

Homework 6: Phys 7230 (Spring 2022)

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Problem 1 (Classical 1d Ising model via transfer matrix): Consider a 1d Ising model with Hamiltonian, $\mathcal{H}_{\text{1d-Ising}} = -\sum_{i=1}^N J\sigma_i\sigma_{i+1}$, with nearest neighbors exchange interactions, in zero external field, and with periodic boundary conditions (i.e., closed spin-1/2 chain on a ring), with N spins and $\sigma_{N+1} = \sigma_1$.

Use transfer matrix methods discussed in the lectures to compute and plot the total energy $E(T)$ and the corresponding heat capacity $C(T)$, verifying that they are smooth functions (no singularities) as a function of temperature and thus demonstrating that classical 1d Ising model exhibits no phase transition and only has a paramagnetic field.

Note: To really show that it is a paramagnet we would need to compute its magnetization $m(h)$ as a function of field and show that it is always zero in $h \rightarrow 0$ limit and exhibits Curie susceptibility of effectively independent spins. This is worked out in the lecture notes so I will spare you the extra work, but encourage you to explore it further if you are interested.

Solution.

Given the Hamiltonian, the canonical partition function is

$$Z = \sum_{\{\sigma_i\}} \exp \left(\sum_{i=1}^N J\sigma_i\sigma_{i+1} \right) = \sum_{\{\sigma_i\}} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} \dots T_{\sigma_N\sigma_1} = \text{tr}[\hat{T}^N], \quad (1.1)$$

where $\beta J \mapsto J$ and

$$\hat{T}_{\sigma\sigma'} = e^{J\sigma\sigma'} = \begin{pmatrix} e^J & e^{-J} \\ e^{-J} & e^J \end{pmatrix}. \quad (1.2)$$

The eigenvalues of \hat{T} are roots of the characteristic polynomial

$$\det(\hat{T} - \lambda \mathbb{1}) = \det \begin{pmatrix} e^J - \lambda & e^{-J} \\ e^{-J} & e^J - \lambda \end{pmatrix} = \lambda^2 - 2\lambda e^J + e^{2J} - e^{-2J} = 0, \quad (1.3)$$

which are $\lambda_{\pm} = e^J \pm e^{-J}$. Thus, it follows that

$$Z = \lambda_+^N + \lambda_-^N = (2 \cosh J)^N + (2 \sinh J)^N = (2 \cosh(\beta J))^N + (2 \sinh(\beta J))^N \approx (2 \cosh(\beta J))^N, \quad (1.4)$$

where we have unpacked J back into units of energy in the last equality and assumed the thermodynamic limit $N \gg 1$. Now, by definition, the energy is

$$E(T) = -\frac{\partial \ln Z}{\partial \beta} = -NJ \tanh(\beta J). \quad (1.5)$$

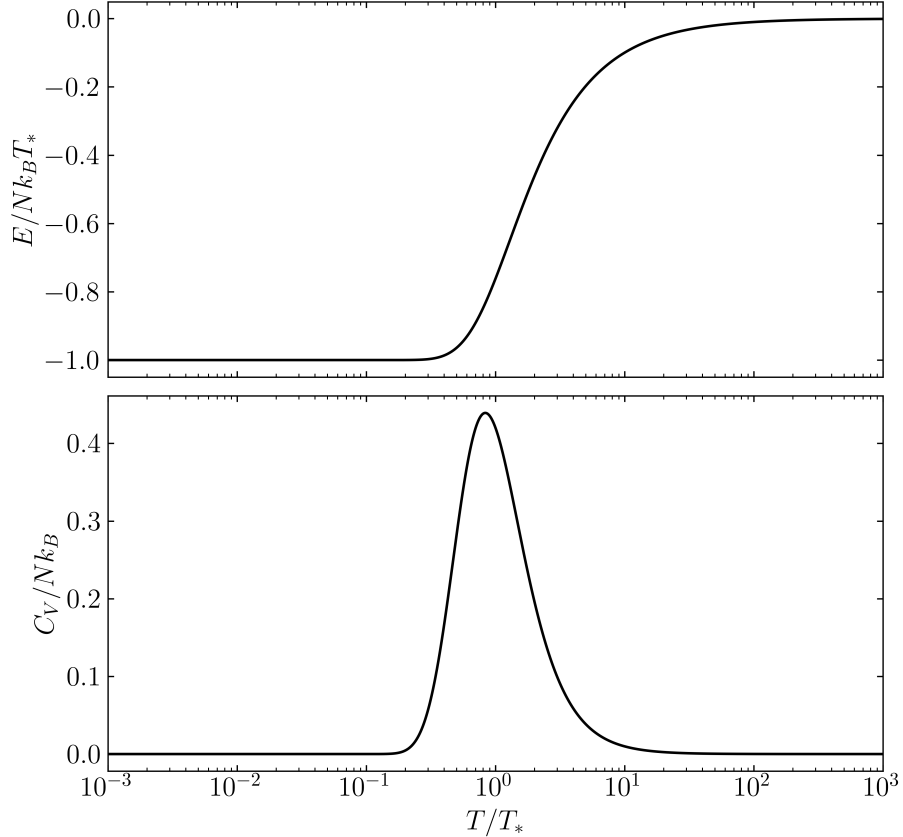
Also, the heat capacity is

$$C_V(T) = \frac{\partial E}{\partial T} = -k_B \beta^2 \frac{\partial E}{\partial \beta} = Nk_B (\beta J)^2 \operatorname{sech}^2(\beta J). \quad (1.6)$$

Letting the crossover temperature be $T_* = J/k_B$, these results can be rewritten as

$$E(T) = -Nk_B T_* \tanh\left(\frac{T_*}{T}\right), \quad \text{and} \quad C_V(T) = Nk_B \left(\frac{T_*}{T}\right)^2 \operatorname{sech}^2\left(\frac{T_*}{T}\right). \quad (1.7)$$

A plot of them is included below. As expected, $E \rightarrow 0$ at high temperature and saturates at $-Nk_B T_*$ at low temperature, and C_v exhibits the Schottky peak form, which crosses over at $T = T_*$.



□

Problem 2 (Ising model in a field via Weiss mean-field theory):

(a) Estimate very roughly the strength of Coulomb interaction in solids, thereby verifying that $E_{\text{Coulomb}} \gg E_{\text{dipole}}$, comparing it also to room temperature. (*Hint*: no complicated calculations are really needed, just reference to a familiar result in e.g., quantum mechanics, where you know the result well in eV).

Solution.

The Coulomb potential energy is

$$E_{\text{Coulomb}} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_0} \approx 27 \text{ eV}, \quad (2.1)$$

where e is the charge of an electron and r_0 is the Bohr radius. Thus, compared to $E_{\text{dipole}} \approx 10^{-4} \text{ eV}$, the Coulomb interaction dominates in a solid. This is also much larger than thermal motion at room temperature $k_B T \sim 0.03 \text{ eV}$. \square

(b) Using Weiss mean-field approximation, rederive the implicit self-consistent MFT equation for the magnetization in $m(T, B)$.

Solution.

First, the classical Heisenberg Hamiltonian with external field is

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \mu \mathbf{S} \cdot \mathbf{B}. \quad (2.2)$$

Now, we write $\mathbf{S}_i = \langle \mathbf{S}_i \rangle + \delta \mathbf{S}_i$, where $\delta \mathbf{S}_i = \mathbf{S}_i - \langle \mathbf{S}_i \rangle$. Plugging this into (2.2), ignoring the $\mathcal{O}(\delta \mathbf{S}^2)$ terms, we get

$$\begin{aligned} \mathcal{H} &= -\frac{1}{2} \sum_{ij} J_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - \frac{1}{2} \sum_{ij} J_{ij} (\langle \mathbf{S}_i \rangle \cdot \delta \mathbf{S}_j + \langle \mathbf{S}_j \rangle \cdot \delta \mathbf{S}_i) - \mu \mathbf{B} \cdot \sum_i \mathbf{S}_i \\ &= -\frac{1}{2} \sum_{ij} J_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - \sum_{ij} J_{ij} \langle \mathbf{S}_j \rangle \cdot (\mathbf{S}_i - \langle \mathbf{S}_i \rangle) - \mu \mathbf{B} \cdot \sum_i \mathbf{S}_i \\ &= \frac{1}{2} \sum_{ij} J_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - \sum_{ij} J_{ij} \langle \mathbf{S}_j \rangle \cdot \mathbf{S}_i - \mu \mathbf{B} \cdot \sum_i \mathbf{S}_i, \end{aligned} \quad (2.3)$$

where we have done a label exchange $i \mapsto j$ and $j \mapsto i$ in the second term in the first equality. Writing the effective Weiss field as $\mathbf{B}_{\text{eff}} = \mathbf{B} + \frac{1}{\mu} \sum_j J_{ij} \langle \mathbf{S}_j \rangle$, we get the same Hamiltonian (31) in the lecture notes

$$\mathcal{H}_{\text{mft}} = \frac{1}{2} \sum_{ij} J_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - \mu \mathbf{B}_{\text{eff}} \cdot \sum_i \mathbf{S}_i. \quad (2.4)$$

\square

(c) Plot both sides of the MFT equation as a function of m for a range of T 's (i) for $B = 0$, thereby solving graphically for $m(T, 0)$ demonstrating that there is a PM-FM phase transition from $m(T > T_c, 0) = 0$ PM to $m(T < T_c, 0) \neq 0$ FM. (ii) Show graphically that for $B \neq 0$ there is a $m(T, B) \neq 0$ solution for any finite T , and that while for $T > T_c$ this solution is smooth, for $T < T_c$ it jumps at $B = 0$ between $m > 0$ to $m < 0$, as B changes sign. Thus, for $T < T_c$ there is a (what's called) a first-order discontinuous phase transition as a function of B at $B = 0$, at which the system jumps between two minima separated by a barrier. This is in contrast to the continuous second-order transition as a function of T at T_c for $B = 0$, where $m > 0$ develops continuously from $m = 0$.

(d) As discussed in the lectures, appreciating that MFT equation for m is actually a saddle-point equation for free-energy density $f(m, B, T)$ with respect to m , i.e., $\partial f / \partial m = 0$, calculate $f(m, B, T)$, plot it for a range of T and B (including $B = 0$), demonstrating how its minima move with these parameters and thereby showing the PM-FM phase transition and its absence for $B = 0$ and $B \neq 0$, respectively.

(e) By Taylor-expanding $f(m, B, T)$ for small m (in fact it may be more convenient to expand the saddle-point MFT equation first and then integrate term by term to obtain the expanded $f(m, B, T)$), show that it exhibits the generic Landau " ϕ " form (i.e., m^4 here, with $\phi = m$) and extract from it the PM-FM transition temperature T_c in terms of the exchange constant J_0 .

(f) By minimizing this Landau ϕ^4 form of $f(m, B, T)$, derive (i) the spontaneous magnetization $m_0(T < T_c, B = 0)$, (ii) $m_0(T_c, B \rightarrow 0)$, (iii) $\chi(T)$, thereby extracting the MF critical exponents β, δ, γ defined in the lecture notes.

(g) Sketch qualitative behavior of the resulting $m(T, B = 0)$ and $m(T, B \neq 0)$ as a function of T through the PM-FM transition.

Note: The MFT results you found are independent of the dimensionality d and therefore for $d = 1$ are in conflict with the exact 1d prediction we found in problem 1 via transfer matrix method. Thus, this should give you caution on noncritically accepting the predictions of MFT approximation.

Solution.

□

Problem 3 (Variational mean-field theory of classical Ising model in external local fields, h_i): Using the variational bound on the free energy, derived in class

$$F \leq F_{\text{var}} = F_{\text{tr}} + \langle \mathcal{H} - \mathcal{H}_{\text{tr}} \rangle_{\text{tr}}, \quad (3.1)$$

with

$$\mathcal{H}_{\text{tr}} = - \sum_{i=1}^N b_i \sigma_i \quad (3.2)$$

as the trial Hamiltonian of independent spins in the presence of N local variationall parameter “fields” b_i , derive mean-field self-consistent (implicit) equations for the local magnetization $m_i(\{h_i/T\})$, by determining variational parameters $b_i(\{h_i/T\})$, that minimize $F_{\text{var}}(\{b_i\})$. By eliminating b_i ’s, show that for uniform $h = h_i$, the self-consistent equation reproduces the Weiss mean-field theory equation for $m(h/T)$.

Solution.

□

Problem 4: The Landau ϕ^4 field theory for Ising ($N = 1$), XY ($O(N = 2)$) and Heisenberg ($O(N = 3)$) models naturally generalizes to $O(N)$ model N component field ϕ ($O(N)$ stands for orthogonal group of rotations, $\phi \rightarrow R \cdot \phi$ under which the model is invariant).

$$H_{O(N)}(\phi) = \int_{\mathbf{x}} \left[\frac{1}{2} K (\nabla \phi)^2 + \frac{1}{2} t |\phi|^2 + \frac{1}{2} u |\phi|^4 + \dots \right], \quad (4.1)$$

An external field \mathbf{h} *explicitly* breaks this $O(N)$ rotational symmetric through a Zeeman term $H_Z = - \int_{\mathbf{x}} \mathbf{h} \cdot \phi$, “telling” ϕ where to point on average. As explored in lectures, $N > 1$ case contains new important physics associated with “massless” (gapless) Goldstone modes. To simplify the analysis, below, let us focus on a mean-field regime where ϕ is spatially uniform, i.e., ignoring the gradient (exchange K) energy above.

(a) Minimize the Landau theory for $t > 0$ and $t < 0$ and find the *spontaneous* order parameter $\phi_0(t)$ for $\mathbf{h} = \mathbf{0}$.

Note: In zero field, its direction is arbitrary and only its magnitude is determined by above minimization.

(b) Note that in the disordered, PM ($T > T_c$) state ϕ fluctuates around 0 and thus a harmonic (quadratic) approximation for the effective Landau Hamiltonian $H_{>} \approx \frac{1}{2} t |\phi|^2$ is sufficient. The effective curvature t of the excitations is sometimes referred to as the “mass-squared” m^2 (not to be confused with magnetization) or a gap-squared Δ^2 (nomenclature going back to application of the $O(N)$ model for quantum phase transitions and in particle physics, where the description corresponds to the Klein-Gordon equation, where it is a mass of a bosonic particle, like the Higgs field). Note that in the PM state $\Delta_{>}^2 = t$ (i denotes $t > 0$, i.e., for $T > T_c$). Using this simple harmonic approximation, calculate the *linear* (uniform) susceptibility χ of ϕ response to small \mathbf{h} in this PM state.

(c) In the ordered FM state, the average order parameter $\langle \phi \rangle_{<} = \phi_0$ is spontaneously nonzero (with arbitrary direction). By taking $\phi = \phi_0 + \delta\phi$ derive the effective Landau theory $\mathcal{H}_{<}$ of small fluctuations $\delta\phi$ about ϕ_0 . Thereby show that (i) longitudinal oscillations, $\delta\phi_L$ along ϕ_0 are gapped (i.e., massive), namely with the corresponding part of the energy going like $\mathcal{H}_L \approx \frac{1}{2} \Delta_{<}^2 |\delta\phi_L|^2 + \dots$ with the gap $\Delta_{<} = \sqrt{2} \Delta_{>}$, (ii) transverse fluctuations, $\delta\phi_T$ perpendicular to ϕ_0 are gapless (i.e., massless), namely with vanishing quadratic term in $\delta\phi_T$, which is the reflection of the underlying rotational symmetry in the spontaneously ordered FM state. Components of these transverse oscillations are the Goldstone modes of the PM-FM “spontaneous symmetry breaking” of the $O(N)$ symmetry of the PM state down to $O(N - 1)$ remaining symmetry of the FM state.

(d) By considering the case of $N = 2$ and $N = 3$ explicitly and thinking geometrically about these oscillations in terms of the “Mexican hat” potential, how many Goldstone modes are there for these two cases? How many Goldstone modes are there for these two cases? How many Goldstone modes are there for the general case of N ? (Just for your future information, more generally, when the symmetry is broken from a disordered state, symmetric under group G down to an ordered state with reduced symmetry group H , the number of Goldstone modes, typically [but with some prominent exceptions, e.g., quantum ferromagnets, that we will discuss later] is the dimension of the coset space G/H .)

Solution.



Problem 6 (XY-model with orthorhombic anisotropy: coupled Ising models): Consider an XY ferromagnet, with additional weak in-plane orthorhombic crystalline anisotropy, due to a *rectangular* unit cell of the crystalline lattice, i.e., the m_x and m_y spin axes are not equivalent.

Aside: Actually, a convenient and well-studied physical system in which such effective model arises is an Ising antiferromagnet with an external field applied parallel or perpendicular to the “easy” Ising axis. The resulting phenomenology (spin-flop transition, etc) has been studied theoretically by M. E. Fisher and D. R. Nelson, Phys. Rev. Lett. **32**, 1350 (1974), and experimentally in MnF_2 and in GdAlO_3 by Y. Shapira and S. Foner, Phys. Rev. **1**, 3083 (1970).

(a) Write down the phenomenological Landau free energy density $f(m_x, m_y)$ for this system.

Hint: You can start out with two independent Ising models, one for m_x component and one for m_y component and then couple them together via a lowest order coupling allowed by symmetry of the problem. Equivalently, you can start out with a rotationally invariant Landau free energy for the XY model and introduce additional terms that appropriately break the spin rotational symmetry, down to a rectangular one.

(b) Give a reason why, given the symmetries of the physical system described above, the coupling such as for example $\delta f_{\text{couple}}^{\text{forbidden}} = 2v_{xy}m_xm_y$ is *not* allowed.

(c) Explore the phase diagram of this model for the quartic couplings satisfying $u_xu_y > u_{xy}^2$. That is,

- (i) make the standard assumption of Landau theory that $t_x = a(T - T_{cx})$ and $t_y = a(T - T_{cy})$ and that all other coupling constants are temperature independent.
- (ii) By varying T , enumerate the possible phases that are allowed and characterize them by the value of the order parameters m_x and m_y in these phases.
- (iii) Display these phases in a two-dimensional phase diagram with t_y and t_x as the two *independent* control parameters (two axes, rather than just one parameter T) in your phase diagram.
- (iv) Compute the expressions for $m_x(t_x, t_y)$ and $m_y(t_x, t_y)$ in these phases.

(d) Repeat above analysis (order parameters, phase diagram) for the case of $u_xu_y < u_{xy}^2$, but still in the range so that the system is stable.

Solution.

□

Bonus problems

Problem 5: The superfluid He^4 order parameter is a complex scalar field, $\psi(\mathbf{x})$ (in the simplest BEC case describing the single-particle wavefunction state that all the He^4 atoms condense into when they undergo a transition into a superfluid BEC phase; you can think of real and imaginary components of ψ as forming a 2-component real vector $\phi = (\psi_r, \psi_i)$ and thus ψ is also an $O(2)$ XY-model order parameter [see problem 4, above]. In the presence of a concentration $c(\mathbf{x})$ of He^3 impurity atoms, the system has the following Landau-Ginzburg Hamiltonian functional,

$$\beta\mathcal{H}_{\text{He}}[\psi(\mathbf{x}), c(\mathbf{x})] = \int_{\mathbf{x}} \left[\frac{1}{2}K(\nabla\psi)^2 + \frac{1}{2}t|\psi|^2 + \frac{1}{2}u|\psi|^4 + \frac{1}{6}v|\psi|^6 + \frac{1}{2}\kappa^{-1}c(\mathbf{x})^2 - \alpha c(\mathbf{x})|\psi|^2 \right], \quad (5.1)$$

where K, u, v, α are constant phenomenological parameters, $t \sim T - T_c$ is a sign-changing reduced temperature, and κ is the He^3 compressibility (but we do not really need to know this to solve the problem); positive v will be needed for the overall energetic stability.

(a) Using Gaussian functional integral calculus in coordinate space \mathbf{x} (at each \mathbf{x} modelled by above ordinary Gaussian integrals), and in particular the identity $\int d\phi e^{-(1/2)a\phi^2 + h\phi} = Z_0 e^{h^2/2a}$, integrate out the concentration field $c(\mathbf{x})$ out of the partition function Z to obtain an effective Landau-Ginzburg Hamiltonian, $\mathcal{H}_{\text{eff}}[\psi(\mathbf{x})]$ involving only the $\psi(\mathbf{x})$ field,

$$Z = \int [D\psi(\mathbf{x})] e^{-\beta\mathcal{H}_{\text{eff}}[\psi(\mathbf{x})]} = \int [D\psi(\mathbf{x})][Dc(\mathbf{x})] e^{-\beta\mathcal{H}_{\text{He}}[\psi(\mathbf{x}), c(\mathbf{x})]}. \quad (5.2)$$

Hint: Do not be intimidated by the functional integral. Because there are no spatial gradients of $c(\mathbf{x})$, these fields decouple in real space, \mathbf{x} , and thus the functional integral reduces to a product $\prod_{\mathbf{x}}$ over \mathbf{x} of decoupled ordinary integral $\int_{-\infty}^{\infty} dc_{\mathbf{x}}$, one at each point \mathbf{x} . Suggestion: think of \mathbf{x} as a discrete variable index, and also neglect the overall multiplicative constant prefactor that results after integration.

(b) Show that the same result (up to the overall multiplicative prefactor that is not important) can be obtained by simply minimizing $\mathcal{H}_{\text{He}}[\psi(\mathbf{x}), c(\mathbf{x})]$ over $c(\mathbf{x})$, thereby eliminating it in favor of $\psi(\mathbf{x})$, to obtain $\mathcal{H}_{\text{eff}}[\psi(\mathbf{x})]$, above.

(c) Show that the resulting effective Landau-Ginzburg Hamiltonian is

$$\beta\mathcal{H}_{\text{eff}}[\psi(\mathbf{x})] = \int_{\mathbf{x}} \left[\frac{1}{2}K(\nabla\psi)^2 + \frac{1}{2}t|\psi|^2 + \frac{1}{4}u_{\text{eff}}|\psi|^4 + \frac{1}{6}v|\psi|^6 \right], \quad (5.3)$$

where your job is to compute u_{eff} in terms of u, α, κ , and note that it can change sign as e.g., κ is varied. Compute the (tri)critical value κ_c at which u_{eff} vanishes.

(d) Show that the resulting $\mathcal{H}_{\text{eff}}(\psi)$ exhibits a *tricritical* point at $t = 0$, $u_{\text{eff}} = 0$, at which the transition as a function of t changes character from a continuous 2nd-order transition to a discontinuous 1st-order transition, as u_{eff} changes sign. Demonstrate this analytically (by finding the behavior of extrema) and graphically by plotting $\mathcal{H}_{\text{eff}}(\psi)$ as function of ψ for various ranges of t and u_{eff} . Which sign of u_{eff} corresponds to the 1st-order transition

Suggestion: Again, don't be intimidated, all you are doing is minimizing a polynomial and finding its minima and maxima points and studying how they behave as function of parameters like t, κ, \dots . So, at mathematical level, it is just an exercise at freshman calculus.

(e) In the 1-st order transition regime, the value of ψ jumps by $\Delta\psi$. Compute how this jump vanishes as the tricritical point $t = 0, u_{\text{eff}} = 0$ is approached from the discontinuous 1st-order side.

(f) At the tricritical point $u_{\text{eff}} = 0$ compute the tricritical exponents β, δ, γ , respectively governing the singularities in “magnetization” (magnitude of ψ) as function of t (for $h = 0$) $\psi(t < 0) \sim |t|^\beta$ and external “field” h (for $t = 0$) $\psi(h) \sim |h|^{1/\delta}$, and linear susceptibility as function of t (at $h = 0$) $\chi(t) \sim |t|^{-\gamma}$.

Solution.

□