

Physics GR6047 Quantum Field Theory I

Assignment # 4

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1 Problem 1

Consider a 1D lattice with a two-state spin at each lattice site. The Hamiltonian is,

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \cdot \sigma_j$$

We have N spins and choose periodic boundary conditions $\sigma_{N+1} = \sigma_1$. The partition function is,

$$Z = \text{Tr} (e^{-\beta H}) = \sum_{\sigma} \prod_{\langle i,j \rangle} e^{-\beta J \sigma_i \sigma_j}$$

Then we use the following trick,

$$e^{-\beta J \sigma_i \sigma_j} = \cosh \beta J + \sigma_i \sigma_j \sinh \beta J$$

If we consider the function,

$$Z^{ij} = \cosh \beta J + \sigma_i \sigma_j \sinh \beta J$$

as a matrix in σ_i and σ_j ,

$$M_{\sigma_1 \sigma_2} = \cosh \beta J + \sigma_1 \sigma_2 \sinh \beta J$$

then we find,

$$Z = \sum_{\sigma_1, \dots, \sigma_N} Z_{12} Z_{23} \cdots Z_{N1} = \sum_{\sigma_1, \dots, \sigma_N} M_{\sigma_1 \sigma_2} M_{\sigma_2 \sigma_3} \cdots M_{\sigma_N \sigma_1} = \text{Tr} (M^N)$$

Therefore, it suffices to compute the eigenvalues of the matrix,

$$M = \begin{pmatrix} \cosh \beta J + \sinh \beta J & \cosh \beta J - \sinh \beta J \\ \cosh \beta J - \sinh \beta J & \cosh \beta J + \sinh \beta J \end{pmatrix} = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}$$

which are $2 \cosh \beta J$ and $2 \sinh \beta J$. Therefore,

$$Z = \text{Tr} (M^N) = (2 \cosh \beta J)^N + (2 \sinh \beta J)^N$$

(COMPUTE CORRELATION LENGTH AND HEAT CAPACITY)

2 Problem 2

Consider a 1D lattice with a unit planar vector at each lattice site. That is there is a vector \mathbf{S}_i with length $\mathbf{S}_i^2 = 1$ which can thus be parametrized by an angle ϕ_i . Then the Hamiltonian is,

$$H(\mathbf{S}) = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j)$$

Therefore, the partition function is,

$$Z = \int_{\mathbf{S}} e^{-\beta H(\mathbf{S})} = \int_{\theta \in [0, 2\pi]^N} e^{-\beta \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j)} d\mathbf{S}$$

with N spins and thus $N - 1$ interaction energies. Now we perform a change of variables, $\theta_i = \phi_{i+1} - \phi_i$ for $1 \leq i \leq N - 1$. To preserve degrees of freedom, we also need to consider as a coordinate,

$$\theta = \sum_{i=1}^N \phi_i$$

so that the θ_i and θ can reproduce the ϕ_i . Therefore,

$$Z = \int_{\theta \in [0, 2\pi]^N} \prod_{i=1}^{N-1} e^{-\beta \cos \theta_i} d^N \theta_i = 2\pi \prod_{i=1}^{N-1} \int_0^{2\pi} e^{-\beta \cos \theta_i} d\theta = 2\pi \left(\int_0^{2\pi} e^{-\beta \cos \theta} d\theta \right)^{N-1}$$

Furthermore,

$$\int_0^{2\pi} e^{-\beta \cos \theta} d\theta =$$

(PERIODIC BOUNDARY CONDITIONS?) (HOW TO DO THIS INTEGRAL?)

3 Problem 3

Consider a free energy functional,

$$F[\theta(\mathbf{r})] = \frac{1}{2} \epsilon_0 \int [\ell^2 (\nabla \theta(\mathbf{r}))^2 - \cos^2 \theta(\mathbf{r})] d^3 r$$

The fixed points are found by minimizing the free energy,

$$\frac{\delta F}{\delta \mathbf{r}} = -\epsilon_0 [\ell^2 \nabla^2 \theta(\mathbf{r}) - \sin \theta(\mathbf{r}) \cos \theta(\mathbf{r})] = 0$$

This gives the PDE,

$$\ell^2 \nabla^2 \theta - \sin \theta \cos \theta = 0$$

First, lets consider a domain-wall transition along the z -axis homogenous in the x - y plane. Then we need to solve,

$$\ell^2 \frac{d^2 \theta}{dz^2} = \sin \theta \cos \theta$$

This does not have a solution in terms of elementary functions in general. However, we can solve it for the specific boundary conditions $\theta(z \rightarrow -\infty) = 0$ and $\theta(z \rightarrow +\infty) = \pi$ as follows. First, consider the first integral,

$$\mathcal{E} = \ell^2 \left(\frac{d\theta}{dz} \right)^2 + \cos^2 \theta$$

which is conserved. Therefore,

$$\frac{d\theta}{dz} = \frac{1}{\ell} \sqrt{\mathcal{E} - \cos^2 \theta}$$

For our boundary conditions, $\mathcal{E} = 1$ and thus,

$$\frac{d\theta}{dz} = \frac{1}{\ell} \sqrt{1 - \cos^2 \theta} = \frac{\sin \theta}{\ell}$$

and thus we find,

$$z = \ell \int_{\frac{\pi}{2}}^{\theta} \frac{d\theta}{\sin \theta} = \log \tan \frac{\theta}{2}$$

Inverting gives,

$$\theta(z) = 2 \arctan(e^{z/\ell})$$

From this we may compute the free energy stored in the surface per surface area,

$$\frac{\Delta F}{A} = \int_{-\infty}^{\infty} \left[\ell^2 \left(\frac{d\theta}{dz} \right)^2 - \cos^2 \theta + 1 \right] dz$$

We know that,

$$\mathcal{E} = \ell^2 \left(\frac{d\theta}{dz} \right)^2 + \cos^2 \theta = 1$$

and therefore,

$$\frac{\Delta F}{A} = 2 \int_{-\infty}^{\infty} \sin^2 \theta(t) dz = 4 \int_0^{\infty} \sin^2 \theta(t) dz$$

Now we perform a change of variables,

$$u = \sin \theta(t)$$

Then recall that,

$$\frac{du}{dz} = -\sin \theta \frac{d\theta}{dz} = -\frac{\sin^2 \theta}{\ell}$$

therefore,

$$\frac{\Delta F}{A} = 4\ell \int_0^1 du = 4\ell$$

4 Problem 4

Consider a gas with equation of state,

$$P = \frac{k_B T}{v - b} \exp \left[-\frac{a}{k_B T v} \right]$$

where $v = V/N$. The critical point occurs for a critical isotherm,

$$\begin{aligned}\left(\frac{\partial P}{\partial V}\right)_T &= 0 \\ \left(\frac{\partial^2 P}{\partial V^2}\right)_T &= 0\end{aligned}$$

Computing these derivatives, we find,

$$\begin{aligned}N \left(\frac{\partial P}{\partial V}\right)_T &= -\frac{k_B T}{(v-b)^2} \exp\left[-\frac{a}{k_B T v}\right] + \frac{k_B T}{v-b} \left(\frac{a}{k_B T v^2}\right) \exp\left[-\frac{a}{k_B T v}\right] \\ &= \left[-\frac{1}{v-b} + \frac{a}{k_B T v^2}\right] \frac{k_B T}{v-b} \exp\left[-\frac{a}{k_B T v}\right] \\ &= \left[\frac{a}{v^2} - \frac{k_B T}{v-b}\right] \frac{1}{v-b} \exp\left[-\frac{a}{k_B T v}\right]\end{aligned}$$

Taking a second derivative gives,

$$N^2 \left(\frac{\partial^2 P}{\partial V^2}\right)_T = [a^2(v-b)^2 + 2(k_B T)^2 v^4 - 2a(k_B T)v(b^2 - 3bv + 2v^2)] \frac{1}{(k_B T)v^4(v-b)^3} \exp\left[-\frac{a}{k_B T v}\right]$$

Therefore, we need to set,

$$\frac{a}{v^2} = \frac{k_B T}{v-b}$$

and,

$$a^2(v-b)^2 + 2(k_B T)^2 v^4 - 2a(k_B T)v(b^2 - 3bv + 2v^2) = 0$$

Using the first relation, we find,

$$a^2(v-b)^2 + 2a^2(v-b)^2 - 2a^2(v-b)v^{-1}(b^2 - 3bv + 2v^2) = 0$$

Therefore,

$$3v(v-b) = 2(b^2 - 3bv + 2v^2)$$

Rearranging,

$$v^2 - 3bv + 2b^2 = 0$$

which has a solutions,

$$v = \frac{3b \pm \sqrt{(3b)^2 - 8b^2}}{2} = \frac{3b \pm b}{2} = \begin{cases} b \\ 2b \end{cases}$$

However, we require that $v > b$ else there is a divergence in the equation of state. Thus, $v_c = \frac{3}{2}b$. Then, at the critical point,

$$\frac{a}{4b^2} = \frac{k_B T_c}{b}$$

and thus,

$$k_B T_c = \frac{a}{4b}$$

Therefore, plugging in,

$$\frac{P_c v_c}{k_B T_c} = \frac{a}{4b^2} e^{-4}$$