Quantum harmonic oscillator

We first consider a single one-dimensional harmonic oscillator with Hamiltonian

$$\mathcal{H} = \hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$$

where $\hat{a}$ and $\hat{a}^+$ are the lowering and raising operators, respectively. The stationary states are denoted by $|n\rangle$ for $n = 1, 2, \ldots$ and satisfy

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle, \quad \hat{a}^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

such that

$$\hat{n} \equiv \hat{a}^+ a \quad \Rightarrow \quad \hat{n}\,|n\rangle = n\,|n\rangle$$

is the number operator. The energy is then given by

$$\mathcal{H}\,|n\rangle = \varepsilon_n\,|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle .$$

We want to consider now N such harmonic osc. with total Hamiltonian

$$\mathcal{H}_{tot} = \sum_{i=1}^{N} \overset{\text{single harm. osc.}}{\mathcal{H}_i} = \sum_{i=1}^{N} \hbar\omega\left(\hat{a}_i^+\hat{a}_i + \frac{1}{2}\right).$$

Note that the harm. osc. are not interacting. The stationary states are tensor products of the single harm. osc. stationary states

$$|n_1, \dots, n_N\rangle = |n_1\rangle \otimes \dots \otimes |n_N\rangle$$

with $n_1, \dots, n_N = 1, 2, \dots$ such that

$$\mathcal{H}_{tot} |n_1, \dots, n_N\rangle = \sum_{i=1}^{N} \hbar\omega \left(n_i + \frac{1}{2}\right).$$

How can we describe the thermodynamic of such a system? In the classical case, the connection between the statistical (microscopic) and the thermodynamical (macroscopic) description is provided by the definition of the entropy as

$$S = k_B \log \omega(E) \qquad (*)$$

where $\omega(E)$ is the number of states (microscopic) with a prescribed energy. In the quantum case it is hence pertinent to define $\omega(E)$ as the number of stationary states with prescribed energy E, that is

$$\mathcal{H} |\psi_i\rangle = \varepsilon_i |\psi_i\rangle \qquad \left(\begin{array}{c}\text{stationary}\\\text{states}\end{array}\right)$$

$$\omega(E) = \sum_i \delta(E - \varepsilon_i) = tr\Big(\sum_{E \leq \varepsilon_i \leq E+\delta} |\psi_i\rangle\langle\psi_i|\Big)$$

and still define the entropy using eq. $(*)$.

Going back to our harmonic oscillators, this means that we have to compute

$$w(E) = \sum_{n_1=0}^{\infty}{}' \cdots \sum_{n_N=0}^{\infty}{}' \, \delta\Big(E - \sum_{i=1}^{N}{}' \hbar\omega\big(n_i + \tfrac{1}{2}\big)\Big) .$$

In order to compute this nested sum, we rewrite the δ-function using the identity

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \, e^{ikx}$$

to obtain

$$w(E) = \sum_{n_1=0}^{\infty}{}' \cdots \sum_{n_N=0}^{\infty}{}' \frac{1}{2\pi} \int dk \; e^{ik\left(E - \sum_{i=1}^{N} \hbar\omega (n_i + \frac{1}{2})\right)}$$

$$= \frac{1}{2\pi} \int dk \; e^{ikE} \prod_{i=1}^{N} \frac{e^{-ik\frac{\hbar\omega}{2}}}{1 - e^{-ik\hbar\omega}} = \frac{1}{2i \sin\left(k \frac{\hbar\omega}{2}\right)}$$

using the harmonic (sic) expansion $\frac{1}{1-x} = \sum_{n=0}^{\infty}{}' x^n$.
This can be rewritten as

$$w(E) = \int \frac{dk}{2\pi} \; e^{N\left(ik \underbrace{\frac{E}{N}}_{\equiv e} - \log\left(2i \sin\left(k\frac{\hbar\omega}{2}\right)\right)\right)}$$

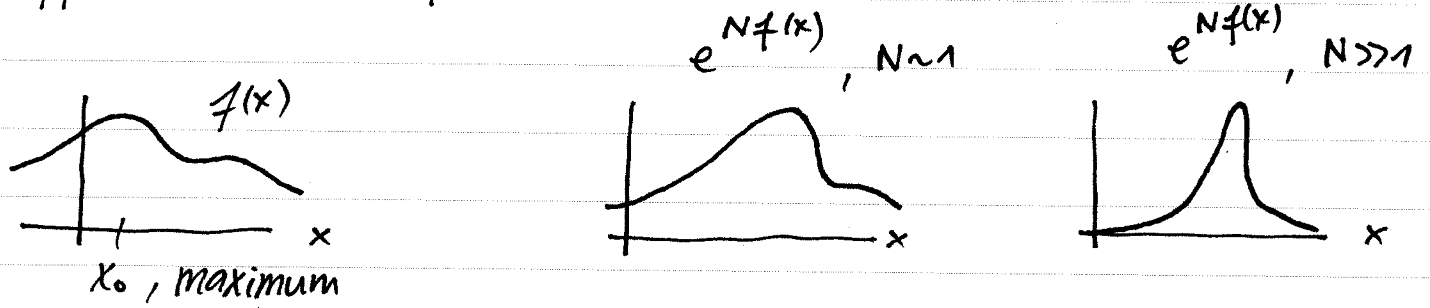
We are here interested in the asymptotic expansion for $N \to \infty$ of this integral, for $e = E/N$ fixed.

Interlude: saddle point approximation
a.k.a. steepest descent
stationary phase

We consider the integral

$$\int_{-\infty}^{\infty} dx \; e^{N f(x)}$$

as $N \to \infty$. Let us consider the situation pictorialy for different values of N:



Intuitively: as $N \to \infty$ the function $e^{Nf(x)}$ tend to $\delta(x_0)$, where x_0 is the position of the maximum of f. Hence for N big we can approximate $f(x)$ as

$$f(x) = f(x_0) + (x-x_0)\cancelto{0}{f'(x_0)} + \frac{1}{2}(x-x_0)^2 f''(x_0)$$

such that we obtain

$$\int_{-\infty}^{\infty} dx \; e^{N f(x)} \sim e^{N f(x_0)} \underbrace{\int_{-\infty}^{\infty} dx \; e^{\frac{N}{2}(x-x_0)^2 f''(x_0)}}_{= \sqrt{\frac{2\pi}{-N f''(x_0)}}}$$

Here we define

$$f(k) = ike - \log\left(2i \sin\left(k \frac{\hbar\omega}{2}\right)\right).$$

The maximum point k_0 is given by the equation

$$0 = f'(k_0) = ie - \frac{\cancel{2i}\cos\left(k_0 \frac{\hbar\omega}{2}\right)}{\cancel{2i}\sin\left(k_0 \frac{\hbar\omega}{2}\right)} \cdot \frac{\hbar\omega}{2}$$

This equation can be solved by noting that

$$\frac{\cos(-i\log(x))}{\sin(-i\log(x))} = i\,\frac{e^{\log x} + e^{-\log x}}{e^{\log x} - e^{-\log x}} = i\,\frac{x + \frac{1}{x}}{x - \frac{1}{x}} = (-i)\,\frac{1+x^2}{1-x^2}$$

such that if we set $k_0 = -i\frac{2}{\hbar\omega}\log(x)$ we obtain

$$0 = ie - (-i)\frac{\hbar\omega}{2}\left(\frac{1+x^2}{1-x^2}\right) \Rightarrow x = \left(\frac{e + \frac{\hbar\omega}{2}}{e - \frac{\hbar\omega}{2}}\right)^{1/2}$$

such that

$$k_0 = \frac{-i}{\hbar\omega}\log\left(\frac{e + \frac{\hbar\omega}{2}}{e - \frac{\hbar\omega}{2}}\right).$$

We need to compute

$$f(k_0) = ik_0 e - \log\left(2i \sin\left(k_0 \frac{\hbar\omega}{2}\right)\right)$$

$$= ik_0 e - \log\left(2i \sin\left(\frac{-i}{2}\log\left(\frac{e + \frac{\hbar\omega}{2}}{e - \frac{\hbar\omega}{2}}\right)\right)\right)$$

$$\sin(-i\log(x)) = \frac{x - 1/x}{2i}$$

$$= ik_0 e - \log\left(\left(\frac{e+\frac{\hbar\omega}{2}}{e-\frac{\hbar\omega}{2}}\right)^{1/2} - \left(\frac{e-\frac{\hbar\omega}{2}}{e+\frac{\hbar\omega}{2}}\right)^{1/2}\right)$$

$$= ik_0 e - \log\left(\frac{\hbar\omega}{\sqrt{(e+\frac{\hbar\omega}{2})(e-\frac{\hbar\omega}{2})}}\right)$$

$$= \frac{e}{\hbar\omega}\log\left(\frac{e+\frac{\hbar\omega}{2}}{e-\frac{\hbar\omega}{2}}\right) + \frac{1}{2}\log\left(\frac{(e+\frac{\hbar\omega}{2})(e-\frac{\hbar\omega}{2})}{(\hbar\omega)^2}\right)$$

$$= \frac{e+\frac{\hbar\omega}{2}}{\hbar\omega}\log\left(\frac{e+\frac{\hbar\omega}{2}}{\hbar\omega}\right) - \frac{e-\frac{\hbar\omega}{2}}{\hbar\omega}\log\left(\frac{e-\frac{\hbar\omega}{2}}{\hbar\omega}\right).$$

Hence using the saddle point approximation we finally obtain

$$(E) \sim e^{Nf(k_0)} \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{\frac{N}{2}(k-k_0)f''(k_0)}$$

With $f(k_0)$ given by ⊛. As show earlier the gaussian integral will contribute as $N^{-1/2}$ and hence we obtain for the entropy

$$S = k_B \log w(E) \sim N k_B f(k_0) + O(\log N$$

giving us the thermodynamical description of our system.

We can now obtain the caloric equation of state via

$$\left(\frac{\partial S}{\partial E}\right) = \frac{1}{T}$$

which gives

$$\frac{E}{N} = e = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} .$$

Comparing with the Hamiltonian $\mathcal{H}_{tot} = \sum_i \hbar\omega(n_i + \frac{1}{2})$ we see that the distribution of states must be given by

$$\langle n \rangle = \frac{1}{e^{\beta\hbar\omega} - 1} ,$$

which corresponds to the Bose-Einstein distribution. Hence we can interpret the excitations of our harm. oscillators as bosonic particles occupying the mode ω. This correspondence is at the basis of the quantization of field theories.

Having determined $E \equiv U$ we can directly get the heat capacity

$$C = \frac{\partial E}{\partial T} = -k_B \cdot \beta \cdot \frac{\partial E}{\partial \beta} = N k_B \left(\beta \frac{\hbar\omega}{2}\right)^2 \frac{1}{\sinh^2\left(\beta \frac{\hbar\omega}{2}\right)}$$

with the limiting properties

$$C = \begin{cases} N k_B & , \beta \hbar \omega \ll 1 \quad \text{(High T.)} \\ N k_B (\beta \hbar \omega)^2 e^{-\beta \hbar \omega} & , \beta \hbar \omega \gg 1 \quad \text{(Low T.)} \end{cases}$$

In the high-temperature limit, the heat capacity approaches a constant value as for the one-dim. classical oscillators. In the low-temperature limit the heat capacity tends (exponentially) to 0, as required by the third law of thermodynamics.

Hence, we see an illustration of the general fact that the correct low-temperature behaviour of a system, where quantum effects are becoming dominant, is only obtained by a quantum mech. description.