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Answer to Exercise Set #3 of Critical Phenomena

1- (Cardy book exercise 2-1):

Feynman inequality is:

$$\langle e^X \rangle \geq e^{\langle X \rangle}$$

We take $X = \mathcal{H}' - \mathcal{H}$ and we use $\langle A \rangle = \langle A \rangle_{\mathcal{H}'}$ (A is an observable) we have:

$$\begin{aligned} \langle e^{\mathcal{H}' - \mathcal{H}} \rangle_{\mathcal{H}'} &\geq e^{\langle \mathcal{H}' - \mathcal{H} \rangle_{\mathcal{H}'}} \\ \frac{\text{Tr} [e^{\mathcal{H}' - \mathcal{H}} e^{-\mathcal{H}'}]}{\text{Tr} [e^{-\mathcal{H}'}]} &\geq e^{\langle \mathcal{H}' - \mathcal{H} \rangle_{\mathcal{H}'}} \\ \text{Tr} [e^{-\mathcal{H}}] &\geq e^{\langle \mathcal{H}' - \mathcal{H} \rangle_{\mathcal{H}'}} \text{Tr} [e^{-\mathcal{H}'}] \\ \text{Tr} [e^{-\mathcal{H}}] &\geq \text{Tr} [e^{-\mathcal{H}'} e^{\langle \mathcal{H}' - \mathcal{H} \rangle_{\mathcal{H}'}}] \\ \text{Tr} [e^{-\mathcal{H}}] &\geq \text{Tr} [e^{-\mathcal{H}' - \langle \mathcal{H}' - \mathcal{H} \rangle_{\mathcal{H}'}}] \end{aligned}$$

We know that $e^{\langle \mathcal{H}' - \mathcal{H} \rangle_{\mathcal{H}'}}$ is a constant because of averaging.

2- (Cardy book exercise 2-2):

This problem is like problem 2-2 of Goldenfeld book, solution is as follows:

(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:

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

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:

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

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:

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

We have interactions between all agents so we can write:

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

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

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

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

Plug in above result in 1:

$$\begin{aligned}
\mathcal{Z}_\Omega &= \text{Tr} \exp \left[\beta HS + \frac{\beta J}{2N} S^2 \right] \\
&= \text{Tr} \exp \left[\beta HS \right] \exp \left[\frac{\beta J}{2N} S^2 \right] \\
&= \text{Tr} \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} \exp \left[-\frac{N\beta J}{2} y^2 + \beta(Jy + H)S \right] dy \\
&= \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} \exp \left[-\frac{N\beta J}{2} y^2 \right] \text{Tr} \left(\exp[\beta(Jy + H)S] \right) dy \\
&= \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} \exp \left[-\frac{N\beta J}{2} y^2 \right] \left[\sum_{\{s_i\}} \exp[\beta(Jy + H)S] \right] dy \\
&= \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} \exp \left[-\frac{N\beta J}{2} y^2 \right] \left[\sum_{s_1=\pm 1} e^{\beta(Jy+H)s_1} \dots \sum_{s_N=\pm 1} e^{\beta(Jy+H)s_N} \right] dy \\
&= \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} \exp \left[-\frac{N\beta J}{2} y^2 \right] \left[e^{\beta(Jy+H)} + e^{-\beta(Jy+H)} \right]^N dy \\
&= \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} \exp \left[-\frac{N\beta J}{2} y^2 \right] \left[2 \cosh(\beta(Jy + H)) \right]^N dy \\
&= \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} \exp \left[-\frac{N\beta J}{2} y^2 + N \log \left(2 \cosh(\beta(Jy + H)) \right) \right] dy
\end{aligned}$$

We take definition of L as:

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

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:

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

For finding L 's extremums, we take derivation:

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

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

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

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

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:

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

For the last part we use 2.

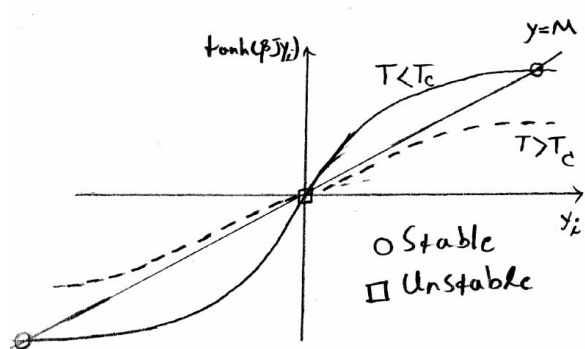
(e) We can deal with this part by using self-consistent method like Goldenfeld book page 106. We know that equation for y_i is:

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

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:

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

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:

$$M = \tanh(H/k_B T + \tau M) = \frac{\tanh H/k_B T + \tanh M \tau}{1 + \tanh H/k_B T \tanh M \tau}$$

Thus:

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

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

$$H/k_B T \approx M(1 - \tau) + M^3(\tau - \tau^2 + \tau^3/3) \quad (3)$$

We take derivate with respect to H we have:

$$1/k_B T \approx \chi_T(1 - \tau) + 3M^2 \chi_T(\tau - \tau^2 + \tau^3/3) \quad (4)$$

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

$$\chi_T \approx \frac{1}{k_B T_c} \frac{1}{t}$$

This show that χ_T diverge as $T \rightarrow T_c^+$ with critical exponent $\gamma = 1$. For $T \rightarrow T_c^-$ 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:

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

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

3- (Cardy book exercise 2-3):

In this model we have spin with two component according to $\mathbf{s}_i = (\cos \theta_i, \sin \theta_i)$. We have external magnetic field $\mathbf{H}_i = H_i(\cos \theta_i, \sin \theta_i)$. Exchange interaction energy is $J_{ij} = J/(i-j)^\sigma$. For simplicity we take $\sigma = 0$ (we consider nearest neighbor) and we have constant magnetic field \mathbf{H} . Hamiltonian for XY model is:

$$\mathcal{H}_{XY} = -J \sum_{\langle ij \rangle} \hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_j - \mathbf{H} \cdot \sum_i \hat{\mathbf{s}}_i$$

Now we consider mean field approximation. Like Ising model we consider a constant magnetic field that generated from other spins and we can approximate first term in Hamiltonian as follows:

$$\mathcal{H}_{XY} = -2Jd\mathbf{M} \cdot \sum_i \hat{\mathbf{s}}_i - \mathbf{H} \cdot \sum_i \hat{\mathbf{s}}_i = -(2Jd\mathbf{M} + \mathbf{H}) \cdot \sum_i \hat{\mathbf{s}}_i$$

If we are in d-dimensional hypercubic lattice the number of neighbors is $2d$. If we apply an external field on system all spins on average have direction aligned with external field so we can take \mathbf{M} and \mathbf{H} in one direction, we have:

$$\mathcal{H}_{XY} = -(2JdM + H) \sum_i \cos \theta_i$$

For partition function we have:

$$\begin{aligned} \mathcal{Z}_{xy} &= \int_0^{2\pi} \int_0^{2\pi} \dots \int_0^{2\pi} d\theta_1 d\theta_2 \dots d\theta_N e^{\beta(2JdM+H) \cos \theta_1} e^{\beta(2JdM+H) \cos \theta_2} \dots e^{\beta(2JdM+H) \cos \theta_N} \\ &= \prod_{i=1}^N \int d\theta e^{\beta(2JdM+H) \cos \theta} = \left[\int d\theta e^{\beta(2JdM+H) \cos \theta} \right]^N = \left[2\pi I_0 \left(\frac{2JdM + H}{k_B T} \right) \right]^N \end{aligned}$$

$I_0(x)$ is modified Bessel function for the first kind³. For free energy we have:

$$\mathcal{F}_{XY} = -k_B T \log \mathcal{Z}_{xy} = -k_B T N \log \left[2\pi I_0 \left(\frac{2JdM + H}{k_B T} \right) \right]$$

and Magnetization:

$$M = -\frac{1}{N} \frac{\partial \mathcal{F}_{XY}}{\partial H} = k_B T \frac{\partial}{\partial H} \left(\log \left[2\pi I_0 \left(\frac{2JdM + H}{k_B T} \right) \right] \right) = \frac{I_1 \left(\frac{2JdM + H}{k_B T} \right)}{I_0 \left(\frac{2JdM + H}{k_B T} \right)}$$

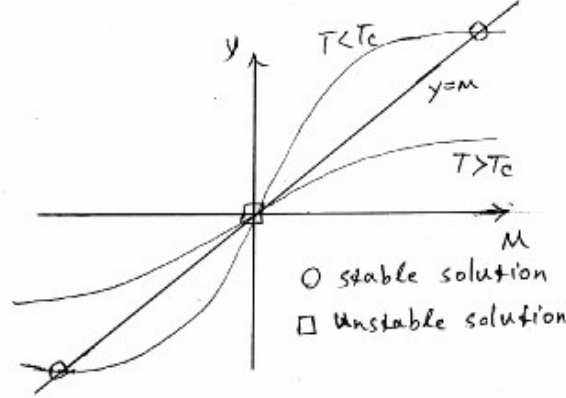
If we use self-consistent method (like Ising model) we can find Ising like results. If we put $H = 0$ and expand above equation right hand side for small M we have:

$$M \approx \frac{1}{2} \frac{2dJM}{k_B T_c} \Rightarrow T_c = \frac{dJ}{k_B}$$

If $T > T_c$ the only intersection is $M = 0$ and if $T < T_c$ we have three intersections, two of them are stable solution and one of them is unstable. The stable solutions are parallel

³For more information see <http://mathworld.wolfram.com/ModifiedBesselFunctionoftheFirstKind.html>

or anti-parallel with mean magnetization of all spins \mathbf{M} . Solution $M = 0$ is stable when $T > T_c$ and unstable when $T < T_c$.



In above figure I plot function of M correspond to M self consistently. I used Mathematica. For critical exponent we should expand above for small M and h if We define $\tau = T_c/T$, we have:

$$\begin{aligned}
 M &= \frac{I_1 (2M\tau + H/k_B T)}{I_0 (2M\tau + H/k_B T)} \\
 &\approx \left(\frac{H}{2k_B T} - \frac{1}{16} \left(\frac{H}{k_B T} \right)^3 + \mathcal{O}(H^4) \right) + M \left(\tau - \frac{3}{8} \tau \left(\frac{H}{k_B T} \right)^2 + \mathcal{O}(H^4) \right) \\
 &+ M^2 \left(-\frac{3}{4} \tau^2 \frac{H}{k_B T} + \frac{5}{12} \tau^2 \left(\frac{H}{k_B T} \right)^3 + \mathcal{O}(h^4) \right) + M^3 \left(-\frac{\tau^3}{2} + \frac{5}{6} \tau^3 \left(\frac{H}{k_B T} \right)^2 + \mathcal{O}(h^4) \right) + \mathcal{O}(M^4) \\
 &= M \left(\tau - \frac{3}{8} \tau \left(\frac{H}{k_B T} \right)^2 \right) + M^2 \left(\frac{5}{12} \tau^2 \left(\frac{H}{k_B T} \right)^3 - \frac{3}{4} \tau^2 \frac{H}{k_B T} \right) + M^3 \left(\frac{5}{6} \tau^3 \left(\frac{H}{k_B T} \right)^2 - \frac{\tau^3}{2} \right) \\
 &\quad + \frac{H}{2k_B T} - \frac{1}{16} \left(\frac{H}{k_B T} \right)^3
 \end{aligned}$$

We throw away terms with order bigger than three for M and bigger than one for H :

$$M \approx M\tau - \frac{3}{4} M^2 \left[\frac{H}{k_B T} \right] \tau^2 - \frac{1}{2} M^3 \tau^3 + \frac{H}{2k_B T} + \mathcal{O}(M^4)$$

We can find equation of states as follows:

$$\begin{aligned}
 \frac{H}{2k_B T} \left(1 - \frac{3}{2} M^2 \tau^2 \right) &\approx M(1 - \tau) + \frac{1}{2} M^3 \tau^3 + \dots \\
 &= \left(M(1 - \tau) + \frac{1}{2} M^3 \tau^3 \right) \left(1 - \frac{3}{2} M^2 \tau^2 \right)^{-1} \\
 &\approx \left(M(1 - \tau) + \frac{1}{2} M^3 \tau^3 \right) \left(1 + \frac{3}{2} M^2 \tau^2 \right)
 \end{aligned}$$

Finally:

$$\frac{H}{2k_B T} \approx M(1 - \tau) + M^3 \left(\frac{3}{2} \tau^2 - \tau^3 \right) \quad (5)$$

For $H = 0$ and $T \rightarrow T_c^-$ we have:

$$M^2 \approx 2 \frac{(T_c - T)}{T} + \dots$$

where the dots indicate corrections to this leading order formula. We can read off the critical exponent β : $\beta = 1/2$. The critical isotherm is the curve in the $H - M$ plane corresponding to $T = T_c$. Its shape near the critical point is described by the critical exponent δ :

$$H \sim M^\delta$$

Setting $\tau = 1$ in the equation of state 5 , we find:

$$\frac{H}{k_B T} \sim M^3$$

Showing that the mean field value of δ is 3. The isothermal magnetic susceptibility χ_T also diverges near T_c :

$$\chi_T \equiv \left. \frac{\partial M}{\partial H} \right|_T$$

Differentiating the equation of state 5, gives:

$$\frac{1}{2k_B T} \approx \chi_T (1 - \tau) + \chi_T \left(\frac{3}{2} \tau^2 - \tau^3 \right) 3M^2 \quad (6)$$

For $T > T_c$, $M = 0$ and $\tau \rightarrow 1$ we have:

$$\chi_T = \frac{1}{2k_B} \frac{1}{T - T_c} + \dots$$

Comparing with the definition of the critical exponent γ :

$$\chi_T \sim |T - T_c|^\gamma$$

we conclude that $\gamma = 1$. For $T < T_c$, we have:

$$M \approx \sqrt{2} \left(\frac{T_c - T}{T} \right)^{1/2} + \dots$$

Substituting into 6 gives:

$$\begin{aligned} \frac{1}{2k_B T} &\approx \chi_T \left(\frac{T - T_c}{T_c} \right) + 3\chi_T \left(\frac{T_c - T}{T} \right) \\ &= 2\chi_T \left(\frac{T_c - T}{T} \right) \\ \chi_T &= \frac{1}{4} \frac{1}{k_B |T_c - T|} \Rightarrow \chi_T = \frac{1}{4k_B} \frac{1}{T_c - T} + \dots \end{aligned}$$

which shows that the divergence of the susceptibility below the transition temperature is governed by the critical exponent $\gamma' = \gamma = 1$.

This is my Mathematica code.

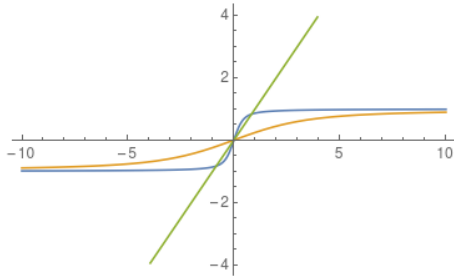
Integrate[Exp[(h + 2 d m J) / (K T) * Cos[θ]], {θ, 0, 2 Pi}]

$$2 \pi \text{BesselI}\left[0, \frac{h + 2 d J m}{K T}\right]$$

K T θ_h (Log[2 π BesselI[0, $\frac{2 D m J + h}{K T}$]])

$$\frac{\text{BesselI}\left[1, \frac{h + 2 D J m}{K T}\right]}{\text{BesselI}\left[0, \frac{h + 2 D J m}{K T}\right]}$$

Plot[{{BesselI[1, 4 m], BesselI[1, 0.5 m]}, {BesselI[0, 4 m], BesselI[0, 0.5 m]}}, {m, -10, 10}]



In[1]= Series[BesselI[1, 2 m τ + h / (K T)], {m, 0, 3}, {h, 0, 3}]

$$\text{Out[1]} = \left(\frac{h}{2 K T} - \frac{h^3}{16 (K^3 T^3)} + 0[h]^4 \right) + \left(\tau - \frac{3 \tau h^2}{8 (K^2 T^2)} + 0[h]^4 \right) m + \left(-\frac{3 \tau^2 h}{4 (K T)} + \frac{5 \tau^2 h^3}{12 K^3 T^3} + 0[h]^4 \right) m^2 + \left(-\frac{\tau^3}{2} + \frac{5 \tau^3 h^2}{6 K^2 T^2} + 0[h]^4 \right) m^3 + 0[m]^4$$

In[2]= Normal[%1]

$$\text{Out[2]} = -\frac{h^3}{16 K^3 T^3} + \frac{h}{2 K T} + m \left(\tau - \frac{3 h^2 \tau}{8 K^2 T^2} \right) + m^2 \left(\frac{5 h^3 \tau^2}{12 K^3 T^3} - \frac{3 h \tau^2}{4 K T} \right) + m^3 \left(-\frac{\tau^3}{2} + \frac{5 h^2 \tau^3}{6 K^2 T^2} \right)$$

4- (Cardy book exercise 2-4):

First, we define the two-point function:

$$G(\mathbf{r}_i - \mathbf{r}_j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$$

Partition function is:

$$\mathcal{Z}_\Omega = \text{Tr} e^{-\beta \mathcal{H}_\Omega} = \text{Tr} \exp \left[\beta J \sum_{\langle ij \rangle} S_i S_j + \beta H \sum_i S_i \right]$$

We can obtain averages by differentiating from partition function:

$$\begin{aligned} \sum_i \langle S_i \rangle &= \frac{1}{\mathcal{Z}_\Omega} \text{Tr} \left[\sum_i S_i \right] e^{-\beta \mathcal{H}_\Omega} = \frac{1}{\beta \mathcal{Z}_\Omega} \frac{\partial \mathcal{Z}_\Omega}{\partial H} \\ \sum_{ij} \langle S_i S_j \rangle &= \frac{1}{\mathcal{Z}_\Omega} \text{Tr} \left[\sum_{ij} S_i S_j \right] e^{-\beta \mathcal{H}_\Omega} = \frac{1}{\beta^2 \mathcal{Z}_\Omega} \frac{\partial^2 \mathcal{Z}_\Omega}{\partial H^2} \end{aligned}$$

Now we want to calculate susceptibility:

$$\begin{aligned} \chi_T &= \frac{\partial M}{\partial H} = -\frac{\partial^2 \mathcal{F}}{\partial H^2} = \frac{1}{N\beta} \frac{\partial^2 \log \mathcal{Z}_\Omega}{\partial H^2} \\ &= \frac{1}{N\beta} \frac{\partial}{\partial H} \left[\frac{1}{\mathcal{Z}_\Omega} \frac{\partial \mathcal{Z}_\Omega}{\partial H} \right] \\ &= \frac{1}{N\beta} \left[\frac{1}{\mathcal{Z}_\Omega} \frac{\partial^2 \mathcal{Z}_\Omega}{\partial H^2} - \left(\frac{1}{\mathcal{Z}_\Omega} \frac{\partial \mathcal{Z}_\Omega}{\partial H} \right)^2 \right] \\ &= \frac{\beta}{N} \left[\sum_{ij} \langle S_i S_j \rangle - \left(\sum_i \langle S_i \rangle \right)^2 \right] \\ &= \frac{\beta}{N} \sum_{ij} G(\mathbf{r}_i - \mathbf{r}_j) = \beta \sum_i G(\mathbf{x}_i) = \frac{\beta}{a^d} \int_\Omega d^d r G(r) \end{aligned}$$

In last step we take our space to be continuous and summation become integral as follows:

$$\sum_i \longrightarrow \frac{1}{a^d} \int_\Omega$$

Volume of a spin is a^d . Now we use correlation function relation which derived in Goldenfeld book (eq. 5.109):

$$G(\mathbf{r}) \sim \frac{e^{-r/\xi}}{r^{(d-1)/2} \xi^{(d-3)/2}}$$

We calculate integral(I used Mathematica):

$$\int \frac{r^{d-1} e^{-r/\xi}}{r^{(d-1)/2} \xi^{(d-3)/2}} dr = \xi^2 \Gamma\left(\frac{d+1}{2}\right)$$

We consider susceptibility near critical temperature, we have ⁴ :

$$\begin{cases} \frac{1}{k_B} \frac{1}{T-T_c} + \dots = \frac{\beta}{a^d} \xi^2 \Gamma\left(\frac{d+1}{2}\right) & \text{if } T \rightarrow T_c^+ \\ \frac{1}{2k_B} \frac{1}{T-T_c} + \dots = \frac{\beta}{a^d} \xi^2 \Gamma\left(\frac{d+1}{2}\right) & \text{if } T \rightarrow T_c^- \end{cases}$$

From above we can find that $\nu = 1/2$ for both side of critical temperature and ratio of amplitudes is $1/\sqrt{2}$.

⁴I used equation 3.148 and 3.151 of Goldenfeld book.

5- System always want to maximize it's entropy or want to reach equilibrium state, so depend on system thermodynamic constants or variables we can define **thermodynamic potential** (abstract of class discussion). Greiner⁵ discuss about this topic in chapter 4.

We start from the internal energy $U(S, V, N, \dots)$ as a function of the natural variables. The variable S , the entropy, shall be replaced by the temperature $T = \partial U / \partial S|_{v, N, \dots}$. To this end, one uses the Legendre transform:

$$F = U - TS = -pV + \mu N$$

Which is called the *free energy* or *Helmholtz potential*. Here we have employed Euler's equation. The total differential of U reads:

$$dU = TdS - pdV + \mu dN + \dots$$

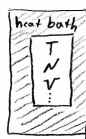
Correspondingly, the total differential of F is:

$$\begin{aligned} dF &= dU - SdT - TdS \\ &= -SdT - pdV + \mu dN + \dots \end{aligned}$$

Hence, the free energy is a function of T, V, N, \dots , which contains exactly the same information as the internal energy U , but which now depends on the temperature instead of the entropy. In particular one obtains from above the equations of state:

$$-S = \left. \frac{\partial F}{\partial T} \right|_{V, N, \dots}, \quad -p = \left. \frac{\partial F}{\partial V} \right|_{T, N, \dots}, \quad \mu = \left. \frac{\partial F}{\partial N} \right|_{T, V, \dots}, \quad \dots$$

To understand the importance of the free energy we consider a non-isolated system in a heat bath of constant temperature T (Figure below).



The total system (including the heat bath) must be isolated. Thus, the second law can be directly applied to the total system. Accordingly, irreversible processes happen in this total system, until in equilibrium the entropy has a maximum and does not change any more:

$$dS_{tot} = dS_{sys} + dS_{bath} \geq 0 \tag{7}$$

Here we have split the total entropy into that of the heat bath and that of the system under consideration.

Since the system and the heat bath are in mutual contact, they may exchange heat and, eventually, also work. This leads, according to the first law, to a change of the

⁵ *Thermodynamics and Statistical Mechanics*, Authors: Greiner, Walter, Neise, Ludwig, Stöcker, Horst

internal energy of the partial systems. Let δQ_{sys} be the heat exchanged with the heat bath (as seen from the system) and δW_{sys} the remaining work exchanged with the heat bath. Then we have, according to the first law, for the change in internal energy of the partial systems:

$$dU_{sys} = \delta Q_{sys} + \delta W_{sys}, \quad dU_{bath} = \delta Q_{bath} + \delta W_{bath}$$

Since the total system is isolated, for reversible processes it must hold that:

$$\delta Q_{sys} = -\delta Q_{bath}, \quad \delta W_{sys} = -\delta W_{bath}$$

When discussing the second law we have discussed the following inequalities, which are also valid for partial systems:

$$TdS = \delta Q_{rev} > \delta Q_{irr}, \quad \delta W_{rev} \leq \delta W_{irr}$$

As seen from the system we therefore have:

$$dU_{sys} - TdS_{sys} = \delta W_{sys}^{rev} < \delta W_{sys}^{irr} \Rightarrow dF_{sys} = dU_{sys} - TdS_{sys} = \delta W_{sys}^{rev} < \delta W_{sys}^{irr}$$

The change of free energy dF_{sys} of the system at constant temperature (isothermal process) represents the work done by or performed on the system in a reversible process. This work is always smaller (including sign) than that in irreversible processes.

For reversible processes the equality sign holds in Equation D.40), so that with $dU_{sys} = TdS_{sys} + \delta W_{sys}^{irr}$:

$$dS_{bath} = -dS_{sys} = -\frac{\delta Q_{sys}}{T} = -\frac{1}{T} \left(dU_{sys} - \delta W_{sys}^{rev} \right)$$

If we insert this into Equation 7, it follows for isothermal reversible processes ($dS_{tot} = 0$) that

$$TdS_{tot} = TdS_{sys} - dU_{sys} + \delta W_{sys}^{rev} = -dF_{sys} + dW_{sys}^{rev} = 0$$

or for irreversible processes, respectively,

$$TdS_{tot} = -dF_{sys} + dW_{sys}^{irr} \geq 0$$

Here it becomes quite evident that for isothermal systems the free energy has an importance quite analogous to the entropy for isolated systems. Let the work performed be $\delta W_{sys} = 0$, then the entropy of the isolated total system has a maximum if and only if the free energy of the isothermal partial system has a minimum. In particular, processes which diminish the free energy happen spontaneously and irreversibly in an isothermal system. Since

$$dF = d(U - TS) = dU - TdS \leq 0 \quad \text{for} \quad \delta W = 0 \quad \text{and} \quad T = \text{const.}$$

the free energy yields a combination of the principle of maximum entropy and minimum energy. Isothermal systems, which can exchange only heat, but not work with their surroundings, try to minimize their free energy; i.e., they try to minimize their energy and simultaneously maximize their entropy! This has the consequence that, for

instance, isothermal processes which actually increase the internal energy, i.e., which require energy input, nevertheless happen spontaneously, if for a given temperature the gain in entropy TdS is larger than the expense in energy dU —the energy is here extracted from the heat bath.

In general, an isothermal system which does not exchange work with its surroundings strives for a minimum of the free energy. Irreversible processes happen spontaneously, until the minimum

$$dF = 0 \quad F = F_{min}$$

is reached.