<u>Problem 1.</u> (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.

<u>**a**</u> 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}.

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

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

where $\omega + \alpha m = \beta B_{\text{eff}}$, thus giving an expression for Y(x). $\beta = 1/k_B T$, k_B is Boltzmanns 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.)

<u>**c**</u> 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 $Y'(x) = dY(x)/dx$.

<u>**d**</u> 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 <u>**b**</u>, 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.

<u>Problem 2.</u> (Points: 10+10+10=30)

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

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

where $c^\dagger_{\mathbf{k}}$ 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

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

$\beta = 1/k_B T$, k_B is Boltzmanns 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.

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

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

<u>**b**</u> 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.

<u>**c**</u> Compute the second virial-coefficient $B_2(T)$ of this system, defined via

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

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

$$\begin{aligned} Z &= \frac{1}{h^N N!} \int d\Gamma \; e^{-\beta H} \\ d\Gamma &\equiv \prod_{i=1}^{N} dp_i dx_i \end{aligned}$$

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

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

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

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

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:

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

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

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

$$\begin{aligned}
\sum_{\mathbf{k}} F(\varepsilon_{\mathbf{k}}) &= \int_{-\infty}^{\infty} de \; g(e) \; F(e) \\
g(e) &\equiv \sum_{\mathbf{k}} \delta(e - \varepsilon_{\mathbf{k}}) \\
\sum_{\mathbf{k}} &= \frac{V}{(2\pi)^d} \, \Omega_d \int_0^{\infty} dk \; k^{d-1} \\
\int d^{\nu}\mathbf{r} \; F(|\mathbf{r}|) &= \Omega_{\nu} \int dr \; r^{\nu-1} \; F(r); \quad \Omega_{\nu} = \frac{2\pi^{\nu/2}}{\Gamma(\nu/2)} \\
\int_{-\infty}^{\infty} dx \; x^{2n} \; e^{-\alpha x^2} &= \left(-\frac{d}{d\alpha}\right)^n \sqrt{\frac{\pi}{\alpha}} \\
\Gamma(z) &\equiv \int_0^{\infty} dx \; x^{z-1} \; e^{-x} \\
\Gamma(z+1) &= z \; \Gamma(z) \\
\zeta(z) &\equiv \sum_{l=1}^{\infty} \frac{1}{l^z} \\
\int_0^a dx \; x^{\nu-1} \; e^{-x^{\nu}} &= \frac{1}{\nu} \int_0^{a^{\nu}} du \; e^{-u} \\
\int_0^{\infty} dx \; \frac{x^z}{e^x - 1} &= \zeta(z+1) \; \Gamma(z+1) \\
\int_0^{\infty} dx \; x \; e^{-x} &= 1
\end{aligned}$$

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.