Problem set 1

1) Spinzão

$$E_s = -hs, \qquad s = S, S-1, \dots, -S+1, -S$$

(a) $$Z = \sum_{s=-S}^{S} e^{\beta h s}$$

$m = s + S \rightarrow 0, \quad s = -S$

$\rightarrow 2S, \quad s = S$

$$= e^{-\beta h S} \sum_{m=0}^{2S} e^{\beta h m}$$

Using $\sum_{m=0}^{L} x^m = \frac{1 - x^{L+1}}{1-x}$

$$= e^{-\beta h S} \left(\frac{1 - e^{\beta h (2S+1)}}{1 - e^{\beta h}} \right)$$

(b) $$M = \langle s \rangle = \frac{1}{Z} \sum_s s\, e^{\beta h s}$$

$$= \frac{1}{Z} \frac{1}{\beta} \frac{\partial}{\partial h} \sum_s e^{\beta h s}$$

$$= T \frac{\partial}{\partial h} \ln Z$$

$$= -\frac{\partial F}{\partial h} \qquad \text{where} \quad F = -T \ln Z$$

(c) Using the result from (a):

$$M = T \frac{\partial}{\partial h} \ln \left(\frac{e^{-\beta h S}\left(1 - e^{\beta h (2S+1)}\right)}{1 - e^{\beta h}} \right)$$

$$= -S + T\left[\frac{-\beta(2S+1)\, e^{\beta h(2S+1)}}{1 - e^{\beta h(2S+1)}} \right] - T\left[\frac{-\beta e^{\beta h}}{1 - e^{\beta h}} \right]$$

$$= \cancel{-S} + \frac{(2S+1)}{2}\left\{ \cancel{1+} \coth\left[\frac{(2S+1)\beta h}{2} \right] \right\} - \frac{1}{2}\left\{ \cancel{1+} \coth\left(\frac{\beta h}{2} \right) \right\}$$

$$\therefore \quad M = \frac{(2S+1)}{2} \coth\left[\frac{(2S+1)\beta h}{2} \right] - \frac{1}{2} \coth\left(\frac{\beta h}{2} \right)$$

We can write this in terms of the Brillouin function

$$B_S(x) = \frac{2S+1}{2S} \coth\left[\frac{(2S+1)}{2S} x \right] - \frac{1}{2S} \coth\left(\frac{x}{2S} \right)$$

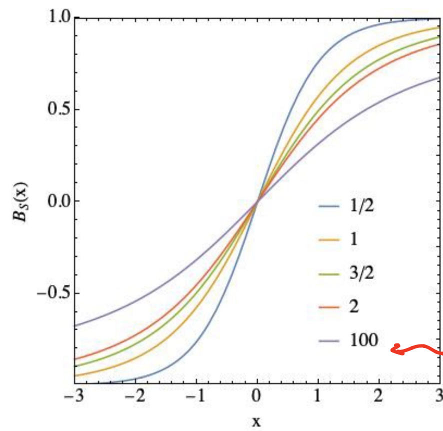
We then get

$$M = S\, B_S(\beta h S)$$

(d) Clearly, it is more convenient to analyze the normalized magnetization

$$m = \frac{M}{S} = B_S(\beta h S)$$

This will then depend only on $\beta h S$, so it suffices for us to analyze $B_S(x)$:



← different values of S

← Langevin function essentially.

Brillouin function

Close to $x = 0$, we can use

$$\coth(x) \simeq \frac{1}{x} + \frac{x}{3}$$

to get

$$B_S(x) \simeq \frac{(2S+1)}{2S}\left[\frac{2S}{2S+1}\frac{1}{x} + \frac{2S+1}{2S}\frac{x}{3}\right]$$

$$- \frac{1}{2S}\left[\frac{2S}{x} + \frac{1}{3}\frac{x}{2S}\right]$$

$$= \frac{(2S+1)^2}{(2S)^2}\frac{x}{3} - \frac{1}{(2S)^2}\frac{x}{3}$$

$$= \frac{1}{4S^2}(4S^2 + 4S)\frac{x}{3}$$

$$= \frac{S+1}{S}\frac{x}{3}$$

Thus

$$B_S(x) \simeq \frac{S+1}{3S}x \qquad x \ll 1$$

Thus, for low enough fields we get

$$m \approx \frac{S+1}{3S}\beta h S = \frac{S+1}{3}\frac{h}{T}$$

This is again Curie's law: $m \propto h$ with a coefficient $1/T$. The coefficient in front is seen to increase with S: larger spins imply larger responses.

(e) $m = \frac{M}{S} = B_S(\beta h S)$. Keeping m and hS finite, we essentially have to take the limit $S \to \infty$ in the Brillouin function:

$$B_S(x) = \frac{(2S+1)}{2S}\coth\left(\frac{2S+1}{2S}x\right) - \frac{1}{2S}\coth\left(\frac{x}{2S}\right)$$

← Taylor expand $\coth(y) \sim 1/y$ (for S large)

$$\simeq \frac{2S}{2S}\coth\left(\frac{2S}{2S}x\right) - \frac{1}{2S}\frac{2S}{x}$$

Thus

$$\lim_{S\to\infty} B_S(x) = \mathcal{L}(x) = \coth(x) - \frac{1}{x}$$

In the classical limit the magnetization thus becomes

$$m = \frac{M}{S} = \mathcal{L}(\beta h S)$$

the linear response for low fields become

$$m \simeq \frac{\beta h S}{3}$$

2) Classical spins

$$\vec{s} = S(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

$$E = -hS\cos\theta$$

(a) $$Z = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \; e^{\beta h S\cos\theta}$$

$z = \cos\theta$

$$= 2\pi \int_{-1}^{1} dz \; e^{\beta h S z}$$

$$= 2\pi \; \frac{e^{\beta h S} - e^{-\beta h S}}{\beta h S}$$

$$\therefore \quad Z = 4\pi \frac{\sinh(\beta h S)}{\beta h S}$$

(b) $$M = T \frac{\partial}{\partial h} \ln Z$$

$$= T\left\{ \beta S \frac{\cosh(\beta h S)}{\sinh(\beta h S} - \frac{1}{h} \right\}$$

$$= S\coth(\beta h S) - \frac{1}{\beta h}$$

$$\therefore \quad m = \frac{M}{S} = \coth(\beta h S) - \frac{1}{\beta h S} = \mathcal{L}(\beta h S)$$

where $\mathcal{L}(x)$ is the Langevin function.

(c) $E = -hS\cos\theta - \frac{kS\cos^2\theta}{2}$

$$Z = 2\pi \int_{-1}^{1} dz \; e^{\beta h S z + \beta k S z^2/2}$$

No analytical solution.

For low field we can expand

$$Z = 2\pi \int_{-1}^{1} dz \; e^{\beta k S z^2/2} + 2\pi \, \beta h S \underbrace{\int_{-1}^{1} dz \; z \, e^{\beta k S z^2/2}}_{= 0 \text{ due to parity}} + 2\pi \frac{(\beta h S)^2}{2} \int_{-1}^{1} dz \; z^2 e^{\beta k S z^2/2}$$

Let

$$R_m = \int_{-1}^{1} dz \; z^m \, e^{\beta k S z^2/2}$$

Then

$$Z = 2\pi \left\{ R_0 + \frac{(\beta h S)^2}{2} R_2 \right\}$$

the magnetization then becomes

$$M = T \frac{\partial}{\partial h} \ln Z = T \frac{(\beta S)^2 h R_2}{R_0 + (\beta h S)^2 R_2/2}$$

To leading order in h, this reduces to

$$M = \frac{S^2}{T} \frac{R_2}{R_0} h$$

this is no longer in the form of curie's law since R_n depends on T.

3) LMG, part 1:

For $S=1$, we have 3 states $|1\rangle$, $|0\rangle$ and $|-1\rangle$. Using (14)

$$S_+|s\rangle = \sqrt{(1-s)(2+s)}\,|s+1\rangle$$

Thus

$$S_+|1\rangle = 0 \qquad S_+|0\rangle = \sqrt{2}\,|1\rangle \qquad S_+|-1\rangle = \sqrt{2}\,|0\rangle$$

$$\Rightarrow \qquad S_+ = \begin{array}{cc} \begin{array}{ccc} |1\rangle & |0\rangle & |-1\rangle \end{array} & \\ \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} & \begin{array}{c} \langle 1| \\ \langle 0| \\ \langle -1| \end{array} \end{array}$$

From this its easy to get

$$S_- = S_+^\dagger = \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

then

$$S_x = \frac{S_+ + S_-}{2} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$S_y = \frac{S_+ - S_-}{2i} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

And, of course

$$S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(b)

$$H = -hS_z - \frac{k}{2S} S_x^2 = - \begin{pmatrix} h+k/4 & 0 & k/4 \\ 0 & k/2 & 0 \\ k/4 & 0 & h-k/4 \end{pmatrix}$$

The eigenvalues are

$$E_\pm = -\frac{k}{4} \pm \sqrt{h^2 + (k/4)^2} \qquad E_0 = -k/2$$

Thus

$$Z = \sum_m e^{-\beta E_m}$$

$$= e^{-\beta E_0} + e^{-\beta E_+} + e^{-\beta E_-} \qquad \Omega = \sqrt{h^2+(k/4)^2}$$

$$= e^{\beta k/2} + e^{\beta k/4}\left(e^{\beta\Omega} + e^{-\beta\Omega} \right)$$

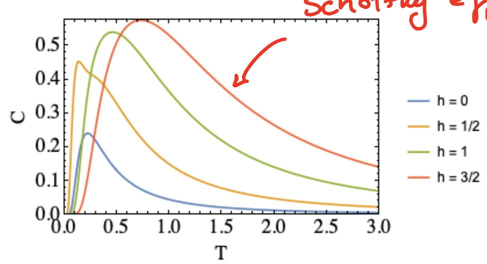
$$\therefore \quad Z = e^{\beta k/2} + 2e^{\beta k/4}\cosh(\beta\Omega)$$

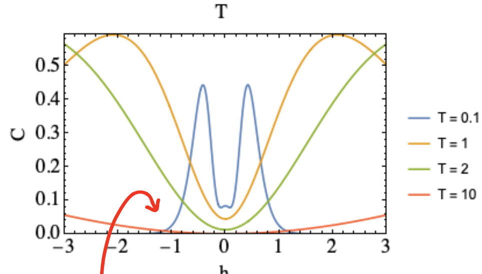
(c)

$$U = -\frac{\partial}{\partial\beta} \ln Z$$

$$C = \frac{\partial U}{\partial T}$$

Schottky effect.



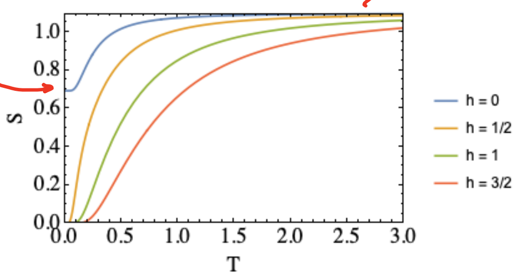


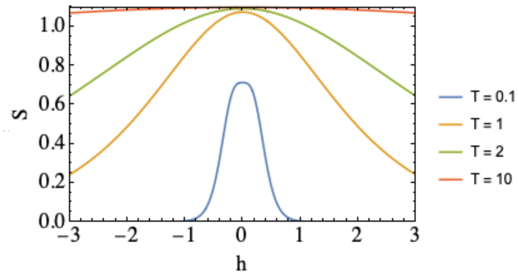
For low T, the heat capacity is only significant around h=±1

(d) $S = \dfrac{U - F}{T}$ $\qquad F = -T\ln Z$

$\ln 2$

$\ln 2$





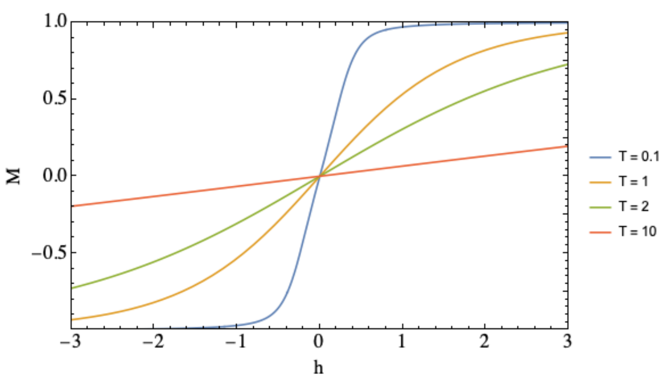
T = 0: entropy tends to the degenerecy of the GS.

GS is non-degenerate for $h \neq 0$ and doubley degenerate for $h = 0$, so $S = \ln 2$.

$T \to \infty$: S tends to the dimension of the Hilbert space, $S = \ln 3$.

(e)

$$M = T\frac{\partial}{\partial h}\ln Z = \frac{h}{\Omega}\,\frac{(e^{2\beta\Omega} - 1)}{1 + e^{2\beta\Omega} + e^{\beta\Omega + \beta k/4}}$$



Typical paramagnetic response. Becomes softer when T is high

4) Spin coherent states

A sandwich like $e^{i\phi S_z}(\ldots)e^{-i\phi S_z}$ performs a rotation around the z axis by a value ϕ. We can see this using the BCH formula to compute

$$e^{i\phi S_z} S_x e^{-i\phi S_z} = S_x + i\phi\,[S_z, S_x] + \frac{(i\phi)^2}{2!}[S_z,[S_z,S_x]] + \cdots$$

$$= S_x + i\phi\,(iS_y) + \frac{(i\phi)^2}{2!} S_x + \frac{(i\phi)^3}{3!}(iS_y) + \cdots$$

$$= S_x\left(1 - \frac{\phi^2}{2!} + \frac{\phi^4}{4!} \cdots\right) - S_y\left(\phi - \frac{\phi^3}{3!} + \cdots\right)$$

$$\therefore \quad e^{i\phi S_z} S_x e^{-i\phi S_z} = S_x \cos\phi - S_y \sin\phi$$

By symmetry one may guess that

$$e^{i\phi S_z} S_y e^{-i\phi S_z} = S_x \sin\phi + S_y \cos\phi.$$

Similarly $e^{-i\theta S_y}$ will rotate by θ around y:

$$e^{i\theta S_y} S_z e^{-i\theta S_y} = S_z + i\theta\,[S_y, S_z] + \cdots$$

$$= S_z - \theta S_x + \cdots$$

which will give

$$e^{i\theta S_y} S_z e^{-i\theta S_y} = S_z \cos\theta - S_x \sin\theta$$

and, again by symmetry

$$e^{i\theta S_y} S_x e^{-i\theta S_y} = S_z \sin\theta + S_x \cos\theta \quad //$$

we now use these results to compute:

$$\langle S_x \rangle = \langle \theta, \phi | S_x | \phi, \phi \rangle$$

$$= \langle S | e^{i\theta S_y} e^{i\phi S_z} S_x e^{-i\phi S_z} e^{-i\theta S_y} | S \rangle$$

$$= \langle S | e^{i\theta S_y} \left[S_x \cos\phi - S_y \sin\phi \right] e^{-i\theta S_y} | S \rangle$$

$$= \cos\phi \langle S | e^{i\theta S_y} S_x e^{-i\theta S_y} | S \rangle - \sin\phi \underbrace{\langle S | S_y | S \rangle}_{0}$$

$$= \cos\phi \langle S | \left[S_z \sin\theta + S_x \cos\theta \right] | S \rangle$$

$$= \sin\theta \cos\phi \underbrace{\langle S | S_z | S \rangle}_{S} + \cos\phi \cos\theta \underbrace{\langle S | S_x | S \rangle}_{0}$$

$$\therefore \quad \langle S_x \rangle = S \sin\theta \cos\phi \quad //$$

Proceeding analogously:

$$\langle S_y \rangle = \langle S | e^{i\theta S_y} e^{i\phi S_z} S_y e^{-i\phi S_z} e^{-i\theta S_y} | S \rangle$$

$$= \langle S | e^{i\theta S_y} [S_x \sin\phi + S_y \cos\phi] e^{-i\theta S_y} | S \rangle$$

$$= \sin\phi \langle S | e^{i\theta S_y} S_x e^{-i\theta S_y} | S \rangle + 0$$

$$= \sin\phi \langle S | [S_z \sin\theta + S_x \cos\theta] | S \rangle$$

$$\therefore \quad \langle S_y \rangle = S \sin\theta \sin\phi$$

And finally

$$\langle S_z \rangle = \langle S | e^{i\theta S_y} e^{i\phi S_z} S_z e^{-i\phi S_z} e^{-i\theta S_y} | S \rangle$$

$$= \langle S | e^{i\theta S_y} S_z e^{-i\theta S_y} | S \rangle$$

$$= \langle S | [S_z \cos\theta - S_x \sin\theta] | S \rangle$$

$$\therefore \quad \langle S_z \rangle = S \cos\theta$$

5) LMG, part 2

$$H = -h S_z - \frac{k}{2S} S_x^2$$

Using the results from the previous exercise, we get

$$E(\theta,\phi) = \langle\theta,\phi| H |\theta,\phi\rangle = -hS\cos\theta - \frac{kS}{2}\sin^2\theta\cos^2\phi.$$

We now minimize this with respect to θ and ϕ.

$$\frac{\partial E}{\partial\theta} = hS\sin\theta - kS\sin\theta\cos\theta\cos^2\phi = 0$$

$$\frac{\partial E}{\partial\phi} = kS\sin^2\theta\cos\phi\sin\phi = 0$$

It suffices to consider $h>0$, since the problem is symmetric with respect to $h \to -h$

This gives two equations

$$\sin\theta\,(h - k\cos\theta\cos^2\phi) = 0$$

$$\sin^2\theta\,\sin 2\phi = 0$$

One solution is

$$\theta_1 = 0, \quad \phi_1 = \text{arbitrary}.$$

That is, the spin is in the north pole.

But if $h/k \leq 1$ there can also be a solution with

For $\frac{h}{k} < 1$

$$\phi_2 = 0 \text{ or } \pi \quad \text{and} \quad \cos\theta_2 = h/k.$$

This solution is 2-fold degenerate, since we can have either $\phi_2 = 0$ or $\phi_2 = \pi$.

The fact that one of the solutions only exist for $h<k$ signals the critical field

$$h_c = k$$

at which the quantum phase transition occurs.

The energy at the two solutions is

$$E_1 = E(\theta_1, \phi_1) = -hS$$

$$E_2 = E(\theta_2, \phi_2) = -hS\,(h/k) - \frac{kS}{2}\left[1 - (h/k)^2\right]$$

$$= -\frac{h^2 S}{k} - \frac{kS}{2} + \frac{h^2 S}{2k}$$

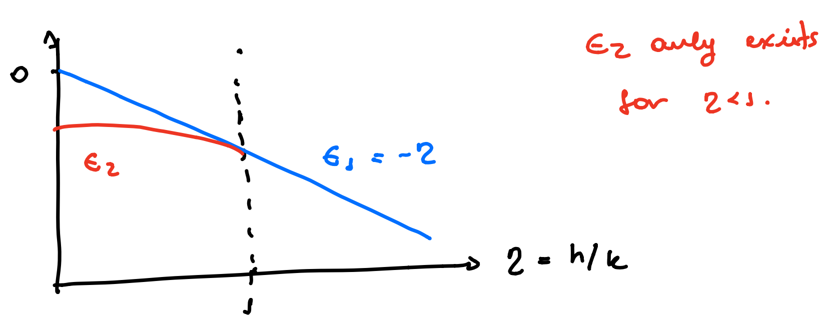
$$= -\frac{h^2 S}{2k} - \frac{kS}{2}$$

It is better to define

$$\epsilon = \frac{E}{kS} \qquad \eta = h/k$$

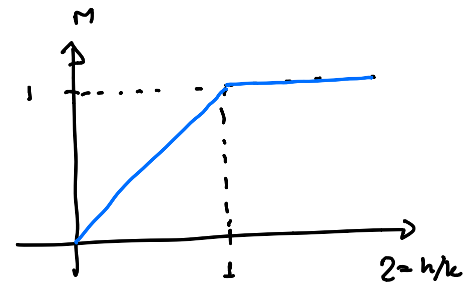
then

$$\epsilon_1 = -\eta \qquad \epsilon_2 = -\frac{1}{2}(1+\eta^2)$$



For $h > h_c$ the system remains magnetized with $\theta = \theta_1 = 0$. But below $h = h_c$ the magnetization becomes $\cos\theta_2 = h/\kappa$. Thus

$$M = \langle S_z \rangle = S\cos\theta = \begin{cases} S & h > h_c \\ S h/\kappa & h < h_c \end{cases}$$



Compare this with the blue curve in the fig of exercise 2e. There we used $S = 1$, so M was a smooth function. When $S \to \infty$ this is replaced by a sharp transition.

The phase $h < h_c$ is called the "broken phase". The reason is because in this phase a symmetry is broken. The Hamiltonian is symmetric under the change

$$S_x \to -S_x$$

or, what is equivalent,

$$\phi \to \phi + \pi$$

When $h > h_c$ this remains true for the ground state. But for $h < h_c$ the ground-state is degenerate and has <u>either</u> $\phi = 0$ <u>or</u> $\phi = \pi$. Thus, if the system is in, e.g., $\phi = 0$, the original symmetry in the Hamiltonian has been broken.