This statement is proofed by a straightforward calculation and will be very important later on.

16.2 BASICS OF DENSITY FUNCTIONAL THEORY

After the two preparing sub-chapters we finally return to our original task: Find a new formalism for the electronic problem. This problem can be defined as finding the ground state (GS) energy of N strictly non-relativistic electrons for arbitrary positions of M nuclei within the Born-Oppenheimer approximation. Furthermore, we consider only the time-independent, non-degenerate and spin unpolarized case. To simplify notation, we'll choose atomic units where $m_e = \hbar = e = 4\pi\epsilon_0 = 1$. Expressed in these units and in Born-Oppenheimer approximation the Hamiltonian of our problem reads

$$\hat{H} = \underbrace{-\frac{1}{2} \sum_{i=1}^N \nabla_i^2}_{=: \hat{T}} + \underbrace{\frac{1}{2} \sum_{i \neq j}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{=: \hat{U}} - \underbrace{\sum_{i=1}^N \sum_{j=1}^M \frac{Z_j}{|\mathbf{r}_i - \mathbf{R}_j|}}_{=: \hat{V}} = \hat{T} + \hat{U} + \hat{V} \quad (16.4)$$

The variables Z_i and \mathbf{R}_i denote the nuclear charges and positions, respectively, and the \mathbf{r}_i indicate the positions of the electrons. The operators \hat{T} and \hat{U} are universal (i.e. system independent) operators whereas the operator \hat{V} is known as the external potential and carries specific information about the system. Usually, one would try to solve the many-body SE, derive the wave function as functional of the external potential and consequently express all observables as expectation value. However, this is often not a practicable way since the many-body wave function is not a handy quantity (see introduction) and the SE is very hard to solve. The following two theorems, the pillars of DFT, open the door to a new but equivalent formalism.

Theorem (Hohenberg-Kohn I, 1964):

Let $\hat{H} = \hat{T} + \hat{U} + \hat{V}$ be the Hamiltonian of a N -particle system. The operators \hat{T} and \hat{U} are fixed and $c \in \mathbb{R}$ is a constant. Then there's a one-to-one mapping between $(V \bmod c)$ and the ground state density n_0 .

Proof of HK I. The usual way of solving the electronic problem and deriving the GS density can be summarized as follows:

$$V(\mathbf{r}) \xrightarrow[A]{SE} \psi[V](\mathbf{r}_1, \dots, \mathbf{r}_N) \xrightarrow[B]{(16.2)} n_0(\mathbf{r}) \quad (16.5)$$

The mapping $B \circ A : V(\mathbf{r}) \longrightarrow n_0(\mathbf{r})$ is invertible if A and B can be inverted. By considering two different systems, we can easily proof that mapping A is invertible. For this purpose we show that two different external potentials are mapped onto two different states. The two systems are described by the Hamiltonians $\hat{H}_i = \hat{T} + \hat{U} + \hat{V}_i$ and different potentials means (in this context) that $\Delta\hat{V} = \hat{V}_1 - \hat{V}_2 \neq \text{const.}$ almost everywhere. We assume by contradiction that $|\psi_1\rangle = |\psi_2\rangle =: |\psi\rangle \neq 0$ and have a look at

$$\begin{aligned} (\hat{H}_1 - \hat{H}_2) |\psi\rangle &= (E_1 - E_2) |\psi\rangle \\ \Leftrightarrow \Delta\hat{V} |\psi\rangle &= (E_1 - E_2) |\psi\rangle. \end{aligned} \quad (16.6)$$

The right hand side of the last equation is a constant, but $\Delta\hat{V} \neq \text{const.}$ by assumption and $|\psi\rangle \neq 0$. Contradiction! We conclude that the two systems have no common eigenstates and that mapping A can be inverted. The inverse mapping A^{-1} can (formally) be found by solving the SE equation for V , i.e.

$$V = \frac{1}{\psi} \hat{T} \psi - U. \quad (16.7)$$

This follows from the multiplicativity of the potential operators and the fact that potentials differing by a constant are regarded as equal and thus the constant energy E can be ignored (gauge freedom).

For the inversion of B we have to proof $|\psi_1\rangle \neq |\psi_2\rangle \Rightarrow n_{0,1} \neq n_{0,2}$ and consider thus again two different N -particle systems. Assume by contradiction that $|\psi_1\rangle \neq |\psi_2\rangle$ produce the same GS density n_0 . Then calculate the GS energy of system 1.

$$\begin{aligned} E_1 &= \langle \psi_1 | \hat{H}_1 | \psi_1 \rangle \stackrel{\text{a)}}{<} \langle \psi_2 | \hat{H}_1 | \psi_2 \rangle \\ &= \langle \psi_2 | \hat{H}_2 + \hat{V}_1 - \hat{V}_2 | \psi_2 \rangle \stackrel{\text{b)}}{=} E_2 + \int n_0(\mathbf{r})(v_1(\mathbf{r}) - v_2(\mathbf{r})) d^3r. \end{aligned} \quad (16.8)$$

The strict inequality a) holds because of the Rayleigh-Ritz principle and the fact that the \hat{H}_i have no common ground eigenstates. The integral appearing in b) is the rule given in (16.3). An analogue inequality holds for E_2 : $E_2 < E_1 + \int n_0(\mathbf{r})(v_2(\mathbf{r}) - v_1(\mathbf{r})) d^3r$. By subtracting the two inequalities we obtain

$$E_1 + E_2 < E_1 + E_2 \quad (16.9)$$

which is clearly a contradiction. We conclude that different ground states produce different densities and thus B can be inverted. This completes the proof. \square

16.2 Basics of Density Functional Theory

The first Hohenberg-Kohn theorem (HK I) allows us to construct the mapping

$$n_0 \xrightarrow{(B \circ A)^{-1}} V[n_0] \xrightarrow{SE} \psi[n_0] \quad (16.10)$$

and by taking expectation values $\langle \psi[n_0] | \hat{O} | \psi[n_0] \rangle = O[n_0]$ we recognize that every observable can be expressed as functional of the GS density. This implies that we can replace the wave function and the GS density becomes the fundamental quantity of our theory. However, we still need to solve the many-body SE to get the wave function to calculate the GS density. So, if we really want to get rid of the wave function, we have to find an alternative to the SE. Such an alternative will be provided by the following theorem.

Theorem (Hohenberg-Kohn II, 1964):

There exists a functional $E[n]$ with $E[n] \geq E_0$, where E_0 is the exact GS energy. Equality holds only for $n = n_0$, where n_0 is the GS density. Moreover, the variational equation

$$\frac{\delta E[n]}{\delta n(\mathbf{r})} = 0$$

yields the exact GS density n_0 .

Proof of HK II. The functional $E[n]$ is simply the energy functional defined by

$$\begin{aligned} E[n] &:= \langle \psi[n] | \hat{T} + \hat{U} + \hat{V} | \psi[n] \rangle = T[n] + U[n] + V[n] \\ &= F_{HK}[n] + \int n(\mathbf{r})v(\mathbf{r})d^3r. \end{aligned} \quad (16.11)$$

The functional $F_{HK}[n]$ is known as Hohenberg-Kohn functional and is a universal quantity (it's the expectation value of the two universal operators \hat{T} and \hat{U}). The theorem follows by applying Rayleigh-Ritz's principle to $E[n]$. \square

The variational equation of the second Hohenberg-Kohn theorem (HK II) replaces the many-body SE and in principle we developed a new formalism. According to HK I, we can calculate all observables from the GS density and this density can be found using HK II. However, the variational equation is hard to solve and no analytic expression for $F_{HK}[n]$ is known.

Nevertheless, we can try to understand an easy system. Following the idea of Kohn and Sham, we consider a virtual system of N non-interacting spin 1/2 electrons which move in some unknown potential $V_s(\mathbf{r})$. To have a link to our

physical system, we require that both, virtual and real system have the same GS density n_0 . The equation to solve and the side condition then read

$$\frac{\delta E[n]}{\delta n(\mathbf{r})} = \frac{\delta T_s[n]}{\delta n(\mathbf{r})} + \frac{\delta V_s[n]}{\delta n(\mathbf{r})} =: \frac{\delta T_s[n]}{\delta n(\mathbf{r})} + v_s(\mathbf{r}) = 0 \quad (16.12)$$

$$N = \int n_0(\mathbf{r}) d^3r.$$

Since the kinetic energy of non-interacting particles $T_s[n]$ and the potential $V_s[n]$ are not known, this equation can't be solved directly. However, we can write down the wave function of our system as Slater determinant consisting of orbitals $\phi_i(\mathbf{r})$ and derive

$$n(\mathbf{r}) = \sum_{i=1}^N |\phi_i(\mathbf{r})|^2 \quad (16.13)$$

as expression for the density. Further, $T_s[n]$ can be calculated as expectation value of the kinetic energy operator and is given by

$$T_s[n] = -\frac{1}{2} \sum_{i=1}^N \langle \phi_i | \nabla_i^2 | \phi_i \rangle. \quad (16.14)$$

The minimization can now be performed indirectly, i.e. by taking the variation with respect to the $\phi_i^*(\mathbf{r})$. The new equation to solve is

$$\frac{\delta}{\delta \phi_i^*(\mathbf{r})} \left(T_s[n] + V_s[n] - \epsilon_i (\langle \phi_i | \phi_j \rangle - \delta_{ij}) \right) = 0 \quad (16.15)$$

where the Lagrange multipliers ϵ_i were introduced to take into account the orthonormality condition of the orbitals. By performing the variation explicitly, we are led to the equation

$$\left(-\frac{1}{2} \nabla_i^2 + v_s(\mathbf{r}) \right) \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r}) \quad (16.16)$$

which is satisfied by each electron of the virtual Kohn-Sham system. This N single-body SE solve (in principle) the electronic problem for the virtual system. By solving (16.16) for the ϕ_i 's one can calculate the GS density by using (16.13) and thus find all observables. In particular, the GS energy is simply given by the sum over the ϵ_i . But where is the link to a real system? Remember that we required from our virtual system, that it produces the same GS density like our physical system. This means that by solving (16.16) in connection with (16.13) one finds the GS density of the physical system and consequently all observables. Further, the following one-to-one mapping relation holds due to HK I:

$$v_s \longleftrightarrow n_0 \longleftrightarrow v_{eff} \quad (16.17)$$

16.2 Basics of Density Functional Theory

where v_{eff} denotes the effective potential of the physical system (we will define it below). To find the one-to-one mapping between the two potentials, we rewrite the kinetic energy of the real system as $T[n] = T_s[n] + T_c[n]$ where $T_s[n]$ represents the energy contribution of non-interacting particles of density n and $T_c[n]$ is the remainder coming from the interacting particles. The energy $E[n]$ is then typically rewritten as

$$E[n] = T_s[n] + V[n] + U_H[n] + E_{XC}[n] \quad (16.18)$$

where the expectation value of \hat{U} is approximated by the Hartree potential $U_H[n]$

$$U[n] \approx U_H[n] = \frac{1}{2} \int \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r d^3r' \quad (16.19)$$

which can be understood as a classical mean value. The exchange-correlation (XC) energy E_{XC} is introduced to fix the approximation, absorb $T_c[n]$ and make equation (16.18) exact again. The variational equation now reads

$$\begin{aligned} \frac{\delta E[n]}{\delta n(\mathbf{r})} &= \frac{\delta T_s[n]}{\delta n(\mathbf{r})} + \frac{\delta V[n]}{\delta n(\mathbf{r})} + \frac{\delta U_H[n]}{\delta n(\mathbf{r})} + \frac{\delta E_{XC}[n]}{\delta n(\mathbf{r})} \\ &= \frac{\delta T_s[n]}{\delta n(\mathbf{r})} + \underbrace{v(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r' + v_{xc}[n](\mathbf{r})}_{=: v_{eff}} = 0. \end{aligned} \quad (16.20)$$

The last line is obtained by defining $\delta_{n(\mathbf{r})} E_{XC}[n] =: v_{XC}[n](\mathbf{r})$ and performing the variation of the other terms concretely. By comparing (16.20) with (16.12) we immediately recognize that they have the same form and we have to define $v_s := v_{eff}$. So we found our one-to-one mapping and to study a physical system we have to solve the so-called Kohn-Sham (KS) equations:

$$\left(-\frac{1}{2} \nabla_i^2 + v(\mathbf{r}) + \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r' + v_{xc}[n](\mathbf{r}) \right) \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r}). \quad (16.21)$$

These equations are completely equivalent to the many-body SE of the electronic problem and imply that DFT is (so far) an exact theory and can be regarded as alternative formalism. Moreover, it turns out that it's easier to solve the N KS equations several times than solve the many-body SE once and there's no storing problem when using the KS equations. That's because by discretizing real space into M points, the needed storage grows as M^N (N = number of electrons) for the SE, but only as MN for the KS equations.

However, since the XC energy functional is not known, one has to find approximations for this term. The simplest ansatz for $E_{XC}[n]$ is called local density

approximation (LDA) and the idea is once again to study a simpler system and to apply it to a real physical system. The toy system in LDA is the well-known homogeneous electron gas (HEG). Even though there is no analytic expression for the XC energy $\epsilon_{XC}^{HEG}(n)$ of the HEG, it can be calculated numerically using Monte Carlo calculations and there are numerical parameterizations of $\epsilon_{XC}^{HEG}(n)$. The idea is now to approximate the XC energy of the physical system locally (i.e. around a point \mathbf{r}) by $\epsilon_{XC}^{HEG}(n^{HEG})|_{n^{HEG}=n(\mathbf{r})}$. Note that n^{HEG} is a constant and we choose this constant to be equal to the density of the real system at the (fix) point \mathbf{r} . By summing up all contributions over all space, we're led to the expression

$$E_{XC}^{LDA}[n] = \int \epsilon_{XC}^{HEG}(n(\mathbf{r}))n(\mathbf{r})d^3r. \quad (16.22)$$

The LDA was originally invented for slow varying densities, however, it turned out that it works also very good for other densities. Of course LDA is a rather rough approximation and there are more sophisticated ones, but nevertheless, now we have everything we need to make DFT work in practice: To solve a real problem, we first have to choose an approximation for $E_{XC}[n]$ and make an initial guess for $n(\mathbf{r})$ (for example by using a fast but less accurate approximation method). Then $v_{eff}(\mathbf{r})$ is calculated and inserted into the KS equation. By solving the N KS equations for the orbitals, we can calculate a new GS density by using (16.13). The new density is then compared to the initial guess. If the two densities are not equal, the new one is taken as new initial guess and the whole cycle is repeated until it converges. This self-consistent cycle is called the Kohn-Sham scheme. Usually, the KS scheme converges very quickly and provides very good results, but there's no criterion if the found GS density is the correct one and everything depends on the chosen approximation for the XC energy. Moreover, the formalism developed so far has strong limitations (treats only GS, time-independent systems, not degenerate GS,...). In the following, we will have a look at extensions of DFT.

16.3 TIME-DEPENDENT DFT

Density functional theory has many applications in solid-state physics, chemistry, biology and mineralogy. But as already mentioned, the basic theory of Hohenberg and Kohn is limited and there are different generalizations, which are used in the different fields. Important extensions are for instance degenerate ground state DFT, spin / magnetic orbitals DFT to describe paramagnetism / diamagnetism, relativistic DFT and time-dependent DFT (TDDFT). The last one can comparatively easy be developed from the basic theory and will be discussed in

16.3 Time-dependent DFT

this chapter.

Again, we restrict our discussion to non-relativistic and non-degenerate systems. But this time we're not bound to the GS and we require our systems to satisfy the time-dependent SE. Then the first thing to do is of course to redefine the electronic density $n(\mathbf{r})$ to $n(\mathbf{r}, t)$, where the time-dependency comes from the explicit time-dependency of the wave function. The next step is to recognize the differences between a static and a time-dependent quantum mechanical problem. In the first case the GS of the system can be found by minimization of the total energy functional $E[\psi] = \langle \psi | \hat{H} | \psi \rangle$. In time-dependent systems the energy is not conserved and thus there is no minimization principle. However, a new quantity, the quantum mechanical action

$$\mathcal{D}[\psi] := \int_{t_0}^{t_1} dt \langle \psi(t) | i\partial_t - \hat{H}(t) | \psi(t) \rangle \quad (16.23)$$

can be introduced by analogy. As to expect, the first variation of $\mathcal{D}[\psi]$ with respect to ψ^* equated to zero yields the tdSE. So the minimization principle gets substituted by a stationary principle. For stationary points (i.e. for solutions of the tdSE) the action becomes equal to zero and we can't assign any physical meaning to it. This two properties (stationary principle and $\mathcal{D} = 0$ for stationary points) make the action a less useful quantity than the total energy functional (minimizing point yield GS and GS energy).

Another important point is that a time-dependent problem in quantum mechanics is, mathematically, an initial value problem. This means that we have to fix an initial state and that the density depends on the initial state. Further, we have to restrict the set of admissible potential to Taylor expandable potentials:

$$V(\mathbf{r}, t) = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k}{dt^k} V(\mathbf{r}, t) \Big|_{t=t_0} (t - t_0)^k. \quad (16.24)$$

It is easy to show that two potentials that only differ by a purely time-dependent constant produce two states, which only differ by a time-dependent phase. Thus we have to consider potentials that differ by more than a time-dependent constant and we require

$$w_k := \frac{\partial^k}{\partial t^k} [V(\mathbf{r}, t) - V'(\mathbf{r}, t)] \Big|_{t=t_0} \neq \text{const.} \quad (16.25)$$

for some $k > 0$. Considering all this differences, we can proof the following two theorems:

Theorem (Runge-Gross, 1984):

Let $\hat{H}(t) = \hat{T} + \hat{W} + \hat{V}(t)$ be the Hamiltonian of a N -particle system, $\hat{V}(t)$ Taylor-expandable in time. Fix the initial state $|\psi(t_0)\rangle$. Then there is a one-to-one mapping between $(V(\mathbf{r}, t) \text{ mod } c(t))$ and the time-dependent density n .

Proof. We consider two systems (primed and unprimed) and first show that $V \neq V' + c(t) \Rightarrow \mathbf{J} \neq \mathbf{J}'$. The current density is simply given by

$$\mathbf{J}(\mathbf{r}, t) = \langle \psi(t) | \hat{\mathbf{J}}(\mathbf{r}, t) | \psi(t) \rangle \quad (16.26)$$

where $\hat{\mathbf{J}}(\mathbf{r}, t)$ is the paramagnetic current density operator

$$\hat{\mathbf{J}}(\mathbf{r}) = \frac{1}{2i} \sum_{j=1}^N \{ \nabla_{r_j} \delta(\mathbf{r} - \mathbf{r}_j) + \delta(\mathbf{r} - \mathbf{r}_j) \nabla_{r_j} \}. \quad (16.27)$$

Using the quantum mechanical equation of motion for the expectation value of an operator and the fact that $\partial_t \hat{\mathbf{J}}(\mathbf{r}) = 0$, we obtain the following equation for the current density:

$$\frac{\partial}{\partial t} \mathbf{J}(\mathbf{r}, t) = -i \langle \psi(t) | [\hat{\mathbf{J}}(\mathbf{r}), \hat{H}(t)] | \psi(t) \rangle. \quad (16.28)$$

Exactly the same equation holds for \mathbf{J}' with $\psi'(t)$ and $\hat{H}'(t)$. The initial state is fixed (i.e. $\psi(t_0) = \psi'(t_0) \equiv \psi_0$ and thus $n(\mathbf{r}, t_0) = n'(\mathbf{r}, t_0) \equiv n_0(\mathbf{r})$) and we can write

$$\begin{aligned} \frac{\partial}{\partial t} (\mathbf{J}(\mathbf{r}, t) - \mathbf{J}'(\mathbf{r}, t)) \Big|_{t=t_0} &= -i \langle \psi_0 | [\hat{\mathbf{J}}(\mathbf{r}), \hat{H}(t_0) - \hat{H}'(t_0)] | \psi_0 \rangle \\ &= -n_0(\mathbf{r}) \nabla (V(\mathbf{r}, t_0) - V'(\mathbf{r}, t_0)). \end{aligned} \quad (16.29)$$

If condition (16.25) is satisfied for some $k > 0$ and if we apply ∂_t k times to (16.29), we obtain

$$\left(\frac{\partial}{\partial t} \right)^{k+1} (\mathbf{J}(\mathbf{r}, t) - \mathbf{J}'(\mathbf{r}, t)) \Big|_{t=t_0} = -n_0(\mathbf{r}) \nabla w_k(\mathbf{r}) \neq 0 \quad (16.30)$$

and we conclude that $\mathbf{J}(\mathbf{r}, t) \neq \mathbf{J}'(\mathbf{r}, t)$ for $t > t_0$. The next step is to proof $\mathbf{J}(\mathbf{r}, t) \neq \mathbf{J}'(\mathbf{r}, t) \Rightarrow n(\mathbf{r}, t) \neq n'(\mathbf{r}, t)$. For this purpose we write down the continuity equation

$$\frac{\partial}{\partial t} (n(\mathbf{r}, t) - n'(\mathbf{r}, t)) = -\nabla \cdot (\mathbf{J}(\mathbf{r}, t) - \mathbf{J}'(\mathbf{r}, t)) \quad (16.31)$$

and take the $(k+1)$ th time derivative of this equation at $t = t_0$:

$$\left(\frac{\partial}{\partial t} \right)^{k+2} (n(\mathbf{r}, t) - n'(\mathbf{r}, t)) \Big|_{t=t_0} = \nabla \cdot (n_0(\mathbf{r}) \nabla w_k(\mathbf{r})). \quad (16.32)$$

16.4 Summary

Now we have to demonstrate that the right hand side of (16.32) can't be identical to zero. We'll prove it by reductio ad absurdum: Assume

$$\nabla \cdot (n_0(\mathbf{r})\nabla w_k(\mathbf{r})) \equiv 0 \quad (16.33)$$

and apply Green's theorem to obtain

$$\begin{aligned} \int n_0(\mathbf{r})(\nabla w_k(\mathbf{r}))^2 d^3r = & + \oint n_0(\mathbf{r})w_k(\mathbf{r})\nabla w_k(\mathbf{r}) \cdot d\mathbf{a} \\ & - \underbrace{\int w_k(\mathbf{r})\nabla \cdot (n_0(\mathbf{r})\nabla w_k(\mathbf{r}))}_{=0 \text{ by assumption}}. \end{aligned} \quad (16.34)$$

The surface integral has to vanish as well for potentials arising from normalizable external charge densities because the quantity $w_k(\mathbf{r})$ falls off at least as $1/r$. The integral on the left hand side is obviously non-negative and thus we conclude

$$n_0(\mathbf{r})(\nabla w_k(\mathbf{r}))^2 \equiv 0 \quad (16.35)$$

which contradicts $w_k(\mathbf{r}) \neq \text{const.}$ This completes the proof. \square

The Runge-Gross theorem is obviously related to HK I and by using (16.23) we could also derive the time-dependent KS equations:

$$i\partial_t\phi_i(\mathbf{r},t) = \left(-\frac{1}{2}\nabla_i^2 + v(\mathbf{r},t) + \int \frac{n(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}d^3r' + v_{XC}[n](\mathbf{r},t) \right)\phi_i(\mathbf{r},t) \quad (16.36)$$

So TDDFT looks formally like basic DFT, but of course TDDFT is less restricted and expands the field of applications.

16.4 SUMMARY

Starting from the traditional formulation of the electronic problem, we developed a new formalism which allows us to solve the problem more efficiently than by struggling with the SE. We saw that the first Hohenberg-Kohn theorem allows us to replace the wave function by the GS density and that both are equivalent to each other. This means that all observables can be derived from the GS density. By proofing the second Hohenberg-Kohn theorem we replaced the SE by a variational equation that is independent from wave functions and provides the exact GS density as solution. Since the variational equation is still not a very practicable way to solve the electronic problem, we studied a virtual system of non-interacting spin 1/2 electrons and derived the KS equations. These equations

are not only satisfied by the virtual system, but also by a real system. The KS equations, together with an appropriate approximation for the XC energy functional, are the key to find the GS density of a system and thus to derive observables. Furthermore, we saw that the formalism of TDDFT looks formally like basic DFT. Different extensions of the basic theory open the door to a wide range of applications.

16.4 Summary

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CHAPTER 17

MEAN FIELD THEORY: EXPLICIT DERIVATIONS

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(DATE: 14 MAY, 9:45)

We want to give an overview about mean-field constructions in theoretical physics, their applicability and weaknesses. Special focus is laid on Ising model as example spin system and Bose-Einstein condensates by means of Bogoliubov transformation. Physical arguments why and when mean-field techniques are applicable for such systems, as well as heuristic arguments for condensation are gathered but we will also pay attention to the drawbacks.

17.1 INTRODUCTION

In general mean-field techniques and theories (*MFT*), also known as self-consistent or molecular-field theories, are methods to analyze physical many body systems (like those appearing in statistical physics).

A Bose-Einstein condensate (*BEC*) is a state of matter of a dilute gas of weakly interacting Bosons confined in an external potential and cooled to temperatures close to 0 K. Thus a large fraction of the Bosons occupy the ground state (lowest accessible quantum state) revealing quantum effects up to macroscopic scales.

According to [1] this state of matter was predicted first by S. N. Bose and A. Einstein back in 1925. The result of their efforts was the concept of Bose gases governed by Bose-Einstein statistics, which describes the distribution of identical

17.2 Mean-field constructions in spin systems

particles with integer spin (allowed to share quantum states). Einstein demonstrated the effect of cooling bosonic particles below a critical temperature causing them to fall (or "condense") into the ground state, resulting in a new state of matter. The first experimental realization, namely a gaseous condensate was produced by E. Cornell and C. Wieman in 1995 at the University of Colorado for which they received the 2001 Nobel Prize in Physics together with Wolfgang Ketterle at MIT.

17.2 MEAN-FIELD CONSTRUCTIONS IN SPIN SYSTEMS

The basic concept of *MFT* is to replace all interactions in a body with an effective interaction (e.g. average over it's neighbors). This reduces a N -body problem into an effective one-body problem with external field. The study of this effective problem allows insights into the behavior of the original system, for instance by exact computation of the partition function and of the *Helmholtz free energy*. This leads to a qualitative description of phase transitions (which may or may not be in agreement with the behavior of the original system) and provides a simple way to approximately compute the corresponding critical exponents¹.

The field theory description allows to *expand the Hamiltonian in terms of the magnitude of fluctuations* around the mean of the field. In this context, MFT can be viewed as the "zeroth-order" expansion of the Hamiltonian in fluctuations. Physically, this means an MFT system has no fluctuations, which coincides with the idea that one is replacing all interactions with one "mean field". This provides a convenient launch-point for studying first or second order fluctuations.

In general, dimensionality plays a strong role in determining whether a mean-field approach will work for any particular problem.

17.2.1 ISING MODEL

Probably one of the most simple example of a solid state N -body problem one can think of is the *Ising model* described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i \quad \text{with} \quad s_i = \pm s = \pm 1 \quad (17.1)$$

whose exact analytic solution is known for 1 dimension by Ising itself and for 2 dimensions later by Onsager. A straight forward solution for the 1 dimensional case

¹The divergence of a few selected physical observables, such as the specific heat C_V or the magnetic susceptibility χ , signals the presence of a phase transitions. These quantities typically diverge as $|T - T_C|^x$, where T_C is the critical temperature (critical point) and x the critical exponent (which takes characteristic values, e.g. $C_V \rightarrow x = \alpha$, $\chi \rightarrow x = \gamma$, $m \rightarrow x = \beta$, ...)

involving linear algebra can be done by the transfer matrix method as described in [3] sec. 28 and [4] sec. 5-3.

The Ising model is a very good example to demonstrate several mean-field techniques.

The straight way is, according to [2] (sec. 5.2f), to write

$$s_i = \langle s_i \rangle + (s_i - \langle s_i \rangle) = m + (s_i - m) = m + \delta s_i \quad (17.2)$$

and insert this together with the (uniform) mean-field (all spins not just neighbors)

$$m = \langle s_i \rangle = \frac{1}{Z} \sum_{\{s_i\}} s_i e^{-\beta \mathcal{H}} = \frac{1}{Z} \sum_{s_i=\pm 1} s_i e^{-\beta \mathcal{H}}, \quad \forall i \quad (17.3)$$

into the Hamiltonian in order to get the mean-field approximation (it is a long-range approximation since each spin interacts via the mean-field with all other spins)

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} (m^2 + m(s_i - m) + m(s_j - m) + \delta s_i \delta s_j) - H \sum_i s_i \quad (17.4)$$

$$= -J \sum_{\langle i,j \rangle} (-m^2 + m s_i + m s_j + \delta s_i \delta s_j) - H \sum_i s_i \quad (17.5)$$

$$= -J \sum_{i=1}^N (2d m s_i - d m^2) - H \sum_{i=1}^N s_i - J \underbrace{\sum_{\langle i,j \rangle} \delta s_i \delta s_j}_{\text{small b. } \langle \delta s_i \delta s_j \rangle \ll m^2} \quad (17.6)$$

$$\approx - \sum_{i=1}^N \underbrace{(2d J m + H)}_{=H_{\text{eff}}} s_i + N d J m^2 = \mathcal{H}_{\text{mf}} \quad (17.7)$$

with d : dimension of the system considered. Important to notice; this is an *approximation* to the exact Ising model and *becomes better the higher the dimension* is (more neighbors give smaller fluctuations and a better defined mean field). This approximation is reasonable for short range potential in infinite dimensions or very long range potential in finite dimensions (c.f. "Kac type" potential discussion in the Curie-Weiss sec. 17.2.2 model later).

Using this new approximated Hamiltonian the (canonical) partition sum becomes

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straight forward to calculate (with $\beta^{-1} = k_B T$)

$$Z(T, m, H) = \sum_{\{s_i\}} e^{-\beta \mathcal{H}_{\text{mf}}} \quad (17.8)$$

$$= e^{-\beta N J d m^2} \sum_{\{s_i\}} e^{\beta \sum_{i=1}^N H_{\text{eff}} s_i} \quad (17.9)$$

$$= e^{-\beta N J d m^2} \sum_{\{s_i\}} \prod_{i=1}^N e^{\beta H_{\text{eff}} s_i} \quad (17.10)$$

$$= e^{-\beta N J d m^2} \prod_{i=1}^N \sum_{\{s_i\}} e^{\beta H_{\text{eff}} s_i} \quad (17.11)$$

$$= e^{-\beta N J d m^2} (2 \cosh(\beta H_{\text{eff}}))^N \quad (17.12)$$

and thus the Helmholtz free energy is

$$F(T, m, H) = -k_B T \ln(Z) \quad (17.13)$$

$$= N J d m^2 - N k_B T \ln(2 \cosh(\beta H_{\text{eff}})) \quad (17.14)$$

with

$$m = 0, \quad (H = 0) \quad \text{and} \quad F(\beta) = -\frac{N}{\beta} \ln 2 \quad (17.15)$$

a plot is given in fig. 17.1 and in order to find the equilibrium condition we have

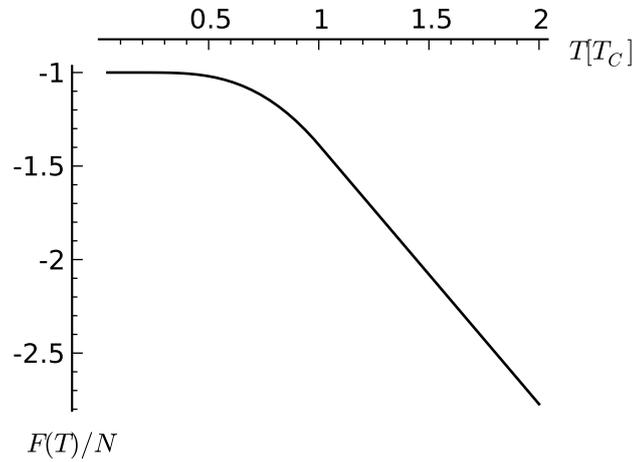


Figure 17.1: Free energy for the Ising model as given by eq. 17.14 (with self-consistence relation 17.17 to get $m(T)$ needed).

to *minimize* F with respect to m giving (remember $H_{\text{eff}} = H_{\text{eff}}(m)$)

$$0 = \frac{\partial F}{\partial m} = N J (2d) m - N J (2d) \tanh(\beta H_{\text{eff}}) \quad (17.16)$$

which is equivalent to the so-called *self-consistence condition*

$$\langle s_i \rangle = m = \tanh(\beta H_{\text{eff}}) = \tanh(2\beta Jmd + \beta H) = -\frac{1}{N} \left(\frac{\partial F}{\partial H} \right)_{T,m}. \quad (17.17)$$

from m (or directly by minimizing) we get the free-energy F and through it all other thermodynamic properties eventually, including critical temperature T_C . This equation in the regime $H = 0$ can be solved numerically and resembles the picture given in fig. 17.2 with the solutions (crossings between \tanh and the linear function) $m = 0$ and $m = \pm m_0(\beta)$. To be able to understand this we have

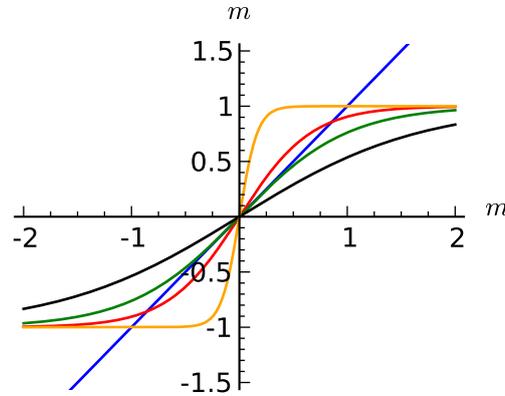


Figure 17.2: Visualization of the self-consistence relation 17.17 and its solutions: *red* is for $T < T_C$, *green* at $T = T_C$ and *black* for $T > T_C$ (*yellow* is $T \ll T_C$).

to look at the *susceptibility*, which is a *good indicator for phase transitions* and it is an observable that can be measured in experiments (in order to check the theory)

$$\chi(T) = -\frac{d^2 F}{(dH)^2} \Big|_{H=0} = -\frac{d}{dH} \left(\frac{\partial F}{\partial H} + \frac{\partial F}{\partial m} \frac{\partial m}{\partial H} \right) \Big|_{H=0} \quad (17.18)$$

$$= -\frac{d}{dH} \frac{\partial F}{\partial H} \Big|_{H=0} = N \frac{dm}{dH} \Big|_{H=0} \approx \frac{N}{k_B T} \left(J(2d) \frac{dm}{dH} \Big|_{H=0} + 1 \right) \quad (17.19)$$

$$= \frac{J(2d)}{k_B T} \chi(T) + \frac{N}{k_B T} = \frac{N}{k_B T - J(2d)} \quad (17.20)$$

were we used the approximation² $m(H=0) = 0$ (and thus it is valid for $T \geq T_C$ as we will see later). χ becomes singular at $1 = \beta J(2d)$ which is called the *critical point* or more precisely here the *critical temperature* T_C (through β) and thus the plot shows a peak as shown in fig. 17.3, this is the phase transition. In

²by using the Taylor's series for \tanh around T_C we can also get critical exponents for m and χ

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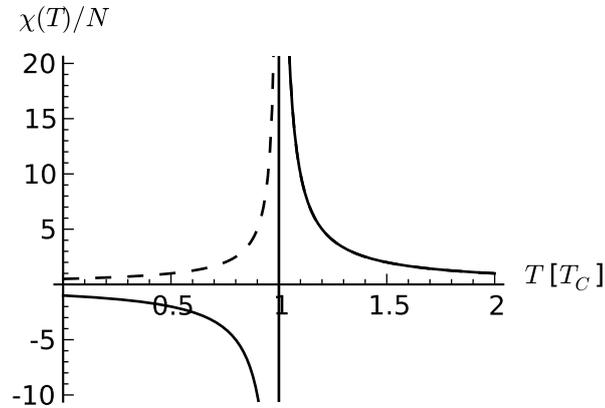


Figure 17.3: Susceptibility for the Ising model according to 17.20.

order to complete the picture we look at the magnetization curve (solution of self-consistence relation for several temperatures) fig. 17.4 were the phase transition

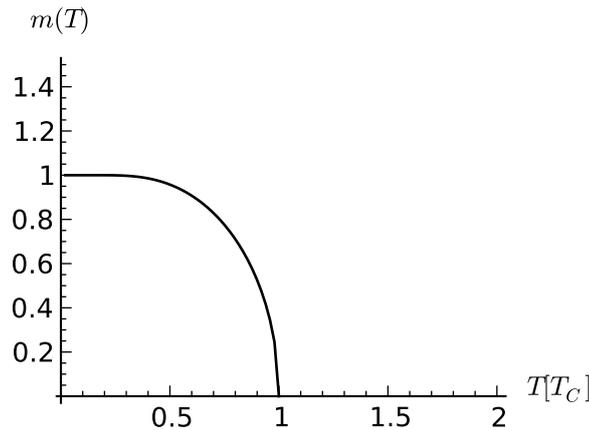


Figure 17.4: Magnetization for the Ising model according to the self-consistence relation 17.17 (the critical point/temperature is also called the *Curie temperature*).

from ordered phase (below T_C or $2\beta J > 1$) with non-vanishing *magnetization* ($m = 1$ at $T = 0$) to a disordered phase (above T_C or $2\beta J < 1$) with zero total magnetization $m = 0$. Looking at the self-consistence relation; the first solution $m = 0$ exist for all temperatures on the other hand the solution with $m = m_0 \neq 0$ exists for $T < T_C$ only.

The *spontaneous magnetization* observed is coupled with a spontaneous *symmetry breaking* in the free energy (according to the famous *Landau theory* of a contin-

uous phase transition). Expanding eq. 17.14 as a Taylor series around $m = 0$ (small m) we find $T \approx T_C$

$$\frac{F(T, m, H = 0)}{N} \approx -k_B T \log(2) \quad (17.21)$$

$$+ \left(Jd - \frac{(\beta H_{\text{eff}}|_{m=H=0})^2}{2} k_B T \right) m^2 \quad (17.22)$$

$$+ \frac{(\beta H_{\text{eff}}|_{m=H=0})^4}{12} k_B T m^4 + \mathcal{O}(m^5) \quad (17.23)$$

a behavior as sketched in fig. 17.5 with 0th, 2nd and 4th order terms. Because of

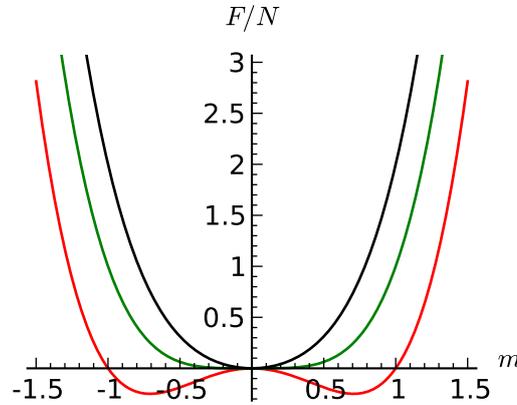


Figure 17.5: Landau free energy for the Ising model according eq. 17.23 (colors like in fig. 17.2). It is visible that for the red curve two minima away from zero exist and the convex envelope has to be taken in order to become a physical valid result.

their signs the 4th order term is always positive but the 2nd order term changes sign at T_C giving either 1 or 3 extrema (from which 1 or 2 are stable minima, especially $m = 0$ is not stable for $T < T_C$) and representing the magnetizations retrieved by self-consistence relation. In order to understand the fact that one of the two possible solutions $\pm m$ is selected consider the fact that this holds for the case $H > 0$ too but then fig. 17.2 is not symmetric anymore and the positive solution $+m_0$ is favored and the unique solution

$$\lim_{H \rightarrow +0} m(H) = +m_0 \quad (17.24)$$

which is after taking the limit the same as before, but clearly preferred³.

³this can be motivated by the fact that there will always be an infinitesimal magnetic field present - this can be e.g. the intrinsic field of the sample itself caused by thermal fluctuations

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So you should note here that there exist three different regimes; long-range order below T_C , short range order above T_C (or even no order at all for $T \rightarrow \infty$) and a fractal structure at the critical point T_C itself with power law scaling (instead of exponential), fractal dimension (a real instead of integer value) and self-similar structure.

A more systematic approach is to use *Gaussian transformation* (Hubbard-Stratonovich transformation) to retrieve (essentially) the same result and tackle the discussion of fluctuation in a rigorous way in the context of field theory. Essentially the idea is to switch from a particle theory description into its respective field theory by linearizing the density operator (matrix) in the many-body interaction term of the Hamiltonian and introducing a scalar auxiliary field, the mean-field. That way we can retrieve a self-consistent field approximation that is renormalizable regarding the critical (or Curie) temperature and exponents⁴. Following the discussion from [2], sec. 5.2.4f we can introduce a auxiliary field ϕ_i and write

$$Z = \sum_{\{s_i\}} e^{-\beta \frac{1}{2} \sum_{i,j} J_{ij} s_i s_j + \beta \sum_i s_i H_i} \quad (17.25)$$

$$= C \int_{-\infty}^{\infty} \left(\prod_{i'} d\phi_{i'} \right) e^{\frac{\beta}{2} \sum_{i,j} (J^{-1})_{ij} (\phi_i - H_i)(\phi_j - H_j)} \underbrace{\sum_{s_i = \pm s} e^{\beta \sum_i s_i \phi_i}}_{= e^{\sum_i \ln(2 \cosh(\beta s_i \phi_i))}} \quad (17.26)$$

with $J_{ij} = -J$ if $\langle i, j \rangle$ are nearest neighbors and 0 otherwise as well as the constant $C = [(2\pi k_B T)^{N/2} \sqrt{\det J}]^{-1}$. By using the identity

$$\int_{-\infty}^{\infty} d\phi e^{-\frac{\phi^2}{2a} + s\phi} = e^{\frac{a}{2}s^2} \int_{-\infty}^{\infty} d\phi e^{-\frac{(\phi - sa)^2}{2a}} = \sqrt{2\pi a} e^{\frac{a}{2}s^2} \quad (17.27)$$

with any real valued field ϕ and constant a , thus

$$\int_{-\infty}^{\infty} \left(\prod_{i'} d\phi_{i'} \right) e^{-\frac{1}{2} \sum_{i,j} \phi_i (A^{-1})_{ij} \phi_j + \sum_i s_i \phi_i} = (2\pi)^{N/2} \sqrt{\det A} e^{\frac{1}{2} \sum_{i,j} s_i A_{ij} s_j} \quad (17.28)$$

(with matrix A_{ij}) is called Gaussian or Hubbard-Stratonovich transformation and allows us to write (with constant C)

$$Z = C \int_{-\infty}^{\infty} \left(\prod_{i'} d\phi_{i'} \right) e^{-\beta S(\phi_i, H_i)} = e^{-\beta F} \quad (17.29)$$

⁴this means; above the critical dimension the mean field exponents are correct, and the only effect of fluctuations is to renormalize certain quantities such as the critical temperature

and this can now be solved by saddle point approximation (sometimes also called method of steepest descent a variant of Laplace's method, confer sec. 17.5.1). The resulting self-consistence relation and thus the thermodynamics retrieved this way are the same as before. The advantage of this method is that we can calculate the correlation function

$$\chi = \beta \sum_{i,j} (\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle) =: \beta \sum_{i,j} \Gamma_{ij} \quad (17.30)$$

with Γ_{ij} the correlation between spins i and j . Varying the distance between i and j allows us to go beyond mean field level and check the validity of the approximation. By using Fourier transformation and other calculations we can then derive an expression showing that at the critical point the correlation length diverges with a power law and can thus be described by a characteristic critical exponent. This allows us to get deeper insight into short and long range ordering.

17.2.2 CURIE-WEISS MODEL

The *classical Curie-Weiss theory* of magnetic transitions⁵ according to [4] sec. 4-5 (and 4-4) considers the Hamiltonian (assuming an interaction potential symmetric in particle exchange)

$$\mathcal{H} = \sum_{1 \leq i < j \leq N} \Phi(|\vec{r}_i - \vec{r}_j|) s_i s_j - H \sum_{i=1}^N s_i \quad (17.32)$$

$$\approx -\frac{\alpha}{N} \sum_{1 \leq i < j \leq N} s_i s_j - H \sum_{i=1}^N s_i \quad (17.33)$$

$$= -\frac{\alpha}{2N} \sum_i \sum_{j \neq i} s_i s_j - H \sum_{i=1}^N s_i \quad (17.34)$$

$$= -\frac{\alpha}{2N} \left(\sum_{i=1}^N s_i \right)^2 + \frac{\alpha}{2} - H \sum_{i=1}^N s_i = \mathcal{H}_{\text{mf}} \quad (17.35)$$

⁵also referred to as the *Weiss-Ising model*, mentioned by [3] sec. 29

$$\mathcal{H}^{\text{WI}} = -\frac{J^{\text{WI}}}{N-1} \sum_i \sum_{j \neq i} s_i s_j - H \sum_i s_i \quad (17.31)$$

The crucial fact is that the Weiss-Ising model can be solved exactly, in contrast to Ising model, for which the mean-field description is an approximation. The free energy of this model is dimension and lattice structure independent. By using the theory of large deviations and random variables we can write the partition sum as an integral, which can be solved by Varadhan's lemma, a fancy kind of Laplace's method (in context of random variables and corresponding distribution functions) in order to retrieve the self-consistence relation similar to the one before.

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can be approximated as mean-field theory with $s_i = \pm 1$ ($s = 1$) and when you compare eq. 17.33 with eq. 17.1 and 17.31 you can see that this approximation yields the same models as before, since the interaction potential term is replaced by the approximation

$$\Phi(r) \approx \frac{1}{N} \int \Phi(r) d\mathbf{r} =: -\frac{\alpha}{N} \leq 0. \quad (17.36)$$

Thus the symmetrized Hamiltonian eq. 17.35 can then be used to write the partition function as (with help of identity eq. 17.27 with $a = 1$)

$$Z(T, N) = \sum_{\{s_i\}} e^{-\beta \mathcal{H}_{\text{mf}}} \quad (17.37)$$

$$= \exp \left[-\frac{\beta \alpha}{2} \right] \sum_{\{s_i\}} \exp \left[\frac{\beta \alpha}{2N} \left(\sum_{i=1}^N s_i \right)^2 - \beta H \sum_{i=1}^N s_i \right] \quad (17.38)$$

$$= \exp \left[-\frac{\beta \alpha}{2} \right] \sum_{\{s_i\}} (2\pi)^{-1/2} \times \quad (17.39)$$

$$\times \int_{-\infty}^{\infty} d\phi \exp \left[-\frac{1}{2} \phi^2 + \left(\phi \sqrt{\frac{\beta \alpha}{N}} + \beta H \right) \sum_{i=1}^N s_i \right] \quad (17.40)$$

$$= e^{-\frac{\beta \alpha}{2}} 2^N \left(\frac{\beta \alpha N}{2\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx \left(e^{-\frac{\beta \alpha x^2}{2}} \cosh(\beta \alpha x + \beta H) \right)^N \quad (17.41)$$

$$\approx e^{-\frac{\beta \alpha}{2}} 2^N \left(\frac{\beta \alpha N}{2\pi} \right)^{1/2} C_N \exp \left[N \max_{-\infty < m < \infty} f(m) \right] \quad (17.42)$$

which involves a Gaussian transformation that allows to completely decouple all spins and enables to carry out the sum over configurations and then a change of variables in order to use Laplace's method as $N \rightarrow \infty$ were (f could be any function that fulfills the needs to apply Laplace's method, but here it is the free energy per particle $f = F/N$)

$$f(m) = -\frac{\beta \alpha m^2}{2} + \log \cosh(\beta \alpha m + \beta H). \quad (17.43)$$

Thus we can write the free energy as

$$\frac{F}{N} = -k_B T \lim_{N \rightarrow \infty} N^{-1} \log Z(N, T) = -\frac{1}{\beta} \log 2 - \frac{1}{\beta} \max_{-\infty < m < \infty} f(m) \quad (17.44)$$

which yields (after some substitutions) the same self-consistence relation and gives the *same thermodynamics* with phase transition and critical-point exponents *as the Ising model*, sec. 17.2.1 with $\alpha = J(2d)$.

A lot more interesting here is to *consider the original problem* eq. 17.32 and try to handle this. In fact, after doing the mean-field approximation, the interaction strength α/N depends on the system size, which is unphysical and is infinite range. A way to rigorously reproduce some of the predictions of the mean field approximation is by re-scaling the original interaction potential v as follows ("Kac type" potential)

$$\Phi(r) = \gamma^d v(\gamma r) \quad (17.45)$$

(with $\gamma > 0$ is a constant and v is the original interaction potential). This means in the case of a "Kac type" (Kac et al. back in 1963 with $v(x) = \exp(-|x|)$) look at them first) interaction $\Phi(r)$ the mean field theory and its solution becomes exact, since

$$\frac{\alpha}{N} = - \int \Phi(r) d\mathbf{r} = -\gamma^d \int_0^\infty r^{d-1} dr v(\gamma r) \underbrace{\int d\sigma_d}_{=C_d} = -C_d \int_0^\infty x^{d-1} v(x) dx \quad (17.46)$$

(with C_d the d-dim. solid angle) is independent of γ (γ^{-1} correspond to the range of the potential, while γ measures its strength), as well as *Lebowitz and Penrose* were able to obtain upper (convex envelope, minimal convex function not less than the given) and lower bounds for $Z(V, N, T)$ and hence for the free energy $F(V, N, T)/N$ by first taking the thermodynamic limit $N \rightarrow \infty$ and second the limit $\gamma \rightarrow 0$ (infinitely weak long-range attraction)

$$F = \text{CE}[F_{\text{MF}}] \quad (17.47)$$

(CE: convex envelope) which is the free energy together with the *Maxwell (or double tangent) construction*, see also e.g. fig. 17.6 (b) (a full version of Lebowitz and Penrose' proof for 1 dimension can be found in [4] app. C and there are more recent results on Kac type potentials and interactions described by them)

For e.g. "Kac type" potentials (eq. 17.45), the zero-field free energy

$$-\frac{F(H=0)}{k_B T} = \begin{cases} \log 2 & \text{when } T \geq T_C \\ \log 2 - \frac{\beta \alpha m_0^2}{2} + \log \cosh(\beta \alpha m_0) & \text{when } T < T_C \end{cases} \quad (17.48)$$

is exact.

The example potential given allows e.g. to interpret the sum over the potential as a Riemann sum and thus as integral. Also eq. 17.45 is much too restrictive and can be relaxed to potential of type $\Phi(r) = \gamma \alpha / r^{d+\gamma}$ accordingly. Last but not least [5] was able to extend this result to quantum-mechanical systems.

17.2 Mean-field constructions in spin systems

17.2.3 LATTICE GAS MODEL

The Lattice Gas (or Binary Alloy) model as described e.g. in [3] sec. 30 and [4] sec. 5-2 consists out of lattice of sites that can be occupied by t_i 1 or 0 particles each - in this sense *very much like the Curie-Ising model* described before, see sec. 17.2.1.

The potential is a hard-core interaction (maximal 1 particle per site, with coupling A)

$$\Phi(r_i - r_j) = \begin{cases} \infty & \text{if } i = j \text{ and both occupied (thus excluded from sum)} \\ -A & \text{if } i, j \text{ nearest-neighbors and occupied} \\ 0 & \text{otherwise} \end{cases} \quad (17.49)$$

which can be described short range interaction (with sum $\sum_{\langle i,j \rangle}$) and is therefore much Ising like. Now we take the same mean-field approximation ($\sum_{j \neq i}$)

$$\mathcal{H}^{\text{LG}} = \sum_i \sum_{j \neq i} \Phi(r_i - r_j) t_i t_j = -A \sum_{\langle i,j \rangle} t_i t_j \quad (17.50)$$

$$\approx -\lambda \sum_i t_i \left(\frac{1}{V-1} \sum_{j \neq i} t_j \right) \quad (17.51)$$

$$= -\frac{\lambda}{4(V-1)} \sum_i \sum_{j \neq i} s_i s_j - \frac{1}{2}(\lambda + \mu) \sum_i s_i - \frac{1}{4}(\lambda + 2\mu)V \quad (17.52)$$

$$= \mathcal{H}_{\text{mf}}^{\text{LG}} \quad (17.53)$$

(the last term is in F of order $\log V \approx \log N$, compare to eq. 17.7 and 17.14) with *constraint*

$$\sum_i t_i = N \quad (17.54)$$

the number of cells occupied, V the total number of lattice sites and by using one of the *substitutions* (+ or -)

$$\pm s_i = 1 - 2t_i \quad \Longleftrightarrow \quad t_i = \frac{1}{2}(1 \mp s_i) \quad s_i \in \{-1, +1\}, t_i \in \{0, 1\}. \quad (17.55)$$

it becomes visible (may be not obvious thought) that it is the same Hamiltonian as eq. 17.34 (after some variable substitutions) and thus *equivalent to the Ising model*. To account for the restriction given in eq. 17.54 we shall consider the Grand canonical partition sum (because the number of particles in the system is allowed change, remember $z = e^{\beta\mu}$)

$$Z_G(T, V, z) = \sum_{N=0}^{\infty} z^N Z(T, N, V) = \sum_{N=0}^V z^N Z(T, N, V) = \sum_{\{t_i\}} z^{\sum_i t_i} e^{-\beta\mathcal{H}} \quad (17.56)$$

and can now it can be shown that in fact it is up to substitutions and constants (that do not change thermodynamics) the same as the Canonical partition sum for the Ising model eq. 17.12 by writing the free-energy in terms of those from Ising as

$$-\frac{1}{\beta} \ln Z_G(T, V, z) = \frac{1}{N} F(\beta, J = \frac{1}{4}\lambda, H = \frac{1}{2}(\lambda + \mu)) - \frac{1}{4}\lambda - \frac{1}{2}\mu \quad (17.57)$$

Therefore in the same way as for the Ising model there exist analytic solutions as well as mean-field approximations, everything told for the Ising model does also apply here. Thus we can retrieve the usual gas observables by

$$\Omega = -pV = -\frac{1}{\beta} \ln Z_G, \quad \frac{N}{V} = \rho = \frac{z}{V} \frac{\partial}{\partial z} \ln Z_G, \quad 1 - 2\rho = m = \frac{1}{V} \frac{\partial}{\partial(\beta H)} \ln Z \quad (17.58)$$

with $Z = Z(T, N = V)$ the canonical partition sum of Ising and Ω the grand (canonical) potential, all other quantities in a similar fashion.

Also interesting to notice might be the fact that this model is able to describe binary alloys of two different atoms too, after some further transformations.

Considering mean-field approximations we can use the *same as for the Ising model too* (e.g. *Weiss-Ising, Curie-Weiss before*) or we can follow a new path.

According to [3] the result is very similar to Van-der-Waals' equation for gases and reproduces e.g. the ideal gas law. This underlines the fact that *Van-der-Waals theory is also a mean-field theory*, thus and because of the relation to Ising anyway it seems feasible to compare the results and consider again the fig. 17.5, see fig. 17.6

Please note: there is no simple mapping or relation between lattice gases and quantum lattice gases mentioned later.

17.2.4 ISSUES / PROBLEMS

Now after we have seen what results can be correctly retrieved within mean field theory for the Ising model (all other are essentially the same) we have to consider the issues that arise due to mean field approximation:

- you get a *phase transition* (existence of critical exponents) which is good *but you will always get one* even if no one is there, e.g. Ising model in 1 dimension
- the *critical exponents* retrieved for the phase transition (at T_C) are - in general - *different* from those of the original model; since they are still close, a quantitative analysis of the original model at the critical point can be done by using the renormalization group

17.2 Mean-field constructions in spin systems

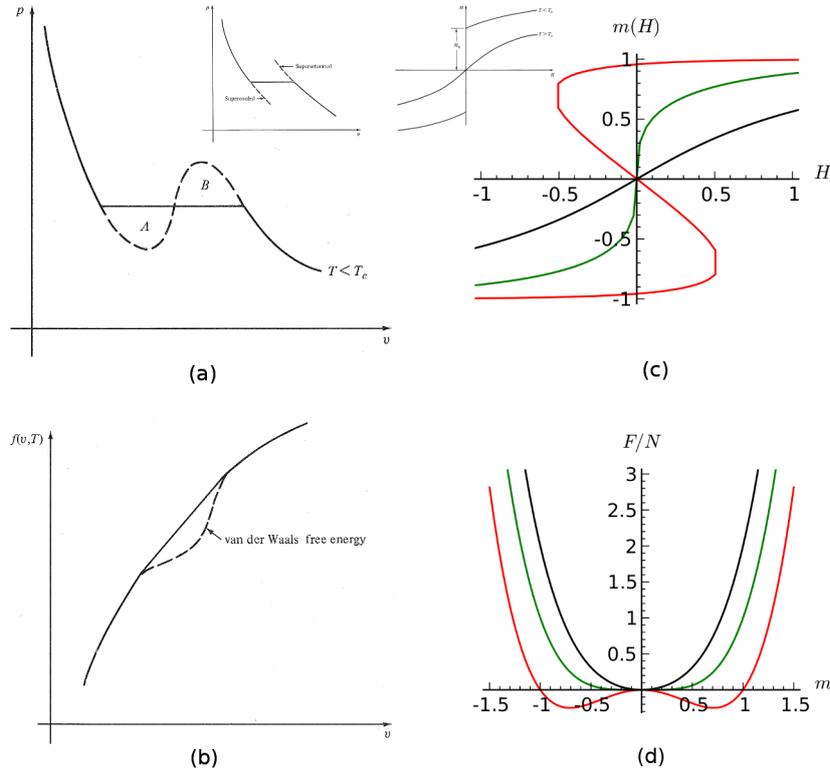


Figure 17.6: The thermodynamic similarities between Van-der-Waals' gas and Ising model by taking $(V, P) \rightarrow (M, -H)$ ($v = V/N = 1/\rho$). (a) Maxwell equal-area construction ($A=B$) to avoid meta-stable states (from [4] fig. 4.6). (b) Double tangent construction or convex envelope (from [4] fig. 4.7) is same as Legendre transformation. (c) Magnetization with hysteresis (like 90 deg. rotated (a)). (d) Landau free energy without (needed) convex envelope.

- the dependence of the critical exponents from system (lattice) dimension is also wrong (they are independent of d)
- the *result is not physical* in the sense of we have to take the convex envelope (in some cases) in order to fix that
- (thermal) fluctuations are not taken into account appropriately (this was the main simplification when switching to the mean field instead of using single spins)

Essentially all those issues are related to the last one, the (thermal) fluctuations not taken into account appropriately or assumed to be very small (in order of $\langle \delta s_i \delta s_j \rangle / \langle \delta s_i \rangle \langle \delta s_j \rangle = \langle \delta s_i \delta s_j \rangle / m^2 \ll 1$) which is not true close to the critical point (phase transition) or for systems of low dimension and thus origin of the so-called

critical phenomena. There are results that show for $d > 4$ the critical exponents at T_C are exact (this must not be true for the thermodynamic properties). Another weakness is the self-consistence relation that has to be solved (transcendental non-linear equation; has to be solved numerically). As mentioned by [2] sec. 7; while the mean field approximation describes second-order phase transitions in a very handy way, we have seen that it treats fluctuations poorly so that the critical behavior is not adequately reproduced.

Since *many interactions are replaced by one*, it naturally follows that if the field or particle exhibits many interactions in the original system, MFT will be *more accurate* for such a system. This is true in cases of *high dimensionality*, or when the Hamiltonian includes *long-range forces*. The Ginzburg criterion is the formal expression of how fluctuations render MFT a poor approximation, depending upon the number of spatial dimensions in the system of interest.

17.3 MEAN-FIELD CONSTRUCTIONS FOR BOSE-EINSTEIN CONDENSATES

In general field theories (which mean-field are a sort of) are retrieved by second quantization (but we use first too) and dealt with in the framework of QFT.

17.3.1 BOSE-EINSTEIN CONDENSATION

To briefly introduce or remind what BEC is we will closely follow the path of [6] sec. 1.1, [2] sec. 3 and 4 as well as [7] sec. 8 and 12 (and [3] sec. 23 should be mentioned for completeness too). The *ideal classical gas* of particles consists of the following ingredients: a collection of $N \gg 1$ non-interacting particles in a large box $\Lambda \subset \mathbb{R}^3$ and volume $V = L^3$. Since we are interested in the thermodynamic limit, we will take the *limits*

$$N \rightarrow \infty \quad \text{and} \quad L \rightarrow \infty \quad \text{such that} \quad \rho = N/V = \text{const.} \quad (17.59)$$

in a way that the density ρ stays constant.

Since we have non-interacting particles, the Hamiltonian consists of kinetic energy only

$$\mathcal{H} = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} \quad (17.60)$$

with particle mass m and momentum \vec{p}_i . The ground state energy is 0 and the

17.3 Mean-field constructions for Bose-Einstein condensates

thermodynamics are given by the partition function

$$Z_N = \frac{1}{h^{3N} N!} \underbrace{\int_{\Lambda^N} \prod_{i=1}^N d\vec{x}_i}_{=V^N} \underbrace{\int_{\mathbb{R}^{3N}} \prod_{i=1}^N d\vec{p}_i e^{-\beta\mathcal{H}}}_{=(\int_{\mathbb{R}^3} d\vec{p} e^{-\beta\mathcal{H}})^N} = \frac{1}{h^{3N} N!} V^N \left(\frac{2\pi m}{\beta} \right)^{3N/2} = \frac{1}{N!} Z_1^N \quad (17.61)$$

from this we immediately go on to the next step, calculating all important thermodynamic quantities among them the free energy, pressure and internal energy

$$F = -\frac{1}{\beta} \ln Z_N, \quad p = -\frac{\partial F}{\partial V} \approx \rho k_B T, \quad U = -\frac{\partial}{\partial \beta} \ln Z_N = \frac{3}{2} N k_B T \quad (17.62)$$

by using Stirling's $\ln N! = N \ln N - N + \mathcal{O}(\log N)$ approximation ($\log N$ dropped, see also eq. 17.52 resp. 17.7 and 17.14).

In quantum mechanics, the Hamiltonian is an operator obtained by *first quantization*, replacing each \vec{p}_j by $-i\hbar\vec{\nabla}_j$, acting on the Hilbert space $L^2(\Lambda)$, with appropriate boundary conditions. The eigenvalues of $\vec{p}^2 = -\hbar^2\Delta$ (with $\Delta = \text{Laplacian} = \vec{\nabla}^2$), for a box with periodic boundary conditions, are $(2\pi\hbar)^2 \vec{n}^2 / L^2$, where \vec{n} is a vector with integer components $n_{\vec{p}}$. If the statistics of the particles is disregarded, the partition function, which in the quantum case is given by ($z = e^{\beta\mu}$)

$$Z_G = \text{tr} e^{-\beta(\mathcal{H}-\mu N)} = \sum_{N \geq 0} z^N Z_N \quad (17.63)$$

the last expression is the same as for the classical (non QM) case thus we write the most general expression (taking the statistics into account again)

$$g_{\{n_{\vec{p}}\}} = \begin{cases} 1 & \text{indistinguishable particles (Fermions and Bosons)} \\ \prod_{\vec{p}} \frac{1}{n_{\vec{p}}!} & \text{classical particles (Boltzmann)} \end{cases} \quad (17.64)$$

and

$$E = \sum_{\vec{p}} \epsilon_{\vec{p}} n_{\vec{p}}, \quad N = \sum_{\vec{p}} n_{\vec{p}} \quad (17.65)$$

thus eq. 17.63 yields finally

$$Z_G = \sum_{\{n_{\vec{p}}\}} g_{\{n_{\vec{p}}\}} z^{\{n_{\vec{p}}\}} Z_{\{n_{\vec{p}}\}} = \sum_{\{n_{\vec{p}}\}} g_{\{n_{\vec{p}}\}} e^{-\beta(E-\mu N)_{\{n_{\vec{p}}\}}} \quad (17.66)$$

$$= \sum_{n_{\vec{p}_1}, n_{\vec{p}_2}, \dots} \left[\left(g_{n_{\vec{p}_1}} z e^{-\beta \epsilon_{\vec{p}_1}} \right)^{n_{\vec{p}_1}} \left(g_{n_{\vec{p}_2}} z e^{-\beta \epsilon_{\vec{p}_2}} \right)^{n_{\vec{p}_2}} \dots \right] \quad (17.67)$$

$$= \begin{cases} \sum_{N=0}^{\infty} z^N \frac{1}{N!} \left(\sum_{\vec{p}} e^{-\beta \epsilon_{\vec{p}}} \right)^N & = \sum_{N=0}^{\infty} z^N Z_N^{\text{class}} & \text{classical} \\ \prod_{\vec{p}} \sum_{n_{\vec{p}}=0,1} (z e^{-\beta \epsilon_{\vec{p}}})^{n_{\vec{p}}} & = \prod_{\vec{p}} (1 + z e^{-\beta \epsilon_{\vec{p}}}) & \text{Fermions} \\ \prod_{\vec{p}} \sum_{n_{\vec{p}}=0,1,2,\dots} (z e^{-\beta \epsilon_{\vec{p}}})^{n_{\vec{p}}} & = \prod_{\vec{p}} \frac{1}{1 - z e^{-\beta \epsilon_{\vec{p}}}} & \text{Bosons} \end{cases} \quad (17.68)$$

since we are looking at BEC we are interested in the bosonic case only. Thus we have further (similar to eq. 17.58)

$$\Omega = -pV = -\frac{1}{\beta} \ln Z_G, \quad N = z \frac{\partial}{\partial z} \ln Z_G = \sum_{\vec{p}} \frac{1}{e^{\beta \epsilon_{\vec{p}}} z^{-1} - 1} \quad (17.69)$$

and thus retrieved the familiar Bose-Einstein statistics as needed. Now by taking the *thermodynamic limit* $N \rightarrow \infty$ we replace the sums over \vec{p} by an integral $L^{-3} \sum_{\vec{p}} \rightarrow h^{-3} \int d^3p$ and we get (for $s = 0$)

$$\frac{p}{k_B T} = -\frac{4\pi}{h^3} \int_0^{\infty} dp p^2 \ln(1 - z e^{-\beta \epsilon_{\vec{p}}}) = \frac{1}{\lambda^3} \sum_{l=1}^{\infty} \frac{z^l}{l^{5/2}} = \frac{1}{\lambda^3} g_{5/2}(z) \quad (17.70)$$

$$\rho = \frac{N}{V} = \frac{4\pi}{h^3} \int_0^{\infty} dp p^2 \frac{1}{e^{\beta \epsilon_{\vec{p}}} z^{-1} - 1} = \frac{1}{\lambda^3} \sum_{l=1}^{\infty} \frac{z^l}{l^{3/2}} = \frac{1}{\lambda^3} g_{3/2}(z) \quad (17.71)$$

with⁶ $\lambda = h/\sqrt{2\pi m k_B T}$ (the thermal de Broglie wavelength) and

$$g_u(1) = \zeta(u) \quad \implies \quad g_{5/2}(1) = \zeta(5/2) \approx 1.342, \quad g_{3/2}(1) = \zeta(3/2) \approx 2.612 \quad (17.77)$$

look also at plot fig. 17.7. This is a monotonously increasing function of μ , which is bounded as the chemical potential $\mu \rightarrow 0$ ($z \rightarrow 1$) by the critical density

$$\rho_C = \lambda^{-3} g_{3/2}(1) \quad (17.78)$$

⁶by using the Taylor series

$$-\log(1-x) = \sum_{k=1}^{\infty} \frac{x^k}{k} \quad \implies \quad \frac{\partial}{\partial x} [-\log(1-x)] = \frac{1}{1-x} = \sum_{k=0}^{\infty} x^k \quad (17.72)$$

17.3 Mean-field constructions for Bose-Einstein condensates

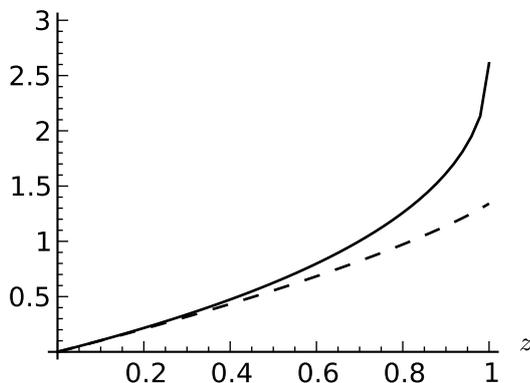


Figure 17.7: The g-functions $g_{3/2}(z)$ (straight line) and $g_{5/2}(z)$ (please note that $g'_{3/2}(z \rightarrow 1) \rightarrow \infty$).

and thus the *density seems to be upper bounded* by a (constant!) value (for all z). Consider that the chemical potential μ is a measure on how much energy it costs to add or remove a particle to/from the system. This (absurd) phenomenon - as the density should become free and not fixed in this limit, since there is no physical reason to expect the density of a Bose gas to be bounded from above - was discovered by Einstein, and the *resolution* is that the particles exceeding the critical number all go into the lowest energy state. In mathematical terms, this means that we have to let $\mu \rightarrow 0$ simultaneously with $L \rightarrow \infty$ to fix the density at some number $> \rho_C$. In this case, we have to be more careful in replacing the sum in eq. 17.71 by an integral (coming from eq. 17.68 and 17.69). It turns out to be

you can see that

$$-\int_0^\infty \log(1 - ze^{-\beta\epsilon_{\vec{p}}})p^2 dp = \sum_{k=1}^\infty \frac{z^k}{k} \int_0^\infty e^{-\beta\epsilon_{\vec{p}}k} p^2 dp \quad (17.73)$$

$$= \sum_{k=1}^\infty \frac{z^k}{k} \left(-\frac{2m}{k}\right) \frac{\partial}{\partial \beta} \underbrace{\int_0^\infty e^{-\beta p^2 k/2m} dp}_{=(1/2)\sqrt{2m\pi/\beta k}} \quad (17.74)$$

$$= \frac{1}{4\pi} \underbrace{\left(\frac{2\pi m}{\beta}\right)^{3/2}}_{=(h/\lambda)^3} \sum_{k=1}^\infty \frac{z^k}{k^{5/2}} \quad (17.75)$$

and analogue with the Taylor series of

$$\frac{1}{x^{-1} - 1} = \sum_{k=1}^\infty x^k = x \frac{\partial}{\partial x} [-\log(1 - x)] \quad (17.76)$$

sufficient to separate the contribution from the lowest energy level (single particle ground state $\vec{p} = 0$), and approximate the contribution from the remaining terms by an integral. The result is that, for $\rho > \rho_C$ we replace eq. 17.71 by

$$\rho = \frac{N}{V} = \underbrace{\lambda^{-3} g_{3/2}(1)}_{=\rho_C} + \rho_0 \quad (17.79)$$

notice that the critical temperature T_C (for fixed ρ) is defined as

$$\text{at } T_C : \rho = \rho_C \Rightarrow 1 = \frac{\rho}{\rho_C} = \frac{\lambda^{-3} g_{3/2}(z)}{\lambda_C^{-3} g_{3/2}(1)} \Rightarrow \frac{g_{3/2}(z)}{g_{3/2}(1)} = \left(\frac{\lambda}{\lambda_C}\right)^3 = \left(\frac{T_C}{T}\right)^{3/2} \quad (17.80)$$

(with $\lambda_C = h/\sqrt{2\pi m k_B T_C}$) which helps us to write for any T

$$\rho_0(\beta) = \frac{N}{V} - \rho_C = \frac{N}{V} \left(1 - \frac{\rho_C}{\rho}\right) = \frac{N}{V} \left(1 - \frac{\lambda^{-3} g_{3/2}(1)}{\lambda^{-3} g_{3/2}(z)}\right) = \frac{N}{V} \left(1 - \left(\frac{T}{T_C}\right)^{3/2}\right) \quad (17.81)$$

(look at fig. 17.8 also) this is the same as

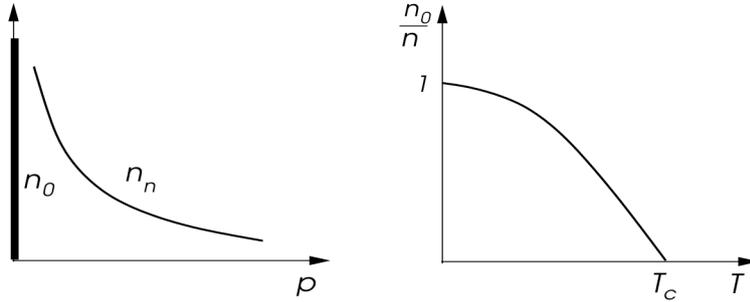


Figure 17.8: (left) shows the distribution of the momenta over the density ($\rho = n$, $\rho_C = n_n$ here). (right) shows the dependence of the $p = 0$ momentum distribution $n_0/n = \rho_0/\rho$ introduced in eq. 17.79 in order to fix the density below the critical temperature. Both figures from [2] p. 80.

$$\rho_0(\beta) = \lim_{L \rightarrow \infty} \frac{1}{V} \frac{1}{e^{\beta(\epsilon_0 - \mu)} - 1} \quad (17.82)$$

and ρ_0 is the density of the "condensate" (the dependence of μ on L is determined by using eq. 17.69 to write $N = L^3 \rho$ with fixed ρ).

The phenomenon that a single particle level has a macroscopic occupation, i.e., a non-zero density in the thermodynamic limit, is called Bose-Einstein condensation

17.3 Mean-field constructions for Bose-Einstein condensates

(BEC). Note that in the model considered there is no condensation into the excited energy levels, and one always has

$$\lim_{L \rightarrow \infty} \frac{1}{V} \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1} = 0 \quad (17.83)$$

for $i \geq 1$, since $\epsilon_i - \mu \geq \epsilon_i - \epsilon_0 = \text{const.} \times L^{-2}$. Note that in the case of zero temperature, i.e., the ground state, all the particles are in the condensate, i.e., $\rho = \rho_0$. In a sector of fixed particle number, the ground state wave function is simply a product of single particle wave-functions in the lowest energy state.

17.3.2 BOSE-EINSTEIN CONDENSATION FOR INTERACTING SYSTEMS

Such systems are described, according to [10] sec. 2 and 3, by a one-particle *density matrix* $\gamma \in L^2(\mathbb{R}^3)$ (acting on Fock space). Note that γ is a positive trace class operator on the one-particle Hilbert space \mathcal{H}_1 , with φ_i a complete basis set, a_i^\dagger, a_i operator valued distributions (creator/annihilator), we have

$$\text{tr } \gamma = \sum_i \langle \varphi_i | \gamma | \varphi_i \rangle = \langle \sum_i a_i^\dagger a_i \rangle = \langle N \rangle \quad (17.84)$$

and γ has the integral kernel⁷ like (specifically, if ψ_0 is the ground state of \mathcal{H}_N the N -particle Hamiltonian)

$$\gamma(x, y) = N \int \psi_0(x, x_2, \dots, x_N) \psi_0(y, x_2, \dots, x_N) dx_2 \cdots dx_N \quad (17.86)$$

According to a criterion by Penrose and Onsager, *BEC is said to occur if γ has an eigenvalue of the order of $\langle N \rangle$* . The corresponding eigenfunction is called the condensate wave function and has to be the constant function $L^{-3/2}$. Since this definition involves large particle numbers $\langle N \rangle$, it refers, strictly speaking, not to a single state but rather a sequence of states for larger and larger system size (and they are not product of single particle states). When one speaks about the occurrence of BEC one hence always has to specify how various parameters depend on this size. The system should be translation invariant and strictly positive which holds for the integral kernel $\gamma(x, y) = \gamma(x - y)$ also, thus following [6] sec. 1.2

$$\frac{1}{V} \int dx dy \gamma(x, y) = \mathcal{O}(N) \propto cN \quad (17.87)$$

⁷with trace

$$\text{tr } \gamma = \int dx \gamma(x, x) \quad (17.85)$$

(with a constant c) has to be true, as stated before. The largest eigenvalue is always associated to the constant eigenfunction, and BEC can only occur in the zero momentum mode. *BEC is extremely hard to establish rigorously.* In fact, the *only known case of an interacting, translation invariant Bose gas* where BEC has been proved in the standard thermodynamic limit is the hard-core *lattice gas* according to [6] sec. 1.2 and 11 BEC in the special case at *half-filling* (i.e., $N =$ half the number of lattice sites). The proof of this relies crucially on a special property of the system known as reflection positivity. Dyson, Lieb, Simon (1978) extend earlier results by [8] on classical spin systems, where this property was first used to prove the existence of phase transitions. Reflection positivity holds only in the case of *particle-hole symmetry*, i.e., $\mu = 0$, and hence the proof is restricted to this particular case.

Besides the hard-core lattice gas, there is also a model (not in mean-field) describing Bosons in optical traps which allowed to retrieve one of the most remarkable recent developments in the study of ultracold Bose gases. BEC has been established in the limit in which the scattering length a is replaced by a/N ($N =$ number of bosons) and $N \rightarrow \infty$, confer [10] sec. 4 this is a *Quantum Phase Transition in an Optical Lattice Model* ([6] sec. 1.2 and 11) in dependence of the periodic trap potential strength λ . This is a reversible transition from a Bose-Einstein condensate to a state composed of localized atoms as the strength of a periodic, optical trapping potential is varied. Lieb et al. rigorously analyzed a model of this phenomenon. The gas is a hard core lattice gas. For small λ and temperature BEC is proved to occur, while at large λ BEC disappears, even in the ground state, which is a Mott insulator state with a characteristic gap. The inter-particle interaction is essential for this effect.

Furthermore [6] shows in app. D, that under quite general assumptions, BEC goes hand in hand with spontaneous gauge symmetry breaking. *Breaking of a continuous symmetry is notoriously difficult to prove*, and in one and two dimensions it is excluded, at least at positive temperature, by the Hohenberg-Mermin-Wagner Theorem. This partly explains why a rigorous proof of BEC for inter-acting systems is still lacking in general. Gauge symmetry breaking corresponds for the magnet to spontaneous magnetization.

This concept of BEC as a large eigenvalue of the one-particle reduced density matrix immediately generalizes to thermal states, both in the canonical and grand-canonical ensembles (or, more generally, to states defined by arbitrary density matrices).

17.3.3 BOGOLIUBOV APPROXIMATION

To treat at BEC in the framework of mean-field theory in quantum mechanics we have in general to use the well developed language of QFT. However the Bogoliubov transformation represents a somehow (simpler) straight forward approach not needing the (whole) QFT machinery (with exception of some details needed in order to e.g. compare to experiments) and still yielding the same results for *the Dilute Bose Gas in 3D*. Bogoliubov is non a non perturbative (in coupling constants) approach for a hard interacting Bose systems⁸.

Consider a dilute Bose gas in 3 dimensions (continuous space in a box L^3), according to [9] sec. 18, 35, [10] sec. 3, [6] sec. 2 and others we first write the non-interacting ground state of N bosons as

$$|\phi_0(N)\rangle = |N, 0, 0, \dots\rangle \quad (17.88)$$

and notice that none of the two ladder or creation/annihilation operators annihilates the ground state (zero momentum)

$$a_0|\phi_0(N)\rangle = N^{1/2}|\phi_0(N-1)\rangle, \quad a_0^\dagger|\phi_0(N)\rangle = (N+1)^{1/2}|\phi_0(N+1)\rangle \quad (17.89)$$

and the usual separation into creation and annihilation operators fails completely. Thus, considering the special role of the zero-momentum state and note, when we *re-scale* them by $V^{-1/2}$ as

$$\xi_0 = V^{-1/2}a_0, \quad \xi_0^\dagger = V^{-1/2}a_0^\dagger \quad \Rightarrow \quad [\xi_0, \xi_0^\dagger] = V^{-1}, \quad \langle\psi_0|\xi_0^\dagger\xi_0|\psi_0\rangle = \frac{N_0}{V} = \rho_0 \quad (17.90)$$

with interacting ground-state ψ_0 wave function and

$$\xi_0|\phi_0(N)\rangle = \left(\frac{N}{V}\right)^{1/2}|\phi_0(N-1)\rangle, \quad \xi_0^\dagger|\phi_0(N)\rangle = \left(\frac{N+1}{V}\right)^{1/2}|\phi_0(N+1)\rangle \quad (17.91)$$

in the thermodynamic limit according to eq. 17.59 the commutator vanishes and thus it seems to be natural to replace the operators a_0 and a_0^\dagger by complex numbers (this is also related to coherent states, as mentioned by [10] sec. 4.5)

$$a_0, a_0^\dagger \rightarrow N_0^{1/2} \in \mathbb{C} \quad (17.92)$$

⁸this can be very handy in cases as mentioned at the beginning of [9] sec. 6 in a discussion why perturbing Bose Einstein condensate is hard to describe, e.g. it may not even be possible to do an expansion, since the ground state does not have a perturbative expansion

The model Hamiltonian we want to consider is a dilute Bose gas with simple multi-particle interaction like⁹

$$\hat{\mathcal{H}} = \sum_{\vec{k}} \vec{k}^2 a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{1}{2V} \sum_{\vec{k}, \vec{k}_3, \vec{k}_4} \mathcal{F}[v](\vec{k}) a_{\vec{k}_4 + \vec{k}}^\dagger a_{\vec{k}_3 - \vec{k}}^\dagger a_{\vec{k}_3} a_{\vec{k}_4} \quad (17.94)$$

$$= \sum_{\vec{k}} \hbar\omega_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{g}{2V} \underbrace{\sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} a_{\vec{k}_1}^\dagger a_{\vec{k}_2}^\dagger a_{\vec{k}_3} a_{\vec{k}_4} \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4}}_{=\hat{\mathcal{H}}_{\text{int}}} \quad (17.95)$$

with pseudo-potential g replacing Fourier transform of the actual one $\mathcal{F}[v](\vec{k})$. Only keeping terms of order N_0 and N_0^2 (because 1st order are of $N_0^{1/2}$ and 3rd order are neglected) and then using eq. 17.92 we get

$$\hat{\mathcal{H}}_{\text{int}} \approx a_0^\dagger a_0^\dagger a_0 a_0 + \quad (17.96)$$

$$+ \sum_{\vec{k} \neq 0} \left[2(a_{\vec{k}}^\dagger a_{\vec{k}} a_0^\dagger a_0 + a_{-\vec{k}}^\dagger a_{-\vec{k}} a_0^\dagger a_0) + a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger a_0 a_0 + a_0^\dagger a_0^\dagger a_{\vec{k}} a_{-\vec{k}} \right] \quad (17.97)$$

$$= N_0^2 + 2N_0 \sum_{\vec{k} \neq 0} (a_{\vec{k}}^\dagger a_{\vec{k}} + a_{-\vec{k}}^\dagger a_{-\vec{k}}) + N_0 \sum_{\vec{k} \neq 0} (a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger + a_{\vec{k}} a_{-\vec{k}}) \quad (17.98)$$

now all interactions of particles outside the condensate $\vec{k} \neq 0$ are neglected, which is valid as long as $N - N_0 \ll N$. The neglected terms do contributed in 3rd order perturbation theory only since at least 3 collisions (Feynman diagram vertices) are needed to excite a particle from condensate above it have a collision/interaction there and go back to condensate. The number operator becomes

$$\hat{\mathcal{N}} = N_0 + \frac{1}{2} \sum_{\vec{k} \neq 0} (a_{\vec{k}}^\dagger a_{\vec{k}} + a_{-\vec{k}}^\dagger a_{-\vec{k}}), \quad N = \langle \hat{\mathcal{N}} \rangle \quad (17.99)$$

and using it the Hamiltonian reads

$$\hat{\mathcal{H}} = \frac{1}{2} V g \rho^2 + \frac{1}{2} \sum_{\vec{k} \neq 0} \left[(\epsilon_{\vec{k}}^0 + \rho g) (a_{\vec{k}}^\dagger a_{\vec{k}} + a_{-\vec{k}}^\dagger a_{-\vec{k}}) + \rho g (a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger + a_{\vec{k}} a_{-\vec{k}}) \right] \quad (17.100)$$

with $n = N/V$ the particle density.

⁹the choice of this Hamiltonian might be better motivated when considering the equivalent but written in first quantization as

$$\hat{\mathcal{H}} \hat{=} \sum_{i=1}^N \Delta_i + \sum_{1 \leq i < j \leq N} v(|x_i - x_j|) \quad (17.93)$$

17.3 Mean-field constructions for Bose-Einstein condensates

The *diagonalization* of $\hat{\mathcal{H}}$ is simplest to be carried out by defining a new set of creation and destruction operators α_k and α_k^\dagger according

$$a_{\vec{k}} = u_k \alpha_{\vec{k}} - v_k \alpha_{-\vec{k}}^\dagger, \quad a_{\vec{k}}^\dagger = u_k \alpha_{\vec{k}}^\dagger - v_k \alpha_{-\vec{k}} \quad (17.101)$$

$$[\alpha_{\vec{k}}, \alpha_{\vec{k}'}^\dagger] = \delta_{\vec{k}\vec{k}'}, \quad [\alpha_{\vec{k}}, \alpha_{\vec{k}'}] = [\alpha_{\vec{k}}^\dagger, \alpha_{\vec{k}'}^\dagger] = 0 \quad (17.102)$$

called the *Bogoliubov transformation* (also used by Holstein and Primakoff). The commutation relations impose the restriction

$$u_{\vec{k}}^2 - v_{\vec{k}}^2 = 1, \quad \forall \vec{k} \implies u_{\vec{k}} = \cosh \varphi_k, \quad v_{\vec{k}} = \sinh \varphi_k \quad (17.103)$$

from which we then may find

$$\hat{\mathcal{H}} = \frac{1}{2} V g \rho^2 + \frac{1}{2} \sum_{\vec{k} \neq 0} [(\epsilon_k^0 + \rho g) v_{\vec{k}}^2 - \rho g u_{\vec{k}} v_{\vec{k}}] + \quad (17.104)$$

$$+ \frac{1}{2} \sum_{\vec{k} \neq 0} [(\epsilon_k^0 + \rho g) (u_{\vec{k}}^2 + v_{\vec{k}}^2) - 2 \rho g u_{\vec{k}} v_{\vec{k}}] \left(a_{\vec{k}}^\dagger a_{\vec{k}} + a_{-\vec{k}}^\dagger a_{-\vec{k}} \right) \quad (17.105)$$

$$+ \frac{1}{2} \sum_{\vec{k} \neq 0} [\rho g (u_{\vec{k}}^2 + v_{\vec{k}}^2) - 2 (\epsilon_k^0 + \rho g) u_{\vec{k}} v_{\vec{k}}] \left(a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger + a_{\vec{k}} a_{-\vec{k}} \right) \quad (17.106)$$

since the parameters u_k, v_k are not fixed yet we chose to eliminate the last line eq. 17.106 of the Hamiltonian which becomes explicitly diagonal in the quasi-particle number operators $\alpha_{\vec{k}}^\dagger \alpha_{\vec{k}}$ then. That allows us to determine all of its eigenvectors and -values (*diagonalize*) and the transformation parameters become

$$\rho g (u_{\vec{k}}^2 + v_{\vec{k}}^2) = 2 (\epsilon_k^0 + \rho g) u_{\vec{k}} v_{\vec{k}} \implies \tanh 2\varphi_k = \frac{\rho g}{\epsilon_k^0 + \rho g} \quad (17.107)$$

The *ground state energy* is then given by $\alpha_{\vec{k}} |\psi_0\rangle = 0 \quad \forall \vec{k} \neq 0$

$$E_k = ((\epsilon_k^0 + \rho g)^2 - (\rho g)^2)^{1/2}, \quad E = \langle \psi_0 | \hat{\mathcal{H}} | \psi_0 \rangle = \frac{1}{2} V \rho^2 g + \frac{1}{2} \sum_{\vec{k} \neq 0} (E_k - \epsilon_k^0 - \rho g) \quad (17.108)$$

note that $|\psi_0\rangle$ is a complicated combination of unperturbed eigenstates since neither a_k nor a_k^\dagger annihilates it. Since all excited states correspond to various numbers of non-interacting Bosons each with an excitation energy E_k the spectrum has the form (same as for a dilute hard-core Bose gas)

$$E_k \approx \begin{cases} \left(\frac{\rho g}{m}\right)^{1/2} \hbar k = \underbrace{\left(\frac{4\pi a \rho \hbar^2}{m^2}\right)^{1/2}}_{=c} \hbar k & k \rightarrow 0 \\ \epsilon_k^0 + \frac{4\pi a \rho \hbar^2}{m} & k \rightarrow \infty \end{cases} \quad (17.109)$$

at long wavelengths, the interacting spectrum is characteristic of a sound wave with velocity given by c for repulsive interaction ($g > 0, a > 0$). Furthermore we even get

$$\frac{E}{N} = \underbrace{\frac{2\pi a \hbar^2 \rho}{m}}_{\text{1. term}} \left[1 + \frac{128}{15} \left(\frac{\rho a^3}{\pi} \right)^{1/2} + 8 \left(\frac{4\pi}{3} - \sqrt{3} \right) (\rho a^3) \log(\rho a^3) + \mathcal{O}(\rho a^3) \right] \quad (17.110)$$

in a *non-perturbative* way fully agreeing with [9] sec. 35 and [6] sec. 2 in the first term. Notice that it matches the naive guess of (# of pairs) \times (energy per pair) of two-body scattering. This result can also be achieved by other means too, e.g. QFT [9] sec. 22 and is thus *first term (order) is well confirmed* (also with models that do not have to assume condensation). The reason for avoiding QFT is not having to find alternatives to Wicks theorem which need annihilation operators to kill the ground-state which is not the case for bosonic system like here. Recently (1998) Lieb and Yngvason were able (according to [10] sec. 2) to derive an lower bound (for the 1st order, no full solution) which is in agreement with eq. 17.110. Using a variational approach Dyson proved the upper bound already (1957) but his the lower bound was 14 times to small. The upper bound can be retrieved by Ritz method (it is a question of good set of functions and a lengthy calculation), whereas the lower bound is a hard problem. The typical wave functions of a particle is necessarily spread out over a region much bigger than the mean particle distance. The particles hence completely lose their individuality, and behave very quantum (i.e., non-classical) in this sense and contrast to e.g. Fermions. There are rigorous results for Two-Dimensional Bose Gas and Bose Gas at Positive Temperatures.

A rigorous derivation of the lowest order contribution to the ground state energy for dilute bosonic gas in 3d (which hints the presence of condensation) can be found in [6] sec. 2 and app. D. This theorem (due to Dyson-Lieb-Yngvason-Seiringer) establishes on a mathematical basis the prediction of the Bogoliubov theory (which is mean-field theory for interacting bosons) in the lowest order.

The ground state distribution function is given by

$$n_k = \langle \psi_0 | \alpha_k^\dagger \alpha_k | \psi_0 \rangle = v_k^2 \langle \psi_0 | \alpha_k \alpha_k^\dagger | \psi_0 \rangle = v_k^2 \approx \begin{cases} k^{-1} & k \rightarrow 0 \\ k^{-4} & k \rightarrow \infty \end{cases} \quad (17.111)$$

At some point during calculation, after clever canceling of all divergences occur-

17.3 Mean-field constructions for Bose-Einstein condensates

ring, we replaced the pseudo-potential g by the scattering length a

$$g = \frac{4\pi\hbar^2 a}{m} \quad (17.112)$$

$$a = \frac{1}{8\pi} \inf_{\phi} \left\{ \overbrace{\int_{\mathbb{R}^3} d^3x (2|\nabla\phi(x)|^2 + v(|x|)|\phi(x)|^2)}^{=L \text{ (Lagrangian)}} : \lim_{|x| \rightarrow \infty} \phi(x) = 1 \right\} \quad (17.113)$$

$=\mathcal{L}$ (Lagrange density)

(L : Lagrangian) this is convenient according to [9] in first order and needed to be able to relate the results to experimental data. Consider sec. 17.5.2 for more info.

Now lets summarize the important assumptions we did here which are in fact at the same time the biggest drawbacks of Bogoliubov also, thus confer sec. 17.3.4. Applications include e.g. *The Charged Bose Gas - Two-Component Case* [6] sec. 10.2, 10.3 may be sec. 5 also.

We have discussed the bosonic mode of Bogoliubov theory, but there is also a description for fermionic modes with the most prominent application by Bogoliubov himself for the BCS theory of superconductivity. The fermionic mode includes the usual trigonometric functions instead of the hyperpolic ones (among other changes as well, confer e.g. [1])

17.3.4 ISSUES / PROBLEMS

Again after we have shown what results are possible to calculate through the methods mentioned, we should now consider their drawbacks.

In general:

- Except for lattice gas with half filling and the optical lattice model; *BEC for interacting particles is a problem!* (in general interacting bosonic QM systems are hard to solve)

Regarding Bogoliubov the biggest drawbacks are also the important assumptions done

- *a-priori condensation* (BEC) has to be assumed, i.e. almost all particles are in the same one-particle state (cannot be proven within this theory) and is related to the next 2 points
- *large number* N of particles in condensate; N_0 large i.e. $N_0 \approx N_{\text{Total}}$
- $a_0^\dagger, a_0 \rightarrow N_0^{1/2}$ and $a_0^\dagger a_0 \rightarrow N_0$ (as mentioned)

- *formally Hamiltonian of free theory* (2 terms only; e.g. $\alpha_{\vec{k}}\alpha_{\vec{k}}^\dagger$) and 2 quasi-particle interaction (4th order terms; like e.g. $\alpha_{\vec{k}}\alpha_{\vec{k}}^\dagger\alpha_{\vec{k}}\alpha_{\vec{k}}^\dagger$) are neglected
- *Bogoliubov transformation* or substitution (as mentioned)

17.4 CONCLUSIONS

We have given some ideas on how to do mean-field approximations on spin systems like Ising (and Lattice gas) model, which lead to the same results (in fact all those systems have the same thermodynamics).

For BEC we have laid out the basic theory and shown one of the well known mean-field techniques, the Bogoliubov approximation. Treating BEC within this framework is very complex and only two fully solved models are known (half filled lattice gas and optical trap potential model).

The applicability for spin systems is strongly related with (the range of) the interaction potential and fluctuations regime considered. There exists rigorous results (e.g. Lebowitz-Penrose theorem, renormalization group) and thus sophisticated methods to tackle this nowadays. For BEC systems the question on applicability is somehow out of scope since it is not possible to show condensation yet (for more than 2 outstanding models). If applied e.g. to dilute gas and assuming condensation, the result are surprisingly good; according to [6] sec. 2 Lenz found the first order for the ground state energy of a single particle in the presence of $N - 1$ randomly placed particles, given in eq. 17.110. This calculation, would give the correct energy, provided the fixed particles are uniformly distributed.

Heuristic arguments for condensation include as most prominent example the spontaneous breaking (of gauge symmetry) which works in all cases. The problem for spin systems is, we retrieve always a phase transition (even for models like 1D Ising for which it is known to be absent). For BEC of interacting particles an eigenvalue of the interaction potential kernel (one particle reduced density matrix) in the order of N has to be present.

I would like to thank my Tutor Marcello Porta and Max Hfliger for their support, assistance and patience during this pro-seminar.

17.5 APPENDIX

17.5.1 LAPLACE'S METHOD, STEEPEST DESCENT AND VARADHAN'S THEOREM

Consider a partition sum containing an arbitrarily complex Hamiltonian. One possible solution to this disaster is to change from summation over discrete variable to the integration over an according continuous set or measure μ

$$Z(\beta) = \sum_{\{s_i\}} e^{-\beta \mathcal{H}(s_i)} = C_N \int_{\Lambda \simeq \mathbb{R}^d} e^{Nf(\vec{x})} d\mu_N(\vec{x}) \quad (17.114)$$

with a function $f(\vec{x})$, $x \in \Lambda$ and the constant C_N , that may (but does not have to) depend on N . Considering the 1 dimensional case, the following theorem called *Laplace's method* holds for $N \rightarrow \infty$ (e.g. in the thermodynamic limit)

$$N \rightarrow \infty: \int_a^b e^{Nf(x)} dx \approx \sqrt{\frac{2\pi}{N|f''(x_0)|}} e^{Nf(x_0)} \text{ with } \max_{x \in \mathbb{R}} f(x) = f(x_0) \quad (17.115)$$

with $f(\vec{x})$ at least 2 times differentiable function with *unique global maximum* at x_0 and fast decaying away from it (confer [1] also). Doing integral calculus attempting to solve an integral of this form we write the Taylor's expansion for $f(x)$ around its global maximum x_0 ($f'(x_0) = 0$, $f''(x_0) < 0$)

$$f(x) = f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + \frac{1}{2}f''(x_0)(\Delta x)^2 + \quad (17.116)$$

$$+ \mathcal{O}((\Delta x)^3) \quad (17.117)$$

$$\approx f(x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 \quad (17.118)$$

$$= f(x_0) - \frac{1}{2}|f''(x_0)|(x - x_0)^2 \quad (17.119)$$

thus we may write

$$\lim_{N \rightarrow \infty} \int_a^b e^{Nf(x)} dx \approx \lim_{N \rightarrow \infty} \int_a^b e^{N(f(x_0) - \frac{1}{2}|f''(x_0)|(x-x_0)^2)} dx \quad (17.120)$$

$$= \lim_{N \rightarrow \infty} e^{Nf(x_0)} \int_a^b e^{-N\frac{1}{2}|f''(x_0)|(x-x_0)^2} dx \quad (17.121)$$

$$\approx \lim_{N \rightarrow \infty} e^{Nf(x_0)} \int_{-\infty}^{\infty} e^{-N\frac{1}{2}|f''(x_0)|(x-x_0)^2} dx \quad (17.122)$$

$$= \lim_{N \rightarrow \infty} e^{Nf(x_0)} \sqrt{\frac{2\pi}{N|f''(x_0)|}} \quad (17.123)$$

$$= \lim_{N \rightarrow \infty} e^{Nf(x_0)} \sqrt{\frac{2\pi}{-Nf''(x_0)}} \quad (17.124)$$

the first approximation was to cut the Taylor's expansion at 2nd order and the second approximation was to expand the integration interval to whole \mathbb{R} since the $f(x)$ is (very) fast decaying and zero there. The later approximation allows to translate to $x_0 = 0$ and evaluate the Gaussian integral (this is a relation, to the Gaussian transformation also). To summarize the idea assume that the function $f(x)$ has a unique global maximum at x_0 . If this function gets multiplied by a large number N , the gap between $Nf(x_0)$ and $Nf(x)$ will increase additionally and then grow exponentially for the function $e^{Nf(x)}$. This means all significant contributions to the integral of this function come from points in a neighborhood of x_0 only, which is what we have estimated. The basic ideas for approximations are also closely related to the *Stationary phase approximation* which is for oscillatory integrals and integrates the function and the point where the exponential becomes constant since that gives the biggest contribution.

An extensions of Laplace's method for complex analysis (in particular together with Cauchy's integral formula), is used to find a contour of *steepest descent* for an (asymptotically with large N) equivalent integral, expressed as a line integral. More precisely, if no point x_0 exists on the real line where the derivative of f vanishes (maxima), it can become handy to deform the integration contour away from the real line into the complex plane, where the simpler integral can be explicitly evaluated.

For a sequence $(\vec{x}_1, \vec{x}_2, \dots)$ of d -dimensional variables \vec{x}_i random variables, the *Varadhan's theorem* is a way to estimate the same kind of integrals as before (explained in full detail in [3] sec. 20).

17.5.2 SCATTERING LENGTH

The scattering length is an experimentally accessible quantity (observable). According to [1] it holds, that the scattering length describes low-energy scattering

$$\lim_{k \rightarrow 0} \sigma = 4\pi a^2 \quad (17.125)$$

where k is the wave number and σ the elastic cross section at low energies. When a slow particle scatters off a short ranged scatterer (e.g. an impurity in a solid or a heavy particle) it cannot resolve the structure of the object since its de-Broglie wavelength is very long. The idea is that then it should not be important what precise potential $V(r)$ one scatters off, but only how the potential looks at long length scales. The formal way to solve this problem is to do a partial wave expansion (somewhat analogous to the multipole expansion in classical electrodynamics), where one expands in the angular momentum components of

17.5 Appendix

the outgoing wave. At very low energy the incoming particle does not see any structure, therefore to lowest order one has only a spherical symmetric outgoing wave, the so called s-wave scattering (angular momentum $l = 0$) without higher momentum p and d-wave ($l=1,2$). The idea of describing low energy properties in terms of a few parameters and symmetries is very powerful, and is also behind the concept of renormalization.

17.6 TABLE OF SYMBOLS

\mathbb{R}, \mathbb{C}	real and complex space, accordingly we have integer space \mathbb{N} and whole numbers \mathbb{Z}
δ_{ij}	Kronecker delta (Levi-Civita-Symbol)
\mathcal{O}	Landau symbol
T, β	system temperature (and $\beta = (k_B T)^{-1}$ with k_B Boltzmann's constant) and e.g. T_C the critical temperature
V, N, ρ	system volume $V = L^d$, size and density (in thermodynamic limit $L, N \rightarrow \infty$ such that $\rho = N/V = \text{const.}$), $N = n$ e.g. $n_{\vec{p}}, n_k$
\hat{N}	Number operator
d	system/space dimension ($2d$ number of bonds per lattice site)
i, j, l, \dots	index variables $\in \mathbb{N}$ may be $\in \mathbb{Z}$
s_i	spin variable, takes values $\pm s$ and has fluctuations δs_i around its mean-field magnetization m
t_i	site occupation variable, takes values $\in \{0, 1\}$
m	system magnetization (per spin $m = M/N$, with M total magnetization) with physical solution $\pm m_0$ or the mass
H	external magnetic field and e.g. H_{eff} the effective field
J, J_{ij}	coupling constant (related to A and λ also) and as a matrix for every single interaction
\mathcal{H}	Hamilton function (Hamiltonian), e.g. \mathcal{H}_{mf} the mean-field one
$\hat{\mathcal{H}}$	Hamilton operator (may also involve a Laplacian or Laplace operator Δ), e.g. $\hat{\mathcal{H}}_{\text{int}}$ the interaction Hamiltonian
Z, Z_N	canonical partition sum, e.g. Z_N the N -particle partition sum (sometimes can be written as $Z_N = Z_1^N$)
Z_G, z	grand canonical partition sum and fugacity $z = e^{\beta\mu}$ with chemical potential μ
F	(Helmholtz) free energy (for whole system; per site is $f = F/N$)
Ω, p	grand potential and pressure (or momentum modulus, see below)
S	entropy
$\langle \cdot \rangle$	thermal/weighted average
χ	susceptibility (also related to $\langle s_i s_j \rangle$ and Γ_{ij})
ϕ_i, ϕ	scalar real valued field, thus e.g. potential field Φ too
$\text{CE}[\cdot]$	convex envelope of any function, e.g. by Legendre transformation
$\vec{p}, \vec{k}, \vec{x}$	momentum vector p_i or k_i and space vector x_i (with $p = \vec{p} $)
h, \hbar	Planck constant with $\hbar = h/2\pi$
E, U	energy (e.g. E_k but also $\epsilon_{\vec{p}}, \epsilon_k^0$) and internal energy
λ, ω	coupling constant in Lattice gas model (related to A) or (thermal) de Broglie wavelength and eigen frequencies, e.g. $\omega_{\vec{k}}$

17.6 Table of symbols

g_u, ζ	g -functions (to simplify notation of free BEC) and Zeta function with $g_u(1) = \zeta(u)$
ρ_C, ρ_0	BEC critical density and ground state (zero momentum) state density with λ_C the according de Broglie wavelength
$ \phi_0(N)\rangle$	bosonic ground state functions (for N bosons), e.g. for BEC
$a_{\vec{k}}^{(\dagger)}$	creation $a_{\vec{k}}^\dagger$ and annihilation $a_{\vec{k}}$ (ladder) operators belonging to momentum state \vec{k} (and basis function $ \phi_{\vec{k}}(N)\rangle$)
$\xi_0^{(\dagger)}$	re-scaled ladder operators (for ground state) with commutator that vanishes in the thermodynamic limit
$[\cdot, \cdot]$	commutator of 2, e.g. ladder operators
$\mathcal{F}(\cdot)$	Fourier transformation (from spatial/real to momentum space)
g, a	pseudo potential g (replacing the actual potential in momentum space - after Fourier transf.) and (s-wave) scattering length a
$\alpha_{\vec{k}}^{(\dagger)}$	Bogoliubov ladder operators with the (real valued) transformation parameters u_k, v_k

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CHAPTER 18

MEAN FIELD THEORY: GENERAL RESULTS

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In this report, we will look at ensembles of one-particle systems. The amount of particles will be finite or infinite. We will in particular look at examples where the one-particle Hilbert space is finite dimensional, but the results still apply to systems with infinite dimensional Hilbert space for each particle. As a result we will see that in the thermodynamical limit of infinitely many particles, the system can be described using classical physics.

18.1 INTRODUCTION

Note added: This talk is based on the following references [1, 2].

First of all, we need definitions for the different kinds of symmetries that we will use. Let us denote D as the space of observables of a one-particle system. The space of observables of a multi-particle system can be written as the tensor product of D with itself: $D_n := \bigotimes^n D$. We call an observable of the n -particle quantum system symmetric, if it is equal to its own symmetrisation. For an observable $A \in D_n$ that can be written as a product $A = A_1 \otimes \cdots \otimes A_n$ we will define the symmetrisation of A as

$$\text{sym}_n(A_1 \otimes \cdots \otimes A_n) = \frac{1}{n!} \sum_{\pi \in S_n} A_\pi(1) \otimes \cdots \otimes A_\pi(n) \quad (18.1)$$

and A will be called symmetric if it satisfies $A = \text{sym}_n(A)$.

18.2 Symmetric sequence

In general, the symmetrisation operator is defined as the continuous linear extension of the definition $\text{sym}_n(A_1 \otimes \cdots \otimes A_n) = 1/n! \sum_{\pi} A_{\pi(1)} \otimes \cdots \otimes A_{\pi(n)}$.

18.2 SYMMETRIC SEQUENCE

We call a sequence of observables a symmetric sequence if the elements of the sequence can be written as symmetrisation of previous elements, apart from the first few elements:

$$\exists n_0 : \quad \forall k \geq n_0, n > k \quad A_n = \text{sym}_n(A_k) \quad (18.2)$$

This is more strict than just requiring that each element is symmetric. We will denote the set of symmetric sequences as \mathcal{Y} . The first elements of the sequence might not fulfil the condition. For example if we are looking at a hamiltonian that includes nearest neighbor interaction (of two particles) as well as next nearest neighbor interaction (of four particles), then we obviously can't write H_4 as the symmetrisation of H_2 .

A sequence X is called approximately symmetric if

$$X_n = \text{sym}_n(X_k) \quad \text{for all } k \text{ and} \quad (18.3)$$

$$\forall \epsilon > 0 \quad \exists Y \in \mathcal{Y} \quad \exists n_0 \quad \forall n > n_0 \quad \|X_n - Y_n\| < \epsilon \quad (18.4)$$

Mean field Hamiltonians are not always symmetric sequences. However, it is sufficient if the Hamiltonian is approximately symmetric. The results will still apply.

18.2.1 EXAMPLES

An example of a symmetric sequence of Hamiltonians are mean field Hamiltonians of the form

$$H_n = \frac{1}{n} \sum_i h_i + \frac{1}{n(n-1)} \sum_{i \neq j} V_{ij} \quad (18.5)$$

where h_i is a one-particle hamiltonian and V_{ij} is the interaction potential. The one-particle hamiltonian can be absorbed in the potential by defining the two-particle potential

$$V = V_{12} + \frac{1}{2}(h \otimes 1 + 1 \otimes h) \quad (18.6)$$

Note that these Hamiltonians are normalized to be intensive quantities. One could regard it as a Hamiltonian density. We have to normalize the Hamiltonians

if we want to take the thermodynamic limit, otherwise there would be an infinite ground state energy.

An example for an approximately symmetric sequence is the classical Ising Hamiltonian, which is of the form

$$H = J \left(\frac{1}{n} \sum_i s_i \right)^2 = \frac{J}{n^2} \sum_{i,j} s_i s_j \quad (18.7)$$

We can rewrite this as

$$H = J \left(\frac{1}{n(n-1)} - \frac{1}{n^2(n-1)} \right) \sum_{i,j} s_i s_j \quad (18.8)$$

The first term can be recognized as a symmetric Hamiltonian. The second term will vanish at the order $1/n$ as there are only n^2 terms in the sum.

18.3 SYMMETRIC PRODUCT

On the space of symmetric sequences \mathcal{Y} we can define two different types of products. One is the normal operator product. The other one is the symmetric product. We will see later that they are asymptotically identical. We define the symmetric product of two observables as follows:

$$\star : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathcal{Y} \quad (18.9)$$

$$X_a \star Y_b = \text{sym}_{a+b}(X_a \otimes Y_b) \quad (18.10)$$

The symmetric product \star is commutative. With this definition, we can write a symmetric sequence as

$$X_n = X_k \star 1_{n-k} \quad (18.11)$$

For the \star product of two symmetric sequence, it does not matter which elements of the sequence we choose.

$$(X \star Y)_n = X_m \star Y_{n-m} = (X_k \star 1_{m-k}) \star Y_{n-m} = X_k \star Y_{n-k} \quad (18.12)$$

Lemma

Let $X, Y \in \mathcal{Y}$ and $k, m \in \mathbb{N}$ Then for $n \geq k + m$

$$\|X_n Y_n - (X \star Y)_n\| \leq k * m/n < \|X_k\| * \|Y_m\| \quad (18.13)$$

Proof

18.3 Symmetric product

Let $\alpha_\pi \in \text{Aut}(D_n)$ denote the action of the permutation π on D_n .

Then

$$X_n = \text{sym}_n(X_k) = \frac{1}{n!} \sum_{\pi} \alpha_\pi(X_k) \quad (18.14)$$

Likewise, Y_n can be written in the same way. The product of the two is

$$X_n Y_n = \left(\frac{1}{n!}\right)^2 \sum_{\pi, \pi'} \alpha_\pi(X_k) \alpha_{\pi'}(Y_m) \quad (18.15)$$

$(X \star Y)_n$ is represented by the sum over only those terms in the same sum, for which $\pi(\{1, k\}) \cap \pi'(\{1, m\}) = \emptyset$.

Let $w_n(k, m)$ denote the relative weight of these terms in the sum. Then

$$\|X_n Y_n - (X \star Y)_n\| \leq |1 - w_n(k, m)| \|X_k\| * \|Y_m\| \quad (18.16)$$

Thus it remains to be shown that $|1 - w_n(k, m)| \leq k \cdot m/n$.

The number of permutations π such that $\pi(1, k) \cap \pi'(1, m) = \emptyset$ does not depend on π' . Therefore $n! \cdot w_n(k, m)$ is the number of permutations $\pi \in S_n$ with

$$\pi(1, \dots, k) \cap 1, \dots, m = \emptyset, \quad (18.17)$$

$$\text{i.e.} \binom{n-m}{k} \cdot k! \cdot (n-k)! \quad (18.18)$$

Hence

$$w_n(k, m) = \frac{(n-k)! \cdot (n-m)!}{n! \cdot (n-k-m)!} \quad (18.19)$$

$$= \frac{(n-m)(n-m-1) \cdots (n-m-k+1)}{n(n-1) \cdots (n-k+1)} \quad (18.20)$$

$$= \prod_{\alpha=0}^{k-1} \frac{n-m-\alpha}{n-\alpha}. \quad (18.21)$$

The bound $w_n(k, m) \leq 1 - k \cdot m/n$ is obviously true for $k = 0$ or $m = 0$. Therefore we may assume $m \geq 1$ and proceed by induction over k . Using the induction hypothesis we find

$$w_n(k+1, m) = w_n(k, m) \cdot (1 - m/(n-k)) \quad (18.22)$$

$$\geq (1 - k \cdot m/n)(1 - m/(n-k)) \quad (18.23)$$

$$= 1 - m(k+1)/n + \frac{k \cdot m(m-1)}{n(n-k)} \quad (18.24)$$

$$\geq 1 - m(k+1)/n, \text{ as long as } n > k. \quad (18.25)$$

In the thermodynamical limit the product of operators converges towards the symmetric product of these. The system therefore behaves classically and we get for observables A and B , the expectation value of $A \cdot B$ is

$$\langle A \cdot B \rangle = \langle A \rangle \cdot \langle B \rangle \quad (18.26)$$

Another corollary is that every state of the infinite particle system can be written as a convex combination of pure states. In the finite particle case, this is of course always the case, however it is not trivial in the infinite particle case. It can also be shown that the physical states of the infinite particle system are equivalent to the one particle mixed-states.

18.4 CONCLUSION

We looked at mean-field systems and saw that in the thermodynamical limit they can be described classically. The density matrix of the infinite system can be collapsed to one of a one particle system, giving us a pure or mixed state describing the entire system.

18.4 Conclusion

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CHAPTER 19

BOSE-EINSTEIN CONDENSATES AND THE GROSS-PITAEVSKII EQUATION

ARNE HANSEN

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This talk is about Bose condensates and their description by the Gross Pitaevskii equation. Once the basic concepts have been introduced, the aim will be to outline a rigorous mathematical proof that the theory developed by Gross Pitaevskii actually yields the physical density and ground state energy. The proof was first published in [1] and later summarized in [2].

19.1 BOSE EINSTEIN CONDENSATION FROM QUANTUM STATISTICAL PHYSICS

A Bose Einstein condensate is an N Boson system, where the particle number N is of the order 10^{23} , that is characterized by a macroscopically occupied quantum state. That is to say the occupation number of one particular quantum state is of the order of the total particle number. The gas is therefore largely coherent and quantum mechanical effects become macroscopically observable.

First I want to sketch, how the macroscopically occupied ground state can be derived from quantum statistical mechanics. In a second step we assume that the system under consideration is characterized by a condensate state. We will use this feature to simplify the Hamiltonian. On this basis one can then introduce the Gross-Pitaevskii approach (in the following denoted by GP) allowing us to describe non-uniform gases in an external potential.

19.1 Bose Einstein Condensation from Quantum Statistical Physics

The challenge is to tackle a large number of particles $N \sim 10^{23}$. To do so we use the technique of statistical mechanics deriving the thermodynamic properties from the appropriate partition function. In our case this is the grand canonical ensemble.

19.1.1 THE GRAND CANONICAL ENSEMBLE

In order to introduce the grand canonical partition function we will need the canonical partition function. For an N particle quantum system the *canonical partition function* is

$$Z_N = \text{tr} e^{-\beta H} \quad (19.1)$$

The canonical partition function is used to describe systems with fixed volume, particle number and temperature. Instead of fixing the particle number we can now restrict the chemical potential μ and introduce the *grand canonical partition function* by summing over the particle number

$$\Xi(\beta, \mu) = \sum_{N=0}^{\infty} z^N Z_N = \sum_{N=0}^{\infty} e^{\beta\mu N} (\text{tr}_N e^{-\beta H}) \quad (19.2)$$

where $z = e^{\beta\mu}$ is the called *fugacity*. The index of the trace indicates that the trace is to be taken in the Hilbertspace $\mathcal{H}^{\otimes N}$, whereas the state corresponding to the grand canonical ensemble is an element of the Fock space since its particle number is not fixed.

The corresponding thermodynamic potential is given by the *grand canonical potential*

$$\Omega = E - TS - \mu \quad (19.3)$$

Ω can be calculated from Ξ using

$$\Omega = -k_B T \log \Xi \quad (19.4)$$

From this we obtain entities such as the average particle number and the entropy

$$S = -\frac{\partial \Omega}{\partial T} \quad (19.5)$$

$$\langle N \rangle = -\frac{\partial \Omega}{\partial \mu} \quad (19.6)$$

19.1.2 THE IDEAL QUANTUM GAS

If we now restrict ourselves to an ideal quantum gas, i.e. to a set N non-interacting particles, the Hamiltonian becomes a sum of N one-particle Hamiltonian $H_i^{(1)}$

$$H = \sum_i H_i^{(1)} \quad (19.7)$$

Reformulating $N = \sum_i n_i$ we can now actually calculate the grand canonical partition function to be

$$\begin{aligned} \Xi &= \sum_{N=0}^{\infty} z^N Z_N = \sum_{N=0}^{\infty} z^N \sum_{\substack{n_1, n_2, \dots \\ n_1 + n_2 + \dots = N}} e^{-\beta \sum_{k=1}^N \epsilon_k n_k} \\ &= \sum_{N \geq 0} \sum_{\substack{n_0, n_1, n_2, \dots \\ n_0 + n_1 + n_2 + \dots = N}} \exp\left(\beta \sum_i n_i\right) \exp\left(-\beta \sum_k \epsilon_k n_k\right) = \prod_{i=0}^{\infty} \sum_{n_i} \exp(-\beta(\epsilon_i - \mu)n_i) \\ &= \prod_i \frac{1}{1 - e^{\beta(\epsilon_i - \mu)}} \end{aligned} \quad (19.8)$$

The first 4 steps are just rewriting the sums and products. The final expression follows by solving the geometric series for each n_i . Equation 19.4 yields a formula for the grand canonical potential

$$\Omega = k_B T \sum_i \log(1 - e^{\beta(\mu - \epsilon_i)}) \quad (19.9)$$

Using 19.6 we obtain for the average particle number

$$\langle N \rangle = \sum_i \frac{1}{\exp[\beta(\epsilon_i - \mu)] - 1} \quad (19.10)$$

Furthermore the average particle number for the individual energy states are

$$\langle n_k \rangle = \frac{1}{\beta} \frac{\partial}{\partial \epsilon_k} \sum_i \log \Xi = \frac{1}{\exp[\beta(\epsilon_k - \mu)] - 1} \quad (19.11)$$

So far we have not specified the form of the Hamiltonian apart from the restriction that the particles do not interact with each other. To proceed we further assume that these are free particles in a box of finite length L with periodic boundary conditions. The Hamiltonian is then explicitly given by

19.2 The weakly-interacting Bose-gas

$$H = \frac{1}{2m} \sum_{i=1}^N \vec{p}_i^2 \quad (19.12)$$

The eigen-states are plain waves with $\vec{p} = 2\pi\hbar\vec{n}/L$ with $\vec{n} \in \mathbb{Z}^3$ and eigen-energies $\vec{p}^2/2m$.

Now we are able to calculate the density in the *thermodynamic limit*, taking $L \rightarrow \infty$ while keeping $\rho := \frac{\langle N \rangle}{L^3}$ fixed. The sum 19.10 can be turned into an integral, $1/L^3 \sum_{\vec{p}} \rightarrow 1/(2\pi\hbar)^3 \int d\vec{p}$. If we restrict $\mu < \epsilon_0 = 0$, we obtain

$$\rho = \frac{\langle N \rangle}{L^3} = \lim_{L \rightarrow \infty} \frac{\langle N \rangle}{L^3} = \frac{1}{(2\pi\hbar)^3} \int d\vec{p} \frac{1}{\exp[\beta(\vec{p}^2/(2m) - \mu)] - 1} \quad (19.13)$$

This is a monotonously increasing function in μ . Consider now the limiting case $\mu \rightarrow 0$.

$$\begin{aligned} \rho_c &:= \lim_{\mu \rightarrow 0} \rho = h^{-3} \int d\vec{p} \frac{1}{\exp(\beta\vec{p}^2/(2m)) - 1} \\ &= \frac{4\pi}{h^3} \int_0^\infty dp \frac{p^2}{\exp(p^2/(2m)) - 1} \\ &= \left(\frac{2\pi\hbar^2\beta}{m} \right)^{-3/2} g_{3/2}(1) \end{aligned} \quad (19.14)$$

Here we use the *Bose function*

$$g_p(z) = \frac{1}{\Gamma(p)} \int_0^\infty dx x^{p-1} \frac{1}{z^{-1}e^x - 1} = \sum_{l=1}^\infty \frac{z^l}{l^p} \quad (19.15)$$

with $z = e^{\beta\mu}$ as above. Thus we get an upper bound to the density $\rho \leq \rho_c$. From a physical perspective this behavior seems awkward. Since we are dealing with non-interacting bosons we would expect that an upper limit to the density.

Einstein solved this dilemma by assuming that additional particles, i.e. those that would have caused the density to exceed this value, go to the ground state. Mathematically this amounts to simultaneously taking the limit $\mu \rightarrow 0$ as $L \rightarrow \infty$ instead of taking the two limits one after another.

19.2 THE WEAKLY-INTERACTING BOSE-GAS

For the following to chapters I will follow chapters 4 and 5 in [3].

So far the particles have been independent from one another. We now want to introduce a weak interaction between them. In case we are dealing with a **dilute**

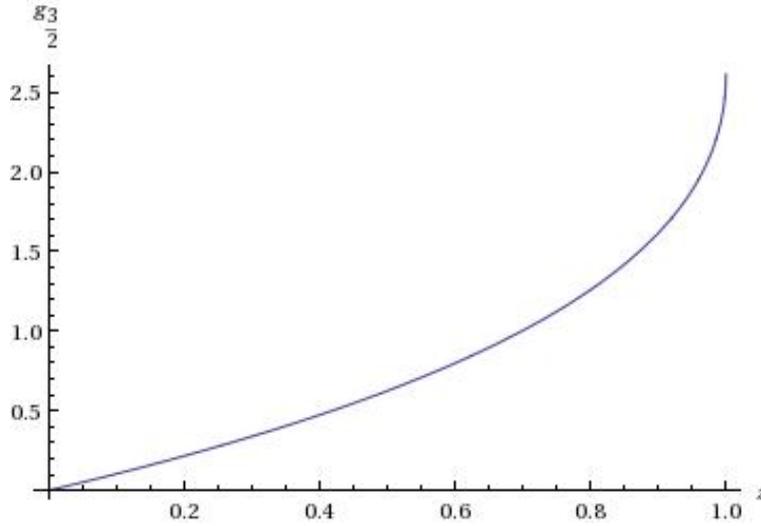


Figure 19.1: The Bose function $g_{3/2}$. For a fixed temperature T we consider the limit $\mu \rightarrow 0$, i.e. $z \rightarrow 1$.

Bose-Einstein condensate, we can apply the Bogoliubov prescription and simplify the interaction potential in order to reduce the complexity of our theory. This will turn out to be the starting point for the Gross-Pitaevskii approach. The Hamiltonian of a system of interacting particle is of the form

$$H = \int d\vec{r} \left(\frac{\hbar^2}{2m} \nabla \hat{\psi}^\dagger \nabla \hat{\psi} \right) + \frac{1}{2} \int d\vec{r} \int d\vec{r}' \left(\hat{\psi}^\dagger \hat{\psi}'^\dagger V(\vec{r}' - \vec{r}) \hat{\psi} \hat{\psi}' \right) \quad (19.16)$$

Since we are dealing with a translation invariant theory the field operator¹ the Fourier transform $\hat{\psi}$ takes the simple form

$$\hat{\psi} = \sum_{\vec{p}} \hat{a}_{\vec{p}}^\dagger \frac{1}{\sqrt{V}} e^{i\vec{p} \cdot \vec{r} / \hbar} \quad (19.17)$$

if we restrict our problem to a finite volume V .

With this we get the Hamiltonian in momentum space

$$H = \sum_{\vec{p}} \frac{p^2}{2m} \hat{a}_{\vec{p}}^\dagger \hat{a}_{\vec{p}} + \frac{1}{2V} \sum_{\vec{p}_1, \vec{p}_2, \vec{q}} V_{\vec{q}} \hat{a}_{\vec{p}_1 + \vec{q}}^\dagger \hat{a}_{\vec{p}_2 - \vec{q}}^\dagger \hat{a}_{\vec{p}_1} \hat{a}_{\vec{p}_2} \quad (19.18)$$

¹Quantum field operators $\hat{\psi}^\dagger(\vec{r})$ ($\hat{\psi}(\vec{r})$) create (annihilate) a particle at position \vec{r} . In order to quantize the theory one postulates the usual commutation (anti-commutation) relations for Bosons (Fermions).

19.2 The weakly-interacting Bose-gas

where $V_{\vec{q}} = \int d\vec{r} V(\vec{r}) e^{-i\vec{p}\cdot\vec{r}/\hbar}$. The aim is now to simplify this for the description of a Bose-Einstein condensate.

19.2.1 REDUCING THE INTERACTION POTENTIAL

Since we are only interested in macroscopic properties of the gas and not what actually happens during the interaction, we assume the gas to be dilute, i.e. that the mean inter-particle distance is much larger than the scattering length of the potential, $|a| \ll n^{-1/3}$. This permits to replace V by an effective soft potential V_{eff} and apply perturbation theory. Further we can assume that only small momenta and hence small momenta differences contribute. Therefore it is sufficient to consider only the term with $q = 0$ for which the potential becomes

$$V_0 = \int d\vec{r} V_{\text{eff}} =: g \quad (19.19)$$

This is just a mean field approximation of the interaction potential.

It turns out that we can express g in terms of the scattering length a

$$g = \frac{4\pi\hbar^2 a}{m} \quad (19.20)$$

19.2.2 BOGOLIUBOV PRESCRIPTION

Bogoliubov's approach allows us to reduce the field operators to classical fields. To motivate this one writes the field operator in terms of the creation and annihilation operators, \hat{a}_i and \hat{a}_i^\dagger , and the single particle eigenfunctions $\phi_i(\vec{r})$ of the Hamiltonian. Further we separate the ground state from the excited states

$$\hat{\psi}(\vec{r}) = \sum_i \phi_i \hat{a}_i = \phi_0 \hat{a}_0 + \sum_{i \neq 0} \phi_i \hat{a}_i \quad (19.21)$$

In the case of BEC we have $N_0 = \langle \hat{a}_0^\dagger \hat{a}_0 \rangle = \langle \phi_{BEC} | \hat{a}_0^\dagger \hat{a}_0 | \phi_{BEC} \rangle \gg 1$, i.e. \hat{a}_0 and \hat{a}_0^\dagger are of order $\sqrt{N_0} \gg 1$ whereas $1 = [\hat{a}_0, \hat{a}_0^\dagger] = \langle \phi_{BEC} | [\hat{a}_0, \hat{a}_0^\dagger] | \phi_{BEC} \rangle$. Therefore we neglect the commutation relations and set the ground state operators to be c -numbers

$$\hat{a}_0 = \sqrt{N_0} \quad \hat{a}_0^\dagger = \sqrt{N_0} \quad (19.22)$$

The actual values $\sqrt{N_0}$ follows from the condition, that the expectation value of the ground state occupation number should still be N_0 .

With this we get

$$\widehat{\psi}(\vec{r}) = \psi_0(\vec{r}) + \delta\widehat{\psi}(\vec{r}) \quad (19.23)$$

where $\psi_0 = \sqrt{N_0}\phi_0$ and $\delta\widehat{\psi} = \sum_{i \neq 0} \phi_i \hat{a}_i$. If the number of particles in excited states is negligible, the operator term can be dropped. This is the case for a dilute Bose gas at low temperatures since the thermal and the quantum depletion are small. What remains is the classical field associated to the ground state.

This approximation is not mathematical sound. Therefore we still have to show that it will yield a reasonable result. This is the subject of the last part.

Note that as we move to a classical field abandoning the commutation relations we fix the total particle number.

$$\int d\vec{r} n(\vec{r}) = \int d\vec{r} \langle \widehat{\psi}^\dagger(\vec{r}) \widehat{\psi}(\vec{r}) \rangle = N_0 \int d\vec{r} |\phi_0(\vec{r})|^2 = N_0 \quad (19.24)$$

In the Bogoliubov prescription the one-particle density matrix takes the simple form

$$\begin{aligned} \rho^{(1)}(\vec{r}, \vec{r}') &= \langle \widehat{\psi}^\dagger(\vec{r}) \widehat{\psi}(\vec{r}') \rangle = \langle \Psi | (\phi_0^*(\vec{r}) \phi_0(\vec{r}') \hat{a}_0^\dagger \hat{a}_0) | \Psi \rangle \\ &= N_0 \phi_0^*(\vec{r}) \phi_0(\vec{r}') \langle \Psi | \Psi \rangle = N_0 \phi_0^*(\vec{r}) \phi_0(\vec{r}') \end{aligned} \quad (19.25)$$

The steps we took above, namely the Bogoliubov prescription and the simplification of the interaction, will be essential in deriving the Gross-Pitaevskii equation. Besides the methodical importance the theory above yields some interesting results. If we insert the simplified field operator $\widehat{\psi} = \sqrt{N}$ into the energy expectation value assuming that the vast majority of the particles is in the condensed state we find the ground energy to be

$$E_0 = \frac{N^2 V_0}{2V} \neq 0 \quad (19.26)$$

This differs from the result in the previous chapter as the value is no longer zero. Furthermore we can consider the pressure of the gas

$$P = -\frac{\partial E_0}{\partial V} = \frac{N^2 V_0}{2V^2} = \frac{V_0 n^2}{2} \quad (19.27)$$

where $n = N/V$ is the *density*. The pressure does therefore not vanish anymore for $T \rightarrow 0$ as it has been the case for the ideal Bose gas.

19.3 THE GROSS-PITAIEVSKII APPROACH

The aim is to develop a theory for a non-uniform dilute Bose gas such as gases in a trap. Most of the steps from above will be repeated. But when applying the

19.3 The Gross-Pitaevskii approach

Bogoliubov prescription we can no longer drop the one-particle wave functions ϕ_i since we lost translation invariance.

19.3.1 THE GROSS-PITAEVSKII EQUATION

Starting from the assumption that the gas will be characterized by a macroscopically occupied ground state, the Bogoliubov prescription 19.2.2 is applied. The ground state annihilation and creation operators, $\hat{\psi}(\vec{r}, t)$ and $\hat{\psi}^\dagger(\vec{r}, t)$, are replaced by classical fields, $\psi(\vec{r}, t)$ and $\psi^*(\vec{r}, t)$. Further the interaction of particles is simplified using a soft potential as above. The crucial difference is to introduce an external potential and to derive equations of motion for the classical fields describing the state of the gas.

FROM THE HEISENBERG PICTURE

The equations of motion for this classical field can be derived from the equations of motions for the field operator $\hat{\psi}(\vec{r}, t)$ in the Heisenberg picture.

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \hat{\psi}(\vec{r}, t) &= \left[\hat{\psi}(\vec{r}, t), \hat{H} \right] \\ &= \left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}}(\vec{r}, t) + \int d\vec{r}' \hat{\psi}^\dagger(\vec{r}', t) V(\vec{r}' - \vec{r}) \hat{\psi}(\vec{r}', t) \right) \hat{\psi}(\vec{r}, t) \end{aligned} \quad (19.28)$$

As above the quantum field operators are now replaced by classical field and the interaction term is approximated by perturbation on an effective soft potential. Further we assume that ψ varies slowly over ranges of the order of the interaction potential. Consequently the integral of the third summand is decoupled. Finally we are left with the Gross-Pitaevskii equation

$$i\hbar \frac{\partial}{\partial t} \psi_0(\vec{r}, t) = \left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}} + g |\psi_0(\vec{r}, t)|^2 \right) \psi_0(\vec{r}, t) \quad (19.29)$$

where $g = \int d\vec{r}' V_{\text{eff}}$.

TIME-INDEPENDENT EQUATION

If we set $\psi_0(\vec{r}, t) = \psi_0(\vec{r}) e^{-i\mu t/\hbar}$, where $\mu = \frac{\partial E}{\partial N}$, the GP equation reduces to

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V_{\text{ext}} - \mu + g |\psi_0(\vec{r})|^2 \right) \psi_0(\vec{r}) = 0 \quad (19.30)$$

The question arises why the time-evolution should be governed by the chemical potential μ and not by the energy. To understand this we have to return to the Bogoliubov prescription. If we consider the expectation value of the field operator $\widehat{\psi}$ after having reduced to classical fields, we obtain on the one hand

$$\langle \widehat{\psi} \rangle = \langle N | \sqrt{N} \phi_0 | N \rangle = \sqrt{N} \phi_0 = \psi \neq 0 \quad (19.31)$$

On the other hand we know the time evolution of the N particle state

$$|N(t)\rangle = e^{-iE(N)t/\hbar} |N\rangle \quad (19.32)$$

Combining these two equations we get the time evolution of the reduced field

$$\begin{aligned} \psi(t) &= \sqrt{N} \phi_0(t) \stackrel{\text{Bog.}}{=} \langle \widehat{\psi} \rangle(t) = \langle N(t) | (N-1)(t) \rangle \\ &= \langle N | N-1 \rangle e^{-i(E(N)-E(N-1))t/\hbar} \end{aligned}$$

If we approximate

$$E(N) - E(N-1) = \frac{E(N) - E(N-1)}{N - (N-1)} \sim \frac{\partial E}{\partial N} = \mu$$

we obtain

$$\psi(t) = \langle \widehat{\psi} \rangle e^{-i\mu t/\hbar} \stackrel{\text{Bog.}}{=} \psi e^{-i\mu t/\hbar} \quad (19.33)$$

Recalling the derivation of BEC from quantum statistical mechanics this is what we should actually expect: the chemical potential is key entity in the description of the Bose gas. We can see that from a slightly different perspective if we use an alternative, variational approach in deriving the time-independent GP equation.

VARIATIONAL APPROACH TO THE TIME-INDEPENDENT EQUATION

Instead of using the Heisenberg equation we could as well consider the energy functional

$$E[\psi] = \int d\vec{r} \left(\frac{\hbar^2}{2m} |\nabla\psi|^2 + V_{\text{ext}}(\vec{r}) |\psi|^2 + \frac{g}{2} |\psi|^4 \right) \quad (19.34)$$

We want to find the minimizing field under the normalizing condition $\int d\vec{r} |\psi|^2 = N$, which we got from the Bogoliubov prescription. To solve this problem we need to introduce a Lagrange multiplier, that will turn out to be μ . The equation we have to deal with is

$$\frac{\delta(E - \mu N)}{\delta\psi^*} = 0 \quad (19.35)$$

19.3 The Gross-Pitaevskii approach

The Lagrange multiplier is determined by

$$\mu = \frac{dE}{dN} \quad (19.36)$$

This is just the definition of the chemical potential from above.

19.3.2 ANALOGY TO ELECTRODYNAMICS

The Bogoliubov prescription has an analogon in electrodynamics. If a large number of photons is in approximately the same quantum state small fluctuations of the photon number do not matter anymore. It is then permitted to consider the classical instead of the quantum field, i.e. to apply classical electrodynamics instead of quantum field theory. The equations of motion for this “large occupation number limit” are given by the Maxwell equations in electrodynamics and correspondingly by Gross-Pitaevskii equation for BEC.

19.3.3 APPLICABILITY OF THE GROSS-PITAEVSKII EQUATION

Applying the Bogoliubov prescription requires a largely occupied ground state. Further the contribution of the remaining eigenstates can only be neglected if these are hardly occupied. This is the case for a dilute, cold Bose gas, as thermal and quantum depletion are small. The diluteness is further required to simplify the interactions.

19.3.4 THE MANY-BODY WAVE FUNCTION AND ONE-PARTICLE DENSITY MATRIX

Assuming the gas to be dilute allows to neglect interactions in a first approximation. The many body wave function is then given by the symmetrized product of wave functions

$$\Psi^{GP}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \left(\frac{1}{\sqrt{N}} \psi^{GP}(\vec{r}_1) \right) \left(\frac{1}{\sqrt{N}} \psi^{GP}(\vec{r}_2) \right) \cdots \left(\frac{1}{\sqrt{N}} \psi^{GP}(\vec{r}_N) \right) \quad (19.37)$$

where ψ^{GP} is the solution of the GP equation. The normalization $\frac{1}{\sqrt{N}}$ is due to choice of ψ while applying the Bogoliubov prescription. From the general formula in the Bogoliubov prescription 19.25, we directly obtain the one-particle density matrix if we set $\phi_0 = \frac{1}{\sqrt{N}} \psi^{GP}$:

$$\tilde{\rho}^{GP}(\vec{r}, \vec{r}') = \psi^{GP}(\vec{r})^* \psi^{GP}(\vec{r}') \quad (19.38)$$

EXAMPLE: THE HOMOGENEOUS BOSE GAS The simplest case is to set $V = 0$. Further we assume the gas to be homogeneous within a box of Volume \mathcal{V} . Therefore the first term drops too. The GP equation 19.30 reduces to

$$\mu = g |\psi^{GP}|^2 = g\tilde{\rho}(\vec{r}, \vec{r}) = g\frac{N}{\mathcal{V}} \quad (19.39)$$

The corresponding energy is

$$E = g\frac{N^2}{\mathcal{V}} \quad (19.40)$$

19.4 MATHEMATICAL RIGOROUS FOUNDATION OF THE GP THEORY

In the preceding part introducing the GP approach approximations have rather been based on physical intuition than mathematical rigorous arguments. Leib, Seiringer, Yngvason addressed this problem in their article *Bosons in a trap: A rigorous derivation of the Gross-Pitaevskii energy functional* [1].

The authors prove for the time-independent case that the ground state energy and the density derived from the GP equation in the thermodynamic limit converges to the physical density matrix.²

Theorem 19.1 (GP limit of the QM ground state energy and density). *If $N \rightarrow \infty$ with Na fixed, with a being the scattering length, then*

$$\lim_{N \rightarrow \infty} \frac{E_0(N, a)}{E^{GP}(N, a)} = 1 \quad (19.41)$$

and

$$\lim_{N \rightarrow \infty} \frac{1}{N} \rho_{N,a}^{QM}(\vec{r}) = \rho_{1,Na}^{GP}(\vec{r}) \quad (19.42)$$

in the weak L^1 sense. The densities are the diagonal elements of the corresponding matrix $\rho_{N,a}^{GP}(\vec{r}) = \tilde{\rho}(\vec{r}, \vec{r})$.

Further the single components of the GP energy, i.e. the kinetic term, the interaction and the external potential contribution, converge separately to the corresponding counterparts of the physical ground state energy.

²The article is summarized in chapter 6 of [2]. In this section I follow mostly this source. For details I took into account the original article [1].

19.4 Mathematical rigorous foundation of the GP theory

SCALING PROPERTIES

Before sketching the proof of the theorem stated above I will briefly remark on scaling properties of the system, particularly as the particle number is varied. The GP energy, i.e. 19.34 evaluated for $\psi_{N,a}^{GP}$, and the GP solution $\psi_{N,a}^{GP}$ itself scale as

$$E^{GP}(N, a) = N E^{GP}(1, Na) \quad (19.43)$$

$$\psi_{N,a}^{GP}(\vec{r}) = \sqrt{N} \psi_{1,Na}^{GP}(\vec{r}) \quad (19.44)$$

Hence it seems natural to fix Na , as done in the theorem. This yields

$$E^{GP} \sim N \quad \psi_{N,a}^{GP} \sim \sqrt{N} \quad (19.45)$$

PROOF

The proof of 19.41 consists of two parts. These are to find upper and lower bounds on E_0 in terms of E_{GP} such that the bounds converge to E_0 in the limit $N \rightarrow \infty$. Once we have shown the convergence of the GP energy, the convergence of the density can be obtained from a variational derivation. Since the proof is very technical I will only sketch the first part here.

In the following we will set \hbar , μ and m to one.

Part 1: Upper bound. In general the expectation value of the energy of any quantum state of the respective Hilbert space is an upper bound to the ground state energy E_0 . The challenge is to find an appropriate state, such that one on the one hand finds a relation to E_{GP} and on the other hand convergence in the thermodynamic limit. In other words we aim to show that

$$E^{QM}(N, a) \leq E^{GP}(N, a)(1 + \mathcal{O}(a\bar{\rho}^{1/3})) \quad (19.46)$$

where

$$\bar{\rho} = \frac{1}{N} \int d\vec{r} |\rho_{N,a}^{GP}(\vec{r})|^2 \quad (19.47)$$

is the mean density. It scales as N^{-2} since $\rho_{N,a}^{GP} \sim N$ and Na fixed i.e. $a \sim N^{-1}$. This yields the desired behavior of 19.46 in the thermodynamic limit.

ANSATZ FOR AN APPROPRIATE TRIAL STATE We start by extending Ψ^{GP} from 19.37. Ψ^{GP} describes a set of independent particles. Now we assume that the particles are inserted one after another and are affected by the closest of the previously inserted particles. The wave functions of the particles that are already present do not change as a new particle is inserted. Like this we take into account the leading term in the energy of dilute systems. This amounts to the following definition

$$\Phi = F(\vec{r}_1, \dots, \vec{r}_N)G(\vec{r}_1, \dots, \vec{r}_N) \quad (19.48)$$

where

$$F(\vec{r}_1, \dots, \vec{r}_N) = \prod_{i=1}^N F_i(\vec{r}_1, \dots, \vec{r}_N) \quad (19.49)$$

$$G(\vec{r}_1, \dots, \vec{r}_N) = \prod_{i=1}^N g(x_i) = \prod_{i=1}^N \frac{\psi^{GP}(\vec{r}_i)}{\|\psi^{GP}\|_\infty} \quad (19.50)$$

The functions F_i depend on the distance to the closest particle with index $j < i$.

$$\begin{aligned} F_i(\vec{r}_1, \dots, \vec{r}_N) &= f(t_i) \\ t_i &= \min \{ |\vec{r}_i - \vec{r}_j|, j = 1, \dots, i-1 \} \\ 0 \leq f \leq 1 \quad f' &\geq 0 \end{aligned} \quad (19.51)$$

Note that while G is inherently symmetric, this is not necessarily true for F . Nevertheless the expectation value

$$\frac{\langle \Phi | H^N | \Phi \rangle}{\langle \Phi | \Phi \rangle} \quad (19.52)$$

is an upper bound to the bosonic ground-state energy since this is the *absolute* ground state energy of any extended Hilbert space also containing non-symmetric states.

THE ENERGY EXPECTATION VALUE The next step is to calculate the energy expectation value 19.52 for

$$H^N = \sum_{i=1}^N (-\nabla_i^2 + V_{\text{ext}}(\vec{r}_i)) + \sum_{i<j} v(|\vec{r}_i - \vec{r}_j|) \quad (19.53)$$

19.5 Conclusion

Using zero energy scattering one can fix the function $f(t)$. This allows to perform the rather tedious steps to explicitly calculate the expectation value yielding the wanted result.

□

19.5 CONCLUSION

With the Gross-Pitaevskii equation we have found a way to describe a Bose condensate with a classical field. In deriving the equation we have approximated the field operators and the interaction. This can be justified as one can proof the convergence of the GP energy and density to the physical entities in the limit $N \rightarrow \infty$.

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CHAPTER 20

TIME EVOLUTION OF OPEN QUANTUM SYSTEMS

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*About the paper of G. Lindblad "On the Generators of Quantum
Dynamical Semigroups" [1]*

20.1 INTRODUCTION

In this chapter we will focus on the mathematical background of the time evolution of an open system in general and not on the solution of a specific physical problem. The main mathematical objects we are going to discuss are (semi-) groups and their generators.

These semigroups are further constrained by physical requirements as for example the conservation of probability. In particular we will take a look at positivity preserving semigroups.

The Paper of G. Lindblad treats all the details, that have to be considered for a rigorous proof in infinite dimensions but for simplicity we will treat only finite Hilbert-spaces in this chapter. So $\mathcal{H} = \mathbb{C}^n$ and $\mathcal{B}(\mathcal{H})$ the space of all linear bounded operators on \mathcal{H} is simply the space of all $n \times n$ matrices.

20.2 TIME EVOLUTION OF A CLOSED QUANTUM SYSTEM

First we want to take a look at the case of a closed system. This will be conducted with the aim to show the different steps we have to take into consideration later when we are going to treat the case of the open system.

To get an insight into the methods we will later use on the open system we will now treat the closed system in the same mathematical way.

We can write our time dependent wave function as

$$\psi(t) = U(t)\psi_0 . \quad (20.1)$$

This implies directly

$$U(t) |_{t=0} = \mathbb{I} . \quad (20.2)$$

Further more we demand $U(t)$ to conserve probability which means that for

$$\begin{aligned} \langle \psi_0 | \psi_0 \rangle &= 1 \\ \langle U(t)\psi_0 | U(t)\psi_0 \rangle &= 1 = \langle \psi_0 | U(t)^*U(t)\psi_0 \rangle . \end{aligned} \quad (20.3)$$

So $U(t)$ is unitary, which means that

$$U(t)^*U(t) = \mathbb{I} \quad \text{and} \quad U(-t) = U(t)^{-1} = U(t)^* . \quad (20.4)$$

We also demand any physical time evolution to fulfil the condition:

$$U(t)U(s) = U(s+t) . \quad (20.5)$$

This is a direct consequence of the requirement for the process to be Markovian. We will later explain the detailed nature of Markovian processes. But Markovianity basically tells us, that if two states at times t_1 and t_2 are equal, the respective states at $t_1 + \Delta t$ and $t_2 + \Delta t$ will be equal. So for $t_1 = t_2$ if

$$\psi_0 = U(-t)\psi_t , \quad (20.6)$$

then we know that at a time $t = s + t$ we get the following equation

$$U(s+t)\psi_0 = U(s)\psi_t \quad (20.7)$$

and we can see that the equation (20.5) holds. We can then prove the following statement:

Theorem of Stone: *Every $U(t)$ that satisfies the conditions (20.1) to (20.5) can be written as*

$$U(t) = e^{-itA} . \tag{20.8}$$

Where $A \in \mathcal{B}(\mathcal{H})$ is a self-adjoint operator.

Proof: $U(t)$ is continuous in t because of (20.5). It follows that $U(t)$ fulfils the following differential equation:

$$\dot{U}(t)\psi = AU(t)\psi , \tag{20.9}$$

where $A = \delta U U^*$ and you can prove using equation(20.5) that such an A is time independent. From equation (20.9) the statement follows. So we have shown that $\{U(t) \mid t \in \mathfrak{R}\} \in \mathcal{B}(\mathcal{H})$ forms a continuous one parameter group. In a Hamiltonian system (20.9) is simply the Schrödinger equation and the self-adjoint operator A is the Hamilton operator $-iH$ of the system.

20.3 GENERAL FORM OF THE TIME EVOLUTION OF AN OPEN QUANTUM SYSTEM

We want to go now from a closed system into an open one, describing irreversible time evolution.

20.3.1 MARKOVIAN STATISTICAL PROCESS

The following discussions are limited to Markovian quantum systems. A Markovian quantum system is a system for which the time evolution does not depend on the history of the system, but only on its current state.

An example for a Markovian statistical process is the so called "drunken sailor":

				x_0				
-4	-3	-2	-1	0	1	2	3	4

Table 20.1: The Drunken sailor is at $t = 0$ at position x_0

The drunken sailor lives in an one dimensional world and in each time step,

20.3 General Form of the Time Evolution of an Open Quantum System

he goes either one step to the left or one step to the right of his current position with equal probability. The probability for the sailor to be at a position x after a certain time t depends only on the probability distribution of the sailor at $t = 0$ and on t . Here it is important to stress again, that the probability does not depend on the way the probability distribution at $t = 0$ was achieved. Furthermore shifting $t = 0$ in time will not change the time evolution for a fixed Δt .

An example of a non-Markovian statistical process would be the following:

Suppose we have 5 black and 5 white balls in a box, and we take them out of the box one after another. After a ball is taken out, it is not put back into the box for the next draw. We can arrive at two situations $\bigcirc \bigcirc \otimes \otimes$ and $\bigcirc \otimes$ where the probability to take a white ball in the next step is 50% in both systems. However in the step after that the probabilities of the two systems differ a lot, because the two systems have a different history.

20.3.2 PROPERTIES OF THE TIME EVOLUTION IN AN OPEN QUANTUM SYSTEM

In general treating the open system as a subsystem of a bigger system $R + S$ of which the time evolution is described by unitary transformations does not lead to a time evolution that is a proper semigroup: Even though we can write

$$\begin{array}{ccc} R \otimes S & \rho_0 & \longrightarrow & U(t)\rho_0U(t)^* \\ & Tr_R(\rho_0) & & Tr_R(U(t)\rho_0U(t)^*) \\ S & \rho'_0 & \longrightarrow & V(t)\rho'_0 \end{array} \quad ,$$

where $V(t)$ is in general not unitary, $V(t)$ is in most cases not a semigroup.

However in applications it is often feasible to use Markovian approximation. We are going to examine the general properties of a dynamical semigroup describing such an irreversible process.

We want to start again with the physical properties we demand of any time evolution. As in the case of a closed system we demand also for the open system the conservation of probability. In the Schrödinger picture we have

$$Tr(\rho) = 1 \quad , \quad (20.10)$$

which has to be conserved under any evolution in time

$$Tr(\phi_t^*(\rho)) = 1 \quad . \quad (20.11)$$

Here it is important to see that instead of a vector ψ the time evolution is now acting on a density matrix ρ . Equivalently we can describe the system in the

Heisenberg picture by looking at the expectation value of any observable X

$$\langle X \rangle_t = \text{Tr}(X \phi_t^*(\rho)) = \text{Tr}(\phi_t(X) \rho) . \quad (20.12)$$

Which then turns the condition (20.11) into

$$1 = \langle \mathbb{I} \rangle_t \implies \phi_t(\mathbb{I}) = \mathbb{I} \quad \forall t . \quad (20.13)$$

Because we are now dealing with density matrices we also have to demand the conservation of positivity. In the Schrödinger picture this reads

$$\rho \geq 0 \implies \phi_t^*(\rho) \geq 0 \quad \forall t . \quad (20.14)$$

For the Heisenberg picture this translates to the condition

$$A \geq 0 \implies \phi_t(A) \geq 0 \quad \forall t , \quad (20.15)$$

where $A \in \mathcal{B}(\mathcal{H})$. As before we also demand the time evolution to be Markovian, so as before in the closed system to fulfil

$$\phi_s \phi_t = \phi_{s+t} \quad (20.16)$$

and we also demand at $t = 0$

$$\phi_0(X) = X \quad (20.17)$$

to be the identical map.

We then get for the Schrödinger picture the following differential equation

$$\dot{\rho} = L^* \rho , \quad (20.18)$$

where

$$\rho(t) = \phi_t(\rho_0) \quad \text{and} \quad \phi_t = \exp(tL^*) . \quad (20.19)$$

In the Hamiltonian case this is simply the Liouville equation

$$\begin{aligned} \dot{\rho} &= -i [H, \rho] \\ \text{where} \quad L^*(\rho) &= -i [H, \rho] \\ \text{giving us} \quad \phi_t(X) &= e^{itH} X e^{-itH} . \end{aligned} \quad (20.20)$$

Where H is the Hamiltonian of the system or, to stress the mathematical picture again, in general a self-adjoint operator on the Hilbert space of the system.

For further considerations we switch now definitely to the Heisenberg picture. So to sum up, we are looking for a one parameter family of maps $\phi_t : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ with:

20.3 General Form of the Time Evolution of an Open Quantum System

- a) ϕ_t is positive
- b) $\phi_t(\mathbb{I}) = \mathbb{I}$
- c) $\phi_s\phi_t = \phi_{s+t}$
- d) $\phi_t(X) \xrightarrow[t \rightarrow 0]{} X$ or for finite dimensions $\phi_0(X) = X$

with $\phi_t = \exp(tL)$. An important remark here: it is the central semigroup property that if $\phi_t \in G$ then $\phi_{-t} = \phi_t^{-1} \notin G$ which is basically directly stating the irreversibility of the time evolution.

20.3.3 THEOREM OF LINDBLAD

We want to show now which general form L takes in a non-Hamiltonian system. To get a better understanding of the steps taken in the proof later on we first what to sketch an overview of the proof and picture how the different steps of the proof are connected to each other.

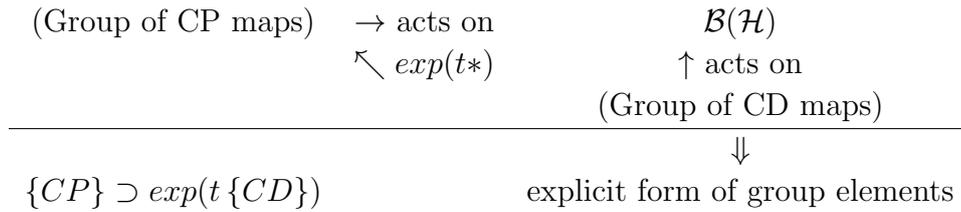


Table 20.2: Overview of the different elements used in the proof and their relations

We showed before that for the time evolution of open systems we have to examine the group of the completely positive (CP) maps, which contains all maps that fulfil the requirements a)- d) from above, except that we replace the condition of positivity by the stronger condition of complete positivity. The difference will be shown in the next section.

What we want to show is, that every element in this group of the CP maps, can be written in terms of a generator $L \in$ Group of the complete dissipative maps (nowadays this property is called Lindbladian because of this paper where Lindblad described this properties for the first time properly), with $\phi_t = \exp(tL)$.

In the first step we are going to examine the properties of the group of CP maps. In a second step we will then examine the properties of CD maps. We will then show, that every element in CD corresponds to a one parameter family in CP and in a final step we will show the general form every element of the group of CD maps takes.

The final statement we want to prove is the following:

Theorem: *Every element of a norm continuous semigroup that fulfils the conditions a)-d) can be written in terms of a generator as $\phi_t = \exp(tL)$ where L is of the following form:*

$$\text{Heisenberg picture } L(X) = \sum_j \left(V_j^\dagger X V_j - \frac{1}{2} \{ V_j^\dagger V_j, X \} \right) + \imath [H, X] \quad (20.21)$$

where $V_j, \sum_j V_j^\dagger V_j \in \mathcal{B}(\mathcal{H}), H$ self-adjoint $\in \mathcal{B}(\mathcal{H})$.

$$\text{Schrödinger picture } L^*(\rho) = \sum_j \left([V_j \rho, V_j^\dagger] + [V_j, \rho V_j^\dagger] \right) - \imath [H, \rho] \quad (20.22)$$

Where we stated the form in the Schrödinger picture just for completeness and $[A, B] = AB - BA, \{A, B\} = AB + BA$ are the usual commutator and anti-commutator.

20.3.4 COMPLETE POSITIVE MAPS

First of all we will show why we need to demand the property of complete positivity instead of simple positivity. To illustrate the problem we take a look at a standard example that was given in [2]. Lets take the transpose operation on a single qubit. This map simply transposes the density operator in the computational basis

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \xrightarrow{T} \begin{pmatrix} a & c \\ b & d \end{pmatrix} \quad (20.23)$$

and conserves the positivity of a single qubit. However suppose this qubit is part of a two qubit system which is initially in the entangled state

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}. \quad (20.24)$$

The transpose is applied to the first of these qubits, while the second one is subject to trivial dynamics. The density operator of the system after the dynamics then is

$$\frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \text{ with Eigenvalues : } \left(\frac{1}{2} \quad \frac{1}{2} \quad \frac{1}{2} \quad -\frac{1}{2} \right). \quad (20.25)$$

So we can see immediately that even though the transpose conserves positivity in the principle system, it does not if applied to a system which contains the principal system as a subsystem.

20.3 General Form of the Time Evolution of an Open Quantum System

Because we are treating an open quantum system, which in general includes an interaction with a reservoir as for example a heat bath, we need to restrict our dynamical semigroup to completely positive maps.

So let's have a look at how we expand the positive map from our subsystem. Suppose S_1 and S_2 are quantum systems, $\phi_{1,t} : \mathcal{B}(\mathcal{H}_1) \rightarrow \mathcal{B}(\mathcal{H}_1)$ the time evolution of S_1 and \mathcal{H}_i the Hilbert-space of S_i .

Consider S_2 to be a closed system with $H_2 = 0$ and extend ϕ_1 to a positive map $\phi : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$, where $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ such that S_2 is unaffected. If S_1 is Hamiltonian then we get from $H = H_1 \otimes \mathbb{I}_2$ that

$$\phi(X \otimes Y) = \phi_1(X) \otimes Y, \quad (20.26)$$

where ϕ_1 has the form

$$\phi_1(X) = U^\dagger X U \quad \text{and} \quad U = e^{tH}. \quad (20.27)$$

If S_1 is non-Hamiltonian equation (20.26) still holds because of the condition

$$\phi(X \otimes \mathbb{I}) = \phi_1(X) \otimes \mathbb{I} \quad \text{and} \quad \phi(\mathbb{I} \otimes Y) = \mathbb{I} \otimes Y. \quad (20.28)$$

For our purpose let \mathcal{H}_2 have finite dimension n . We then have $\mathcal{B}(\mathcal{H}) \simeq M_n(\mathcal{B}(\mathcal{H}_1))$ where $M_n(\mathcal{B}(\mathcal{H}_1))$ denotes the $n \times n$ matrix algebra over $\mathcal{B}(\mathcal{H}_1)$. We can then write

$$\phi_n = \phi \otimes \mathbb{I}_n : M_n(\mathcal{B}(\mathcal{H}_1)) \rightarrow M_n(\mathcal{B}(\mathcal{H}_1)). \quad (20.29)$$

An important remark at this point: \mathbb{I} now denotes the identical map and not the identity matrix.

Definition: $\phi : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ is completely positive iff ϕ_n positive $\forall n$. We then write $\phi \in CP(\mathcal{B}(\mathcal{H}))$.

Proposition: $\phi : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ is CP iff there is a representation π of $\mathcal{B}(\mathcal{H})$ in a Hilbert-space \mathcal{K} and a bounded linear map $F : \mathcal{H} \rightarrow \mathcal{K}$ such that

$$\phi(X) = F^\dagger \pi(X) F. \quad (20.30)$$

This leads to the fact that every normalized $\phi \in CP$ i.e. $\phi(\mathbb{I}) = \mathbb{I}$ fulfils the inequality

$$\phi(X^\dagger) \phi(X) \leq \phi(X^\dagger X), \quad (20.31)$$

which is a generalization of the Cauchy-Schwarz inequality and characterizes every CP map.

Proof:

$$\begin{aligned} (\phi(X^\dagger X) \psi_0, \psi_0) &= (F^\dagger \pi(X)^\dagger \pi(X) \psi_0, \psi_0) \\ &= \|\pi(X) F \psi_0\|^2 \\ &\geq \|F^\dagger \pi(X) F \psi_0\|^2 \\ &= (\phi(X^\dagger) \phi(X) \psi_0, \psi_0). \end{aligned} \quad (20.32)$$

We have used here that from $\phi(\mathbb{I}) = \mathbb{I}$ follows that $\|F^\dagger F\| = 1$ which implies $\|FF^\dagger\| \leq 1$.

So in this section we have learned why complete positivity is important and what the key features of complete positive maps are.

20.3.5 COMPLETELY DISSIPATIVE MAPS (TODAY: LINDBLADIAN MAPS)

As before in the case of the complete positive maps we now want to take a look at the definition of the complete positive maps and their central properties.

Suppose $\phi_t = \exp(tL)$ is a norm continuous semigroup in $\text{CP}(\mathcal{B}(\mathcal{H}))$ with $\phi_t(\mathbb{I}) = \mathbb{I}$. The extension L_n of the generator L to $M_n(\mathcal{B}(\mathcal{H}))$ is defined by $L_n = L \otimes \mathbb{I}_n$ and consequently

$$\phi_t \equiv \phi_t \otimes \mathbb{I} = \exp(tL_n) . \quad (20.33)$$

Differentiation of the inequality (20.32) at $t = 0$ gives

$$L_n(X^\dagger X) - L_n(X^\dagger)X - X^\dagger L_n(X) \geq 0 \quad \forall X \in M_n(\mathcal{B}(\mathcal{H})) . \quad (20.34)$$

It follows directly that $L_n(\mathbb{I}) = 0$ and $L_n(X^\dagger) = L_n(X)^\dagger$. We now introduce the dissipation function $D(L) : \mathcal{B}(\mathcal{H}) \times \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$

$$D(L; X, Y) = L_n(X^\dagger Y) - L_n(X^\dagger)Y - X^\dagger L_n(Y) . \quad (20.35)$$

Definition: *If a bounded map $L : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ satisfies*

$$\begin{aligned} L(\mathbb{I}) &= 0 \\ L(X^\dagger) &= L(X)^\dagger \quad \forall X \in \mathcal{B}(\mathcal{H}) \\ \text{and } D(L_n; X, X) &\geq 0 \quad \forall X \in M_n(\mathcal{B}(\mathcal{H})) \quad \forall n , \end{aligned} \quad (20.36)$$

then L is called completely dissipative and we write $L \in \text{CD}(\mathcal{B}(\mathcal{H}))$.

So now we want to show that

for every $L \in \text{CD} \Rightarrow \phi_t = \exp(tL) \in \text{CP}$ and

for every ϕ_t which is a continuous one parameter semigroup in $\text{CP} \exists L \in \text{CD}$ such that $\phi_t = \exp(tL)$.

Proposition: *Let $L : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ be a bounded map and put $\phi_t = \exp(tL)$ then (1) \Leftrightarrow (2) where*

$$\begin{aligned} (1) \quad &\phi_t(X^\dagger \phi_t(X)) \leq \phi_t(X^\dagger X) \quad \forall X \in \mathcal{B}(\mathcal{H}) \quad \text{with } \phi_t(\mathbb{I}) = \mathbb{I} \\ (2) \quad &D(L; X, X) \geq 0 \quad \forall X \in \mathcal{B}(\mathcal{H}) \quad \text{with } L(\mathbb{I}) = 0 . \end{aligned} \quad (20.37)$$

20.3 General Form of the Time Evolution of an Open Quantum System

We have already shown (1) \Rightarrow (2) in the beginning of this section. (2) \Rightarrow (1) is more difficult and can be found in the original paper from G. Lindblad.

If we apply this to the extension L_n and ϕ_n to $M_n(\mathcal{B}(\mathcal{H})) \forall n$ we get that ϕ_t is a norm continuous semigroup on $\mathcal{B}(\mathcal{H})$ iff $\phi_t = \exp(tL)$ where $L \in \text{CD}(\mathcal{B}(\mathcal{H}))$.

So besides the properties of the group of CD maps we have also found in this section the connection between the CP maps and the CD maps.

20.3.6 GENERAL FORM OF ELEMENTS IN CD

Now in this last section we want to take a look at the general form L takes,

Proposition: $D(L)$ determines L up to a Hamiltonian.

Proof: If $D(L; X, Y) = 0 \forall X, Y \in \mathcal{B}(\mathcal{H})$ then is L called a derivative and we know that $\exists Y \in \mathcal{B}(\mathcal{H})$ such that $L(X) = [Y, X]$. Because we know that $L(X^\dagger) = L(X)^\dagger$ it follows that $Y = \imath H$, where H is a self adjoint operator. So we get $L(X) = \imath[H, X]$ and we find again the well known form for the time evolution:

$$\phi_t = e^{\imath t H} X e^{-\imath t H} . \quad (20.38)$$

Because we know that $[H, X^\dagger Y] = [H, X^\dagger]Y - X^\dagger[H, Y]$ so for an L defined like that we get that $D(L) = 0$ so $D(L) \neq 0$ characterizes the lack of reversibility and the deviation from a Hamiltonian system.

We can show now that there is a $\psi \in \text{CP } \mathcal{B}(\mathcal{H})$ and a self adjoint $H \in \mathcal{B}(\mathcal{H})$ such that

$$L(X) = \psi(X) - \frac{1}{2} \{ \psi(\mathbb{I}), X \} + \imath[H, X] \in \text{CD} . \quad (20.39)$$

The conditions $L(\mathbb{I}) = 0$ and $L(X^\dagger) = L(X)^\dagger$ are obviously fulfilled. We also know that we can write $\psi(X) = F^\dagger \pi(X) F$ where we can choose $\pi(\mathbb{I}) = \mathbb{I}$ and we get

$$\psi(X^\dagger X) + X^\dagger \psi(\mathbb{I}) X - \psi(X^\dagger) X - X^\dagger \psi(X) = (\pi(X) F - F X)^\dagger (\pi(X) F - F X) \geq 0 . \quad (20.40)$$

If we rearrange the terms we get $D(L; X, X) \geq 0$. To show that we can find such a representation $\forall L(X) \in \text{CD}$ is more difficult and again it can be found in the original paper.

To get to the form we headed out for, we need the following statement:

Theorem by Kraus: $\phi \in \text{CP } (\mathcal{B}(\mathcal{H}))$ iff it can be written in the following form

$$\phi(X) = \sum_j V_j^\dagger X V_j , \quad (20.41)$$

where $V_j, \sum_j V_j^\dagger V_j \in \mathcal{B}(\mathcal{H})$.

If we plug this into equation (20.39) we get the general form of the generator as

we proposed in the beginning.

$$L(X) = \sum_j \left(V_j^\dagger X V_j - \frac{1}{2} \{ V_j^\dagger V_j, X \} \right) + i [H, X] , \quad (20.42)$$

where $V_j, \sum_j V_j^\dagger V_j \in \mathcal{B}(\mathcal{H}), H$ self-adjoint $\in \mathcal{B}(\mathcal{H})$.

We have now shown, that any generator of a quantum dynamical semigroup can be written in this specific form. This makes it now a lot easier to calculate the time evolution of an arbitrary open quantum system because the only thing that is left to do now is to find the appropriate V_j 's and H .

20.4 CONCLUSION

In his paper "On the Generators of Quantum Dynamical Semigroups" G. Lindblad treated the mathematical form of the time evolution of open quantum systems rigorously. In this Section we got an overview of the proof and carried out most of the key steps of the proof for the case of a finite dimensional Hilbert-space.

Knowing this general form one can compute now the time evolution of an open system if we find the correct form of the V_j 's and H . To finish the report let's have a look at how these look like in the case of photons in a cavity:

$$H = (a^\dagger a + \frac{1}{2}) \quad V^\dagger = a^\dagger \quad V = a , \quad (20.43)$$

where H is just the usual Hamiltonian for an electro-magnetic field, V^\dagger is the creation and V is the annihilation operator for photons.

20.4 Conclusion

BIBLIOGRAPHY

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