<u>Problem 1.</u> Non-relativistic fermions in $2D$ (Points: 10+10+10 = 30)

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

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

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

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}.$$

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

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

$$\begin{aligned} \beta p V &= \int d\varepsilon \; g(\varepsilon) \; \ln\left(1 + e^{-\beta(\varepsilon - \mu)}\right), \\ \langle N \rangle &= \int d\varepsilon \; \frac{g(e)}{e^{\beta(\varepsilon - \mu)} + 1}, \end{aligned}$$

where $g(\varepsilon) = \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}})$ and $\delta(x)$ is the δ-function. Show also that the internal energy $U = \langle H \rangle$ is given by

$$U = \int d\varepsilon \; \frac{g(e)\; \varepsilon}{e^{\beta(\varepsilon - \mu)} + 1}.$$

<u>b</u>. For this particular system, we have

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

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

$$U = K \; pV,$$

and determine the purely numerical constant K.

c. Calculate the pressure of this system at $T = 0$. Express the answer in terms of the density ρ of the system, where $\rho = \langle N \rangle / V$. Explain on physical grounds why this non-interacting system has a non-zero pressure at $T = 0$.

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 two cases of model. i) The Ising model, defined by spins with only one component, $\mathbf{S}_i = (S_{ix}, S_{iy}, S_{iz}) = S(0, 0, \sigma_i), \sigma_i = \pm 1$. ii) The Heisenberg model, defined by spins with three components, $\mathbf{S}_i = S(\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i)$. Here, $\theta_i \in [0, \pi\rangle$ is the polar angle the spins take relative to the direction of $\mathbf{h}$, while $\phi_i \in [0, 2\pi\rangle$ is the azimuthal angle describing the direction of the spin in the plane perpendicular to $\mathbf{h}$.

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

$$\begin{aligned} H &= -\mathbf{h} \cdot \sum_{i=1}^{N} \mathbf{S}_i, \\ Z &= \sum_{\{\mathbf{S}_i\}} e^{-\beta H}. \end{aligned}$$

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

a. Show that the partition functions for the two variants of the spin-model both are given on the form

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

with $F(x) = 2\cosh(x)$ for the Ising case and $F(x) = 4\pi \sinh(x)/x$ for the Heisenberg case.

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, $C_{\mathbf{h}}$

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

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 the difference in the results you find for $C_{\mathbf{h}}$ for the Ising and Heisenberg cases when $S\beta h \gg 1$.

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

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

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

$$Z = \frac{1}{N! h^{2N}} \int .. \int d\Gamma \; e^{-\beta H},$$

$$d\Gamma = \prod_{i=1}^{N} d^2\mathbf{p}_i \; d^2\mathbf{r}_i.$$

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 $R_0 \equiv 1/(\beta V_0)$.

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

$$Z = \frac{1}{N!} \frac{1}{\lambda^{2N}} Q_1^N,$$

$$\lambda \equiv \frac{h}{\sqrt{2\pi m k_B T}},$$

$$Q_1 \equiv \int d^2\mathbf{r} \; e^{-\beta V_0 r}.$$

c. Calculate U in the limits $R/R_0 \ll 1$ and $R/R_0 \gg 1$.

d. Consider now the limit $R/R_0 \gg 1$. A naive application of the generalized equipartition principle would yield $\langle \mathbf{p}^2/2m \rangle = k_B T$ and $V_0 \langle r \rangle = k_B T$, such that $U = 2Nk_BT$. Explain why this yields the wrong result for U.

Useful formula:

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

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:

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

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