Exercises for Quantum Mechanics 3
Set 10 (module 1)

Exercise 21: ideal gases contained inside a harmonic trap

This is how gaseous Bose–Einstein condensates can be realized in the lab

Consider a 3-dimensional many-particle system consisting of a very large, constant number N of non-interacting identical spin-s particles with mass m. The particles are contained inside a harmonic trap with potential $V(x,y,z) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$. The corresponding (spatial) 1-particle energy eigenvalues are given by

$$E_{\nu_x,\nu_y,\nu_z} = E_0 + \hbar\big(\nu_x\omega_x + \nu_y\omega_y + \nu_z\omega_z\big) \qquad (\nu_{x,y,z} = 0,1,2,\cdots)\ ,$$

with E_0 and $\omega_{x,y,z}$ positive real constants. If we include spin, the density of 1-particle quantum states at energy E can be written in delta-function form:

$$D(E) = (2s+1)\sum_{\nu_x=0}^{\infty}\sum_{\nu_y=0}^{\infty}\sum_{\nu_z=0}^{\infty}\delta(E - E_{\nu_x,\nu_y,\nu_z})\ .$$

The amount of energy $E - E_0$ that the particle has in excess of the zero-point energy E_0 will be called the excitation energy of the particle.

(i) If the number of occupied states is sufficiently high, we can replace these sums by integrals (continuum limit). Show that the density of states then changes into

$$D(E) \equiv (2s+1)\int_0^{\infty}\mathrm{d}\nu_x\int_0^{\infty}\mathrm{d}\nu_y\int_0^{\infty}\mathrm{d}\nu_z\ \delta(E - E_{\nu_x,\nu_y,\nu_z})$$

$$= \begin{cases} \dfrac{2s+1}{2\hbar^3\bar{\omega}^3}(E-E_0)^2 & \text{if} \quad E \geq E_0 \\ 0 & \text{if} \quad E < E_0 \end{cases}\ , \qquad \text{with} \quad \bar{\omega} = (\omega_x\omega_y\omega_z)^{1/3}.$$

Assume the system to be in thermal equilibrium with a very large heat bath at temperature $T = (k_{\mathrm{B}}\beta)^{-1}$. Contrary to the case of particles in a box, the volume V will play no role in the spectrum of energy eigenvalues of the system. As such, the volume can be left out in the discussion without invalidating the canonical and grand-canonical ensemble approaches that were worked out in the lecture notes. Employ the grand-canonical ensemble approach to answer the following questions.

Scenario 1: the particles have $s = 1/2$ and the temperature is given by $T = 0$.

(ii) Determine the maximum value for the excitation energy $E - E_0$ of such a particle.

(iii) Show that the average excitation energy per particle amounts to a fraction $3/4$ of this maximum.

Scenario 2: the particles have $s = 0$ and it is given that $\int_0^\infty \mathrm{d}x\, x^2/[\exp(x) - 1] = 2.404$

(iv) Assume that $k_{\mathrm{B}}T > \hbar\bar{\omega}\,\big(N/1.202\big)^{1/3}$. Show that the total number of particles can be written as

$$\bar{N} \;=\; \frac{1}{2}\Big(\frac{k_{\mathrm{B}}T}{\hbar\bar{\omega}}\Big)^3 \int_0^\infty \mathrm{d}x\, \frac{x^2}{\exp(x + \alpha + \beta E_0) - 1} \;\equiv\; N$$

and explain why $\alpha > -\beta E_0$.

(v) Suppose we lower the temperature to the regime $k_{\mathrm{B}}T < \hbar\bar{\omega}\,\big(N/1.202\big)^{1/3}$.
- Which quantum mechanical phenomenon will occur in that case?
- Explain what you know about α in this situation.
- Determine the fraction of particles with 1-particle energy E_0.

Experimental realization of Bose–Einstein condensates: *it took rougly 70 years to realize a Bose–Einstein condensate in a nearly ideal gas. The main problem was to refrigerate the gas without creating a liquid or solid and without the atoms binding into molecules. To achieve this dilute, neutral gases had to be used and any contact with walls had to be evaded in order to avoid freezing. This meant that the dilute gas had to be refrigerated to extremely low temperatures without physical contact with the outside world. To this end the gas was contained inside a magneto-optical trap (harmonic trap) and cooled down to the nano-kelvin regime by means of laser-cooling and evaporative-cooling techniques. The resulting many-particle system is precisely of the type that we have just investigated.*

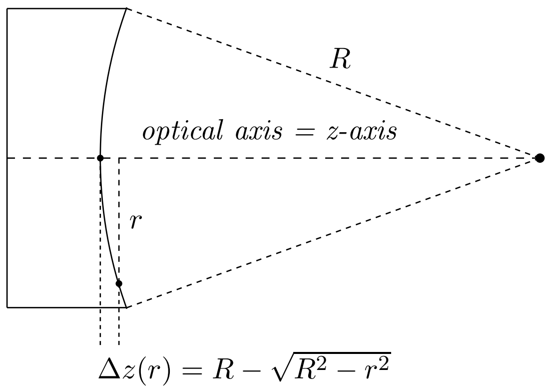
Bose–Einstein condensation for photons (group challenge): *now consider the 2-dimensional photon gas inside the microresonator described on the next page, for which $D(E) \propto E - E_0$. As a result of the perfectly reflecting mirrors, this photon gas possesses two crucial properties that make the formation of a Bose–Einstein condensate of photons possible. Your task is to figure out what these decisive properties are.*

The curved-mirror microresonator (University of Bonn, 2010)

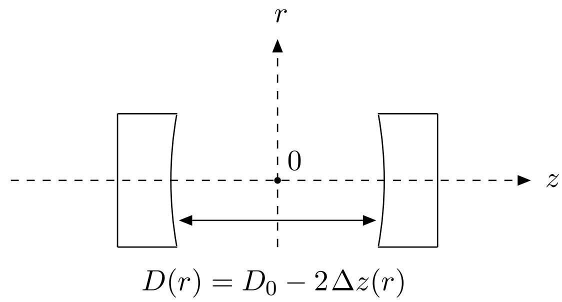
Klaers et al., Nature **468***, 545-548 (25 November 2010)*

Consider a microresonator consisting of two spherically curved, perfectly reflecting dielectric mirrors. These mirrors impose a rigid-wall boundary condition (quantization condition) on the allowed photon modes inside the resonator (see later). In order to analyse the implications of the boundary condition we first have a look at the geometrical aspects of the mirrors and the resonator, as sketched in the 2-dimensional illustration given below. The spherical mirrors have a radius of curvature $R = \mathcal{O}(1\,\text{m})$ and an optical axis that is positioned along the z-direction. The transverse distance with respect to the optical axis is denoted by r. The distance between the two mirrors in the resonator is very small: $D_0 \approx 1.56\,\mu\text{m} \ll R$.

Spherical mirror



Microresonator



The resulting wave-vector quantization in the z-direction is then given by (see §2.5):

$$k_z(r) \;=\; \nu\,\frac{\pi}{D(r)} \qquad (\nu = 1, 2, \cdots) \quad \Rightarrow \quad k_{z_{\min}}(r) \;=\; \frac{\pi}{D(r)} \;\geq\; \frac{\pi}{D_0} \;=\; k_{z_{\min}}(0)\ .$$

The spectrum of 2-dimensional transverse wave vectors $k_{x,y}$ with $k_r = \sqrt{k_x^2 + k_y^2}$ is continuous. Inside the microresonator we have $r \ll R$, so that $\Delta z(r) \approx \frac{1}{2}\, r^2/R$. For the low-energy modes we can take $\nu = 1$ and $k_r \ll k_{z_{\min}}(r)$, which allows us to approximate the corresponding energies by

$$E_{\text{low}} \;=\; \hbar c\,\sqrt{k_{z_{\min}}^2(r) + k_r^2} \;=\; \hbar c\,\sqrt{\pi^2/D^2(r) + k_r^2} \;\approx\; \frac{\hbar c \pi}{D_0 - r^2/R}\left[1 + \frac{k_r^2 (D_0 - r^2/R)^2}{2\pi^2}\right]$$

$$\approx\; \frac{\hbar c \pi}{D_0} + \frac{\hbar c k_r^2 D_0}{2\pi} + \frac{\hbar c \pi r^2}{R D_0^2} \;\equiv\; \boxed{m_\gamma c^2 + \frac{(\hbar k_r)^2}{2 m_\gamma} + \frac{1}{2} m_\gamma \Omega^2 r^2 \;\approx\; E_{\text{low}}}\ .$$

So, we end up with a transverse 2-dimensional bosonic gas with certain special properties.