

4. Second quantization

4.2 Field operators

... but before we start...

RECAP

- \mathcal{H} Hilbert space

example: for spin- $\frac{1}{2}$ particles

$$\mathcal{H} = \mathbb{C}^2 \otimes L^2(\mathbb{R}^3)$$

$$\begin{pmatrix} \text{spin} \\ (\alpha(r)) \\ (\beta(r)) \end{pmatrix}$$

functions over \mathbb{R}^3 that are
"square-integrable", ie

$$f, g \in L^2(\mathbb{R}^3) \Leftrightarrow \int d^3\vec{r} f(\vec{r}) g(\vec{r}) < \infty$$

↳ example: $\psi_k(\vec{r}) = \frac{1}{V} e^{\frac{i\vec{k} \cdot \vec{r}}{V}}$

turns out $\mathcal{H} \cong L^2(\mathbb{R}^3 \otimes \{ \uparrow, \downarrow \})$

so instead of $\mathcal{H} \ni \Psi = \begin{pmatrix} \Psi_\uparrow(\vec{r}) \\ \Psi_\downarrow(\vec{r}) \end{pmatrix}$

we can write $\mathcal{H} \ni \Psi(\vec{r}, s) =: \Psi_s(\vec{r})$

- kets and bras

- ... are functions:

$$|\psi\rangle: \mathbb{C} \longrightarrow \mathbb{H}$$

$$\alpha \longmapsto \alpha \psi$$

$$(\psi \in \mathbb{H}, \text{eg } \psi(\vec{x}) = \frac{1}{\nu} e^{\frac{i \vec{k} \cdot \vec{x}}{\hbar}})$$

$$\langle \phi |: \mathbb{H} \longrightarrow \mathbb{C}$$

$$\psi \longmapsto \cancel{\langle \phi, \psi \rangle}$$

$$, \phi \in \mathbb{H}$$

example: if $\mathbb{H} = L^2(\mathbb{R}^3)$

$$\langle \phi |: \cancel{\psi} \rightarrow \int d^3 \vec{r} \phi^*(\vec{r}) \psi(\vec{r})$$

So the "inner product" between bra and ket is also a function

$$\langle \phi | \psi \rangle: \mathbb{C} \rightarrow \mathbb{C}$$

$$\alpha \longmapsto \alpha \langle \phi, \psi \rangle$$

$$\text{eg } \alpha \longmapsto \alpha \int d^3 \vec{r} \phi^*(\vec{r}) \psi(\vec{r})$$

↳ if $\{\psi_i\}_i$ form an orthonormal basis of \mathbb{H} ,

$$\langle \psi_i | \psi_j \rangle: \mathbb{C} \rightarrow \mathbb{C}$$

$$\alpha \longmapsto \delta_{ij} \alpha$$

$\Rightarrow \delta_{ij}$, delta function

- Commutators

$$[A, B]_{\mp} := AB \mp BA \quad (\text{we'll use } - \text{ for Bosons and } + \text{ for Fermions})$$

- Permutations

$$\mathcal{P}_{\pm} := \sum_{P \in S_n} (\pm 1)^{|P|} P \quad (+ \text{ for Bosons, } - \text{ for Fermions})$$

↳ Bosons always on top!
(alphabetical order)

Differential operators (differential)

- a especially convenient basis for $\mathcal{B} = L^2(\mathbb{R}^3)$

function: $\delta_{\vec{y}}(\vec{x}) := \delta(\vec{y} - \vec{x})$ (delta function)

In particular:

$$\begin{aligned}\langle \delta_y | \psi \rangle &= \int d^3x \delta(\vec{y} - \vec{x}) \psi(\vec{x}) \\ &= \psi(\vec{y})\end{aligned}$$

→ this notation will allow us to skip many annoying calculations
 (↑ mean simplify)

e.g. to prove Eq. 4.2.5 (page 58 of the script):

$\{\psi_i\}$: on. basis of \mathcal{B}

$$\sum_i \psi_i^*(\vec{y}) \psi_i(\vec{x}) = \cancel{\sum_i \psi_i^*(\vec{y}) \psi_i(\vec{x})}, \sum_i \langle \psi_i | \delta_x \rangle \langle \delta_y | \psi_i \rangle$$

$$= \sum_i \langle \delta_y | \psi_i \rangle \langle \psi_i | \delta_x \rangle$$

$$= \langle \delta_y | \underbrace{\left(\sum_i |\psi_i\rangle \langle \psi_i| \right)}_{\mathbb{I}} | \delta_x \rangle$$

$$= \langle \delta_y | \delta_x \rangle = \int d^3x \delta(y-x) \delta(x-y)$$

$$= \delta(y-x)$$

Now we can define the Field operators

$\{\psi_i\}$ basis of $L^2(\mathbb{R}^3)$

$$\Psi_s(\vec{x}) = \sum_i \psi_i(\vec{x}) a_{is}$$

(Capital Psi
(I know...))

$$= \sum_i \langle \delta_x | \psi_i \rangle a_{is}$$

$\{a_{is}\}_{is}$ for Bosons or Fermions

$$\Psi_s^\dagger(\vec{x}) = \sum_i \cancel{\text{star}} \quad \psi_i^*(\vec{x}) a_{is}^\dagger$$

$$= \sum_i \langle \psi_i | \delta_x \rangle a_{is}^\dagger$$

Physical interpretation: creates (ψ^\dagger) or destroys (ψ) a particle at position \vec{x} (with spin s)

Commutation relations

$$[\Psi_s(x), \Psi_z(y)]_+ = [\sum_i \langle \delta_x | \psi_i \rangle a_{is}, \sum_j \langle \delta_y | \psi_j \rangle a_{jz}]_+$$

$$= \sum_{ij} \langle \delta_x | \psi_i \rangle \langle \delta_y | \psi_j \rangle [a_{is}, a_{jz}]_+$$

$$= 0 \quad \text{since } [a_{is}, a_{jz}]_+ = 0 \quad (\text{again, we're doing - for Bosons, + for Fermions})$$

$$[\Psi_s^\dagger(x), \Psi_z^\dagger(y)]_+ = 0 \quad (\text{same: } [a_{is}^\dagger, a_{jz}^\dagger]_+ = 0)$$

$$[\Psi_s(x), \Psi_z^\dagger(y)]_+ = \sum_{ij} \langle \delta_x | \psi_i \rangle \langle \psi_j | \delta_y \rangle [a_{is}, a_{jz}^\dagger]_+$$

$$= \sum_{ij} \langle \delta_x | \psi_i \rangle \langle \psi_j | \delta_y \rangle \delta_{sz} \delta_{ij}$$

$$= \delta_{sz} \delta(\vec{x} - \vec{y})$$

Generalization

We can use field operators to create states of many particles:

$$|x_1, s_1; x_2, s_2; \dots; x_n, s_n\rangle = \frac{1}{\sqrt{n!}} \Psi_{s_n}^+(x_n) \dots \Psi_{s_2}^+(x_2) \Psi_{s_1}(x_1) |0\rangle$$

↳ meaning: 1st I create a particle with spin s_1 at x_1 ,
then a particle with spin s_2 at x_2, \dots ,
finally a particle with spin s_n at x_n

↳ Does the order of creation matter?

(see 2-part. example in footer of page 7.)

$$|x_1, s_1; x_2, s_2; \dots; x_n, s_n\rangle = \frac{1}{\sqrt{n!}} \Psi_{s_n}^+(x_n) \dots \Psi_{s_2}^+(x_2) \Psi_{s_1}^+(x_1) |0\rangle$$

$$\begin{aligned} &= \frac{1}{\sqrt{n!}} \Psi_{s_n}^+(x_n) \dots \left([\Psi_{s_2}^+(x_2), \Psi_{s_1}^+(x_1)]_+ - \Psi_{s_2}^+(x_2) \Psi_{s_1}^+(x_1) \right) |0\rangle \\ * &\quad \curvearrowleft \\ &= \pm \frac{1}{\sqrt{n!}} \Psi_{s_n}^+(x_n) \dots [\Psi_{s_2}^+(x_2), \Psi_{s_1}^+(x_1)]_+ |0\rangle \\ &= \pm |x_2, s_2; x_1, s_1; \dots; x_n, s_n\rangle \end{aligned}$$

∴ The order matters only for Fermions

$$* [\Psi_{s_2}^+(x), \Psi_{s_1}^+(y)]_+ = \begin{cases} 0, \text{ for Bosons} \\ 2 \Psi_{s_2}(x) \Psi_{s_1}^+(y), \text{ for Fermions} \end{cases}$$

$$\begin{aligned} [\bar{A}, \bar{B}]_+ &= 0 \rightarrow [\bar{A}, \bar{B}]_+ = AB + BA = AB - BA + 2BA \\ &= 2BA = 2AB \end{aligned}$$

What happens when you add another particle to an n -particle state?
You get a non-normalized $(n+1)$ -particle state!

$$\Psi_s(x) |x_1, s_1; \dots; x_n, s_n\rangle = \frac{1}{\sqrt{n!}} \Psi_s(x) \Psi_{s_1}(x_1) \dots \Psi_{s_n}(x_n) |0\rangle$$

$$= \sqrt{n+1} |x_1, s_1; \dots; x_n, s_n; x, s\rangle$$

\downarrow
goes to the end!

What happens when you try to destroy a particle?

$$\Psi_s(x) |x_1, s_1; \dots; x_n, s_n\rangle = \dots \text{you'll prove this in the exercise}$$

(Series 9, Ex. 2)

What is the inner product between two n -particle states?

~~$\langle y_1, \dots, y_n | x_1, \dots, x_n \rangle = \delta_{nm} \sum_{P \in S_n} \frac{(-1)^P}{P!} \delta(x_{p_1} - y_1) \dots \delta(x_{p_n} - y_n)$~~

notice that
we're ignoring
spin for now

you'll also prove
this in the Exercise

$$\frac{\delta_{nm}}{n!} \sum_{P \in S_n} (-1)^P [\delta(x_1 - y_1) \dots \delta(x_n - y_n)]$$

P acting on x (experimental notation)

meaning:

meaning $\{x_i\} \neq \{y_j\}$

- if $\exists i : x_i \neq y_j \forall j$ $\rightarrow \langle y_1, \dots, y_n | x_1, \dots, x_n \rangle = 0$

- if (x_1, \dots, x_n) is an even permutation of $(y_1, \dots, y_n) \rightarrow \langle \dots | \dots \rangle = \frac{1}{n!}$

- if (x_1, \dots, x_n) is an odd permutation of $(y_1, \dots, y_n) \rightarrow \langle \dots | \dots \rangle = -\frac{1}{n!}$

Now, since $\{\psi_i\}$ are a basis for $L^2(\mathbb{R}^3)$, the $\{|x_1, \dots, x_n\rangle_{x_1, \dots, x_n}\}$ form a basis for the n -particle space.

↳ sticking to ket notation
for convenience

we can expand any other wave function ϕ as

$$|\phi\rangle = \int d^3x_1 d^3x_2 \dots d^3x_n \langle x_1, \dots, x_n | \phi \rangle |x_1, \dots, x_n\rangle$$

where $\langle x_1, \dots, x_n | \phi \rangle = \frac{1}{n!} \sum_{P \in S_n} (\pm)^{|P|} \langle x_{P(1)}, \dots, x_{P(n)} | \phi \rangle$

$|x_1, \dots, x_n\rangle$ has the same role
as $|x\rangle$, for many particles:

$\langle x_1, \dots, x_n | \phi \rangle := \phi(x_1, \dots, x_n)$

*

$$= \frac{1}{n!} P_x^\pm [\langle x_1, \dots, x_n | \phi \rangle]$$

$$\begin{cases} 1, & \text{if } |\phi\rangle \text{ even perm. of } \langle x_1, \dots, x_n \rangle \\ -1, & \text{if } |\phi\rangle \text{ odd perm. of } \langle x_1, \dots, x_n \rangle \\ 0, & \text{otherwise} \end{cases}$$

4.2.1 Fockspace

(there should be a space between Fock and space)

Let \mathcal{H}_n be the Hilbert space for n particles (Bosons or Fermions). Then

$$\Psi_s^+(x) : \mathcal{H}_n \rightarrow \mathcal{H}_{n+1}, \quad \Psi_s^-(x) : \mathcal{H}_n \rightarrow \mathcal{H}_{n-1}$$

We can define the Fock space,

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{H}_n, \quad \mathcal{H}_0 = \{|0\rangle\}, \quad \bigoplus \text{ means direct sum:}$$

$$\mathcal{H}_n \bigoplus \mathcal{H}_m = \emptyset, \quad m \neq n$$

and together they "span" \mathcal{F}

* in fact $\langle x_1, s_1 | x_2, s_2 \rangle = \Psi_{s_2}^+(x_2) |0\rangle = \sum_i \langle \psi_i | 0 \rangle a_i^\dagger |0\rangle = \sum_i \langle \psi_i | 0 \rangle |0\rangle \otimes |s_2\rangle = \left(\sum_i |\psi_i\rangle \otimes |\psi_i\rangle \right) |0\rangle \otimes |s_2\rangle = 1 |0\rangle \otimes |s_2\rangle$

~~WTF~~ ~~WTF~~ ~~WTF~~ ~~WTF~~ ~~WTF~~

The elements of \mathcal{F} have the form

$$|\Psi\rangle = \{ |\psi_0\rangle_{\mathbb{R}_0}, |\psi_1\rangle_{\mathbb{R}_1}, \dots, |\psi_n\rangle_{\mathbb{R}_n}, 0, 0, \dots \}$$

\hookrightarrow stops here
(somewhere)

With inner product

$$\langle \Psi^* | \Psi \rangle = \sum_{n=0}^{\infty} \langle \psi_n^* | \psi_n \rangle_{\mathbb{R}_n} < \infty$$



4.3 Observables

4.3.1 Density op. particles

just like in the 1-particle case, we define the operator

$$\hat{\rho}(\vec{x}) = \sum_{i=1}^{n \xrightarrow{\text{max # particles (may as well go to } \infty\text{)}}} \delta(\vec{x} - \vec{x}_i)$$

\hookrightarrow operator \hat{x} for \vec{x}_i
 \hookrightarrow 3D delta function, area δ^3

Let $|\phi\rangle, |\chi\rangle$ be two n -particle states, ie

$$|\phi\rangle = \int d^3x_1 \dots d^3x_n \langle x_1, \dots, x_n | \phi \rangle |x_1, \dots, x_n \rangle$$

(same for $|\chi\rangle$)

$$\begin{aligned} \langle \chi | \hat{\rho}(\vec{x}) | \phi \rangle &= \langle \chi | \hat{\rho}(\vec{x}) | \phi \rangle \\ &= \langle \chi | \left[\int d^3x_1 \dots d^3x_n |x_1, \dots, x_n \rangle \langle x_1, \dots, x_n| \right] \hat{\rho}(\vec{x}) | \phi \rangle \\ &= \int d^3x_1 \dots d^3x_n \langle \chi | x_1, \dots, x_n \rangle \langle x_1, \dots, x_n | \sum_i \delta(\vec{x} - \vec{x}_i) | \phi \rangle \end{aligned}$$

$$\sum_i \int d^3x_1 \dots d^3x_n \delta(\vec{x} - \vec{x}_i) \langle \chi | x_1, \dots, x_n \rangle \langle x_1, \dots, x_n | \phi \rangle$$

Identical particles: $F(x_1) = \dots = F(x_n)$

~~for particles that can't be distinguished~~

?

(-> phase?)
(absorbed later!)

$$\delta(x - x_i) = \dots = \delta(x - x_n)$$

$$\langle x | \hat{p}(x) | \phi \rangle = \sum_{i=1}^n \int d^3x_1 \dots d^3x_n \delta(x - x_i) \langle x | x_1, \dots, x_n \rangle \langle x_1, \dots, x_n | \phi \rangle$$

~~$= n \int d^3x_1 \dots d^3x_n \langle x | x_1, \dots, x_n, x \rangle \langle x_1, \dots, x_n, x | \phi \rangle$~~

~~$= n \int d^3x_1 \dots d^3x_n \delta(x - x_1, \dots, x_n, x) \langle x_1, \dots, x_n | \phi \rangle$~~

↳ this "counts" the number of particles, n

Just like before we had

$$\hat{n} = a^\dagger a,$$

now we have

$$\hat{p}(x) = \Psi^+(x) \Psi(x) \dots \text{and we'll prove it!}$$

$$\langle x | \Psi^+(x) \Psi(x) | \phi \rangle = \langle x | \Psi^+(x) \Psi(x) | \phi \rangle$$

$$= \langle x | \Psi^+(x) \left[\int d^3x_1 \dots d^3x_{n-1} \langle x_1, \dots, x_{n-1} | \right] \Psi(x) | \phi \rangle$$

$$= \left\langle \int d^3x_1 \dots d^3x_{n-1} \langle x | (\Psi^+(x) | x_1, \dots, x_{n-1} \rangle) \langle x_1, \dots, x_{n-1} | \Psi(x) \rangle | \phi \rangle \right\rangle$$

$$= \int d^3x_1 \dots d^3x_{n-1} \langle x | (\sqrt{n} | x_1, \dots, x_{n-1}, x \rangle) (\sqrt{n} \langle x_1, \dots, x_{n-1}, x |) | \phi \rangle$$

$$= n \int d^3x_1 \dots d^3x_{n-1} \langle x | x_1, \dots, x_{n-1}, x \rangle \langle x_1, \dots, x_{n-1}, x | \phi \rangle$$

$$= \langle x | \hat{p}(x) | \phi \rangle$$

Scattered state $\langle x | \psi_{\text{in}} \rangle$

$$a_i^+ \psi_i^*(x) \quad \left. \right\} \psi_i(x) a_j$$

$$= a_i^+ \langle \psi_i | x \rangle \quad \left. \right\} \langle x | \psi_i \rangle a_j$$

$$= \langle \psi_i | x \rangle \quad \left. \right\} \langle x | \psi_i \rangle a_i^+ a_j$$

1 particle : $-\frac{\hbar^2}{2m} \nabla^2 \langle x |$

?

?

$$[B, C] = BC - CB$$

$$[A, B, C] = \cancel{[A, [B, C]]} + ABC - CAB \quad BC = [B, C] + CB$$

$$= A(CB + [B, C]) - CAB$$

$$= A[B, C] + [A, C]B$$

$$\psi^+(y) \underbrace{[\nabla^2 \psi(y), \psi(x)]}_0 + [\psi^+(y), \psi(x)] \nabla^2 \psi(x)$$

Now $\hat{\rho}(\vec{x})$ gives you the density of particles at position \vec{x} .

For the total number of particles, simply integrate over \vec{x} :

$$\begin{aligned}\hat{N} &= \int d^3\vec{x} \hat{\rho}(\vec{x}) \\ &= \int d^3x \Psi^*(x) \Psi(x) \\ &= \sum_{ij} \int d^3x \cancel{\text{cancel}} \langle \psi_i | x \rangle \langle x | \psi_j \rangle a_i^* a_j \\ &= \sum_{ij} \langle \psi_i | \left[\int d^3x |x\rangle \langle x| \right] |\psi_j \rangle a_i^* a_j \\ &= \sum_{ij} \langle \psi_i | \psi_j \rangle a_i^* a_j \quad \rightarrow \text{looks familiar?}\end{aligned}$$

4.3.2 Other operators

We want to relate this field formalism to quantities we know (and can measure). Take for instance the kinetic energy operator \hat{T}

$$1 \text{ particle: } \hat{T} = -\frac{\hbar^2}{2m} \int d^3x |x\rangle \nabla^2 \langle x|$$

$$\text{so that } \langle x | \hat{T} | \phi \rangle = -\frac{\hbar^2}{2m} \int d^3x \langle x | x \rangle \nabla^2 \langle x | \phi \rangle$$

$$= -\frac{\hbar}{2m} \int d^3x \cancel{\Psi(x)} \Psi^*(x) \nabla^2 \phi(x)$$

$$\text{field operator: } \hat{T} = \sum_{ij} a_i^* \langle \psi_i | \hat{T} | \psi_j \rangle a_j = \sum_{ij} a_i^* a_j \langle \psi_i | \hat{T} | \psi_j \rangle$$

~~$\hat{T} = \sum_{ij} a_i^* \langle \psi_i | \hat{T} | \psi_j \rangle a_j$~~

\downarrow if \hat{T} takes $|\psi_j\rangle$ to $|\psi_i\rangle$

\downarrow creates $|\psi_i\rangle$

\downarrow destroys $|\psi_j\rangle$

So that

$$\langle x | \hat{T} | \phi \rangle = \sum_{ij} \langle x | a_i^\dagger \langle \psi_i | \hat{T} | \psi_j \rangle a_j | \phi \rangle$$

~~if $\langle \psi_i | \hat{T} | \psi_j \rangle = \langle \psi_i | a_i^\dagger a_j | \phi \rangle$~~

~~$\hat{T} = \frac{-\hbar^2}{2m} \nabla^2$~~

$$= \langle x | \left(\sum_i a_i^\dagger \langle \psi_i | x \rangle \right) \left(\frac{-\hbar^2}{2m} \nabla^2 \right) \left(\sum_j a_j \langle x | \psi_j \rangle \right) | \phi \rangle$$

$$= \langle x | \Psi^+(x) \left(\frac{-\hbar^2}{2m} \nabla^2 \right) \underline{\Psi^-(x)} | \phi \rangle$$

where we had $|x\rangle$, now we have $\Psi(x)$

$$\hookrightarrow \hat{T} = \frac{-\hbar^2}{2m} \int d^3x \Psi^+(x) \nabla^2 \Psi^-(x)$$

This applies to other operators too. Eg potential energy:

$$\hat{U} = \int d^3x U(x) |x\rangle \langle x|$$

becomes

$$\hat{U} = \sum_{ij} \langle \psi_i | \hat{U} | \psi_j \rangle a_i^\dagger a_j$$

$$= \int d^3x U(x) \Psi^+(x) \Psi^-(x)$$

(more examples in the script)

Eg 2-particle interaction described by potential $V(x-y)$

$$\hat{H}_{ww} = \frac{1}{2} \sum_{s_1, s_2} \int d^3x d^3y \Psi_{s_1}^+(x) \Psi_{s_2}^+(y) V(x-y) \Psi_{s_2}^-(y) \Psi_{s_1}^-(x)$$

normalization just in case you had forgotten about spin! ..

4.3.3 Field equations

Heisenberg picture: operators evolve in time

$$\Psi(x, t) = e^{i\hat{H}t/\hbar} \Psi(x) e^{-i\hat{H}t/\hbar}$$

Equations of motion

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = - [\hat{H}, \Psi(x, t)] \\ = -e^{i\hat{H}t/\hbar} [\hat{H}, \Psi(x)] e^{-i\hat{H}t/\hbar}$$

\downarrow we have to compute this commutator!

Dosons

Kinetic energy:

$$[\hat{T}, \Psi(x)] = -\frac{\hbar^2}{2m} \int d^3y [\psi^+(y) \nabla^2 \psi(y), \psi(x)] \\ = -\frac{\hbar^2}{2m} \int d^3y \psi^+(y) [\nabla^2 \psi(y), \psi(x)] + [\psi^+(y), \psi(x)] \nabla^2 \psi(y) \\ = -\frac{\hbar^2}{2m} \int d^3y \psi^+(y) \cdot 0 = \delta(\mathbf{y}-\mathbf{x}) \nabla^2 \psi(y) \\ = \frac{\hbar^2}{2m} \nabla^2 \psi(x)$$

$$[\hat{H}_{\text{int}}, \Psi(x)] = \frac{1}{2} \int d^3y_1 d^3y_2 V(\mathbf{y}_2 - \mathbf{y}_1) [\psi^+(y_1) \psi^+(y_2) \psi(y_1) \psi(y_2), \Psi(x)]$$

$$= \frac{1}{2} \int d^3y_1 d^3y_2 V(\mathbf{y}_2 - \mathbf{y}_1) \underbrace{[\psi^+(y_1) \psi^+(y_2), \Psi(x)]}_{\text{other term}} \psi(y_1) \psi(y_2) + 0$$

$\frac{1}{2} \int d^3y_1 d^3y_2$

\downarrow let's just look at this

$$\begin{aligned}
 [\psi^+(y_1), \psi^+(y_2), \psi(x)] &= \psi^+(y_2) [\psi^+(y_2), \psi(x)] \\
 &\quad + [\psi^+(y_2), \psi(x)] \psi^+(y_2) \\
 &= -\psi^+(y_2) \delta(x-y_2) - \delta(x-y_2) \psi(y_2)
 \end{aligned}$$

$$[H_{\text{int}}, \psi(x)] = - \int d^3y \psi^+(y) V(x-y) \psi(y) \psi(x)$$