Exercises for Quantum Mechanics 3
Set 7

In the next two exercises we analyse polarization effects of spin-1/2 ensembles

Exercise 11: Polarization of a spin-1/2 ensemble

Consider a mixed ensemble of spin-1/2 particles. One third of these spin-1/2 particles is completely polarized in the positive x-direction, one third is completely polarized in the positive y-direction, and one third is completely polarized in the positive z-direction.

(i) Show that the corresponding density matrix in spin space is given by

$$\rho = \begin{pmatrix} 2/3 & 1/6 - i/6 \\ 1/6 + i/6 & 1/3 \end{pmatrix}.$$

Hint: make use of the fact that each of the indicated three subensembles is pure and can thus be characterized by a pure polarization vector.

(ii) Determine the degree of polarization $|\vec{P}|$ of the mixed ensemble.

(iii) Determine the direction of polarization.

Exercise 12: A spin-1/2 ensemble belonging to a pure spin state

Consider an ensemble consisting of spin-1/2 particles that can be described by a pure spin state (spin vector). We are thus dealing with a pure spin ensemble. Assume the following to be known about the spin expectation values of the pure ensemble:

$$\langle \hat{S}_x \rangle = 0 \quad , \quad \langle \hat{S}_y \rangle > 0 \qquad \text{and} \qquad \langle \hat{S}_z \rangle = \lambda \frac{\hbar}{2} \qquad (0 < \lambda < 1) .$$

(i) – Use this to determine the polarization vector $\vec{P}$ of the pure ensemble and the corresponding density matrix ρ in spin space.
– Why do we not need to know the precise value of $\langle \hat{S}_y \rangle$?

(ii) – What is the simplest way to identify the spin vector of the system?
Hint: first figure out what you know at this point about the properties of the density matrix ρ.
– Determine this spin vector up to a phase.

The next exercise can be treated as a practice exercise. You don't have to hand it in.

Exercise 13: Canonical ensemble for a spin-0 particle in a box
Quantum mechanical approach versus classical approach: the similarities

Consider a canonical ensemble of systems that each consist of a single free spin-0 particle with mass m that is contained in a large cubic enclosure with volume $V = L^3$. The fully specified energy levels of the particle are given by

$$E_\nu = \frac{\hbar^2\pi^2}{2mL^2}\,\nu^2 , \qquad \text{with} \quad \nu^2 = \nu_x^2 + \nu_y^2 + \nu_z^2 \qquad \text{and} \qquad \nu_{x,y,z} = 1, 2, \cdots .$$

Since L is large, the energy levels are very closely spaced and it makes good sense to switch to a continuum limit and to replace sums by integrals:

$$\sum_{\nu_x=1}^{\infty} \exp(-C\nu_x^2) \quad \xrightarrow{k_x = \nu_x\pi/L} \quad \frac{L}{\pi}\int_0^\infty \mathrm{d}k_x \exp\Big(-\frac{CL^2}{\pi^2}\,k_x^2\Big) = \frac{1}{2}\sqrt{\frac{\pi}{C}} \qquad (C > 0) ,$$

with similar continuum limits for ν_y and ν_z.

(i) Prove that the canonical partition function of the ensemble is given by

$$Z_1(T) = V/\lambda_T^3 , \qquad \text{with} \quad \lambda_T \equiv \frac{h}{\sqrt{2\pi m k_{\mathrm{B}} T}} = \underline{\text{thermal de Broglie wavelength}} .$$

(ii) Calculate the average energy per particle.

(iii) Use the classical principle of equipartition of energy (see p. 64 of the lecture notes) to determine the number of kinetic and elastic degrees of freedom per particle

(iv) In spite of the fact that we are explicitly working out a quantum mechanical example here, we nevertheless expect classical behaviour to prevail. Why is that?

From this explicit example we infer that the quantum mechanical definitions of entropy, temperature and Boltzmann constant that we are using here are at least consistent with their classical thermodynamic counterparts.

<u>Exercise 14</u>: Canonical ensemble for a linear harmonic oscillator

Quantum mechanical approach versus classical approach: the differences

Consider a canonical ensemble of systems that each consist of a single linear harmonic oscillator with energy levels $\{E_n = \hbar\omega\left(n+\frac{1}{2}\right),\ n=0,1,\cdots\}$ for $\omega > 0$.

(i) Prove that the canonical partition function of this ensemble is given by

$$Z_1(T) \;=\; \frac{\exp(-\beta\hbar\omega/2)}{1-\exp(-\beta\hbar\omega)}\ .$$

(ii) Use this to derive that the average energy per oscillator amounts to

$$\bar{E} \;=\; \frac{1}{2}\hbar\omega\,\frac{1+\exp(-\beta\hbar\omega)}{1-\exp(-\beta\hbar\omega)} \;=\; \frac{\hbar\omega/2}{\tanh(\beta\hbar\omega/2)}\ .$$

(iii) Argue that this corresponds to an average value

$$\bar{n} \;=\; \frac{1}{\exp(\beta\hbar\omega)-1}$$

for the quantum number n.

(iv) What <u>many-particle interpretation</u> can be assigned to the result in part (iii)?

(v) First consider the high-temperature limit $k_{\rm B}T \gg \hbar\omega$. Apply this limit to the result in part (ii) and use the classical principle of equipartition of energy (see p. 64 of the lecture notes) to determine the number of kinetic and elastic degrees of freedom that such a linear harmonic oscillator effectively possesses.

(vi) Next consider the low-temperature limit $k_{\rm B}T \ll \hbar\omega$. Apply also this limit to the result in part (ii).

(vii) – What influence will this low-temperature phenomenon have on the thermal response (such as heat conductance) of such an oscillator system?

– What has happened to the classical degrees of freedom mentioned in part (v)?

(viii) Suppose we have a collection of oscillators with frequency range $\omega \in (\omega_c, \infty)$. Is it possible to effectively prevent the thermal excitation of oscillator modes

– if $\omega_c = 0$ (as is the case for an ideal photon gas inside a black body),

– if $\omega_c > 0$ (as is the case for a photon gas inside a microresonator [see later])?

This example covers the essential features of the quantum statistics of wave phenomena, such as lattice vibrations and electromagnetic waves. It will be used explicitly for deriving Planck's law of black-body radiation.