

Problem 1. (Points: 10+10+10+10 = 40)

A system of classical interacting spins $\{\sigma_i\}$ in a uniform externally controlled magnetic field B is defined by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i$$

Here, $\langle i, j \rangle$ denotes a sum over all lattice sites i and their nearest neighbors j , while the spin-variables take on the values $\sigma_i \in (0, \pm 1, \pm 2)$. The number of lattice sites is N , and the number of nearest neighbors is taken to be z . $J > 0$ is the strength of the spin-spin coupling in the system.

a Show that, by introducing $\sigma_i = m + \delta\sigma_i$ and disregarding terms that are quadratic in $\delta\sigma_i$, the Hamiltonian may be written on the form

$$H = JNzm^2 - B_{\text{eff}} \sum_i \sigma_i$$

where $B_{\text{eff}} \equiv B + 2Jzm$. Here, $|\delta\sigma_i/m| \ll 1$, and $\langle \delta\sigma_i \rangle = 0$. Give a physical interpretation of m and B_{eff} .

b Within this approximation, compute the partition function $Z = \sum_{\{\sigma_i\}} e^{-\beta H}$. Show that the Gibbs energy is given

$$G = JNzm^2 - \frac{N}{\beta} \ln(1 + Y(\omega + \alpha m))$$

where $\omega + \alpha m = \beta B_{\text{eff}}$, thus giving an expression for $Y(x)$. $\beta = 1/k_B T$, k_B is Boltzmann's constant, T is the temperature. Explain on physical grounds why $Y(x) = Y(-x)$. (A check on your result for $Y(x)$: $Y(0) = 4$, and $Y(x)$ is an analytic function of x .)

c State the principle by which to determine m . Show that the equation for m is given by

$$m = \frac{Y'(\omega + \alpha m)}{1 + Y(\omega + \alpha m)}$$

where $Y'(x) = dY(x)/dx$.

d This treatment of the system predicts that it undergoes a phase-transition at $B = 0$ from a high-temperature state with no magnetic ordering (a paramagnetic state), to a low-temperature state with magnetic ordering (a ferromagnetic state). The transition occurs at a critical temperature T_c . Within the approximation used above, determine T_c . If you did not find $Y(x)$ explicitly in **b**, you should still be able to deduce T_c , up to one purely numerical multiplicative constant. In that case, you are asked to provide an explicit expression for that numerical constant, based on the information given above.

Problem 2. (Points: 10+10+10=30)

A d -dimensional ideal quantum system in contact with an infinite particle reservoir is defined by the Hamiltonian

$$H = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}$$

where $c_{\mathbf{k}}^{\dagger}$ and $c_{\mathbf{k}}$ are creation and destruction operators respectively of single-particle states with quantum number $\mathbf{k}$, $\varepsilon_{\mathbf{k}}$ is the single-particle energy of that same state, and μ is the chemical potential of the system. The grand canonical partition function of the system is given by

$$Z_g = \prod_{\mathbf{k}} (1 + e^{-\beta(\varepsilon_{\mathbf{k}} - \mu)})$$

$\beta = 1/k_B T$, k_B is Boltzmann's constant, T is temperature. For $\varepsilon_{\mathbf{k}} = \hbar c |\mathbf{k}|$, $g(\varepsilon)$ is given by

$$g(\varepsilon) = V \frac{\Omega_d}{(hc)^d} \varepsilon^{d-1} \Theta(\varepsilon)$$

where $\hbar = h/2\pi$, h is Planck's constant, c is the speed of light, and $\Theta(x)$ is the Heaviside step-function $\Theta(x) = 0, x < 0$, $\Theta(x) = 1, x > 0$. Ω_d is the solid angle in d dimensions.

a Show that the pressure p and density $\rho = \langle N \rangle / V$ of this system are given by

$$\begin{aligned} p &= \frac{1}{d} \frac{\Omega_d}{(hc)^d} \int_0^{\infty} d\varepsilon \frac{\varepsilon^d}{e^{\beta(\varepsilon - \mu)} + 1} \\ \rho &= \frac{\Omega_d}{(hc)^d} \int_0^{\infty} d\varepsilon \frac{\varepsilon^{d-1}}{e^{\beta(\varepsilon - \mu)} + 1} \end{aligned}$$

b Introduce the fugacity $z = e^{\beta\mu}$ and show that the exact equation of state for this system, $\beta p = F(\rho)$, may be written on the following parametric form

$$\begin{aligned} \beta p &= \frac{1}{\lambda^d} \sum_{l=1}^{\infty} b_l z^l \\ \rho &= \frac{1}{\lambda^d} \sum_{l=1}^{\infty} l b_l z^l \end{aligned}$$

where it is given that the coefficients b_l only depend on (l, d) . Thus, give an expression for the ultra-relativistic thermal de Broglie wavelength λ .

c Compute the second virial-coefficient $B_2(T)$ of this system, defined via

$$\beta p = \rho + B_2(T) \rho^2 + \dots$$

Give an expression for the dimensionless parameter that determines the importance of the correction term to the ideal gas case, and thus give a physical interpretation of this correction term.

Problem 3. (Points: 10+10+10=30)

A system of N one-dimensional anharmonic classical oscillators is described by a Hamiltonian given by

$$H = \sum_{i=1}^N \left[\frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 x_i^2 + \alpha x_i^4 \right]$$

The canonical partition function of this system is given by

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

$$d\Gamma \equiv \prod_{i=1}^N dp_i dx_i$$

In this problem, we will treat the anharmonic term as a small correction to the harmonic Hamiltonian. That, is, we will use the approximation

$$e^{ax^2+bx^4} \approx e^{ax^2} (1 + bx^4)$$

a Within this approximation, show that the partition function of the system is given by

$$Z = \frac{1}{h^N N!} \left(\frac{2\pi}{\beta\omega} \right)^N \left[1 - \frac{3}{4} \frac{\beta\alpha}{\gamma^2} \right]^N$$

where $\gamma \equiv \beta m \omega^2 / 2$. For which temperature range do you expect this to be a valid approximation?

b Compute the internal energy $U = \langle H \rangle$ and specific heat $C_V = (\partial U / \partial T)_V$ of this system.

c Use the classical equipartition principle to compute the average of the potential energy U_p of the system within the approximation used above

$$\langle U_p \rangle = \left\langle \sum_{i=1}^N \left[\frac{1}{2} m \omega^2 x_i^2 + \alpha x_i^4 \right] \right\rangle$$

Useful formulae:

Partition function in the canonical ensemble:

$$Z = e^{-\beta F}$$

Partition function in the Gibbs ensemble:

$$Z = e^{-\beta G}$$

Partition function in the grand canonical ensemble:

$$Z_g = e^{\beta p V}$$

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

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

$$\sum_{\mathbf{k}} F(\varepsilon_{\mathbf{k}}) = \int_{-\infty}^{\infty} de g(e) F(e)$$

$$g(e) \equiv \sum_{\mathbf{k}} \delta(e - \varepsilon_{\mathbf{k}})$$

$$\sum_{\mathbf{k}} = \frac{V}{(2\pi)^d} \Omega_d \int_0^{\infty} dk k^{d-1}$$

$$\int d^{\nu} \mathbf{r} F(|\mathbf{r}|) = \Omega_{\nu} \int dr r^{\nu-1} F(r); \quad \Omega_{\nu} = \frac{2\pi^{\nu/2}}{\Gamma(\nu/2)}$$

$$\int_{-\infty}^{\infty} dx x^{2n} e^{-\alpha x^2} = \left(-\frac{d}{d\alpha} \right)^n \sqrt{\frac{\pi}{\alpha}}$$

$$\Gamma(z) \equiv \int_0^{\infty} dx x^{z-1} e^{-x}$$

$$\Gamma(z+1) = z \Gamma(z)$$

$$\zeta(z) \equiv \sum_{l=1}^{\infty} \frac{1}{l^z}$$

$$\int_0^a dx x^{\nu-1} e^{-x^{\nu}} = \frac{1}{\nu} \int_0^{a^{\nu}} du e^{-u}$$

$$\int_0^{\infty} dx \frac{x^z}{e^x - 1} = \zeta(z+1) \Gamma(z+1)$$

$$\int_0^{\infty} dx x e^{-x} = 1$$

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.