8.334: Statistical Mechanics II Problem Set # 10 Due: 4/23

Functional integrals in statistical mechanics.

1. Ring diagrams. a) Consider a partition function for a real-valued *n*-component field $\eta_i(\mathbf{x})$ with gaussian probability distribution

$$Z = \int \mathcal{D}\{\eta\} \exp(-\mathcal{H}), \quad \mathcal{H}(\eta) = \int \frac{1}{2} \left(\tau \eta^2 + K(\nabla \eta)^2\right) d^d x \tag{1}$$

This is a gaussian integral, and it can be evaluated explicitly in terms of the determinant det $(\tau - K\nabla^2)$. Obtain a general expression for Z, without evaluating integrals over \mathbf{q} , and expand $\ln Z$ in powers of τ .

b) As a technical exercise, it is interesting to compute the series in τ for the partition function (1) directly. For that, split the hamiltonian, $\mathcal{H} = \mathcal{H}_0 + \delta \mathcal{H}$, where

$$\mathcal{H}_0 = \int \frac{1}{2} K(\nabla \eta)^2 d^d x \,, \quad \delta \mathcal{H} = \frac{1}{2} \tau \int \eta^2 d^d x \tag{2}$$

Use Taylor series expansion of $\exp(-\delta \mathcal{H})$ in powers of $\delta \mathcal{H}$. In each term, average over $e^{-\mathcal{H}_0}$ using Wick's theorem.

To show that the resulting expression is identical to that in part a), one has to go through some combinatorics. Classify the terms in the average $\langle \delta \mathcal{H}^n \rangle_0$ according to the number of "connected components," i.e. the number of rings in the corresponding Feynman diagram. Show that there is only one connected diagram in each order, usually denoted as $\langle \langle \delta \mathcal{H}^n \rangle \rangle_0$. Obtain an expression for this diagram, and use the relation between $\langle \delta \mathcal{H}^n \rangle_0$ and $\langle \langle \delta \mathcal{H}^m \rangle \rangle_0$, $m \leq n$, to show that the partition function is an exponential of a sum of all connected diagrams,

$$Z = \exp\left(\sum_{n=1}^{\infty} \frac{(-)^n}{2n} \langle \langle \delta \mathcal{H}^n \rangle \rangle_0\right)$$
(3)

Use this formula to establish correspondence¹ with the result of part a).

2. Instantons and Ising model.

a) Let us consider a 1D scalar field problem with

$$\mathcal{H}(\eta) = \int \left(\frac{1}{2}\dot{\eta}^2 - \mu\eta^2 + u\eta^4\right) dx \tag{4}$$

where $\dot{\eta} = \partial_x \eta$. For $\mu > 0$, there are two minima of the hamiltonian, $\eta_{\pm} = \pm \sqrt{\mu/2u}$. Find a solution to the variational problem

$$\frac{\delta \mathcal{H}}{\delta \eta} = 4u\eta^3 - \mu\eta - \ddot{\eta} = 0 \tag{5}$$

¹We have demonstrated the "connected ring summation rule" (3) for gaussian integrals. However, it is a very general rule which is true for any statistical field theory, with arbitrary interactions in the hamiltonian. To show that, one can either use Wick's theorem and combinatorics for generic hamiltonian (see any field theory text), or use a general argument for volume power counting presented in Problem 2, PS#8.

with the asymptotic behavior $\eta(x \to \pm \infty) = \eta_{\pm}$. A saddle point field configuration like that, interpolating between two minima, is known as *instanton*.

Find the energy of an instanton, i.e. the difference between total system energy with and without an instanton.

b) For a large system of size L at low temperature, the problem can be analyzed by assuming that a typical field configuration consists of zero, one or several instantons far apart from each other, $Z = Z_0 + Z_1 + Z_2 + \dots$ Show that the contribution Z_n with n instantons is an L^n function of system size, i.e. each instanton has an entropy $\ln L$ associated with its position within the system. Estimate typical concentration of instantons as a function of temperature.

Using the above estimate, argue that at low temperature one can use a noninteracting instanton gas approximation. Adopt this approximation to interpret $Z_0 + Z_1 + Z_2 + ...$ as a grand canonical ensemble partition function and evaluate it.

c) Consider a 1D Ising model $\mathcal{H} = -J \sum_i s_i s_{i+1}, s_i = \pm 1$. Using Habbard-Stratonovich transformation, decouple the interaction using an auxiliary field η , and sum over s_i in the partition function.

Using gradient expansion for slowly varying field $\eta(x)$, derive a hamiltonian

$$\mathcal{H} = \int \left(\frac{1}{2}K\dot{\eta}^2 + U(\eta)\right)dx \tag{6}$$

and show that at low temperature the effective potential $U(\eta)$ is of a symmetric doublewell form.

Apply the results of parts a), b) to this problem. Interpret instantons in the Ising model language. Evaluate partition function using the method of part b) and compare the the known result for 1D Ising model.

3. Phase transition on a compressible lattice. Consider how a second order phase transition in D=3 is affected by compressibility of the lattice. Assume that² the only important deformation mode is $\xi = \partial_i u_i$ with $\mathbf{q} = 0$,

$$\mathcal{H}(\eta(x), u) = \int \left[\frac{1}{2}\left(\tau\eta^2 + K(\nabla\eta)^2\right) + g\xi\eta^2 + u\eta^4\right] d^3x + \frac{1}{2}\xi^2 V \tag{7}$$

with the coupling to deformation ξ described by the $g\xi\eta^2$ term. (The last term is the elastic energy of the deformation mode.) The partition function can be evaluated by summing over η at each value of ξ , and then integrating over ξ in

$$Z = \left(V\beta/\pi\right)^{1/2} \int_{-\infty}^{+\infty} \exp\left(-\beta V\xi^2 - \beta F(\tau - 2g\xi, u)\right) d\xi \tag{8}$$

where $F(\tau + 2g\xi, u)$ is the free energy of the problem for η , with critical point shifted by $2g\xi$. Using the scaling theory result, $F \propto \tau^{2-\alpha}$, evaluate the integral over ξ in the saddle point approximation. Show that the second order transition is changed into a first order transition. How does the transition width (e.g. measured by latent heat) depend on g?

 $^{^{2}}$ It can be shown by starting with a generic hamiltonian for coupling between order parameter and lattice deformation that only the spatially uniform mode is relevant near phase transition (Larkin and Pikin, 1969).