باسمه تعالی

درس پدیده‌های بحرانی

تمرینات سری دوم

زمان تحویل: ۹۷/۷/۲۵

۱- تمرین ۲ فصل دوم کتاب Goldenfeld

۲- تمرین ۱و ۲و ۳و ۴ فصل اول کتاب Cardy

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تحصیل علم و دانش مایه‌ی تقویت و تأیید عقل آدمی است. "حضرت علی(ع)"

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Answer to Exercise set 2 of Critical Phenomena

1- (**Goldenfeld book exercise 2-2**):

(a) We know that free energy and entropy related to N as follows:

$$\begin{aligned} F &= E - S \\ &= J_0 \frac{N^2}{2} - kT \log 2^N \\ &= J_0 \frac{N^2}{2} - kTN \log 2 \end{aligned}$$

We know that below limit should be existed for free energy per site:

$$f = \lim_{N\to\infty} \frac{F}{N} = \lim_{N\to\infty} \left(J_0 \frac{N}{2} - kT \log 2 \right)$$

Above equation implies that we should have $J_0 = J/N$ otherwise free energy in thermodynamic limit become infinity or independent of J.

(b)

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi/Na}} e^{-\frac{Na}{2}y^2 + axy} &= \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi/Na}} e^{-\left(y\sqrt{\frac{Na}{2}} - \frac{ax}{2}\sqrt{\frac{2}{Na}}\right)^2 + \frac{a^2x^2}{4}\frac{2}{Na}} \\ &= e^{\frac{a^2x^2}{4}\frac{2}{Na}} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi/Na}} e^{-\left(y\sqrt{\frac{Na}{2}} - \frac{ax}{2}\sqrt{\frac{2}{Na}}\right)^2} \end{aligned}$$

By changing the variables we have:

$$\int_{-\infty}^{\infty} \frac{du\sqrt{\frac{2}{Na}}}{\sqrt{2\pi/Na}} e^{-u^2} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} du\ e^{-u^2 1} = 1, \qquad u = y\sqrt{\frac{Na}{2}} - \frac{ax}{2}\sqrt{\frac{2}{Na}}$$

So we have:

$$\int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi/Na}} e^{-\frac{Na}{2}y^2 + axy} = e^{\frac{ax^2}{2N}}$$

(c) For partition function we have:

$$\mathcal{Z}_\Omega = Tr\left[\exp\left[\beta H \sum_i s_i + \frac{\beta J}{2N} \sum_{ij} s_i s_j \right] \right] \tag{1}$$

We have interactions between all agents so we can write:

$$\sum_{ij} s_i s_j = \left(\sum_i s_i \right)^2 \equiv S^2$$

[1] $\int_{-\infty}^{\infty} dx\ e^{-x^2} = \sqrt{\pi}$

With the result of previous part we can write particle to fields relation which is:

$$\sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}\exp\Big[-\frac{N\beta J}{2}y^2+\beta JyS\Big]dy=\exp\Big[\frac{\beta J}{2N}S^2\Big]$$

Plug in above result in 1:

$$\begin{aligned}
\mathcal{Z}_\Omega &= Tr\exp\Big[\beta HS+\frac{\beta J}{2N}S^2\Big]\\
&= Tr\exp\Big[\beta HS\Big]\exp\Big[\frac{\beta J}{2N}S^2\Big]\\
&= Tr\sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}\exp\Big[-\frac{N\beta J}{2}y^2+\beta(Jy+H)S\Big]dy\\
&= \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}\exp\Big[-\frac{N\beta J}{2}y^2\Big]Tr\Big(\exp[\beta(Jy+H)S]\Big)dy\\
&= \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}\exp\Big[-\frac{N\beta J}{2}y^2\Big]\Big[\sum_{\{s_i\}}\exp[\beta(Jy+H)S\Big]dy\\
&= \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}\exp\Big[-\frac{N\beta J}{2}y^2\Big]\Big[\sum_{s_1=\pm1}e^{\beta(Jy+H)s_1}\cdots\sum_{s_N=\pm1}e^{\beta(Jy+H)s_N}\Big]dy\\
&= \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}\exp\Big[-\frac{N\beta J}{2}y^2\Big]\Big[e^{\beta(Jy+H)}+e^{-\beta(Jy+H)}\Big]^N dy\\
&= \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}\exp\Big[-\frac{N\beta J}{2}y^2\Big]\Big[2\cosh(\beta(Jy+H))\Big]^N dy\\
&= \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}\exp\Big[-\frac{N\beta J}{2}y^2+N\log\Big(2\cosh\big(\beta Jy+\beta H\big)\Big)\Big]dy
\end{aligned}$$

We take definition of L as:

$$L\equiv\frac{J}{2}y^2-\frac{1}{\beta}\log\Big(2\cosh[\beta(H+Jy)]\Big)$$

We can write desired result as:

$$\mathcal{Z}_\Omega=\sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty}e^{-N\beta L}dy$$

(d) We can approximate integral of previous part by steepest descents or saddle point approximation [2] . We want that integrand be very large, so we have:

$$\frac{J}{2}y^2<\frac{1}{\beta}\log\Big(2\cosh[\beta(H+Jy)]\Big)$$

For finding L's extremums, we take derivation:

$$\frac{\partial L}{\partial y}=Jy-J\tanh[\beta(H+Jy)]=0\Rightarrow y=\tanh[\beta(H+Jy)] \tag{2}$$

[2] *For more information see this page* `https://en.wikipedia.org/wiki/Method_of_steepest_descent`

If we have several y that make $e^{-N\beta L}$ very large number, we can approximate partition function by:

$$\mathcal{Z}(\beta, H, J) = \sum_i e^{-N\beta L(H,J,\beta,y_i)}$$

y_i is state that have very large $\exp[-N\beta L(H, J, \beta, y_i)]$ and we can approximate partition function by summation of this large numbers. The probability of finding system in state y_i is:

$$P(y_i) = \frac{e^{-N\beta L(H,J,\beta,y_i)}}{\sum_i e^{-N\beta L(H,J,\beta,y_i)}}$$

We have some important states that dominates others (because of thermodynamic limit) so we can ignore them and use above equation as Boltzmann weight factor.

For magnetization we should take this limit:

$$\begin{aligned}
M &\equiv \lim_{N(\Omega)\to\infty} \frac{1}{\beta N(\Omega)} \frac{\partial \log \mathcal{Z}_\Omega}{\partial H} \\
&= \lim_{N(\Omega)\to\infty} \frac{1}{\beta N(\Omega)} \sqrt{\frac{N(\Omega)\beta J}{2\pi}} \frac{\partial}{\partial H}\left(\log \int_{-\infty}^{\infty} e^{-N(\Omega)\beta L} dy\right) \\
&= \lim_{N(\Omega)\to\infty} -\frac{\beta N(\Omega)}{\beta N(\Omega)} \frac{\int_{-\infty}^{\infty} \frac{\partial L}{\partial H}\, e^{-N(\Omega)\beta L} dy}{\int_{-\infty}^{\infty} e^{-N(\Omega)\beta L} dy} \\
&= -\frac{\int_{-\infty}^{\infty} \tanh[\beta(H + Jy)]\, e^{-N(\Omega)\beta L} dy}{\int_{-\infty}^{\infty} e^{-N(\Omega)\beta L} dy} \\
&\approx -\frac{\tanh[\beta(H + Jy_0)]\, e^{-N(\Omega)\beta L_0}}{e^{-N(\Omega)\beta L_0}} = \tanh[\beta(H + Jy_0)] \\
&= y_0
\end{aligned}$$

For the last part we use 2.

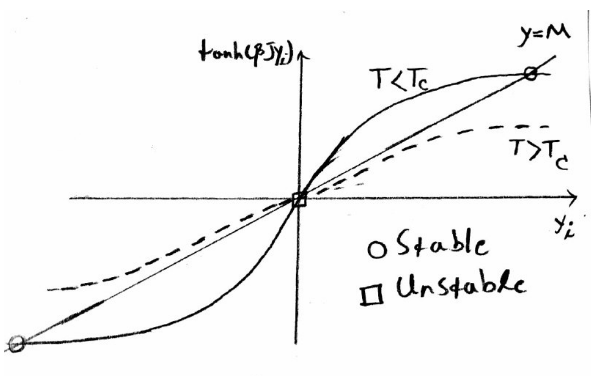
(e) We can deal with this part by using self-consistent method like Goldenfeld book page 106. We know that equation for y_i is:

$$y_i = \tanh[\beta(H + Jy_i)]$$

For $H = 0$ we have:

$$y_i = \tanh\,(\beta J y_i)$$

We can use graphics to solve above. Consider below image and we can have one y_i or two, for different β:



If we expand tanh function for small y_i we can find:

$$y_i = \beta J y_i + \cdots \Rightarrow \beta J = 1 \Rightarrow T_c = \frac{J}{k_B}$$

If the slope of function for small y_i is bigger than one, we have three solution and if slope be smaller than unity we have one solution, critical temperature that specifies this behavior is T_c.

(f) Let $\tau = T_c/T$ and we know $y_0 = M$, we can the equation of state as below:

$$M = \tanh\left(H/k_BT + \tau M\right) = \frac{\tanh H/k_BT + \tanh M\tau}{1 + \tanh H/k_BT \tanh M\tau}$$

Thus:

$$\tanh H/k_BT = \frac{M - \tanh M\tau}{1 - M\tanh M\tau}$$

For small M and H we can expand above, I use Mathematica and answer is:

$$H/k_BT \approx M(1-\tau) + M^3(\tau - \tau^2 + \tau^3/3) \tag{3}$$

We take derivate with respect to H we have:

$$1/k_BT \approx \chi_T(1-\tau) + 3M^2\chi_T(\tau - \tau^2 + \tau^3/3) \tag{4}$$

For $T > T_c$ we know $M = 0$ so we have:

$$\chi_T \approx \frac{1}{k_BT_c}\frac{1}{t}$$

This show that χ_T diverge as $T \longrightarrow T_c^+$ with critical exponent $\gamma = 1$. For $T \longrightarrow T_c^-$ we begin from equation 3 and put $H = 0$ so we have:

$$M^2 \approx 3\frac{\tau - 1}{\tau} \Rightarrow M \approx \sqrt{3}\left(\frac{T_c - T}{T_c}\right)^{1/2}$$

Put above in 4 we have:

$$\begin{aligned}
1/k_BT &\approx \chi_T(1-\tau) + 9\left(\frac{\tau - 1}{\tau}\right)\chi_T(\tau - \tau^2 + \tau^3/3) \\
1/k_BT &\approx \chi_T(1-\tau) + 9\chi_T\,(\tau - 1)\,(1 - \tau + \tau^2/3) \\
\chi_T &\approx \frac{1}{k_BT}\frac{1}{1-\tau}\frac{1}{1 - \tau + \tau^2/3} \\
\chi_T &\propto \frac{1}{k_B}\frac{1}{T - T_c} = \frac{1}{k_BT_c}\frac{1}{t}
\end{aligned}$$

This show that χ_T diverge as $T \longrightarrow T_c^-$ with critical exponent $\gamma' = 1$ and $\gamma = \gamma' = 1$. You can find this calculation in Goldenfeld book page 107 and 108.

2- (**Cardy book exercise 1-1**):
We can write Hamiltonian as below:

$$
\begin{aligned}
\mathcal{H} = \sum_{rr'} \Bigg[& J_{AA}(r-r')\frac{1}{2}\left[1+s(r)\right]\frac{1}{2}\left[1+s(r')\right] \\
& + J_{BB}(r-r')\frac{1}{2}\left[1-s(r)\right]\frac{1}{2}\left[1-s(r')\right] \\
& + J_{AB}(r-r')\frac{1}{2}\left[1+s(r)\right]\frac{1}{2}\left[1-s(r')\right] \Bigg]
\end{aligned}
$$

If there is a particle type A in r we have $[1+s(r)]/2$ and if we have particle type B in r we have $[1-s(r)]/2$, we can write expanded Hamiltonian as below:

$$
\begin{aligned}
\mathcal{H} = \frac{1}{4}\sum_{rr'} \Bigg[& \Big(J_{AA}(r-r') + J_{BB}(r-r') - J_{AB}(r-r')\Big)s(r)s(r') \\
& \Big(J_{AA}(r-r') - J_{BB}(r-r') + J_{AB}(r-r')\Big)s(r) \\
& \Big(J_{AA}(r-r') - J_{BB}(r-r') - J_{AB}(r-r')\Big)s(r') \Bigg] + \text{const.}
\end{aligned}
$$

The last two term can be combined together because summation on r and r' is identical. So Hamiltonian is:

$$
\begin{aligned}
\mathcal{H} = \frac{1}{4}\sum_{rr'} & \Big(J_{AA}(r-r') + J_{BB}(r-r') - J_{AB}(r-r')\Big)s(r)s(r') \\
& + \frac{1}{2}\sum_{rr'}\Big(J_{AA}(r-r') - J_{BB}(r-r')\Big)s(r') + \text{const.}
\end{aligned}
$$

we can map above Hamiltonian to Ising model by below definition:

$$
\begin{aligned}
J_{\text{eff}}(r-r') &= \frac{1}{4}\Big(J_{AA}(r-r') + J_{BB}(r-r') - J_{AB}(r-r')\Big) \\
H_{\text{eff}}(r-r') &= \frac{1}{2}\Big(J_{AA}(r-r') - J_{BB}(r-r')\Big)
\end{aligned}
$$

Finally:

$$
\mathcal{H} = \sum_{rr'} J_{\text{eff}}(r-r')s(r)s(r') + \sum_{rr'} H_{\text{eff}}(r-r')s(r)
$$

If we have $J > 0$ we should expect Ising critical behavior when effective magnetic field vanish at some length scale. It could be somewhere when spin magnetic field of atoms doesn't interact with each other.

3- (**Cardy book exercise 1-2**):
In Ising model, we have two important symmetries first time-reversal symmetry (which tell us $Z_\Omega(-H, J, T) = Z_\Omega(H, J, T)$) and second sub-lattice symmetry. In second (if we have $H = 0$) we divide hypercubic lattice up into two sub-lattices which when we add up them we construct original hypercubic lattice. Ising model Hamiltonian is:

$$\mathcal{H}_\Omega(0, J, \{S_i\}) = -J \sum_{\langle ij \rangle} S_i S_j$$

$\langle ij \rangle$ means sum over nearest neighbors. With two sub-lattices A and B Hamiltonian becomes:

$$\mathcal{H}_\Omega(0, J, \{S_i^A\}, \{S_i^B\}) = -J \sum_{\langle ij \rangle} S_i^A S_j^B$$

We can find for above Hamiltonian below symmetries:

$$\mathcal{H}_\Omega(0, -J, \{S_i^A\}, \{S_i^B\}) = \mathcal{H}_\Omega(0, J, \{-S_i^A\}, \{S_i^B\}) = \mathcal{H}_\Omega(0, J, \{S_i^A\}, \{-S_i^B\})$$

We know that $J > 0$ in Ising model means ferromagnetic and $J < 0$ means anti-ferromagnetic. Now we want to show that if our Hamiltonian has above symmetries the partition function for ferromagnetic and anti-ferromagnetic is identical, we have:

$$\begin{aligned}
\mathcal{Z}_\Omega(0, -J, T) &= Tre^{-\beta\mathcal{H}_\Omega(0,-J,T)} \\
&= \sum_{\{S_i^A\}} \sum_{\{S_i^B\}} e^{-\beta\mathcal{H}_\Omega(0,-J,T,\{S_i^A\},\{S_i^B\})} \\
&= \sum_{\{S_i^A\}} \sum_{\{S_i^B\}} e^{-\beta\mathcal{H}_\Omega(0,J,T,\{-S_i^A\},\{S_i^B\})} \\
&= \sum_{\{S_i^A\}} \sum_{\{S_i^B\}} e^{-\beta\mathcal{H}_\Omega(0,J,T,\{S_i^A\},\{S_i^B\})} \\
&= \mathcal{Z}_\Omega(0, J, T)
\end{aligned}$$

In above I use $\mathcal{H}_\Omega(0, J, T, \{-S_i^A\}, \{S_i^B\}) = \mathcal{H}_\Omega(0, J, T, \{S_i^A\}, \{S_i^B\})$, this means that we have all configuration for S_i^A that contain all opposite configurations too, this is coming from time-reversal symmetry. In zero magnetic field, the ferromagnetic Ising model ($J > 0$) and anti-ferromagnetic Ising model ($J < 0$) on hypercubic lattice have same thermodynamics. This conclusion relies on the fact that a hypercubic lattice is **bipartite**: it can be subdivided into two equivalent sub-lattices. The theorem does not apply on a triangular lattice, which is not bipartite.

<u>For detail information see Goldenfeld book section 2-7.</u>

4- (**Cardy book exercise 1-3**):
Up to now, we have considered classical dipoles, which can assume all possible orientations. However, the magnetic moment of atoms is caused by electrons moving around the nucleus; i.e., it is a quantum mechanical quantity. Therefore we want to perform the same considerations once again for quantum mechanical dipoles. Assume again a magnetic field H in z-direction. In quantum mechanics, μ is an operator which is defined by:

$$\hat{\boldsymbol{\mu}} = (g_l \hat{\boldsymbol{l}} + g_s \hat{\boldsymbol{s}}) \tag{5}$$

Here $\hat{\boldsymbol{l}}$ is the angular momentum operator and $\hat{\boldsymbol{s}}$ is the spin operator, all of which are now dimensionless. The factor $\hbar$ has been incorporated into the Bohr magneton $\mu_B = e\hbar/(2mc)$. Equation 5 is motivated by the fact that the magnetic moment of an electron rotating on a sphere is classically proportional to the angular momentum of the electron.

We know that $\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$ and we know the projection of $\boldsymbol{\mu}$ on $\boldsymbol{j}$ is conserved quantity we can define:

$$\begin{aligned}
\boldsymbol{\mu}_P &= \frac{\boldsymbol{\mu}\cdot\boldsymbol{j}}{|\boldsymbol{j}|^2}\,\frac{\boldsymbol{j}}{|\boldsymbol{j}|} = (g_l \boldsymbol{l}\cdot\boldsymbol{j} + g_s \boldsymbol{s}\cdot\boldsymbol{j})\,\mu_B\,\frac{\boldsymbol{j}}{|\boldsymbol{j}|^2}, \qquad \boldsymbol{l}\cdot\boldsymbol{s} = \frac{1}{2}(|\boldsymbol{j}|^2 - |\boldsymbol{l}|^2 - |\boldsymbol{s}|^2)\\
&= \left[g_l(|\boldsymbol{l}|^2 + \boldsymbol{l}\cdot\boldsymbol{s}) + g_s(|\boldsymbol{s}|^2 + \boldsymbol{l}\cdot\boldsymbol{s})\right]\mu_B\,\frac{\boldsymbol{j}}{|\boldsymbol{j}|^2}\\
&= \left[(g_l + g_s)\boldsymbol{l}\cdot\boldsymbol{s} + |\boldsymbol{l}|^2 g_l + |\boldsymbol{s}|^2 g_s\right]\mu_B\,\frac{\boldsymbol{j}}{|\boldsymbol{j}|^2}\\
&= \frac{1}{2}\left[(g_l + g_s)(|\boldsymbol{j}|^2 - |\boldsymbol{l}|^2 - |\boldsymbol{s}|^2) + 2|\boldsymbol{l}|^2 g_l + 2|\boldsymbol{s}|^2 g_s\right]\mu_B\,\frac{\boldsymbol{j}}{|\boldsymbol{j}|^2}\\
&= \frac{1}{2}\left[(g_l + g_s)|\boldsymbol{j}|^2 + (g_l - g_s)|\boldsymbol{l}|^2 + (g_s - g_l)|\boldsymbol{s}|^2\right]\mu_B\,\frac{\boldsymbol{j}}{|\boldsymbol{j}|^2}
\end{aligned}$$

Put eigenvalues of operators is above we find:

$$\boldsymbol{\mu}_P = g\mu_B \boldsymbol{j}, \qquad g = \left(\frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)}\right) \tag{6}$$

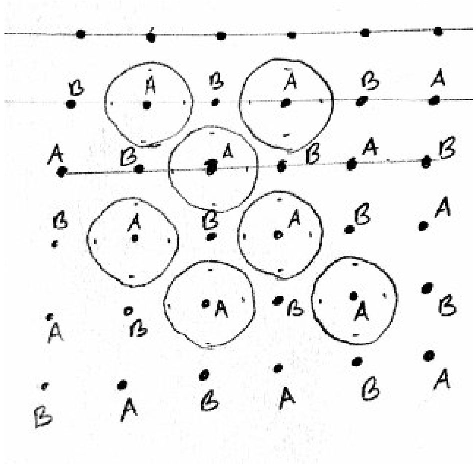
where the values $g_l = 1$ and $g_s \approx 2$ for electrons have been inserted. The projection factor g is the *gyro magnetic ratio or Lande factor.*

Now we can define our Ising like spins to be $\boldsymbol{\mu}_P$ and interaction between them is J_{ij}, Hamiltonian is:

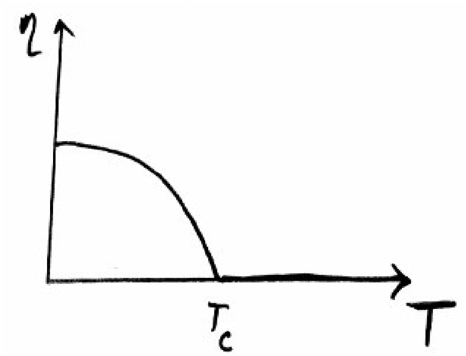
$$\mathcal{H} = -\sum_{\langle uv\rangle} J_{uv}\, S_u S_v$$

We consider interaction between spins is $J_{uv} = g_u g_v$, g_u and g_v can be calculated with equation 6. In high temperature spins are up or down randomly and their energy is maximized, so we can consider their exchange energy interaction between them is maximized or g_u and g_v are maximum, this implies that orbital and spin angular momentum be their maximum value of their options.

3- (**Cardy book exercise 1-4**):
We can find two degenerate ground state with same energy, by setting atoms on A sites or on B sites like figure below:



They are actually one state and their energies are identical. We can define order parameter as $\eta = |N_A - N_B|/N$, this parameter is zero when temperature is high and become one in low temperature like below figure (instead M_s put η):



The pair correlation function g(r) can be measured experimentally using quasi elastic scattering. If a sample is illuminated with a monochromatic beam of x-rays, neutrons, visible light, and so on, the scattered intensity as a function of the angle from the incident beam direction is proportional to the Fourier transform of $g(r)$ (two point correlation function). We can derive this relation:

$$S(\boldsymbol{k}) = {}^{3}\frac{1}{N}\left\langle \sum_{i,j} exp\left[-i\boldsymbol{k}.(\boldsymbol{r}_i - \boldsymbol{r}_j)\right]\right\rangle$$
$$= 1 + \frac{N}{V}\int [1 - g(r)]\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} d\boldsymbol{r} + \frac{N}{V^2}\left|\int e^{i\boldsymbol{k}\cdot\boldsymbol{r}} d\boldsymbol{r}\right|^2$$

For more information see section 10.7.A of Pathria third edition. Structure factor of two above states are equal in law temperature, in high temperature we don't have a lattice or structure.

[3] Structure factor