

Problem 1. Ultra-relativistic bosons in 2D (Points: 10+10+10 = 30)

In this problem, we consider non-interacting ultra-relativistic bosons in two dimensions (2D) in a 2D “volume” V , in contact with an external particle reservoir, and in thermal equilibrium with the surroundings. The system has a grand canonical partition function Z_g given by

$$Z_g = \prod_k \left(1 - e^{-\beta(\varepsilon_k - \mu)}\right)^{-1} = e^{\beta pV}.$$

Here, $\beta = 1/k_B T$, where k_B is Boltzmann's constant and T is temperature, while μ is the chemical potential of the system. Furthermore, p is the pressure of the system. For ultra-relativistic particles, the energy of a particle in a single-particle state specified by specifying $\mathbf{k} = (k_x, k_y)$, is given by

$$\varepsilon_k = \hbar c k.$$

where c is the speed of light, $\hbar = h/2\pi$, h is Planck's constant, and $k \equiv |\mathbf{k}|$. The Hamiltonian of the system is given by $H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} n_{\mathbf{k}}$, with $n_{\mathbf{k}} = 0, 1, 2, \dots$

a. Show that the pressure of the system and the average number of particles in the system, $\langle N \rangle$, are given by

$$\begin{aligned} \beta pV &= - \int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) \ln \left(1 - e^{-\beta(\varepsilon - \mu)}\right), \\ \langle N \rangle &= N_0 + \int_{-\infty}^{\infty} d\varepsilon \frac{g(\varepsilon)}{e^{\beta(\varepsilon - \mu)} - 1}, \end{aligned}$$

where $g(\varepsilon) = \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}})$ and $\delta(x)$ is the δ -function. Here, N_0 is the number of particles in the lowest-energy state. Show also that the internal energy $U = \langle H \rangle$ is given by

$$U = \int_{-\infty}^{\infty} d\varepsilon \frac{g(\varepsilon) \varepsilon}{e^{\beta(\varepsilon - \mu)} - 1}.$$

b. For this particular system, we have

$$g(\varepsilon) = V \frac{2\pi}{(hc)^2} \varepsilon \Theta(\varepsilon),$$

where $\Theta(x) = 0, x < 0$, $\Theta(x) = 1, x > 0$. Show that

$$U = K pV,$$

and determine the purely numerical constant K .

c. Let $\mu \rightarrow 0^-$, and compute the temperature T_λ below which we may have a *macroscopic* occupation of the ground state (Bose-Einstein condensation).

d. In a $2D$ non-relativistic system of particles with mass m , with $\varepsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$, one cannot have Bose-Einstein condensation at any temperature $T_\lambda > 0$. In problem 1 **c**, you found a $T_\lambda > 0$. Explain on physical grounds why an ultra-relativistic non-interacting $2D$ boson system can feature Bose-Einstein condensation at finite temperature, while a corresponding non-relativistic system cannot.

Useful formula:

$$\langle N \rangle = \frac{\partial \ln Z_g}{\partial(\beta\mu)}.$$

Problem 2. Non-interacting classical spins (Points: 10+10+10+10=40)

Consider N classical spins $\mathbf{S}_i = (S_{ix}, S_{iy}, S_{iz})$ in a constant external magnetic field $\mathbf{h} = (0, 0, h)$. Let $|\mathbf{S}_i| = S$ be the length of the spins, which we take to be equal on all lattice sites, and ignore couplings between spins. Consider a particular case of the model, namely a system of three-state Ising spins, defined by $\mathbf{S}_i = (S_{ix}, S_{iy}, S_{iz}) = S(0, 0, \sigma_i)$, $\sigma_i = 0, \pm 1$.

The Hamiltonian H and the canonical partition function Z of this spin-system are given by

$$H = -\mathbf{h} \cdot \sum_{i=1}^N \mathbf{S}_i,$$

$$Z = \sum_{\{\mathbf{S}_i\}} e^{-\beta H}.$$

Here, $\beta = 1/k_B T$, where k_B is Boltzmann's constant and T is temperature.

a. Show that the partition functions for this spin-model is given on the form

$$Z = (F(S\beta h))^N,$$

where the functional form of $F(x)$ is given by $F(x) = 1 + 2 \cosh(x)$.

b. Calculate the enthalpy, H_e , of the systems, where

$$H_e = -\frac{\partial \ln Z}{\partial \beta}.$$

c. Show that in general, we have for the specific heat at constant magnetic field, $C_{\mathbf{h}} \equiv (\partial H_e / \partial T)_{\mathbf{h}}$

$$C_{\mathbf{h}} = k_B \beta^2 [\langle H^2 \rangle - \langle H \rangle^2],$$

where $\langle \mathcal{O} \rangle \equiv (1/Z) \sum_{\{\mathbf{S}_i\}} \mathcal{O} e^{-\beta H}$.

d. Compute $C_{\mathbf{h}}$ in the limit $S\beta h \gg 1$. Explain on physical grounds the result you find.

Problem 3. Classical particles in 2D (Points: 5+5+10+10=30)

Consider N non-relativistic classical particles with mass m moving in the two-dimensional ($2D$) (x, y) -plane with “volume” $V = \pi R^2$, where R is the radius of the circle to which the N particles are confined. These particles are non-interacting, but are subject to an external potential. The Hamiltonian of the system is given by

$$H = \sum_{i=1}^N \left[\frac{\mathbf{p}_i^2}{2m} + V_0 r_i^2 \right].$$

Here, $\mathbf{p}_i = (p_{xi}, p_{yi})$ is the momentum of particle i , while $r_i = \sqrt{x_i^2 + y_i^2}$ is the distance from the center of the volume V of particle i . The canonical partition function Z for this system is given by

$$Z = \frac{1}{N! h^{2N}} \int \dots \int d\Gamma e^{-\beta H}; \quad d\Gamma = \prod_{i=1}^N d^2 \mathbf{p}_i d^2 \mathbf{r}_i.$$

Here, h is a constant with dimension Js, while $\beta = 1/k_B T$, k_B is Boltzmann’s constant, and T is temperature. For later use, we also define the length $R_0 \equiv 1/\sqrt{\beta V_0}$.

a. Show that the internal energy $U = \langle H \rangle$ in general is given by, in the canonical ensemble

$$U = -\frac{\partial \ln Z}{\partial \beta}.$$

b. Show that in this case, the canonical partition function is given

$$\begin{aligned} Z &= \frac{1}{N!} \frac{1}{\lambda^{2N}} Q_1^N, \\ \lambda &\equiv \frac{h}{\sqrt{2\pi m k_B T}}, \\ Q_1 &\equiv \int d^2 \mathbf{r} e^{-\beta V_0 r^2}. \end{aligned}$$

c. Calculate the pressure p that the particles exert on the “walls” of the system (the perimeter of the circle) in the limits $R/R_0 \ll 1$ and $R/R_0 \gg 1$.

d. In polar coordinates, the Hamiltonian may be written

$$H = \sum_{i=1}^N \left[\frac{p_{ri}^2}{2m} + \frac{p_{\theta i}^2}{2mr_i^2} + V_0 r_i^2 \right]$$

Here, p_{ri} is the radial component of the linear momentum of particle i , and $p_{\theta i}$ is its angular momentum. Compute

$$\tilde{u} \equiv \left\langle \frac{p_{\theta i}^2}{2mr_i^2} + V_0 r_i^2 \right\rangle; \quad R/R_0 \ll 1.$$

Useful formula:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \frac{1}{N! h^{2N}} \int \dots \int d\Gamma \mathcal{O} e^{-\beta H}.$$

Useful formulae:

$$\begin{aligned} \sum_{\mathbf{k}} F(\varepsilon_{\mathbf{k}}) &= \int_{-\infty}^{\infty} de g(e) F(e) \\ g(e) &\equiv \sum_{\mathbf{k}} \delta(e - \varepsilon_{\mathbf{k}}) \\ \int d^{\nu} \mathbf{r} F(|\mathbf{r}|) &= \Omega_{\nu} \int dr r^{\nu-1} F(r); \quad \Omega_{\nu} = \frac{2\pi^{\nu/2}}{\Gamma(\nu/2)} \\ \Gamma(z) &\equiv \int_0^{\infty} dx x^{z-1} e^{-x} \\ \Gamma(z+1) &= z \Gamma(z) \\ \zeta(z) &\equiv \sum_{l=1}^{\infty} \frac{1}{l^z} \\ \int_0^a dx x^{\nu-1} e^{-x^{\nu}} &= \frac{1}{\nu} \int_0^{a^{\nu}} du e^{-u} \\ \int_0^{\infty} dx \frac{x^z}{e^x - 1} &= \zeta(z+1) \Gamma(z+1) \\ \int_0^{\infty} dx x e^{-x} &= 1 \\ C_{\mathbf{h}} &= \left(\frac{\partial H_e}{\partial T} \right)_{\mathbf{h}} = -k_B \beta^2 \left(\frac{\partial H_e}{\partial \beta} \right)_{\mathbf{h}} \end{aligned}$$

Generalized Equipartition Principle:

Let the Hamiltonian of a system be given by $H = \alpha|q|^{\nu} + H'$. Here q is a generalized coordinate or momentum which does not appear in H' . Let the partition function be given by

$$Z = \int dq \int d\Gamma' e^{-\beta H},$$

such that we have

$$\langle \alpha|q|^{\nu} \rangle = \frac{1}{Z} \int dq \int d\Gamma' \alpha|q|^{\nu} e^{-\beta H}.$$

Then we have

$$\langle \alpha|q|^{\nu} \rangle = \frac{k_B T}{\nu}.$$

Three-dimensional volume element in spherical coordinates:

$$d^3 r = d\Omega r^2 dr; \quad d\Omega = d\theta \sin \theta d\phi$$

Here, θ is a polar angle and ϕ is an azimuthal angle.