Quantum Magnetism, Condensed Matter Physics 24/25

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Problem (6.2), Blundell:

(6.2) A uniaxial ferromagnet is described by the Hamiltonian

$$\hat{\mathcal{H}} = -\sum_{ij} \mathsf{J}_{ij}\, \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \sum_{ij} K_{ij} \hat{S}_i^z \hat{S}_j^z. \qquad (6.57)$$

(a) Show that the state with all spins fully aligned along the z axis is an eigenstate of the Hamiltonian.

(b) Obtain an expression for the spin wave spectrum as a function of wave vector $\mathbf{q}$.

(c) Simplify the expressions for the case where J_{ij} and K_{ij} are restricted to nearest neighbours, J_0 and K_0, and the ferromagnet is (i) a one-dimensional chain, (ii) a two-dimensional square lattice and (iii) a three-dimensional body–centred cubic material.

(a)

Starting from the original Hamiltonian:

$$\hat{H} = -\sum_{i,j}\left[J_{i,j}\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + K_{i,j}\hat{S}_i^z\hat{S}_j^z\right] = -\sum_{i,j}\left[J_{i,j}(\hat{S}_i^x\hat{S}_j^x + \hat{S}_i^y\hat{S}_j^y + \hat{S}_i^z\hat{S}_j^z) + K_{i,j}\hat{S}_i^z\hat{S}_j^z\right]$$

and using that $S^x \pm iS^y \equiv S^{\pm}$, we get:

$$\hat{H} = -\sum_{i,j}\left[(J_{i,j} + K_{i,j})\hat{S}_i^z\hat{S}_j^z + \frac{J_{i,j}}{2}(\hat{S}_i^+\hat{S}_j^- + \hat{S}_i^-\hat{S}_j^+)\right]$$

where we can see that all pairs of the fully aligned states $|\uparrow\uparrow / \downarrow\downarrow\rangle$, are eigenstates of the last term $(\hat{S}_i^+\hat{S}_j^- + \hat{S}_i^-\hat{S}_j^+)\ |\uparrow\uparrow / \downarrow\downarrow\rangle \propto\ |\uparrow\uparrow / \downarrow\downarrow\rangle$, since for:

- $i \neq j\ \rightarrow$ either i or j cancels: $S^+|\downarrow\rangle \underbrace{S^-|\downarrow\rangle}_{=0} = \underbrace{S^+|\uparrow\rangle}_{=0} S^-|\uparrow\rangle = 0$
- $i = j\ \rightarrow$ one term cancels and the other flips twice, leaving the same state:

$$S^+\underbrace{S^-|\downarrow\rangle}_{=0} + \underbrace{S^-S^+|\downarrow\rangle}_{\propto|\downarrow\rangle\equiv\lambda_{-\downarrow}\lambda_{+\downarrow}|\downarrow\rangle} \propto |\downarrow\rangle\ ; \quad \underbrace{S^+S^-|\uparrow\rangle}_{\propto|\uparrow\rangle\equiv\lambda_{+\uparrow}\lambda_{-\uparrow}|\uparrow\rangle} + S^-\underbrace{S^+|\uparrow\rangle}_{=0} \propto |\uparrow\rangle$$

and since they are eigenstates of S^z by def., they are eigenstates of the full Hamiltonian:

$$\boxed{\hat{H}\,|\uparrow\uparrow ... / \downarrow\downarrow ...\rangle = -\left[\text{Sum}(J+K)\ \lambda^2_{\uparrow/\downarrow} + \frac{Tr(J)}{2}\lambda_{+\uparrow/\downarrow}\lambda_{-\uparrow/\downarrow}\right]|\uparrow\uparrow ... / \downarrow\downarrow ...\rangle}$$

(b)

For low temperature ($\approx$ large spins, $S >> 1$), we can use the Holstein-Primakoff relations:

$$\hat{S}_i^+ = \sqrt{2S}\sqrt{1-\frac{\hat{a}_i^\dagger \hat{a}_i}{2S}}\,\hat{a}_i \approx \sqrt{2S}\hat{a}_i, \quad \hat{S}_i^- = \sqrt{2S}\hat{a}_i^\dagger\sqrt{1-\frac{\hat{a}_i^\dagger \hat{a}_i}{2S}} \approx \sqrt{2S}\hat{a}_i^\dagger, \quad \hat{S}_i^z = S - \hat{a}_i^\dagger \hat{a}_i,$$

where $\hat{a}_i^\dagger, \hat{a}_i$ create/destroy a (bosonic) spin excitation in i. Resulting in:

$$\hat{H} = -\sum_{i,j}\Big[(J_{i,j}+K_{i,j})(S-\hat{a}_i^\dagger \hat{a}_i)(S-\hat{a}_j^\dagger \hat{a}_j) + SJ_{i,j}(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_i \hat{a}_j^\dagger)\Big]$$

which getting rid of terms lower in $O(S)$, due to large spins, ends like:

$$\begin{aligned}\hat{H} &\approx -\sum_{i,j}\Big[(J_{i,j}+K_{i,j})(S^2 - S\hat{a}_i^\dagger \hat{a}_i - S\hat{a}_j^\dagger \hat{a}_j) + SJ_{i,j}(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_i \hat{a}_j^\dagger)\Big] \\ &= H_0 + S\sum_i\Big[\underbrace{2\,\hat{a}_i^\dagger \hat{a}_i \sum_j (J_{i,j}+K_{i,j})}_{\sum_{i,j} J_{i,j}\hat{a}_i^\dagger \hat{a}_i \equiv (1)} - \underbrace{\sum_j (J_{i,j}+J_{j,i})\hat{a}_i^\dagger \hat{a}_j}_{\sum_{i,j} J_{i,j}\hat{a}_i^\dagger \hat{a}_j \equiv (2)}\Big]\end{aligned}$$

And introducing the Fourier transforms:

- $J(\mathbf{q}) = \sum_{i,j} J_{i,j} e^{-i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \;\leftrightarrow\; J_{i,j} = \sum_{\mathbf{q}} J(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}$
- $K(\mathbf{q}) = \sum_{i,j} K_{i,j} e^{-i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \;\leftrightarrow\; K_{i,j} = \sum_{\mathbf{q}} K(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}$
- $\hat{a}_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i}\hat{a}_i \;\leftrightarrow\; \hat{a}_i = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}_i}\hat{a}_{\mathbf{q}}$
- $\hat{a}_{\mathbf{q}}^\dagger = \frac{1}{\sqrt{N}}\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\hat{a}_i^\dagger \;\leftrightarrow\; \hat{a}_i^\dagger = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}_i}\hat{a}_{\mathbf{q}}^\dagger$

we get, that the terms (1) and (2), from the previous expression of $\hat{H}$, become:

$$\begin{aligned}(1) &= \sum_{i,j} J_{i,j}\hat{a}_i^\dagger \hat{a}_i = \sum_{i,j}\sum_{\mathbf{q}} J(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\sum_{\mathbf{q}'} e^{i\mathbf{q}'\cdot\mathbf{r}_i}\hat{a}_{\mathbf{q}'}^\dagger \sum_{\mathbf{q}''} e^{-i\mathbf{q}''\cdot\mathbf{r}_i}\hat{a}_{\mathbf{q}''} = \\ &= \sum_{\mathbf{q},\mathbf{q}'\mathbf{q}''} J(\mathbf{q})\hat{a}_{\mathbf{q}'}^\dagger \hat{a}_{\mathbf{q}''}\underbrace{\sum_i e^{i(\mathbf{q}+\mathbf{q}'-\mathbf{q}'')\cdot\mathbf{r}_i}}_{=\delta_{\mathbf{q}+\mathbf{q}'-\mathbf{q}''}}\underbrace{\sum_j e^{-i\mathbf{q}\cdot\mathbf{r}_j}}_{=\delta_{\mathbf{q}}} = \sum_{\mathbf{q}'} J(0)\hat{a}_{\mathbf{q}'}^\dagger \hat{a}_{\mathbf{q}'}\end{aligned}$$

$$\begin{aligned}(2) &= \sum_{i,j} J_{i,j}\hat{a}_i^\dagger \hat{a}_j = \sum_{i,j}\sum_{\mathbf{q}} J(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\sum_{\mathbf{q}'} e^{-i\mathbf{q}'\cdot\mathbf{r}_i}\hat{a}_{\mathbf{q}'}^\dagger \sum_{\mathbf{q}''} e^{i\mathbf{q}''\cdot\mathbf{r}_j}\hat{a}_{\mathbf{q}''} = \\ &= \sum_{\mathbf{q},\mathbf{q}'\mathbf{q}''} J(\mathbf{q})\hat{a}_{\mathbf{q}'}^\dagger \hat{a}_{\mathbf{q}''}\underbrace{\sum_i e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}_i}}_{=\delta_{\mathbf{q}-\mathbf{q}'}}\underbrace{\sum_j e^{-i(\mathbf{q}-\mathbf{q}'')\cdot\mathbf{r}_j}}_{=\delta_{\mathbf{q}-\mathbf{q}''}} = \sum_{\mathbf{q}} J(\mathbf{q})\hat{a}_{\mathbf{q}}^\dagger \hat{a}_{\mathbf{q}}\end{aligned}$$

which finally, gives:

$$\boxed{\hat{H} = H_0 + \sum_{\mathbf{q}} \hbar\omega(\mathbf{q})\hat{a}_{\mathbf{q}}^\dagger \hat{a}_{\mathbf{q}} \;= H_0 + 2S\sum_{\mathbf{q}}\left[J(0)+K(0) - \frac{J(\mathbf{q})+J(-\mathbf{q})}{2}\right]\hat{a}_{\mathbf{q}}^\dagger \hat{a}_{\mathbf{q}}}$$

showing that the spin-wave dispersion (for a symmetric $J_{i,j}$) is $\boxed{\omega(\mathbf{q}) = 2S\,[J(0)+K(0)-J(\mathbf{q})]}$.

(c)

Restricting the couplings J and K to nearest-neighbors J_0 and K_0, makes that J is now symmetric $J_{i,j} = J_{j,i} = J_0 \leftrightarrow J(\mathbf{q}) = J(-\mathbf{q}) = \sum_{<i,j>} J_0 e^{-i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}$, giving a cleaner:

$$\omega(\mathbf{q}) = 2S\left[J(0) + K(0) - J(\mathbf{q})\right] = 2S\left[J_0 + K_0 - \sum_{<i,j>} J_0 e^{-i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}\right]$$

which now in each case, we just need to sum over the corresponding near-neighbours.

1. In a 1D chain:

The near-neighbours are only the left and right ones, separated at a distance $\delta_x = \pm a$, so:

$$J(\mathbf{q}) = J_0(e^{i\mathbf{q}a} + e^{-i\mathbf{q}a}) = 2J_0\cos(\mathbf{q}a)$$

giving:

$$\boxed{\omega(\mathbf{q}) = 4S\left[J_0(1 - \cos(\mathbf{q}a)) + K_0\right]}$$

2. In a 2D square lattice:

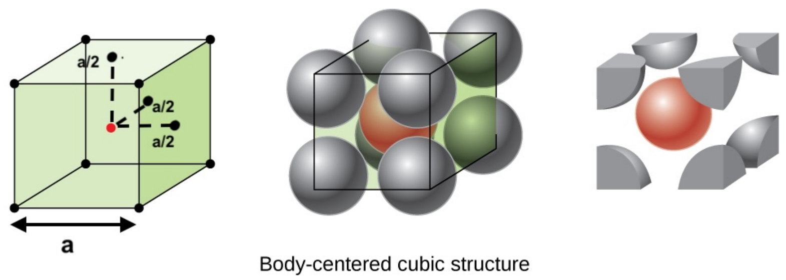
The near-neighbours are the same, but in both directions $\delta_x, \delta_y = \pm a$, getting:

$$J(\mathbf{q}) = J_0(\underbrace{e^{i\mathbf{q}_x a} + e^{-i\mathbf{q}_x a}}_{2\cos(\mathbf{q}_x a)} + \underbrace{e^{i\mathbf{q}_y a} + e^{-i\mathbf{q}_y a}}_{2\cos(\mathbf{q}_y a)}) = 2J_0\left(\cos(\mathbf{q}_x a) + \cos(\mathbf{q}_y a)\right)$$

and:

$$\boxed{\omega(\mathbf{q}) = 8S\left[J_0\left(1 - \frac{\cos(\mathbf{q}_x a) + \cos(\mathbf{q}_y a)}{2}\right) + K_0\right]}$$

3. In a 3D body-centered cubic material:



Body-centered cubic structure

The near-neighbours are all the combinations of $\delta x, \delta y, \delta z = \pm\frac{a}{2}$, which gives:

$$J(\mathbf{q}) = J_0 \sum_{\delta x, \delta y, \delta z = \pm\frac{a}{2}} e^{i(\delta x \mathbf{q}_x + \delta y \mathbf{q}_y + \delta z \mathbf{q}_z)} = \sum_{\delta x = \pm\frac{a}{2}} e^{i\delta x \mathbf{q}_x} \sum_{\delta y = \pm\frac{a}{2}} e^{i\delta y \mathbf{q}_y} \underbrace{\sum_{\delta z = \pm\frac{a}{2}} e^{i\delta z \mathbf{q}_z}}_{2\cos(\frac{\mathbf{q}_z a}{2})}$$

$$= 8J_0 \cos\left(\frac{\mathbf{q}_x a}{2}\right)\cos\left(\frac{\mathbf{q}_y a}{2}\right)\cos\left(\frac{\mathbf{q}_z a}{2}\right)$$

so that, finally the spectrum looks like:

$$\boxed{\omega(\mathbf{q}) = 16S\left[J_0\left(1 - \cos\left(\frac{\mathbf{q}_x a}{2}\right)\cos\left(\frac{\mathbf{q}_y a}{2}\right)\cos\left(\frac{\mathbf{q}_z a}{2}\right)\right) + K_0\right]}$$

Problem (6.3), Blundell:

> (6.3) Using the results of Exercise 6.2 for small wave vectors, deduce the temperature dependence at low temperatures of the number of spin waves for the Heisenberg model ($K_0 = 0$) and the Ising model ($J_0 = 0$) for each of the structures (i), (ii) and (iii) of Exercise 6.2. Show that your results for the Ising model for case (i) agree with the results obtained in Exercise 6.1 and that there is no long range magnetic order above absolute zero for the Heisenberg model in one or two dimensions.

For small wave vectors ($\cos(x) \approx 1 - \frac{x^2}{2} + \cancel{O(x^4)}$), the previous expressions become:

- 1. In a 1D chain: $\omega(\mathbf{q}) = 4S\left[J_0\frac{\mathbf{q}^2a^2}{2} + \cancel{O(\mathbf{q}^4)} + K_0\right] = 2S\left[J_0\mathbf{q}^2a^2 + 2K_0\right]$
- 2. In a 2D square lattice: $\omega(\mathbf{q}) = 8S\left[J_0\frac{(\mathbf{q}_x^2+\mathbf{q}_y^2)a^2}{4} + \cancel{O(\mathbf{q}^4)} + K_0\right] = 2S\left[J_0\mathbf{q}^2a^2 + 4K_0\right]$
- 3. In a 3D bcc material: $\omega(\mathbf{q}) = 16S\left[J_0\frac{(\mathbf{q}_x^2+\mathbf{q}_y^2+\mathbf{q}_z^2)a^2}{8} + \cancel{O(\mathbf{q}^4)} + K_0\right] = 2S\left[J_0\mathbf{q}^2a^2 + 8K_0\right]$

Heisenberg model ($K_0 = 0$):

From the above expression it is clear that our dispersion relation in the Heisenberg model is independent of the dimension, being always:

$$\omega(\mathbf{q}) = 2SJ_0\mathbf{q}^2a^2 \equiv D\mathbf{q}^2 \quad \text{with a spin stiffness:} \quad D = 2SJ_0a^2$$

Now to compute the number of spin waves, we have to use:

$$N_s = \int \frac{d^dq}{e^{\hbar\omega(\mathbf{q})/k_BT} - 1} = \int \frac{d^dq}{e^{D\mathbf{q}^2/k_BT} - 1} \equiv \int \frac{d^dq}{e^{c\mathbf{q}^2} - 1} \propto \left(\frac{\pi}{c}\right)^{\frac{d}{2}} \zeta\left(\frac{d}{2}\right)$$

with $c = D/k_BT = 2SJ_0a^2/k_BT$, where the integral depended basically on $\mathbf{q}^2/T$.

Examining the Riemann zeta function $\zeta\left(\frac{d}{2}\right)$ in the expression, it is clear that N_s automatically diverges for $d \leq 2$ unless c diverges ($T = 0$). Showing that above absolute zero ($T \neq 0$), the isotropic Heisenberg model in 1d and 2d, will have no long-range magnetic order.

Ising model ($J_0 = 0$):

In the Ising model, the dispersion relation becomes independent of $\mathbf{q}$:

$$\omega = zSK_0 \quad \text{where } z = \text{nº of near neighbors in each case: 2, 4, 8...}$$

Making N_s computation trivial. Concretely for low T: $\boxed{N_s \propto (e^{\hbar\omega/k_BT} - 1)^{-1} \approx e^{-\hbar\omega/k_BT}}$, so their energy $E \propto \hbar\omega\, e^{-\hbar\omega/k_BT}$. From where we can compute the heat capacity per spin:

$$c = \frac{C}{N} = \frac{1}{N}\frac{\partial E}{\partial T} \propto \hbar\omega \underbrace{\frac{\partial e^{-\hbar\omega/k_BT}}{\partial T}}_{\frac{+\hbar\omega}{k_BT^2}e^{-\hbar\omega/k_bT}} = \frac{(\hbar\omega)^2}{k_BT^2}e^{-\hbar\omega/k_BT} = \frac{(zSK_0)^2}{k_BT^2}e^{-\hbar\omega/k_BT}$$

agreeing with Problem (6.1) results, where for low T: $\boxed{c \propto e^T/T^2}$.