Assignment on Quantum Magnetism

Submitted by: AATIF KAISAR KHAN

(6.2) A uniaxial ferromagnet is described by the Hamiltonian

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

(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) we can write the Hamiltonian as:

$$\mathcal{H} = -\sum_{i,j} J_{ij}\left(S_i^z S_i^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)\right) - \sum_{i,j} K_{ij}\, S_i^z S_j^z$$

(we used $S^\pm = S^x \pm i\, S^y$)

Now consider a state $|\phi\rangle$ with all spins up

$\therefore\ S_i^- S_j^+ |\phi\rangle = 0$

Now $S_i^+ S_j^- = S_j^- S_i^+$, as $i \neq j$

$\Rightarrow S_i^+ S_j^- |\phi\rangle = 0$

Since every term has $|\phi\rangle$ eigenvector, thus $|\phi\rangle$ is an eigenstate of the Hamiltonian

(b)

For low temperature, we have Holstein-Primakoff relations:

$$S_j^+ \approx \sqrt{2S}\, a_j \quad , \quad S_j^- \approx \sqrt{2S}\, a_j^\dagger \quad , \quad S_j^z \approx S - a_j^\dagger a_j$$

Thus:

$$\mathcal{H} = -\sum_{i,j}\left[(J_{ij} + K_{ij})(S - a_i^\dagger a_i)(S - a_j^\dagger a_j) + J_{ij} S\, a_i a_j^\dagger + J_{ij} S\, a_i^\dagger a_j\right]$$

$$\approx -\sum_{i,j} (J_{ij} + K_{ij})\left(S^2 - S a_i^\dagger a_i - S a_j^\dagger a_j\right) - S\sum_{i,j} J_{ij}\left(a_i a_j^\dagger - a_i^\dagger a_j\right)$$

neglecting quad. term

Let, $J(\vec{q}) = \sum_{i,j} J_{ij}\, e^{-i\vec{q}(\vec{r}_i-\vec{r}_j)}$, $J_{ij} = \sum_{q} J(\vec{q})\, e^{iq(\vec{r}_i-\vec{r}_j)}$,

$K(\vec{q}) = \sum_{i,j} K_{ij}\, e^{iq(\vec{r}_i-\vec{r}_j)}$, $K_{ij} = \sum_{q} K(\vec{q})\, e^{-iq(r_i-r_j)}$,

$a_q = \frac{1}{\sqrt{N}} \sum_j e^{-i\vec{q}\cdot\vec{r}_j} a_j$, $a_q^{+} = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{q}\cdot\vec{r}_j} a_j^{+}$,

$a_j = \frac{1}{\sqrt{N}} \sum_q e^{i\vec{q}\cdot\vec{r}_j} a_q$, $a_j^{+} = \frac{1}{\sqrt{N}} \sum_q e^{-i\vec{q}\cdot\vec{r}_j} a_q^{+}$

Thus,

$$\sum_{i,j} J_{ij}\, a_i^{+} a_j^{+} = \sum_{i,j} \sum_q J(q)\, e^{i\vec{q}(\vec{r}_i-\vec{r}_j)} \sum_{q'} \frac{e^{-i\vec{q}'\cdot\vec{r}_i}}{\sqrt{N}} a_{q'}^{+} \sum_{q''} \frac{e^{i\vec{q}''\cdot\vec{r}_j}}{\sqrt{N}} a_{q''}$$

$$= \frac{1}{N} \sum_{q,q',q''} J(q) \sum_i e^{i(\vec{q}-\vec{q}')\cdot\vec{r}_i} \sum_j e^{j(q''-q)\cdot\vec{r}_j}\, a^{+}_{q'}\, a_{q''}$$

$$= \sum_{q,q',q''} J(q)\, \delta_{qq'}\, \delta_{qq''}\, a^{+}_{q'}\, a_{q''}$$

$$= \sum_q J(q)\, a_q^{+} a_q$$

Similarly, we get, $\sum_{i,j} J_{ij}\, a_i^{+} a_i^{+} = \sum_q J(0)\, a_q^{+} a_q$

we get the same results for K_{ij}.

Also, let $E_0 = \sum_{i,j} (J_{ij} + K_{ij}) s^2$.

Now using these results in the Hamiltonian gives:

$$\mathcal{H} = E_0 + 2S \sum_q \Big(J(0) + K(0) - J(q)\Big)\, a_q^{+} a_q$$

$$\boxed{\therefore\ \hbar\omega = 2S\ \Big(J(0) + K(0) - J(q)\Big)}$$

(c)

Nearest Neighbour Approximation:

For 1D: $J(q) = J_0 \left(e^{-iqa} + e^{iqa}\right) = 2J_0 \cos qa$

similarly $K(q) = 2K_0 \cos qa$

$$\Rightarrow \hbar\omega = 2S\left(2J_0 + 2K_0 - 2J_0 \cos qa\right)$$

$$= \underline{4SK_0 + 4SJ_0(1 - \cos qa)}$$

For 2D square lattice:

$$J(q) = J_0\left(e^{-iq_x a} + e^{iq_x a} + e^{-iq_y a} + e^{iq_y a}\right)$$

$$\Rightarrow J(q) = 2J_0\left(\cos q_x a + \cos q_y a\right)$$

Similarly, $K(q) = 2K_0\left(\cos q_x a + \cos q_y a\right)$

$$\Rightarrow \hbar\omega = 2S\left(4J_0 + 4K_0 - 2J_0\left(\cos q_x a + \cos q_y a\right)\right)$$

$$= \underline{8SK_0 + 4SJ_0\left(2 - \cos q_x a - \cos q_y a\right)}$$

For 3D body-centered cubic material:

$$J(q) = J_0 \sum_{l=\pm 1} \sum_{m=\pm 1} \sum_{n=\pm 1} e^{i(lq_x + mq_y + nq_y)\frac{a}{2}}$$

$$= 8J_0 \cos\left(\frac{q_x a}{2}\right)\cos\left(\frac{q_y a}{2}\right)\cos\left(\frac{q_z a}{2}\right)$$

Similarly, $K(q) = 8K_0 \cos\left(\frac{q_x a}{2}\right)\cos\left(\frac{q_y a}{2}\right)\cos\left(\frac{q_z a}{2}\right)$

$$\therefore \hbar\omega = \underline{16SK_0 + 16SJ_0\left[1 - \cos\left(\frac{q_x a}{2}\right)\cos\left(\frac{q_y a}{2}\right)\cos\left(\frac{q_z a}{2}\right)\right]}$$

(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.

Knowing that : for small x, $\cos x = 1 - \frac{x^2}{2}$

Thus for small wave-vectors :

For 1D : $\hbar\omega = 2S(J_0 q^2 a^2 + 2K_0)$

For 2D : $\hbar\omega = 2S(J_0 q^2 a^2 + 4K_0)$, $q^2 = q_x^2 + q_y^2$

For 3D : $\hbar\omega = 2S(J_0 q^2 a^2 + 8K_0)$, $q^2 = q_x^2 + q_y^2 + q_z^2$

Any power of q_i greater than 2 is neglected

Ising Model ($J_0 = 0$):

$\hbar\omega = 4dSK_0$

$\hookrightarrow$ no. of dimensions

Now,

no. of spin waves , $N \propto e^{-\hbar\omega/k_B T}$

Energy , $E \propto \hbar\omega\, e^{-\hbar\omega/k_B T}$

Heat capacity per spin , $\frac{C}{N} = c \propto \frac{(\hbar\omega)^2}{k_B T^2} e^{-\hbar\omega/k_B T}$

If we take $J = \hbar\omega$ for high temp. in 6.1, we get the same result.

Heisenberg's Model ($K_0 = 0$):

$$\hbar\omega = 2 S J_0 q^2 a^2$$

$$\hbar\omega \equiv D q^2$$

↳ called spin-stiffness

no. of spin wave is given by $\Rightarrow N \propto \int \frac{d^d q}{e^{\hbar\omega/K_B T} - 1}$ → no. of dimensions

$$\Rightarrow N \propto \int \frac{d^d q}{e^{Dq^2/K_B T} - 1} = \int \frac{d^d q}{Dq^2/K_B T}$$

(For low q)

$N \longrightarrow \infty$ for $d = 1, 2$

Thus showing that there is no long range order in 1d & 2d