Problem 6 (10 Points):

A large flat surface is in contact with a mono-atomic gas above it. The volume of gas above the surface acts as an infinite reservoir of gas atoms, but does not otherwise enter into the problem. The suface consist of a square lattice of sites that gas atoms can occupy; denote the number of gas atoms on site i by n_i, where $n_i \in \{0, 1\}$, and the total number of lattice sites by N_s. The energy of the system is given by:

$$E(\{n_i\}) = -\left[\sum_i n_i\,\epsilon + v_0 \sum_i \sum_{j \in n.n.} n_i n_j\right] \tag{1}$$

where ϵ is a binding energy of atom to the substrate, v_0 is an interaction between adjacent atoms, and the sum over j is restricted to the nearest neighbors of i.

a. Write down an expression for the grand canonical partition function $Z(T, \mu)$. Your answer should be in the form of a sum over states. **(2 Points)**

b. Calculate the grand canonical free energy, $\Omega(T, \mu, N_s)$ when $v_0 = 0$. **(2 Points)**

c. Calculate N, the number of gas atoms adsorbed to the surface, as a function of T, μ and N_s when $v_0 = 0$. **(2 Points)**

d. When $v_0 \neq 0$ the problem is in general more difficult. To simplify it, replace n_j in the above sum by $\bar{n}$, a constant that will be set equal to the average occupation of any site. Calculate the number of gas atoms adsorbed to the surface, N, as a function of T, μ, N_s and $\bar{n}$. **(2 Points)**

e. Discuss the possibility of a phase transition in $\bar{n}$ as a function of β. This can be done by graphically investigating the requirement that $N(T, \mu, \bar{n})/N_s = \bar{n}$, or by returning to the expression for the energy given in equation (1) and mapping it on to other well known problems in statistical mechanics. **(2 Points)**

a) $Q = \sum_{n_{tot}=0}^{N_s} \sum_{\{n_i\}} e^{\beta\mu\sum_i n_i} e^{\beta(\sum_i n_i \epsilon + V_0 \sum_i \sum_j n_i n_j)} = \prod_i^{N_s} \sum_{n_i=0}^{1} e^{\beta(\mu+\epsilon')n_i} = \left(1+e^{\beta(\mu+\epsilon')}\right)^{N_s}$

where $\epsilon' = \epsilon + V_0 \bar{n}$

$\bar{n}$ is avg prob of a site having an atom

b) Using $Q = (1+e^{\beta(\mu+\epsilon)})^{N_s}$, $\mathcal{Y} = -\frac{1}{\beta}\ln Q = -\frac{N_s}{\beta}\ln(1+e^{\beta(\mu+\epsilon)})$

c) $N_{tot} = -\frac{\partial \mathcal{Y}}{\partial \mu} = +\frac{N_s}{\beta}\frac{1\, e^{\beta(\mu+\epsilon)}}{1+e^{\beta(\mu+\epsilon)}}\beta = \frac{N_s}{e^{-\beta(\epsilon+\mu)}+1}$ makes sense, shd look like fermions since $n_i = 0,1$

d) All that changes is

$\epsilon \to \epsilon' = \epsilon + V_0\bar{n}$

$n_T = \frac{N_s}{e^{-\beta(\mu+\epsilon+V_0\bar{n})}+1}$

e) We can set $\frac{N_{tot}}{N_s} = \bar{n}$

See for what T we get multiple answers for $\bar{n}$.

$\bar{n} = \frac{1}{e^{-\beta(\mu+\epsilon+V_0\bar{n})}+1}$

$\frac{1}{\bar{n}} = e^{\beta(\,)}+1$ etc

$\bar{n} - n_0 = kT\ln\left(\frac{\bar{n}}{1-\bar{n}}\right)$

where $n_0 = -\frac{(\mu+\epsilon)}{V_0}$

When $n_0 = \frac{1}{2}$: high temp - 1 sol'n

low temp's - multiple sol'ns

6. **Boson Magnetism** Consider a gas of non-interacting spin-1 bosons in 3D, each subject to the Hamiltonian

$$\begin{aligned} H(\vec{p}, s_z) &= \frac{p^2}{2m} - \mu_0 s B \\ &= \frac{\hbar^2 k^2}{2m} - \mu_0 s B \end{aligned}$$

where s takes on one of three possible states, $s \in (-1, 0, +1)$, and $\vec{k} \equiv \vec{p}/\hbar$. In this Hamiltonian B is the z-component of the magnetic field, m is the mass of a particle, and μ_0 is the Bohr magneton. (We will ignore the orbital effect (or Lorentz force) where the momentum $\vec{p}$ would have been replaced, $\vec{p} \rightarrow \vec{p} + e\vec{A}/c$).

a) $f_B(E) = \dfrac{1}{e^{\beta(E-\mu)} - 1}$

$n_s(k) = \dfrac{1}{e^{\beta\left(\frac{\hbar^2 k^2}{2m} - \mu_0 s B - \mu\right)} - 1}$

(a) In a grand canonical ensemble of chemical potential μ (which is **not** to be confused with the Bohr magneton, μ_0, above) and temperature T, write down $n_s(\vec{k})$, the average occupation number of the state with wave vector $\vec{k}$ and spin s. (1 point).

(b) Show that the total number of particles in a given spin state s is given by

$$N_s = \frac{V}{\lambda^3} \qquad g_{3/2}(z e^{\beta \mu_0 s B})$$

where z is the fugacity, $z = e^{\beta\mu}$, λ is the thermal de Broglie wavelength,

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

and $g_p(z)$ is defined on the formula section on page 2 above. (4 points)

b) - See other side

c) $N_+ = \frac{V}{\lambda^3} g_{3/2}\left(z e^{\beta\mu_0 B}\right)$

$N_- = \frac{V}{\lambda^3} g_{3/2}\left(z e^{-\beta\mu_0 B}\right)$

(c) The magnetization for fixed μ and T is given by

$$M(T, \mu) = \mu_0 (N_{(+)} - N_{(-)})$$

Show that the zero field susceptibility, χ, is given by:

$$\chi \equiv \left.\frac{\partial M}{\partial B}\right|_{B=0} = \frac{2\mu_0^2}{k_B T} \qquad \frac{V}{\lambda^3}\, g_{1/2}(z).$$

(5 points).

$\chi = \left.\frac{\partial M}{\partial B}\right|_{B=0} = \left[\frac{\partial}{\partial B}\mu_0 N_+ - \frac{\partial}{\partial B}\mu_0 N_-\right]_{B=0}$

$= \frac{\mu_0 V}{\lambda_3}\left[\frac{\partial g_+}{\partial B} - \frac{\partial g_-}{\partial B}\right] = \frac{\mu_0 V}{\lambda^3}\left[\beta\mu_0 - -\beta\mu_0\right] g_{1/2}(z)$ since $B=0$, $g_{1/2} = g_{+1/2} = g_{-1/2}$ $\Big\}\ \chi = \frac{2\beta\mu_0^2 V}{\lambda^3} g_{1/2}(z)$ ✓

$\frac{dg_+}{\partial B} = \sum_n \frac{d}{\partial B}\frac{(z e^{\beta\mu_0 B})^n}{n^{3/2}} = \sum_n \frac{n\beta\mu_0 (z e^{\beta\mu_0 B})^{n-1}}{n^{3/2}} = \sum_n \beta\mu_0 \frac{(z e^{\beta\mu_0 B})^{n-1}}{n^{3/2-1}\}n^{1/2}} = g_+(1/2)\,\beta\mu_0$

$\frac{\partial g_-}{\partial B} = -\beta\mu_0 g_-(1/2)$

b) $Q = \prod_i \left(\frac{1}{1-e^{-\beta(E-\mu)}} \right)$

$$N = \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Q = \sum_i \frac{1}{e^{\beta(E_i-\mu)}-1}$$ as written for part a

Now we have to sum our states - $\sum_i$ becomes an integral, as we are summing over a "really big box".

$$N = \int \frac{d^3x\, d^3p}{h^3} \frac{1}{e^{\beta(E-\mu)}-1} = \frac{4\pi V}{h^3}\int_0^\infty \frac{p^2\,dp}{e^{\beta(\frac{p^2}{2m}-\mu_0 sB-\mu)}-1}$$ use $\int_0^\infty \frac{x^{n-1}}{z^{-1}e^x-1}\,dx = \Gamma(n)g_n(z)$

$u = \left(\frac{p^2}{2m}\right)\beta$ $\quad du = \frac{\beta}{m}p\,dp$ $\quad p = \sqrt{\frac{2mu}{\beta}}$

$$N = \frac{V}{\lambda^3} g_{3/2}(ze^{\beta\mu_0 sB})$$ (slight typo in answer given)

Problem 4 (10 Points):

This problem involves the mean field Ising model. Consider a solid containing N electrons localized at lattice sites. Each electron has a magnetic moment μ. In a magnetic field H each electron can exist in one of two states, with energies $\pm\mu$ H.

a. Show that for *non-interacting electrons* the total magnetic moment is given by $M = N\mu\tanh(\frac{\mu H}{kT})$. **(2 Points)**

b. In order to add interactions between the electrons, assume that each electron sees an effective magnetic field equal to the applied field plus a local field arising from its neighbors. In this case, $H_{eff} = H + \frac{\alpha}{N}M$, where α is a positive constant. Write down a self consistency equation that determines M. **(2 Points)**

c. Show that there is a spontaneous magnetization (e.g. when $H = 0$) below some critical temperature, T_c, and determine its value. **(3 Points)**

d. Show that the magnetic susceptibility χ, diverges at $T \to T_c$ from the high T side. (Hint: be careful because you will have to take a derivative of a transcendental equation.) **(3 Points)**

d) $M = N\mu\tanh\beta\mu(H + \frac{\alpha M}{N})$

take $\chi = \frac{\partial M}{\partial H}$ of both sides

$$\frac{\partial M}{\partial H} = N\mu\left[\frac{\cosh^2(\ )(\beta\mu + \frac{\alpha\chi}{N}) - \sinh^2(\ )(\beta\mu + \frac{\alpha\chi}{N})}{\cosh^2(\ )}\right]$$

$$\chi = \frac{(\beta\mu + \frac{\alpha\chi}{N})N\mu}{\cosh^2(\ )}$$

$$\chi - \frac{\frac{\alpha\chi \cancel{N}\mu}{\cancel{N}}}{\cosh^2(\ )} = \frac{\beta\mu^2 N}{\cosh^2(\ )}$$

$$\chi = \frac{N\mu^2\beta}{\cosh^2(\ ) - \mu^2\beta\alpha}$$

If I plug in $T = T_c$:

$$\chi = \frac{N}{\alpha\cosh^2(\frac{M}{N\mu}) - \alpha}$$

(for $H=0$)

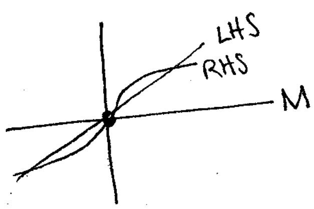
So reasoning for d): For $T > T_c$, $M = 0$. So for $T > T_c$ & $H = 0$ (external field turned off) we see that χ diverges as $T \to T_c$. This is the "zero field" phase transition.

a) $E = \pm\mu H$ so $Z = (e^{\beta\mu H} + e^{-\beta\mu H}) = 2\cosh\beta\mu H \rightarrow Z = (2\cosh\beta\mu H)^N$

$F = -\frac{1}{\beta}\ln Z = -\frac{N}{\beta}\ln(2\cosh\beta\mu H)$ $M = \frac{-\partial F}{\partial H} = \frac{N}{\beta}\frac{1\,(2\sinh\beta\mu H)\beta\mu}{2\cosh\beta\mu H} = \underline{N\mu\tanh\beta\mu H}$ ✓

b) $\underline{M = N\mu\tanh\beta\mu(H + \frac{\alpha M}{N})}$

c) LHS is linear, RHS is tanh }



For values of the RHS that curve enough, we have sol'ns besides at $M=0$

To find T_c analytically... The slope of the RHS must be at least equal to the slope of the LHS at $M=0$. use $\frac{M}{N\mu} = \tanh\frac{\beta\mu\alpha M}{N}$

Slope of LHS at $M=0$ is $\frac{\beta\mu\alpha}{N}$. Slope of RHS is $\frac{1}{N\mu}$

$$\frac{1}{N\mu} = \frac{\beta\mu\alpha}{N} \rightarrow \underline{T_c = \frac{\mu^2\alpha}{k}} \quad \text{crazy.}$$

Problem 5 (10 Points):

A crystal lattice consists of N atoms. Each atom is in a quantum state in which the total orbital angular momentum is zero and the total spin angular momentum is S$=\frac{1}{2}$. The crystal is in an external magnetic field $\mathbf{B}_0 = \mu_0\mathbf{H}$ of magnetic field intensity $\mathbf{H}$, where μ_0 is the permeability of free space. Choosing the z-axis to lie along the field, we can specify a microstate in terms of the site indices σ_i for each lattice site j, which are defined as $\sigma_j = \pm 1$ if $(\mathrm{M}_s)_j = \mp\frac{1}{2}$, respectively. In the Ising model, the energy E_p for a microstate ψ_p of a one-dimensional crystal in this field is,

$$E_p = -J \sum_{(i,j)_{nn}}^{N} \sigma_i\sigma_j - B_0 \sum_{j=1}^{N} \sigma_j.$$

where $\mathrm{J} > 0$ is a constant, and the subscript $(i,j)_{nn}$ means to sum *once* over each nearest neighbor pair of sites. Now, define

$$N_+ = \text{number of atoms with } \sigma_j = 1$$
$$N_- = \text{number of atoms with } \sigma_j = -1$$
$$N_{++} = \text{number of nearest} - \text{neighbor pairs } (i,j) \text{ with } \sigma_i = 1 \text{ and } \sigma_j = 1$$
$$N_{+-} = \text{number of nearest} - \text{neighbor pairs } (i,j) \text{ with } \sigma_i = 1 \text{ and } \sigma_j = -1$$

In terms of these quantities, the microstate energy for E_p can be written

$$E_p = -4JN_{++} + 2(fJ - B_0)N_+ - \frac{1}{2}(fJ - 2B_0)N,$$

where f is defined so that the number of nearest neighbor pairs with at least one $\sigma_i = 1$ is $f\,\mathrm{N}_+ = 2\,\mathrm{N}_{++} + \mathrm{N}_{+-}$.

a. Write down expressions for the I[illegible]
terms of the canonical partition fu
partition function in terms of the m
to evaluate or simplify your expressi

$$E = -\left[B_0 \sum_j \sigma_j + J \sum_j \sum_{i \in nn} \sigma_i \sigma_j\right]$$

$$\sigma_j = \pm 1$$

b. Let m_0 denote the difference between the fraction of atoms with $M_s = \frac{1}{2}$ and the fraction with $M_s = -\frac{1}{2}$; $m_0 = (N_+ - N_-)/N$. Derive the following approximate implicit equation for m_0 in the limit of zero field strength ($H \rightarrow 0$):

$$B_0 + fJm_0 = k_B T \tanh^{-1}(m_0)$$

(2 Points)

c. From the expression in b., derive an expression for the critical temperature T_c for spontaneous magnetization. Express your answer in terms of f, J, and Boltzmann's constant. **(2 Points)**

d. Derive the *value* of the critical exponent β (the degree of the coexistence curve) that describes how the order parameter $M_0(T)$ behaves as the temperature T approaches the critical temperature T_c from below:

$$M_0 \sim (\frac{T - T_c)}{T_c}) \text{ for } T \leq T_c$$

(3 Points)

Problem 4 (10 Points):

A closed system consists of two distinguishable spin 1 magnets. Each magnet can have one of three orientations, ↑, ↔, and ↓, with respect to the z axis. The respective magnetic moments are +m, 0 and -m. There is no applied field. The Hamiltonian, H = B Σm_i.

↑↑ ↔↑ ↓↑

↑↔ ↔↔ ↓↔

↑↓ ↔↓ ↓↓

a. List all the possible microstates of the system. What is the total number of states? **(1 Points)** 9 microstates, 5 states (2m, m, 0, -m, -2m)

b. For B=0 what is the probability that the total magnetic moment, M, of the system is zero?**(1 Points)** $\frac{3}{9} = \frac{1}{3}$

c. For B=0 compute average value of the total magnetic moment, ⟨M⟩, using the list in part (a.). **(1 Points)** $\frac{1}{3}(0) + \frac{2}{9}(+m) + \frac{2}{9}(-m) + \frac{1}{9}(2m) + \frac{1}{9}(-2m) = 0$

d. If $\Delta M = M - \langle M \rangle$, show that $(\Delta M)^2 = \langle M^2 \rangle - \langle M \rangle^2$, and compute $(\Delta M)^2$ for B=0. **(2 Points)**

e. If the spins were *indistinguishable*, what would be the total number of microstates of the system? **(1 Points)** 6 : ↑↑ ↑↔ ↑↓ ↔↔ ↔↓ ↓↓

For the last two parts of this problem consider N of the spins described in the initial part of the problem. These N spins are now in contact with a heat bath at temperature, T, and B≠0.

f. Find the partition function of the N spins. **(2 Points)**

g. What is the Helmholtz free energy of the N spins? **(2 Points)**

f) $Z = \sum_n e^{\beta E_n} = \left(e^{-\beta m B} + e^{0} + e^{+\beta m B}\right)$ $\quad Z = \left(1 + 2\cosh \beta m B\right)^N$ for N particles (distinguishable)

g) $F = -\frac{1}{\beta} \ln Z = -\frac{N}{\beta} \ln\left(1 + 2\cosh \beta m B\right)$

d) $\Delta M = \langle \Delta M \rangle = \langle M - \langle M \rangle \rangle \rightarrow$

$\Delta M^2 = \langle (M - \langle M \rangle)^2 \rangle = \langle M^2 - M\langle M \rangle 2 + \langle M \rangle^2 \rangle$

$= \langle M^2 - \langle M \rangle^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2$ ✓

$\langle M \rangle^2 = 0$

$\langle M^2 \rangle = \dfrac{0^2 + 2m^2 + 2m^2 + 4m^2 + 4m^2}{9} = \underline{\underline{\frac{12}{9} m^2}} = \Delta M^2$