Exercises for Quantum Mechanics 3
Set 9 (module 1)

Exercise 19: **Statistical spread in low-temperature non-interacting systems**

Consider a grand-canonical ensemble of systems that comprise of a large number of non-interacting indistinguishable particles, as described in § 2.6 of the lecture notes. In that paragraph a derivation was given of the average occupation number $[\hat{n}_k] = \bar{n}_k$ belonging to a fully specified 1-particle energy level with energy E_k. In this exercise we want to determine the corresponding statistical spread. To this end we use the identity

$$\hat{\rho}\,\hat{a}_k^\dagger \;=\; \exp(-\beta E_k - \alpha)\,\hat{a}_k^\dagger\,\hat{\rho}$$

for the grand-canonical density operator $\hat{\rho}$, as well as the expressions

$$\exp(\beta E_k + \alpha) \;=\; 1/\bar{n}_k \pm 1$$

for the $\bar{n}_k$ distributions, where the upper (lower) sign refers to bosons (fermions).

(i) Derive the following ensemble average: $[\hat{n}_k^2] = \bar{n}_k\,(\bar{n}_k + 1 \pm \bar{n}_k)$.

(ii) Why could you actually have predicted the fermionic (lower-sign) variant of this result without performing a calculation?

For the statistical spread in the quantum mechanical distributions this implies

$$\Delta n_k \;\equiv\; \sqrt{[\hat{n}_k^2] - \bar{n}_k^2} \;=\; \sqrt{\bar{n}_k\,(1 \pm \bar{n}_k)}\ .$$

Let's now investigate what this means for two extreme low-temperature scenarios.

(iii) What happens to the statistical spread in the fermionic case if $T = 0$?

(iv) What happens to the ground-state statistical spread Δn_0 in the bosonic case if the ground state is occupied macroscopically [$\bar{n}_0 = \mathcal{O}(\text{total number of particles}) \gg 1$]?

Exercise 20: **Bose−Einstein condensation or no Bose−Einstein condensation**

Identifying which enclosed gas systems exhibit Bose−Einstein condensation

Consider a many-particle system consisting of a very large, constant number N of free identical particles with integer spin s. The particles are contained inside a macroscopic d-dimensional enclosure with fixed edges L and impenetrable walls. The dimensionality d

can take the values $1, 2$ or 3. Assume the following to hold for the corresponding quantized 1-particle energy eigenvalues:

$$E_\nu \;=\; \text{constant} * (\hbar\pi\nu/L)^q \;>\; 0 \;, \qquad \text{with} \quad \nu \;\equiv\; \sqrt{\sum_{i=1}^{d} \nu_i^2} \qquad\qquad (\nu_{1,\cdots,d} = 1, 2, \cdots) \;.$$

The positive power q tells us that the energy and momentum of the considered type of particle are linked by the dispersion relation (powerlaw) $E \propto p^q$, bearing in mind that the d-dimensional momenta $\vec{p}$, wave vectors $\vec{k}$ and quantum numbers $\vec{\nu}$ are related according to $\vec{p} = \hbar\vec{k} = \hbar\pi\vec{\nu}/L$.

(i) Argue that the number of 1-particle energy eigenstates with the length of the wave vector smaller than $k = \pi\nu/L$ is given by

$$N(k) \;\propto\; (2s+1) V_d k^d$$

in the continuum limit, with $V_d = L^d$ the "volume" of the d-dimensional enclosure.

(ii) Derive the following expression for the corresponding 1-particle density of states:

$$D(E) \;=\; (2s+1) C V_d E^{d/q-1} \qquad (C > 0 \text{ is a constant that depends on } d \text{ and } q) \;.$$

Assume the system to be in thermal equilibrium with a very large heat bath at temperature $T = (k_{\rm B}\beta)^{-1}$ and answer the following questions.

(iii) Why is it in general acceptable to use the grand-canonical ensemble approach, in spite of the fact that the number of particles of the embedded system is kept fixed?

(iv) Show that the total number of particles and the average total energy of the system can be written as follows:

$$\bar{N} \;=\; (2s+1) C V_d (k_{\rm B}T)^{d/q} \int_0^\infty \mathrm{d}x \, \frac{x^{-1+d/q}}{\exp(x+\alpha) - 1} \;\equiv\; N \;, \tag{1}$$

$$\bar{E}_{\rm tot} \;=\; (2s+1) C V_d (k_{\rm B}T)^{1+d/q} \int_0^\infty \mathrm{d}x \, \frac{x^{d/q}}{\exp(x+\alpha) - 1} \;, \tag{2}$$

and explain why α cannot be negative.

(v) What should hold for the integral in equation (1) if we want the system to exhibit Bose–Einstein condensation at sufficiently low temperatures?

Challenge: substantiate the statement that Bose–Einstein condensation can only occur for enclosed systems that have $d > q$.

(vi) Suppose a Bose–Einstein condensate occurs below the critical temperature T_0. Explain that for $T < T_0$ a fraction $(T/T_0)^{d/q}$ of the bosons will occupy states outside the condensate.