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PH5080 Statistical Physics **Problem Set 9** **26.3.2022**

Quiz 2 reloaded

1. The energy levels of a quantum mechanical one-dimensional anharmonic oscillator is given by

$$\varepsilon_n = \hbar\omega\Big[\left(n+\tfrac{1}{2}\right) - x\left(n+\tfrac{1}{2}\right)^2\Big] \quad n = 0, 1, 2, \ldots \ ,$$

with $0 \leq x \ll 1$. The oscillator is in contact with a thermal heat bath at temperature T.

(a) Determine the canonical partition function to first order in x. In other words, let

$$Z = Z_0 + x\ Z_1 + O(x^2)\ .$$

Show that

$$Z_0 = \frac{1}{2\sinh\xi} \quad , \quad Z_1 = \frac{\xi}{2}\frac{\partial Z_0}{\partial \xi^2}\ .$$

where $\xi = \hbar\omega/(2k_BT)$.

(b) Let us expand the internal energy as follows:

$$U = U_0 + x\ U_1 + O(x^2)\ .$$

Show that

$$U_0 = -\frac{\hbar\omega}{2}\frac{1}{Z_0}\frac{\partial Z_0}{\partial\xi} \quad , \quad U_1 = -\frac{\hbar\omega}{2}\left(\frac{1}{Z_0}\frac{\partial Z_1}{\partial\xi} - \frac{Z_1}{Z_0^2}\frac{\partial Z_0}{\partial\xi}\right)$$

(c) In the limit of high temperature i.e., $\xi \to 0$, show that Z_0 and Z_1 are given by

$$Z_0 = \frac{1}{2}\left(\frac{1}{\xi} - \frac{\xi}{6} + \frac{7\xi^3}{360} + O(\xi^5)\right)$$
$$Z_1 = \frac{1}{4}\left(\frac{2}{\xi^2} + \frac{7\xi^2}{60} + O(\xi^4)\right)$$

(d) Using the above expansion, show that the internal energy takes the following form in the high temperature limit

$$U = k_BT\left[\left(1 + \frac{\xi^2}{3} + O(\xi^4)\right) + x\ \left(\frac{1}{\xi} - \frac{\xi}{6} + O(\xi^3)\right) + O(x^2)\right]\ ,$$
$$= \frac{\hbar\omega}{2}\left[\left(\frac{1}{\xi} + \frac{\xi}{3} + O(\xi^3)\right) + x\ \left(\frac{1}{\xi^2} - \frac{1}{6} + O(\xi^2)\right) + O(x^2)\right]\ .$$

(e) Show that the specific heat is given by

$$\frac{C}{k_B} = \left(1 - \frac{\xi^2}{3} + O(\xi^4)\right) + x\left(\frac{2}{\xi} + O(\xi^3)\right) + O(x^2) \ .$$

2. Consider the Ising model on a lattice where each site has q nearest neighbours. Thus $q = 2$ in the one-dimensional case and $q = 4$ for the two-dimensional square lattice. The Hamiltonian for the system is given by

$$H = -J \sum_{\langle ij \rangle} \sigma_i \ \sigma_j$$

where σ_i takes values ± 1 (not $\pm 1/2$ as in class). We will try to improve on the mean field solution that we considered in class. This is by consider a site and its q nearest neighbours (call this a **cluster**) and setting all the other sites to take a fixed value $m = \langle \sigma_i \rangle$ that we will determine self-consistently.

(a) Show that the effective Hamiltonian for the cluster of $(q+1)$ spins is then given by

$$H_c = -J\left(\sigma_0 + (q-1)m\right) \sum_{i=1}^{q} \sigma_i \ .$$

Here σ_0 is the spin located at the centre of the cluster and σ_i (for $i = 1, \ldots, q$) are its q nearest neighbours.

(b) Show that the canonical partition function of the cluster is given by

$$\begin{aligned} Z &= \sum_{\sigma_0} \left(2\cosh(\tilde{\beta}(\tilde{m} + \sigma_0)\right)^q \\ &= \left(2\cosh(\tilde{\beta}(\tilde{m} + 1)\right)^q + \left(2\cosh(\tilde{\beta}(\tilde{m} - 1)\right)^q \ . \end{aligned}$$

where $\tilde{\beta} = \beta J$ and $\tilde{m} = (q-1)m$.

(c) Hence show that

$$\langle \sigma_0 \rangle = \frac{\left(\cosh(\tilde{\beta}(\tilde{m}+1)\right)^q - \left(\cosh(\tilde{\beta}(\tilde{m}-1)\right)^q}{\left(\cosh(\tilde{\beta}(\tilde{m}+1)\right)^q + \left(\cosh(\tilde{\beta}(\tilde{m}-1)\right)^q}$$

and

$$\langle \sigma_i \rangle = \frac{[\cosh(\tilde{\beta}(\tilde{m}+1)]^{q-1}(\sinh(\tilde{\beta}(\tilde{m}+1)) + [\cosh(\tilde{\beta}(\tilde{m}-1)]^{q-1}(\sinh(\tilde{\beta}(\tilde{m}-1))}{\left(\cosh(\tilde{\beta}(\tilde{m}+1)\right)^q + \left(\cosh(\tilde{\beta}(\tilde{m}-1)\right)^q}$$

(d) Equating the two expressions in the previous part, show that m is determined by the consistency condition

$$\left(\frac{\cosh\tilde{\beta}(\tilde{m}+1)}{\cosh\tilde{\beta}(\tilde{m}-1)}\right)^{q-1} = e^{2\tilde{\beta}\tilde{m}} \ ,$$

where $\tilde{\beta} = \beta J$ and $\tilde{m} = (q-1)m$. It is easy to see that $m = 0$ is always a solution. The appearance of additional solutions determine whether there is a phase transition or not. This is done by studying the behaviour near $m = 0$ graphically as we did in the other case.

(e) Show that the critical temperature is given by the condition

$$\tanh \beta_c J = \frac{1}{q-1} \ .$$

For the one-dimensional lattice, $q = 2$ and we see that $\beta_c \to \infty$ which gives $T_c = 0$ in agreement with the exact solution. Thus, this mean field solution behaves better than the mean field solution that we studied in class.
Hint: Take the logarithm of the consistency condition. The slope of the two sides match at the critical temperature.

3. As discussed in class, the mean number of fermions with energy ε is given by the formula.

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

(a) Show that at zero temperature $n(\varepsilon) = 1$ for $\epsilon < \mu$ and $n(\varepsilon) = 0$ for $\varepsilon > \mu$. What is its value at $\varepsilon = \mu$.

(b) In same plot, plot the function for temperatures $k_B T/\mu = 0, 1/100, 1/10, 1$.

(c) Given the number density (N/V) of a gas of spin-1/2 fermions, obtain a formula for the chemical potential at $T = 0$ by computing the following integral:

$$N = 2\int d\varepsilon\ \rho(\varepsilon)\ n(\varepsilon)\ .$$

Use the semi-classical expression for $\rho(\varepsilon)$