<u>Problem 1.</u> (Points: 10+10+10+10 = 40)

A classical system of N particles is described by specifying a set of generalized coordinates $\{q_i\}$ and generalized momenta $\{p_i\}$, where $i = 1, ..N$. The dynamics of q_i and p_i is governed by Hamilton's equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i}; \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}; \quad \dot{A} \equiv \frac{dA}{dt}$$

where H is the Hamiltonian of the system, $H = H(\{q_i\}, \{p_i\})$. A collection of $\mathcal{N}$ copies of a system with the same Hamiltonian H, but in $\mathcal{N}$ different states, is called an *ensemble*. Furthermore, we define a *phase-space* as a space spanned by $(q, p) = (\{q_i\}, \{p_i\})$. From $\mathcal{N}$ initial states at $t = 0$, the ensemble evolves in phase-space according to Hamilton's equations.

<u>a</u> Show that points in (q, p), where each point describes one of the $\mathcal{N}$ systems in phase-space, do not cross or disappear.

<u>b</u> For a very large number $\mathcal{N}$, we may consider a density $\rho = \rho(t, \{q_i, p_i\}$ of points in phase-space as a continuous function of its variables. Use the result of **<u>a</u>** to show that there is a continuity equation for ρ given by

$$\frac{d\rho}{dt} \equiv \frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0,$$

where $\vec{\nabla}$ is a gradient in phase-space (q, p) and $\vec{v} \equiv (\dot{q}, \dot{p})$ is a velocity in phase-space.

<u>c</u> Use Hamilton's equations to show that the continuity equation for ρ may be written on the form

$$\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0$$

where

$$\{A, B\} \equiv \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right).$$

<u>d</u> For a stationary state, we have $\partial \rho / \partial t = 0$. Show that in this case, we may set

$$\rho(\{q_i, p_i\}) = \rho(H(\{q_i, p_i\})).$$

Give a physical interpretation of ρ. Explain how this equation facilitates a computation of macroscopically measurable quantities from a microscopic description of a system given by H.

Problem 2. (Points: 10+10+10+10=40)

A spin-dimer is a composite object of two spins living on adjacent sites on a lattice. In this problem we will consider a system of N_d *classical* spin-dimers on a two-dimensional square lattice in a uniform external magnetic field B. The spins we will consider are Ising spins $\sigma_i = \pm 1$. The Hamiltonian of a single spin-dimer is given by

$$H = -J\sigma_1 \ \sigma_2 - B \ (\sigma_1 + \sigma_2)$$

where σ_1, σ_2 are the values of the two spins in the dimer. We assume that there are no interactions between *different* spin-dimers. The total number of spins is $N_s = 2N_d$. Moreover, J is the strength of the spin-spin coupling within the dimer.

a Show that for any spin-system with the Hamiltonian

$$H = -\sum_{i,j} J_{ij}\sigma_i\sigma_j - B\sum_i \sigma_i,$$

the enthalpy $H_e = \langle H \rangle$ and the uniform magnetization $M = \sum_i \langle \sigma_i \rangle$ are given by

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

$$M = \frac{\partial \ln Z}{\partial \beta B}$$

where $Z = \sum_{\{\sigma_i\}} \exp(-\beta H)$ is the prescribed-B partition function of the system (Gibbs ensemble).

b Compute the enthalpy H_e and the specific heat C_B of the dimer-system.

c Compute the uniform magnetization M and uniform isothermal magnetic susceptibility χ per spin of the dimer-system.

d Consider now the case $J < 0$. Compute χ at low temperatures for this case, and give a short physical interpretation of the result.

Problem 3. **(Points: 10+10+10+10=40)**

Quite recently, a new type of three-dimensional solid state systems (so-called topological insulators) have been predicted and found that are electrical insulators in their interior (bulk), but they feature very robust metallic quantum states on their surface. These surface states may be described as ultra-relativistic fermions living in two dimensions, $d = 2$, where we may ignore Newtonian forces between the particles. The states are specified by a quantum number $\mathbf{k} = (k_x, k_y)$ and the energy of such a surface state is $\varepsilon_{\mathbf{k}} = \hbar c|\mathbf{k}|$. Here, $\hbar = h/2\pi$, h is Planck's constant, $\beta = 1/k_B T$, k_B is Boltzmann's constant and T is temperature. Finally, c is the velocity of the particle. The density of states $g(\varepsilon) = \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}})$ of the surface states is given by

$$g(\varepsilon) = \frac{A}{(hc)^2}\,\varepsilon; \quad \varepsilon > 0$$

The grand canonical partition function Z_g for this system, contained on a flat surface of area A with pressure p is given by

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

where $z = e^{\beta\mu}$ and μ is the chemical potential of the system. We also introduce the surface density $\rho = \langle N\rangle/A$ where $\langle N\rangle$ is the average number of particles in the system.

a Show that the pressure and density may be written as a power series in z

$$\begin{aligned} \beta p &= \frac{1}{\lambda^2}\sum_{l=1}^{\infty} b_l z^l \\ \rho &= \frac{1}{\lambda^2}\sum_{l=1}^{\infty} l\, b_l z^l \end{aligned}$$

and give expressions for b_l and λ, and a physical interpretation of λ. (Hint: b_l only depends on l and no other parameters of the system.)

b Show that the pressure, to second order in ρ, may be written

$$\beta p = \rho + B_2\,\rho^2 + ...$$

and give an expression for B_2. (If you did not find b_l in **a**, express B_2 in terms of b_1, b_2.) Explain on physical grounds what the sign of B_2 should be.

c Under what conditions does it make sense to truncate the series at second order in ρ?

d Compute the pressure as a function of ρ at $T = 0$.

Formulae that might be useful:

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:

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

Specific heat at constant magnetic field B:

$$C_B = \left(\frac{\partial H_e}{\partial T}\right)_B$$

Uniform isothermal magnetic susceptibility:

$$\chi = \left(\frac{\partial M}{\partial B}\right)_T$$

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

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

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

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\begin{aligned}
\zeta(z) &\equiv \sum_{l=1}^{\infty} \frac{1}{l^z} \\
\eta(z) &\equiv \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l^z} \\
\int_0^\infty dx \, \frac{x^{z-1}}{e^x - 1} &= \zeta(z)\, \Gamma(z) \\
\int_0^\infty dx \, \frac{x^{z-1}}{e^x + 1} &= \eta(z)\, \Gamma(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 \; x \; e^{-x} &= 1 \\
\ln(1+x) &= \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l} \, x^l
\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.