Problem set 3

1. Blume - Capel model

$$H = -J \sum_{i=1}^{N} S_z^i S_z^{i+1} - D \sum_i (S_z^i)^2$$

this Hamiltonian is already diagonal:

$$E = -J \sum_{i=1}^{N} S_i S_{i+1} - D \sum_i S_i^2 \qquad S_i = 1, 0, -1$$

the partition function is

$$Z = \sum_{\{S\}} e^{-\beta E}$$

and can be written as

$$Z = \sum_{\{S\}} V(S_1, S_2)\, V(S_2, S_3) \dots V(S_{N-1}, S_N)\, V(S_N, S_1)$$

where

$$V(S_1, S_2) = e^{\beta J S_1 S_2 + \frac{\beta D}{2}(S_1^2 + S_2^2)}$$

this defines the transfer matrix

$$V = \begin{pmatrix} V_{11} & V_{10} & V_{1,-1} \\ V_{01} & V_{00} & V_{0,-1} \\ V_{-1,1} & V_{-1,0} & V_{-1,-1} \end{pmatrix}$$

or

$$V = \begin{pmatrix} e^{\beta J + \beta D} & e^{\beta D/2} & e^{-\beta J + \beta D} \\ e^{\beta D/2} & 1 & e^{\beta D/2} \\ e^{-\beta J + \beta D} & e^{\beta D/2} & e^{\beta J + \beta D} \end{pmatrix}$$

the partition function then becomes

$$Z = \operatorname{tr} V^N = \lambda_+^N + \lambda_0^N + \lambda_-^N$$

where the eigenvalues of V are

$$\lambda_0 = 2 e^{\beta D} \sinh \beta J$$

$$\lambda_\pm = e^{\beta D} \cosh \beta J + \frac{1}{2} \pm \frac{1}{2} \sqrt{8 e^{\beta D} + (2 e^{\beta D} \cosh \beta J - 1)^2}$$

clearly $\lambda_+ > \lambda_-$. But we can also show that $\lambda_+ > \lambda_0$:

$$\lambda_+ > e^{\beta D} \cosh \beta J + \frac{1}{2} + \frac{1}{2} (2 e^{\beta D} \cosh \beta J - 1)$$

$$= 2 e^{\beta D} \cosh \beta J$$

$$> 2 e^{\beta D} \sinh \beta J$$

$$= \lambda_0$$

thus λ_+ is always the largest eigenvalue. In the limit $N \to \infty$ we then get

$$Z = \lambda_+^N$$

The free energy per particle is

$$f = -\frac{T}{N}\ln Z = -T\ln\lambda_+$$

or

$$f = -T\ln\left\{e^{\beta D}\cosh\beta J + \frac{1}{2} \pm \frac{1}{2}\sqrt{8e^{\beta D} + (2e^{\beta D}\cosh\beta J - 1)^2}\right\}$$

—,,—

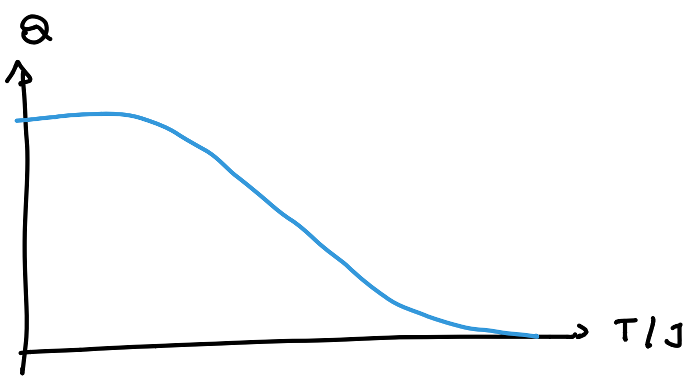
The quadrupole moment is

$$Q = \frac{1}{N}\left\langle \sum_i (S_z^i)^2 \right\rangle = -\frac{\partial f}{\partial D}$$

Thus

$$Q = 1 + \frac{e^{\beta D}\cosh\beta J + \frac{1}{2}}{\sqrt{8e^{\beta D} + (2e^{\beta D}\cosh\beta J - 1)^2}}$$

this looks like

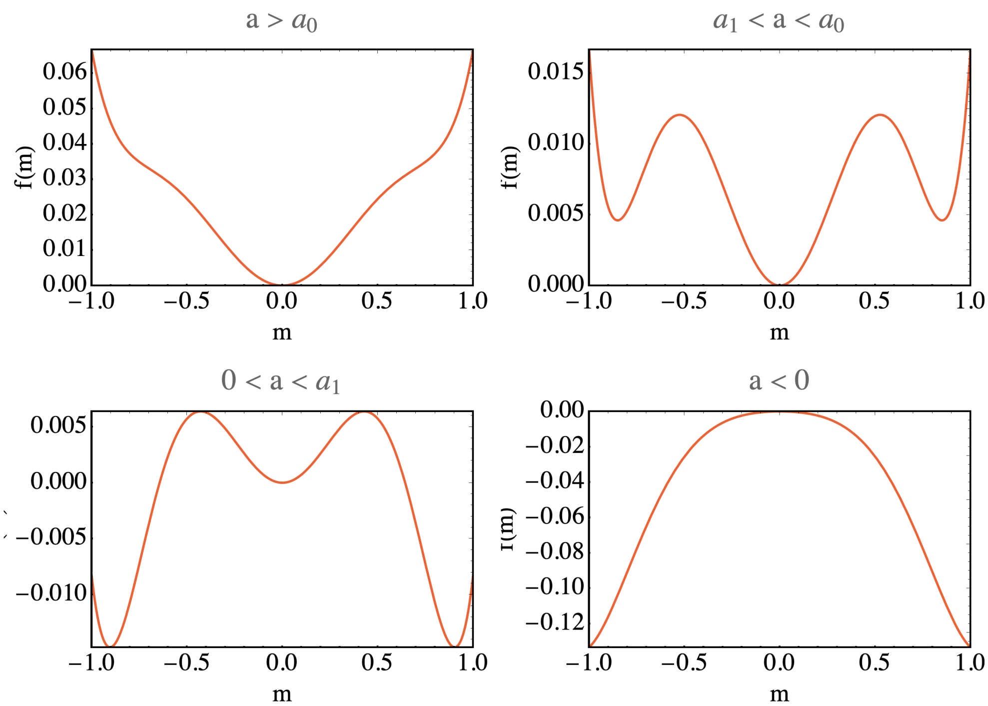


2. Landau theory for discontinuos transitions

$$f(m) = \frac{a}{2} m^2 + \frac{b}{4} m^4 + \frac{c}{6} m^6$$

with $b < 0$ and $a \propto (T - T_c)$.

(a)



$a_0 = \frac{b^2}{4c}$

$a_1 = \frac{3b^2}{16c}$

$$\frac{\partial f}{\partial m} = m\left(a + b m^2 + c m^4\right) = 0$$

$\hookrightarrow \quad m = 0$

$$m^2 = -\frac{b}{2c} \pm \frac{1}{2c}\sqrt{b^2 - 4ac} \quad := m_\pm^2 \qquad (1)$$

$$= -\frac{b}{2c} \pm \frac{1}{\sqrt{c}}\sqrt{a_0 - a}$$

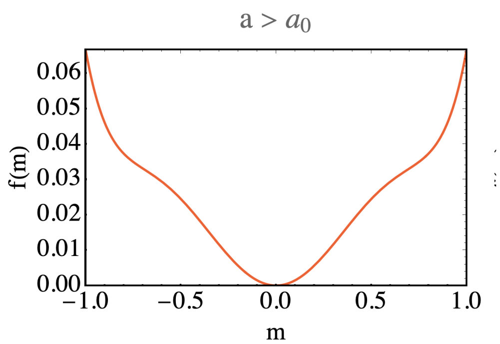
$-b = \sqrt{4ac}$

$$= \frac{1}{\sqrt{c}}\left(-\sqrt{a} \pm \sqrt{a_0 - a}\right)$$

$$\frac{\partial^2 f}{\partial m^2} = a + 3bm^2 + 5cm^4$$

$$= \begin{cases} a & m = 0 \\ -4a + \frac{b}{c}\left(b + \sqrt{b^2 - 4ac}\right) & m = m_- \\ -4a + \frac{b}{c}\left(b - \sqrt{b^2 - 4ac}\right) & m = m_+ \end{cases} \qquad (2)$$

(b) $a > a_0$. The only solution of (1) is $m = 0$. From (2), this is a minimum.



(c) $a_1 < a < a_0$: solutions $m_\pm$ in (1) become real. From (2), m_- is a maximum and m_+ a minimum.

But getting rid of b using a_1, we may write

$$f(m_+) = \frac{1}{6\sqrt{c}}\left(\sqrt{a_0} + \sqrt{a_0 - a}\right)\left(a_0 - 2a + \sqrt{a_0(a_0 - a)}\right)$$

The other minimum at $m = 0$ has $f(0) = 0$. Thus we must compare $f(m_+)$ with 0. The sign of $f(m_+)$ will depend on the last term, since the first is always positive

The last term changes sign when

$$a_0 - 2a = \sqrt{a_0(a_0 - a)}$$

or

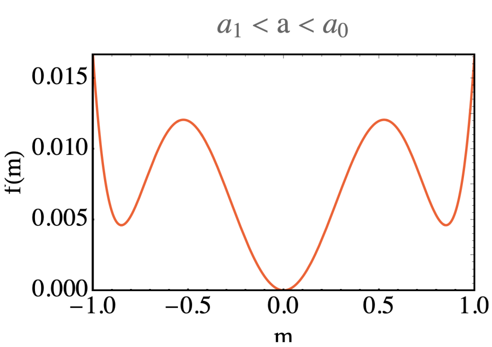
$$\cancel{a_0^2} - 4a_0 a + 4a^2 = \cancel{a_0^2} - a_0 a$$

$$4a^2 - 3a_0 a = 0$$

$$\therefore \quad a = \frac{3a_0}{4} = \frac{3}{4}\frac{b^2}{4c} = \frac{3b^2}{16c} = a_1$$

(d)

Thus, as we lower a below a_1, the points $\pm m_+$ become global minima.



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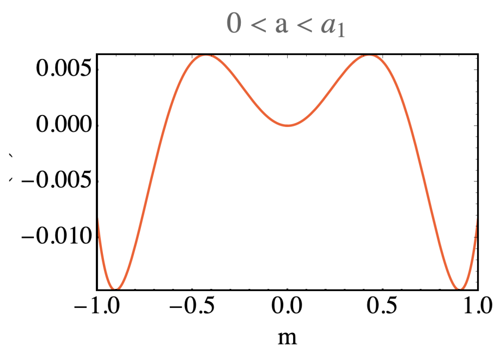
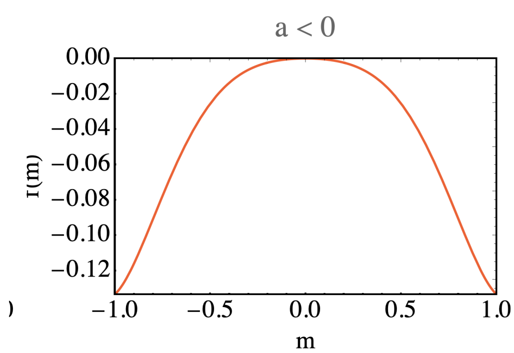
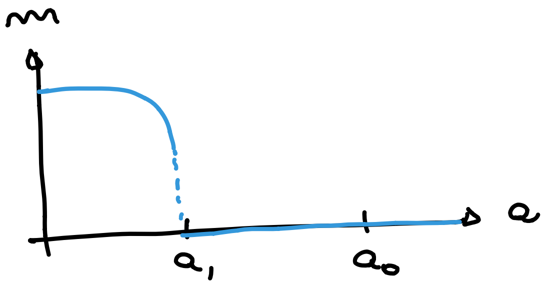


(e) $a < 0$: From Eq (2), at $m = 0$ $\frac{\partial^2 f}{\partial m^2} = a$. Thus, if $a < 0$ this becomes a maximum.



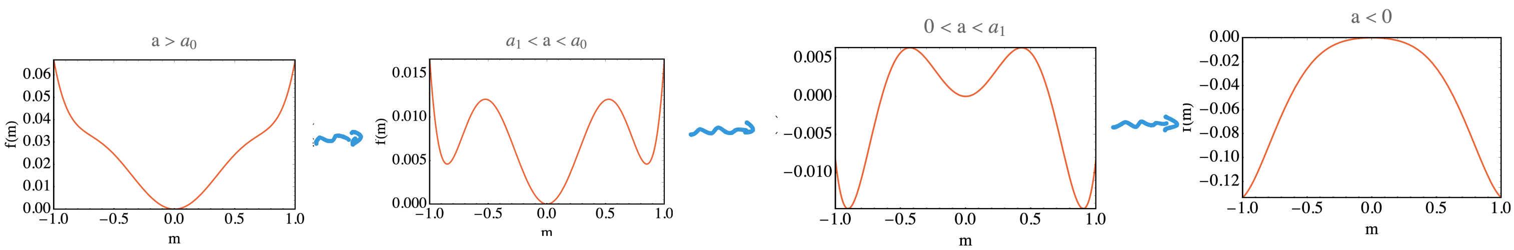
(f) Assuming that the magnetization is always at the global minimum, we should have



The magnetization jumps discontinuously at a_1.

If the experiment is done at finite time, m may be stuck at some local minima. It then becomes important whether we are reducing a or increasing it.

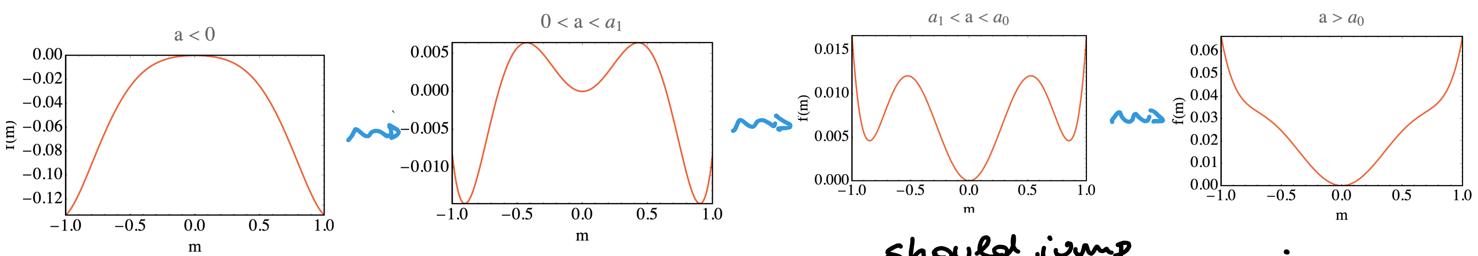
If we start with $a > a_0$ and then start to lower it, we get



$m = 0$ | $m = 0$ | should jump but not enough time | Jumps.

It will therefore jump at some point between $a = a_1$ and $a = 0$

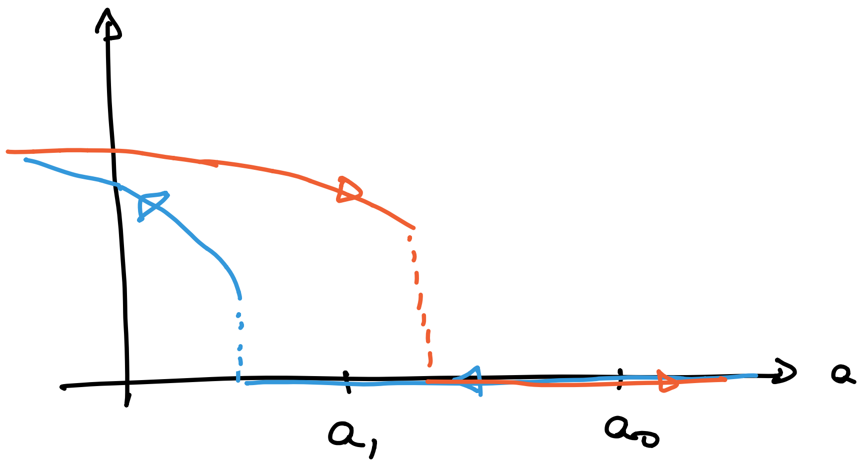
Conversely, if we start at $a < 0$ and then start to increase it



$m \neq 0$ | $m \neq 0$ | should jump but doesn't | jump

The jump will thus take place somewhere within $a = a_1$ and $a = a_0$

The magnetization may thus present hystheresis



3. Mean-field theory for anti-ferromagnetic systems

$$H = J \sum_{ij} \sigma_z^i \sigma_z^j - \sum_i h_i \sigma_z^i$$

(a) Mean-field: $\sigma_z^i = m_i + \delta\sigma_z^i$

$$\sigma_z^i \sigma_z^j = m_i m_j + m_i \delta\sigma_z^j + m_j \delta\sigma_z^i + \underbrace{\delta\sigma_z^i \delta\sigma_z^j}_{\approx 0}$$

$$\simeq m_i m_j + m_i (\sigma_z^j - m_j) + m_j (\sigma_z^i - m_i)$$

$$\therefore \quad \sigma_z^i \sigma_z^j \simeq -m_i m_j + m_i \sigma_z^j + m_j \sigma_z^i$$

We now impose that

$$m_i = \begin{cases} m_a & \text{if } i \in A \\ m_b & \text{if } i \in B \end{cases}$$

Moreover, we use the fact that a site $i \in A$ only interacts with $j \in B$. whence

$$\sum_{\langle i,j \rangle} \sigma_z^i \sigma_z^j \simeq -m_a m_b N d + \sum_{\langle i,j \rangle} (m_i \sigma_z^j + m_j \sigma_z^i)$$

We now write

$$\sum_{\langle i,j \rangle} m_i \sigma_z^i = d \sum_{j \in A} m_b \sigma_z^j + d \sum_{j \in B} m_a \sigma_z^j$$

since each i has d bonds associated to it.

The other term is identical. Thus

$$\sum_{\langle i,j\rangle} \sigma_z^i \sigma_z^j = -Nd\, m_a m_b + 2d\left(\sum_{i\in A} m_b \sigma_z^i + \sum_{i\in B} m_a \sigma_z^i\right)$$

The Hamiltonian in the MF approx. may thus be written as

$$H = -NJd\, m_a m_b + 2dJ\left(\sum_{i\in A} m_b \sigma_z^i + \sum_{i\in B} m_a \sigma_z^i\right) - \sum_i h_i \sigma_z^i$$

We can write this more compactly as

$$H = -NJd\, m_a m_b - \sum_i h_i^{eff} \sigma_z^i$$

where

$$h_i^{eff} = \begin{cases} h_i - 2Jd\, m_b & i \in A \\ h_i - 2Jd\, m_a & i \in B. \end{cases}$$

(b) The Hamiltonian is now a sum of independent terms. Thus

$$Z = e^{\beta NJd\, m_a m_b} \prod_i \left[2\cosh \beta h_i^{eff}\right]$$

The free energy is $F = -T \ln Z$, or

$$F = -NJd\, m_a m_b - T \sum_i \ln\left[2\cosh\left(\beta h_i^{eff}\right)\right]$$

(c) Since each site is assumed to have it's own magnetic field h_i, the magnetization of each site can be computed as

$$m_i = -\frac{\partial F}{\partial h_i} = -\frac{\partial F}{\partial h_i^{eff}} = \tanh(\beta h_i^{eff})$$

Thus

$$m_a = \tanh(\beta h_i - 2\beta Jd\, m_b)$$

$$m_b = \tanh(\beta h_i - 2\beta Jd\, m_a)$$

Now we can set $h_i = h$, leading to

$$m_a = \tanh(\beta h - 2\beta Jd\, m_b)$$

$$m_b = \tanh(\beta h - 2\beta Jd\, m_a)$$

(d) For $h=0$ we can write

$$-2\beta Jd\, m_b = \tanh^{-1}(m_a)$$

$$-2\beta Jd\, m_a = \tanh^{-1}(m_b)$$

Looking for solutions with $m_b = -m_a$, it suffices to focus on one of the equations.

Expanding: $\tanh^{-1}(x) \simeq x + x^3/3$

$$2\beta J d\, m_a = \left(m_a + \frac{m_a^3}{3} \right)$$

or

$$\frac{m_a^3}{3} = m_a \left(\frac{2Jd}{T} - 1 \right)$$

Looking for solutions with $m_a \neq 0$ we get

$$m_a = \pm \sqrt{\frac{3}{T}} \sqrt{T_N - T}$$

where the Neel temperature is

$$T_N = 2Jd$$

(e) For small h and $T > T_N$ we can write

$$\beta h - \beta T_N m_b = \tanh^{-1}(m_a) \simeq m_a$$

$$\beta h - \beta T_N m_a = \tanh^{-1}(m_b) \simeq m_b$$

Adding the two yields

$$2\beta h - \beta T_N M \simeq M$$

where $M = m_a + m_b$. Thus

$$M \simeq \frac{2\beta h}{1+\beta T_N} = \frac{2h}{T+T_N}$$

whence

$$\chi = \frac{\partial M}{\partial h} = \frac{2}{T+T_N}$$