P503 Homework 3 Solutions

October 30, 2023

AF Magnons in 2D

(a) Show that while the ferromagnetic state is an exact eigenstate of the Heisenberg Hamiltonian, this is not true for the antiferromagnetic state.

Let us assume that we have a lattice with a local moment of spin S at each site. The magnetic properties of this lattice are given by the Heisenberg model as follows:

$$H = H_{\text{exchange}} + H_{\text{on-site}} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z, \tag{1}$$

where J is the exchange interaction, h is the on-site magnetization in the z direction, $\sum_{\langle i,j \rangle}$ denotes the summation over nearest neighbors on the lattice. The exchange Hamiltonian can be rewritten as:

$$\begin{aligned} H_{\text{exchange}} &= -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\ &= \hat{S}_i^z \hat{S}_j^z + \frac{1}{2} \left[\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+ \right]. \end{aligned} \tag{2}$$

Here, $\hat{S}_i^{\pm} = \hat{S}_i^x \pm \hat{S}_i^y$ are spin raising ($\hat{S}^+$) and lowering operators ($\hat{S}^-$) at site i. They act on an eigenstate $|S, m\rangle$ as

$$\hat{S}^{\pm} |S, m\rangle = \sqrt{(S \mp m)(S \pm m + 1)} |S, m \pm 1\rangle \tag{3}$$

for any $m = -S, -S+1, ..., S-1, S$. Note that any spin configuration will be an eigenstate of the onsite Hamiltonian (since $S_i^z |S, m\rangle_i = m |S, m\rangle_i$). Hence, we consider only H_{exchange} in the following analysis.

Ferromagnetic order

In a classical ferromagnet, all spins align parallel to one another to minimize energy. Further, if $h > 0$ in $H_{\text{on-site}}$, then the all spins in the $|GS\rangle$ will be aligned in the $z-$direction. We can then guess the ground state to be $|GS\rangle = |+S, +S, +S, ... + S\rangle$. When acting on a pair of spins $|+S, +S\rangle$, the first term in Eq. (2) gives S^2 as the eigenvalue and the second one vanishes, because no spin can be further raised. Hence, we obtain,

$$H_{\text{exchange}} |GS\rangle = -\frac{Nz}{2} J S^2 |GS\rangle, \tag{4}$$

where N is the number of sites and z is the coordination number.

Antiferromagnetic order

In a classical antiferromagnet, $J \to -J$, so the spins now favor an antiparallel alignment. One guess for the ground state would be $|GS\rangle_{AFM} = |+S, -S, +S, -S, ...\rangle$. We can think of the lattice comprising two sublattices, A and B, with spins polarized "upwards" in sublattice A and "downwards" in sublattice B. Applying the operators $\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+$, from H_{exchange}, we notice that a term such as $|..., +S, -S, ...\rangle$ will take the form $|...S-1, -S+1, ...\rangle$. Particularly for spin-$\frac{1}{2}$ systems, this means that any pair of spins can be flipped such that the one that was spin-up originally is now spin-down and vice versa. Therefore, $|GS\rangle_{AFM} = |+S, -S, +S, -S, ...\rangle$ is not an eigenstate. Due to this, we

conclude that the classical AF state is at best an approximate ground state of the quantum Heisenberg Hamiltonian with $J < 0$. [N.B.: In one spatial dimension the exact ground state can be found using the so called Bethe-ansatz technique, but this is quite involved. In $d > 1$ the exact ground state is not known.]

(b) Following the discussion on p. 61-62 of Kittel handout work out the zero-point sublattice magnetization for an antiferromagnet on a 2D square lattice. Assume zero applied field and ignore magnon interaction terms. Hint: To get the final numerical answer you must evaluate the k-space integral numerically using Maple, Mathematica, Wolfram Alpha, MatLab or a similar package. Alternately, you can use the long-wavelength approximation for ω_k and evaluate the integral analytically using the Debye-type approach (but this leads to a less accurate result).

Following the steps on p. 61-62 of Kittel, the zero-point sublattice magnetization for an antiferromagnet is given by

$$\Delta\mathcal{S}_z = \frac{1}{2}\sum_k \left[(1-\gamma_k^2)^{-1/2} - 1\right]. \tag{5}$$

For a two-dimensional square lattice,

$$\gamma_k = \frac{1}{4}\left(\mathrm{e}^{ik_x a} + \mathrm{e}^{-ik_x a} + \mathrm{e}^{ik_y a} + \mathrm{e}^{-ik_y a}\right) = \frac{1}{2}\left(\cos(k_x a) + \cos(k_y a)\right).$$

Setting $a = 1$, for an N spin system, we get

$$\Delta\mathcal{S}_z = -\frac{1}{2}N + \frac{N}{2(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dk_x dk_y (1-\gamma_k^2)^{-1/2}. \tag{6}$$

Solving this using Mathematica, we get the zero-point sublattice magnetization as $\Delta\mathcal{S}_z = 0.1966N$.

(c) Now discuss the temperature dependence of sublattice magnetization in the same setup. What does your result imply for the stability of AF order in low-dimensional solids?

For a 2D square lattice, we derive the temperature dependence of the sublattice magnetization using

$$\langle\mathcal{S}_z(0)\rangle - \langle\mathcal{S}_z(T)\rangle = \sum_{\mathbf{k}}\langle n_{\mathbf{k}}\rangle(1-\gamma_k^2)^{-1/2} \tag{7}$$

$$= \frac{\Omega}{(2\pi)^2}\int_0^{k_{\max}} 2\pi k dk \langle n_k\rangle (1-\gamma_k^2)^{-1/2} \tag{8}$$

where

$$\langle n_{\mathbf{k}}\rangle = \frac{1}{\exp\left(\frac{\omega_k}{k_B T}\right) - 1}.$$

Following Kittel, this can be simplified using $\omega_k \approx \mathrm{k}_B\Theta_N k/k_{\max}$ which modifies $\langle n_{\mathbf{k}}\rangle$ as

$$\langle n_{\mathbf{k}}\rangle = \frac{1}{\exp\left(\frac{\Theta_N}{T}\cdot\frac{k}{k_{\max}}\right) - 1}.$$

If n is the number of atoms on one sublattice per unit volume, then $k_{\max}$ obeys the following relation

$$n = \frac{1}{(2\pi)^2}\pi k_{\max}^2.$$

Assuming $ka \ll 1$, we may also simplify $(1-\gamma_k^2)^{-1/2}$ as follows

$$\begin{aligned}(1-\gamma_k^2)^{-1/2} &= \left(1-\frac{1}{4}(\cos(k_x)+\cos(k_y))^2\right)^{-1/2} \\ &\approx \left(1-\frac{1}{4}(2-k^2/2)^2\right)^{-1/2} \\ &\approx \frac{\sqrt{2}}{k}. \end{aligned} \tag{9}$$

Using these approximations, we obtain,

$$\langle \mathcal{S}_z(0)\rangle - \langle \mathcal{S}_z(T)\rangle \propto \int_0^{k_{\max}} dk k \frac{1}{\exp\left(\frac{\Theta_N}{T}\cdot\frac{k}{k_{\max}}\right)-1}\frac{1}{k}. \tag{10}$$

This integral is of the type $\int_0^{x_{\max}} \frac{1}{e^x-1}$ which is divergent when x approaches the lower bound. This implies that antiferromagnetic order in 2D becomes unstable at any non-zero temperature. A similar analysis shows that 1D antiferromagnetic order becomes unstable even at $T = 0$ and thus, stricly speaking, there are no 1D antiferromagnets.