HW 6

Q1

Ferromagnet in dD (spin wave spectrum)

$$\hat{H} = -2 \sum_{i<j} J_{ij} \hat{S}_i \cdot \hat{S}_j - 2 \sum_{i<j} K_{ij} \hat{S}_{i,z} \hat{S}_{j,z}$$

Restrict to nearest neighbors, $J_{ij} = J$, $K_{ij} = K$

$$\hat{H} = -2J \sum_{\substack{i<j \\ j=i+1}} \hat{S}_i \cdot \hat{S}_j - 2K \sum_{\substack{i<j \\ j=i+1}} \hat{S}_{i,z} \hat{S}_{j,z}$$

Focusing on two spins m and $m+1$

$$\hat{H}_{m,m+1} = -2J \left(\hat{S}_{m,x} \hat{S}_{m+1,x} + \hat{S}_{m,y} \hat{S}_{m+1,y} + \hat{S}_{m,z} \hat{S}_{m+1,z} \right) - 2K \left(\hat{S}_{m,z} \hat{S}_{m+1,z} \right)$$

$$= -2J \left(\frac{\hat{S}_{m,+} \hat{S}_{m+1,-} + \hat{S}_{m,-} \hat{S}_{m+1,+}}{2} + \hat{S}_{m,z} \hat{S}_{m+1,z} \right) - 2K \left(\hat{S}_{m,z} \hat{S}_{m+1,z} \right)$$

$$= -J \left(\hat{S}_{m,+} \hat{S}_{m+1,-} + \hat{S}_{m,-} \hat{S}_{m+1,+} \right) - (2)(J+K) \hat{S}_{m,z} \hat{S}_{m+1,z}$$

Next, we apply Holstein-Primakoff transformations. For convenience, $m = 2$.

$$\hat{H}_{1,2} = -J\left(2S\left(\hat{a}_1 \hat{a}_2^{\dagger} + \hat{a}_1^{\dagger} \hat{a}_2\right)\right) - 2(J+K)\left(S^2 - (\hat{n}_1 + \hat{n}_2)S\right.$$

where $\hat{n}_1 = \hat{a}_1^{\dagger} \hat{a}_1$, $\hat{n}_2 = \hat{a}_2^{\dagger} \hat{a}_2$ and we have dropped biquadratic terms such as $\hat{n}_1 \hat{n}_2$.

Since $[\hat{a}_1, \hat{a}_2^{\dagger}] = 0$

$$\hat{H}_{1,2} = -J\left(2S\left(\hat{a}_2^{\dagger} \hat{a}_1 + \hat{a}_1^{\dagger} \hat{a}_2\right)\right) - 2(J+K)\left(S^2 - (\hat{a}_1^{\dagger}\hat{a}_1 + \hat{a}_2^{\dagger}\hat{a}_2)\right.$$

We now add up all the pair-wise interactions.

$$\cancel{\hat{H} = -2JS \sum_m \left(\hat{a}_{m+1}^{\dagger} \hat{a}_m + \hat{a}_m^{\dagger} \hat{a}_{m+1}\right) - 2(J+K)\sum_m \left(S^2 - (\hat{a}_m^{\dagger}\hat{a}_m + \hat{a}_{m+1}^{\dagger}\hat{a}_{m+1}\right.}$$

$$= -2JS \sum_m \left(\hat{a}_m^{\dagger} \hat{a}_{m+1} + \hat{a}_{m+1} \hat{a}_m\right)$$

$$- \cancel{2}(J+K) S^2 \left(\frac{N}{\cancel{2}}\right) + 2(J+K)S(2) \sum_m \hat{a}_m^{\dagger} \hat{a}_m$$

$$\boxed{\hat{H} = -2JS \sum_m \left(\hat{a}_m^{\dagger} \hat{a}_{m+1} + \hat{a}_{m+1}^{\dagger} \hat{a}_m\right) - (J+K) S^2 N + 4S(J+K) \sum_m \hat{a}_m^{\dagger} \hat{a}_m}$$

We can express the field operators in terms of the Fourier transforms:

$$\hat{a}_m = \frac{1}{\sqrt{N}} \sum_q \hat{b}_q \, e^{+i\vec{q}\cdot\vec{r}_m} \quad *$$

$$\hat{a}_m^{\dagger} = \frac{1}{\sqrt{N}} \sum_q \hat{b}_q^{\dagger} \, e^{-i\vec{q}\cdot\vec{r}_m} \quad *$$

$$\vec{r}_{m+1} = \vec{r}_m + \vec{a}$$

$$\hat{a}_m^{\dagger}\hat{a}_{m+1} = \frac{1}{N}\sum_q \hat{b}_q^{\dagger}\hat{b}_q \, e^{+i\vec{q}\cdot\vec{a}}$$

$$\hat{a}_{m+1}^{\dagger}\hat{a}_m = \frac{1}{N}\sum_q \hat{b}_q^{\dagger}\hat{b}_q \, e^{-i\vec{q}\cdot\vec{a}}$$

$$\hat{a}_m^{\dagger} a_m = \frac{1}{N}\sum_q \hat{b}_q^{\dagger} b_q$$

$$\hat{H} = -2JS\frac{1}{N}\sum_m\left(2\sum_q \hat{b}_q^{\dagger} b_q \cos(\vec{q}\cdot\vec{a})\right) - (J+K)S^2 N + 4\cancel{JS}\,S(J+K)\sum_q \hat{b}_q^{\dagger}\hat{b}_q$$

$$= -4JS\sum_q \hat{b}_q^{\dagger}\hat{b}_q \cos(\vec{q}\cdot\vec{a}) - (J+K)\underline{S^2 N} + 4S(J+K)\sum_q \hat{b}_q^{\dagger}\hat{b}_q$$

$\hbar\omega\left(\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\right)$

$$= H_0 + 4JS\sum_q \hat{b}_q^{\dagger}\hat{b}_q\left(1-\cos(\vec{q}\cdot\vec{a})\right)$$

$$+ 4KS\sum_q \hat{b}_q^{\dagger}\hat{b}_q$$

$$\boxed{\hat{H} = \hat{H}_0 + \sum_q \hat{b}_q^{\dagger}\hat{b}_q\left(\underline{4KS + 4JS\left(1-\cos(\vec{q}\cdot\vec{a})\right)}\right)}$$

$$\boxed{\hbar\omega = E(\vec{q}) = 4KS + 4JS\left(1-\cos(\vec{q}\cdot\vec{a})\right)}$$ – dispersion relation

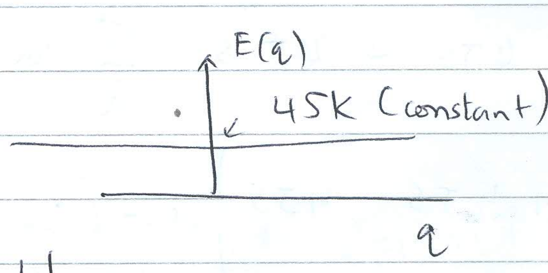
a) <u>For a 1D chain</u>

(i) $\vec{q}\cdot\vec{a} = qa$

$$E(q) = 4S\left(K + J\cdot 2\sin^2\left(\frac{qa}{2}\right)\right)$$

(ii) $J = 0$ — Ising model

$$E(q) = 4SK$$

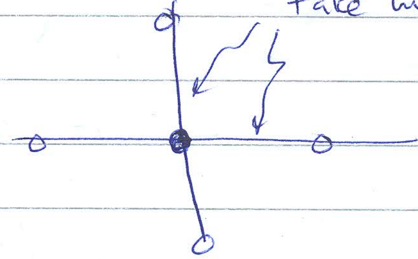


(iii) $K = 0$ — Heisenberg model

$$E(q) = 8SJ\sin^2\left(\frac{qa}{2}\right) \underset{\text{long wavelength}}{\approx} 8SJ\frac{q^2a^2}{4} = 2SJq^2a^2.$$

HW6
Q1

(b) For a square lattice



take into account these nearest neighbor interactions.

$$E(\vec{q}) = 4KS + 4JS\left(1 - \sum_{\vec{a}} \cos(\vec{q}\cdot\vec{a})\right)$$

nearest neighbors (i and $i+1$) are at $\vec{a} = (a,0)^T$ and $(0,a)^T$.

Hence

$$E(\vec{q}) = 4KS + 4JS\left(1 - \cos(q_x a) - \cos(q_y a)\right)$$

If $qa \ll 1$ (long wavelength)

$$\cos(qa) \approx 1 - \frac{q^2a^2}{2}.$$

So

$$E(\vec{q}) \approx 4KS + 4JS\left(1 - \left(1 - \frac{q_x^2a^2}{2}\right) - \left(1 - \frac{q_y^2a^2}{2}\right)\right)$$

$$= 4KS + 4JS\left(\cancel{1} - \cancel{1} + \frac{q_x^2a^2}{2} - 1 + \frac{q_y^2a^2}{2}\right)$$

$$= 4KS + 4JS\left(-1 + \frac{q^2a^2}{2}\right)$$

$$= 4KS - 4JS\left(1 - q^2a^2/2\right)$$

Q2

(a) $$Z = e^{-\beta \mu_B B} + e^{+\beta \mu_B B} = 2\cosh(\beta \mu_B B)$$

$$\langle E \rangle = U = \frac{\sum E_i e^{-\beta E_i}}{Z}$$

Now $$Z = \sum_i e^{-\beta E_i}$$

$$\Rightarrow \frac{\partial}{\partial \beta}(\ln Z) = \frac{1}{Z}\left(\frac{\partial}{\partial \beta} Z\right)$$

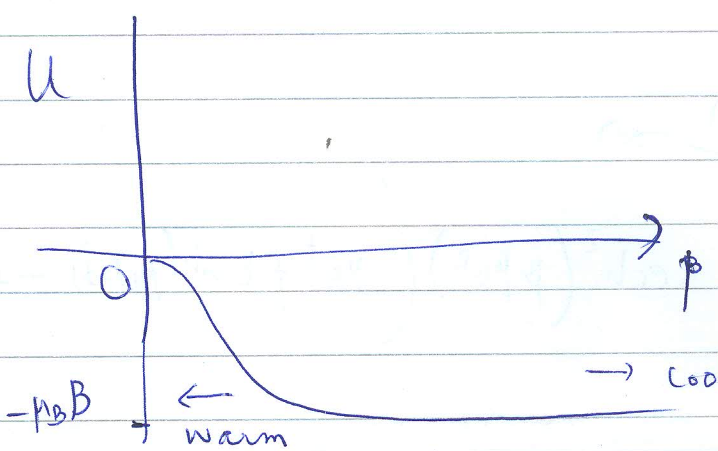
$$= \frac{1}{Z} \sum_i (-E_i)\, e^{-\beta E_i})$$

$$= -U$$

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

$$U = -\frac{\partial}{\partial \beta} \ln\left(2\cosh(\beta \mu_B B)\right) = -\frac{1}{2\cosh(\beta \mu_B B)} \cdot 2\sinh(\beta \mu_B B)\, \mu_B B$$

$$= -\mu_B B \tanh(\beta \mu_B B)$$



(b) $C_v = \dfrac{\partial U}{\partial T} = -\mu_B B \dfrac{\partial}{\partial T} \tanh\left(\dfrac{\mu_B B}{k_B T}\right)$

$\dfrac{d}{dx} \dfrac{\sinh(x)}{\cosh(x)}$

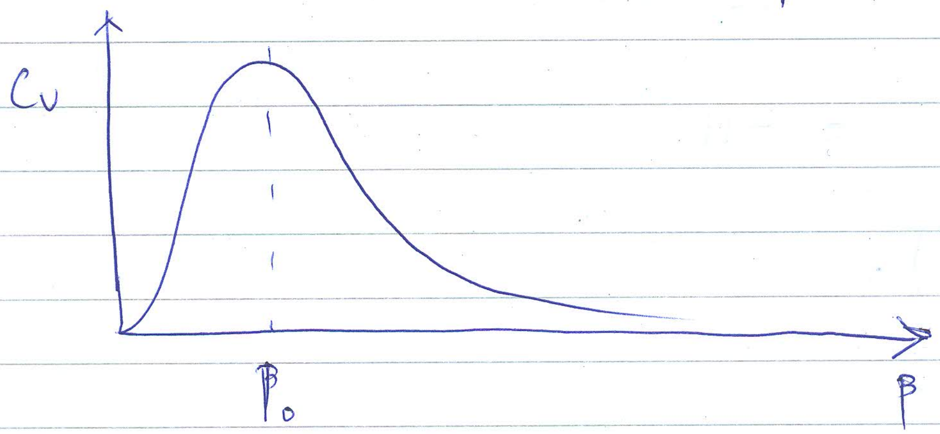
$= \dfrac{\cosh^2 x - \sinh^2 x}{\cosh^2 x}$

$= -\mu_B B \operatorname{sech}^2\left(\dfrac{\mu_B B}{k_B T}\right)\left(\dfrac{\mu_B B}{k_B}\right)\left(-\dfrac{1}{T^2}\right)$

$= \cancel{\phi}\ \operatorname{sech}^2 x$

$= \dfrac{\mu_B^2 B^2}{k_B^2 T^2} k_B \operatorname{sech}^2\left(\dfrac{\mu_B B}{k_B T}\right)$

$C_v = (\mu_B B)^2 k_B \beta^2 \operatorname{sech}^2(\beta \mu_B B)$.



$\dfrac{\partial C_v}{\partial \beta} = (\mu_B B)^3 k_B \left[-2\beta \operatorname{sech}^2(\beta \mu_B B)\ (\beta - 1 \tanh(\beta \mu_B B))\right] = 0$

$\Rightarrow$ ~~$\beta_0 = \tanh(\beta_0 \mu_B B)$~~

$= -2 k_B (\mu_B B)^2 \beta \operatorname{sech}^2(\beta \mu_B B)\left(\mu_B B \beta \tanh(\mu_B B \beta) - 1\right) = 0$

$$\Rightarrow \quad \mu_B B \beta_0 \tanh(\mu_B B \beta_0) = 1.$$

$$\beta_0 \underbrace{\tanh(\mu_B B \beta_0)} = \frac{1}{\mu_B B} \quad \boxtimes.$$

(c) $$F = -Nk_B T \ln(2)$$

$$= -Nk_B T \ln\left(2\cosh(\mu_B B \beta)\right).$$

$$F = U - TS \Rightarrow S = \left\{\frac{U-F}{T}\right\}.$$

$$S = \frac{-N\mu_B B \tanh(\mu_B B / k_B T) + Nk_B T \ln\left(2\cosh(\mu_B B / k_B T)\right)}{T}$$

Q3.

$$\omega_q = \alpha q^n \quad , \quad \hbar = 1$$

$$U = \int \cancel{\hbar}\, d\omega \; \alpha q^n \; g(\omega) \; n(\omega)$$

Let's first find $g(\omega)$ for the d-D case.

Per unit volume, we have $g(k)\,dk = \begin{cases} \frac{4\pi k^2}{(2\pi)^3}\, dk , & d = 3 \text{ (Dim)} \\ \frac{2\pi k}{(2\pi)^2}\, dk , & d = 2 \\ \frac{2\, dk}{2\pi} , & d = 1 \end{cases}$

$\therefore \; g(k) \propto k^{d-1}$ where d is the no. of dimensions.

We are given $\omega = \alpha k^n \Rightarrow k = \left(\frac{1}{\alpha}\right)^{1/n} \omega^{1/n} \Rightarrow k^n = \frac{\omega}{\alpha}$

$$\boxed{d\omega = \alpha n k^{n-1} dk} \qquad k^{n-1} = \left(\frac{1}{\alpha}\right)^{\frac{n-1}{n}} \omega^{\frac{n-1}{n}} .$$

$\rightarrow g(k) = A_d \, k^{d-1}$ where $A_3 = \frac{4\pi k^2}{(2\pi)^3}$,

$$A_2 = \frac{2\pi k}{(2\pi)^2}$$

$$A_1 = \frac{2}{2\pi} = \frac{1}{\pi} .$$

$$g(k)\,dk = A_d \, k^{d-1} \, dk$$

$$= A_d \left(\frac{1}{\alpha}\right)^{\frac{d-1}{n}} \omega^{\frac{d-1}{n}} \frac{d\omega}{\alpha n k^{n-1}}$$

$$g(k)\,dk = A_d \left(\frac{1}{\alpha}\right)^{\frac{d-1}{n}} \omega^{\frac{d-1}{n}} \frac{d\omega \quad (\alpha)^{\frac{n-1}{n}}}{\alpha n \quad \omega^{\frac{n-1}{n}}}$$

$$= A_d \left(\frac{1}{\alpha}\right)^{\frac{d-1}{n}} \frac{(\alpha)^{\frac{n-1}{n}}}{\alpha n} \omega^{\frac{d-1}{n} - \frac{n-1}{n}} d\omega$$

$$= C_d \, \omega^{\frac{d-\cancel{1}-n\cancel{+1}}{n}} d\omega .$$

$$\cancel{g(\omega) = C_d \, \omega^{\frac{d-1-n^2+n}{n}}} .$$

$$g(k)\,dk = C_d \, \omega^{\frac{d-n}{n}} d\omega$$

$$\boxed{g(\omega) = C_d \, \omega^{\frac{d}{n}-1}}$$

$\cancel{\hbar = 1}$

$$U = E_0 + \int_{\omega=0}^{\infty} d\omega \, \hbar \alpha k^n \, C_d \, \omega^{\frac{d}{n}-1} \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

$$= E_0 + \int_{\omega=0}^{\infty} \frac{d\omega \, \hbar\omega \, C_d \, \omega^{\frac{d}{n}-1}}{e^{\hbar\omega/k_B T} - 1} .$$

$$= E_0 + \hbar C_d \int_0^{\infty} d\omega \frac{\omega^{d/n}}{e^{\hbar\omega/k_B T} - 1} , \quad \text{let } \frac{\hbar\omega}{k_B T} = x .$$

$$\omega = \frac{k_B T}{\hbar} x$$

$$d\omega = \frac{k_B T}{\hbar} dx .$$

$$U = E_0 + \hbar C_d \left(\frac{k_B T}{\hbar}\right) \int_{x=0}^{\infty} dx \left(\frac{k_B T}{\hbar}\right)^{\frac{d}{n}} \frac{x^{d/n}}{\{e^x - 1\}}.$$

$$= E_0 + \hbar C_d \left(\frac{k_B T}{\hbar}\right)^{1+\frac{d}{n}} \underbrace{\int_0^{\infty} \frac{x^{d/n}}{e^x - 1} dx}_{\text{a standard integral}}.$$

$$C_V \propto \frac{d}{dT} T^{1+\frac{d}{n}}$$

$$= \left(1 + \frac{d}{n}\right) T^{d/n}, \qquad \boxed{C_V \propto T^{d/n}}.$$

Q4.

(a) $$H = -2J \sum_{i=1}^{N-1} \hat{S}_{i,z} \hat{S}_{i+1,z} \quad , \quad \hbar = 1$$

$$\langle \hat{S}_{i,z} \hat{S}_{i+1,z} \rangle = \pm \frac{1}{4}$$

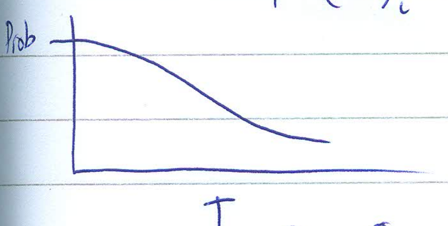
$$Z_1 = e^{-\beta J/2} + e^{+\beta J/2} = 2\cosh(\beta J/2)$$

$$\boxed{Z_{N-1} = 2^{N-1} \cosh^{N-1}(\beta J/2)}$$

(b) Let $\hat{\zeta}_i = \hat{S}_{i,z} \hat{S}_{i+1,z}$

Prob. that ~~a~~ two consecutive spins are pointing in the same direction within a pair is

$$P\left(\zeta_i = \frac{1}{4}\right) = \frac{e^{+\beta J/2}}{e^{\beta J/2} + e^{-\beta J/2}} = \frac{1}{1 + e^{-\beta J}}$$



M consecutive spins
$\Rightarrow$ M − 1 pairs

Prob that M spins, all adjacent have spins pointing together is

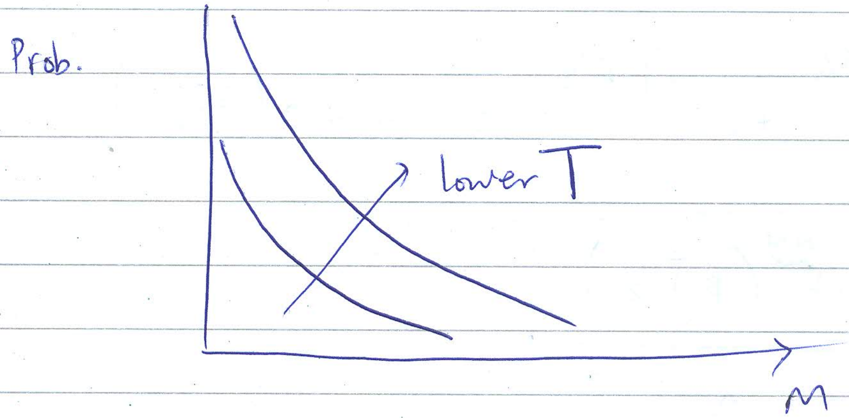
$$P(M) = \left(\frac{1}{1 + e^{-\beta J}}\right)^{M-1} = (1 + e^{-\beta J})^{(1-M)}$$

$$= \exp\left(\ln (1 + e^{-\beta J})^{(1-M)}\right)$$

$$= \exp\left((1-M) \ln (1 + e^{-\beta J})\right)$$

$$= e^{(1-M)\ln\left(1+\underbrace{e^{-\beta J}}\right)}$$

$\Rightarrow$ prob decays exponentially with M.



$\rightarrow$ lower the T, the prob. decays much slower (i.e., over a longer chain length).