

Phys 210A — Spring 2024
Problem Set #4: Phase Transition and Critical Phenomena
Due date: Friday June 7

1. **Liquid-Gas Transition** — Van der Waals' theory of interacting gas can be written in terms of the following equation of state:

$$\left(P + \frac{a}{v^2}\right) \cdot (v - v_0) = k_B T,$$

where $v \equiv V/N$ is the specific volume per particle, for a system of N fixed particles. a and v_0 are two interaction parameters.

- (a) Find the critical point (P_c, v_c, T_c) of this system in terms of the interaction parameters v_0 and a . Compute the dimensionless combination $(P_c v_c)/(k_B T_c)$. Show that in terms of the scaled variables $\tilde{P} \equiv P/P_c$, $\tilde{v} = v/v_c$, $\tilde{T} = T/T_c$, the van der Waals equation of state becomes

$$\left(\tilde{P} + \frac{3}{\tilde{v}^2}\right) (3\tilde{v} - 1) = 8\tilde{T}.$$

- (b) Obtain the variational free energy $\Psi(\tilde{v}; \tilde{P}, \tilde{T})$, and sketch its dependence on \tilde{v} for $(\tilde{P}, \tilde{T}) = (0.5, 0.5)$ and $(\tilde{P}, \tilde{T}) = (1, 1)$.
- (c) Expand Ψ in the vicinity of the critical point, i.e., for $t = (T - T_c)/T_c \ll 1$, $p = (P - P_c)/P_c \ll 1$ and $\nu = (v - v_c)/v_c \ll 1$, to $O(\nu^4)$. Find the phase coexistence line $p_{LG}(t)$ to leading order in t .
- (d) Show that along the coexistence line, the difference in specific volume of the two phases is $\Delta\nu(t) \approx 4(-t)^\beta$ to leading order in $t < 0$, and find the value of the exponent β . From the Clausius-Claperton equation, find the latent heat of evaporation.
- (e) For $t = 0$, find the equation of state to leading order in ν , thereby verifying the scaling law $\nu \sim p^{1/\delta}$. Find the value of the exponent δ .
- (f) For $|t| \ll 1$, find the isothermal compressibility $\kappa_T = -\left(\frac{\partial v}{\partial p}\right)_T$ along the “critical isochore” $\nu = 0$. Show that $\kappa_T \approx A_+ t^{-\gamma}$ for $t > 0$ and $\kappa_T \approx A_- |t|^{-\gamma}$ for $t < 0$. Find the value of the exponent γ and the coefficients A_\pm .
2. **Antiferromagnetism** — Consider an Ising *antiferromagnet* in a uniform magnetic field H , described by the Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i,$$

with $J > 0$, and the spins $s_i \in \{\pm 1\}$ arranged on a 2D square lattice.

- (a) At $T = 0$ and $H = 0$, what is the (pair of) ground state spin configurations? Find the threshold field H_c above which this pair of antiferromagnetic states are no longer the lowest in energy. What is the ground state for $H > H_c$?

- (b) Generalize the Weiss mean-field theory to obtain *two* self-consistent equations relating the average magnetization of *neighboring* spins, \bar{s}_A and \bar{s}_B , at finite temperature T .
- (c) For $H = 0$, find the critical point $T_c(0)$ and find the exponent β describing the onset of antiferromagnetic order for T slightly below $T_c(0)$. It will be helpful to obtain the qualitative behaviors at low and high temperatures by sketching graphical solutions to the equations obtained in part (b).
- (d) For $H \neq 0$, expand the two coupled nonlinear equations involving \bar{s}_A and \bar{s}_B to the third order, and express \bar{s}_A, \bar{s}_B in terms of their mean $\bar{s} \equiv (\bar{s}_A + \bar{s}_B)/2$ and difference $m \equiv \bar{s}_A - \bar{s}_B$. Show that $\bar{s} \propto H$ if $|m| \ll 1$.
- (e) Show that m has a singular dependence on T near some temperature $T_c(H)$, and find explicitly $T_c(H)$ for small H . What is the exponent β describing the emergence of antiferromagnetic order (i.e., $|m| \gtrsim 0$) for $H \neq 0$?
- (f) Sketch the phase diagram in the (T, H) plane, indicating clearly the nature of the different phases, and the order(s) of the phase transition(s).
ferromagnet discussed in class and explain the difference.

3. **Isotropic ferromagnet** — An isotropic ferromagnet may be described by the classical Heisenberg model,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{\sigma}(i) \cdot \vec{\sigma}(j) - \mu \vec{H} \cdot \sum_i \vec{\sigma}(i),$$

where $\vec{\sigma}(i)$ is a 3d unit vector giving the direction of a classical spin vector located on lattice site i , $J > 0$ is the strength of the ferromagnetic interaction energy, $\mu \vec{H} \cdot \vec{\sigma}(i)$ gives the magnetic energy of the spin of magnetic moment μ at site i in an uniform external magnetic field \vec{H} , and $\langle i, j \rangle$ denotes sum over q nearest-neighbor sites.

- (a) Apply Weiss' mean-field approximation and write down the mean-field Hamiltonian in term of a sum of non-interacting single-site Hamiltonian $\tilde{\mathcal{H}}$. Show that a self-consistent equation for the average magnetization per site $\vec{m} \equiv \langle \vec{\sigma} \rangle$ can be obtained as the following,

$$m_\alpha = \frac{\partial}{\partial x_\alpha} \log \tilde{Z}(x)$$

where m_α is the component of \vec{m} in direction α , x_α is the component of $\vec{x} \equiv \mathcal{J} \vec{m} + \vec{h}$ in direction α (with $\mathcal{J} = qJ\beta$, and $\vec{h} = \beta\mu\vec{H}$), and $\tilde{Z} = \int d\vec{\sigma} e^{-\beta\tilde{\mathcal{H}}}$ is the single-site partition function which depends on a single dimensionless combination of parameters, $x \equiv |\vec{x}|$.

- (b) Compute $\log \tilde{Z}(x)$ and its derivative by referring to Lecture #7. To explore behaviors close to the critical point, it will be sufficient to expand $\log \tilde{Z}(x)$ to $O(x^4)$. Show that for a vector \vec{v} with magnitude $|\vec{v}| \equiv v$, $\frac{\partial}{\partial v_\alpha} v = v_\alpha/v$, and use this result to derive the self-consistent equation for m_α to $O(m^2 m_\alpha)$ and $O(h_\alpha)$.

- (c) Find the critical temperature T_c in the absence of the external field (i.e., for $\vec{h} = 0$) as the lowest temperature for which the solution of the self-consistent equation is $m = 0$. Explain why the numerical value of T_c is smaller or larger than the result $T_c = qJ/k_B$ derived in class for the Ising model.
- (d) For $T < T_c$, system enters the ferromagnetic phase where $m > 0$ even with $h = 0$. Obtain the dependence of the spontaneous magnetization, m , on the reduced temperature $t = (T - T_c)/T_c$ in the vicinity of the critical temperature for $h = 0$. How does m depend on the magnitude of the applied field h along $T = T_c$?

For a vector order parameter \vec{m} , the magnetic susceptibility is a tensor:

$$\chi_{\alpha\beta} \equiv \lim_{h \rightarrow 0} \frac{\partial m_\alpha}{\partial h_\beta},$$

and can be generally written in the form

$$\chi_{\alpha\beta} = \lim_{h \rightarrow 0} \left[\chi_L \frac{h_\alpha h_\beta}{h^2} + \chi_T \left(\delta_{\alpha\beta} - \frac{h_\alpha h_\beta}{h^2} \right) \right],$$

where χ_L and χ_T are the longitudinal and transverse susceptibility, respectively. In a Cartesian coordinate system, if a small field \vec{h} is applied in the z-direction, then $\chi_{zz} = \chi_L$ and $\chi_{xx} = \chi_{yy} = \chi_T$, while all off-diagonal components are 0.

In the following, you will calculate χ_L and χ_T by starting with the self-consistent equation for $m_\alpha(h_\alpha)$ derived in part (b).

- (e) Let $\vec{h} = h_0 \hat{z} + \delta h_z \hat{z}$. Correspondingly, we expect $\vec{m} = \vec{m}_0(h_0) \hat{z} + \delta m_z \hat{z}$. Insert these forms of \vec{h} and \vec{m} into the equation of state, and find $\chi_L = \lim_{h_0 \rightarrow 0} \frac{\delta m_z}{\delta h_z}$ in the vicinity of the critical temperature by using the result $m(t, h = 0)$ obtained in part (d). State the results both above and below the critical temperature.
- (f) Now let $\vec{h} = h_0 \hat{z} + \delta h_x \hat{x}$ and $\vec{m} = \vec{m}_0(h_0) \hat{z} + \delta m_x \hat{x}$. Again insert these forms of \vec{h} and \vec{m} into the equation of state, and find $\chi_T = \lim_{h_0 \rightarrow 0} \frac{\delta m_x}{\delta h_x}$ in the vicinity of the critical temperature by using the result $m(t, h = 0)$ obtained in part (d). Why does χ_T behave so differently from χ_L below T_c ?

[Hint: Consider the difference in changing the magnitude and direction of \vec{m} in the ferromagnetic phase.]

4. **Potts model** — Consider the following system defined on a square lattice of N sites. On each lattice site i , there is a discrete spin-like variable $s(i)$ which may take on one of q discrete values, e.g., $s(i) \in \{1, 2, \dots, q\}$. The energetics of the system is given by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i, j \rangle} [q \delta_{s(i), s(j)} - 1]$$

such that if the nearest neighbor spins (indicated by $\langle i, j \rangle$) belong to the same state, there is an energy gain of $-(q - 1)J$, while if the nearest neighbor states are different, there is an energy cost of $+J$. This model is known as the q -state Potts model; it is

a generalization of the Ising model for $q > 2$. Here you are asked to provide a mean-field solution to the Potts model for $q = 3$, which is a model of, e.g., the adsorption of Krypton gas on graphite (where each Krypton atom can occupy one of three equivalent sites on the hexagonal lattice of graphite).

- (a) Let the fraction of sites belonging to state s be x_s , with $x_1 + x_2 + x_3 = 1$. Find the mixing entropy $S(x_1, x_2, x_3)$ by computing first the number of configurations Ω that the N sites have N_1 sites in state 1, N_2 sites in state 2, and N_3 sites in state 3. [Hint: You may assume N_1, N_2, N_3 are all much larger than 1 and use the Stirling approximation, $\ln(x!) \approx x \ln(x) - x$ valid for large x .]
- (b) Write down an expression for the average energy $E(x_1, x_2, x_3)$ assuming that each site may belong to state s with probability x_s independently of the states of the other sites.
- (c) Anticipating spontaneous symmetry breaking at low temperatures, one can describe the fraction x_s 's in terms of a single order parameter m (with $0 \leq m \leq 1$) such that when $m = 0$, the $x_s = \frac{1}{3}$ for all 3 states s (corresponding to the complete lack of ordering), and when $m = 1$, one of the state (e.g., $s = 1$) is selected by all sites such that $x_1 = 1$, and $x_2 = x_3 = 0$. Find the linear functions $x_s(m) = a_s m + b_s$ satisfying the above requirements.
- (d) Using $x_s(m)$ found in part (c) for the entropy S and average energy E obtained earlier to show that the *mean-field* free energy $\psi(m) \equiv E - TS$ is of the form

$$\frac{\psi(m)}{Nk_B T} \approx c_0 + \frac{T - T_0}{T} m^2 - \frac{1}{3} m^3 + \frac{1}{2} m^4$$

for small m , with c_0 being an unimportant constant, and T_0 being a characteristic temperature scale set by J/k_B . In what sense is what we have done the “mean-field approximation”?

- (e) Sketch $\psi(m)/(Nk_B T)$ for $T = T_0$ and $T \gg T_0$, and find the value of m (referred to as m^*) which minimizes $\psi(m)$ for the two cases. Show that there is a phase transition at some temperature $T_c > T_0$ and sketch $\psi(m)$ at T_c . Based on the qualitative behavior of $m^*(T)$ above and below T_c , predict the order of this phase transition.