Homework 8
Due Friday, December 4 in class

1. Consider a Heisenberg antiferromagnet on a 4-site linear chain. The Hamiltonian is:

$$H = J\left(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_4 \cdot \mathbf{S}_1\right),$$

where $J > 0$ and $\mathbf{S}_i$ are spins of magnitude S.

   (a) Assuming the spins are classical vectors, sketch the arrangement of spins that minimizes the energy. Find the classical ground state energy $E_0^{c\ell}$.

   (b) Now assume the spins are quantum and show that the exact quantum mechanical ground state energy is given by:

$$E_0^{qm} = -4JS^2\left(1 + \frac{1}{2S}\right).$$

   Hint: start by showing that the Hamiltonian can be written as:

$$H = \frac{J}{2}\left[(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2 - (\mathbf{S}_1 + \mathbf{S}_3)^2 - (\mathbf{S}_2 + \mathbf{S}_4)^2\right].$$

   Now think how the spins in each of the three terms above should add up to minimize the energy.

   (c) Compare $E_0^{c\ell}$ and E_0^{qm} and comment on the result.

   (d) Now repeat the same calculation for a ferromagnetic chain with $J < 0$. Compare $E_0^{c\ell}$ and E_0^{qm} in this case. Comment on the difference from the antiferromagnetic chain case.

2. *Classical theory of spin waves.*
Consider Heisenberg model on a 3-dimensional cubic lattice:

$$H = -\frac{J}{2}\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where $J > 0$, i and j are nearest-neighbor sites and $\mathbf{S}_i$ are classical vectors of length S, not quantum spin operators. Recall that the equation of motion for a spin can generally be written as:

$$\frac{d\mathbf{S}_i}{dt} = \mathbf{S}_i \times \mathbf{B}_i,$$

Problem 1

$$\mathcal{H} = J\left(\vec{S}_1\cdot\vec{S}_2 + \vec{S}_2\cdot\vec{S}_3 + \vec{S}_3\cdot\vec{S}_4 + \vec{S}_4\cdot\vec{S}_1\right)$$

(a) $\uparrow \quad \downarrow \quad \uparrow \quad \downarrow$

$$E_0^{cl} = -4JS^2.$$

(b) Simple algebra shows that $\mathcal{H}$ can be rewritten as:

$$\mathcal{H} = \frac{J}{2}\left[\left(\vec{S}_1+\vec{S}_2+\vec{S}_3+\vec{S}_4\right)^2 - \left(\vec{S}_1+\vec{S}_3\right)^2 - \left(\vec{S}_2+\vec{S}_4\right)^2\right]$$

Looking at the classical sketch, it is clear that the spins in the first term should add up to total spin 0, while spins in the second and third terms to spin $2S$. Thus we obtain:

$$E_0^{qm} = \frac{J}{2}\left[0 - 2S(2S+1) - 2S(2S+1)\right] =$$

$$= -\frac{J}{2}\left[8S^2+4S\right] = -4JS^2\left(1+\frac{1}{2S}\right)$$

(c) $E_0^{qm} < E_0^{cl}$ – This shows that the classical ground state, which can be written in Dirac notation as: $|\uparrow\downarrow\uparrow\downarrow\rangle$ is not the true ground state, since it is not even an eigenstate of $\mathcal{H}$.

The true quantum mechanical ground state of an antiferromagnet has quantum fluctuations, not reflected in $|\uparrow\downarrow\uparrow\downarrow\rangle$.

However, as the classical limit $S \to \infty$ is taken, $E_0^{qm} \to E_0^{cl}$.

(d) In the ferromagnetic case $J<0$ we have:

$$\uparrow \quad \uparrow \quad \uparrow \quad \uparrow$$

$$E_0^{cl} = -4|J|S^2$$

$$E_0^{qm} = -\frac{|J|}{2}\left[4S(4S+1) - 2S(2S+1) - 2S(2S+1)\right] =$$

$$= -\frac{|J|}{2}\left(16S^2 - 8S^2\right) = -4|J|S^2$$

Thus $E_0^{qm} = E_0^{cl} \Rightarrow |\uparrow\uparrow\uparrow\uparrow\rangle$ is the true ground state.

The difference from the antiferromagnet case is due to the fact that $|\uparrow\uparrow\uparrow\uparrow\rangle$ is an eigenstate of $\mathcal{H}$, while $|\uparrow\downarrow\uparrow\downarrow\rangle$ is not.

Problem 2

$$\mathcal{H} = -\frac{J}{2} \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$\frac{d\vec{S}_i}{dt} = \vec{S}_i \times \vec{B}_i$$

$$\vec{B}_i = -\frac{\partial \mathcal{H}}{\partial \vec{S}_i} = J \sum_{j\,nn\,i} \vec{S}_j$$

Substituting this into the equation of motion, we obtain:

$$\frac{d\vec{S}_i}{dt} = J \sum_{j\,nn\,i} \vec{S}_i \times \vec{S}_j$$

$j\,nn\,i$ ← this means that j and i are nearest neighbors.

let $\vec{S}_i = S\hat{z} + \delta\vec{S}_i$

$\delta\vec{S}_i$ is a small correction.

$$\vec{S}_i^{\,2} = \left(S\hat{z} + \delta\vec{S}_i\right)^2 \simeq S^2 + 2S\hat{z}\cdot\delta\vec{S}_i + \delta\vec{S}_i^{\,2} \simeq$$

$$\simeq S^2 + 2S\hat{z}\cdot\delta\vec{S}_i$$

Thus if $\delta\vec{S}_i \cdot \hat{z} = 0$, $\vec{S}_i^{\,2} = S^2$ to first order in $\delta\vec{S}_i$.

Then we obtain:

$$\frac{d\,\delta\vec{S}_i}{dt} = J \sum_{j\,nn\,i} \left(S\hat{z} + \delta\vec{S}_i \right) \times \left(S\hat{z} + \delta\vec{S}_j \right) \approx$$

$$\approx JS \sum_{j\,nn\,i} \hat{z} \times \left(-\delta\vec{S}_i + \delta\vec{S}_j \right)$$

Writing this in components, we obtain:

$$\frac{d\,\delta S_i^x}{dt} = JS \sum_{j\,nn\,i} \left(\delta S_i^y - \delta S_j^y \right)$$

$$\frac{d\,\delta S_i^y}{dt} = JS \sum_{j\,nn\,i} \left(-\delta S_i^x + \delta S_j^x \right)$$

Take $\delta S_i^{x,y} = \delta_k^{x,y} e^{i\vec{k}\cdot\vec{r}_i - i\omega t}$

let $\vec{r}_j = \vec{r}_i + \vec{\lambda}$, where $\vec{\lambda}$ is a nearest-neighbor vector.

$$-i\omega\,\delta S_k^x = JSz\,\delta S_k^y \left(1 - \gamma_k \right)$$

$$-i\omega\,\delta S_k^y = -JSz\,\delta S_k^x \left(1 - \gamma_k \right)$$

Here $\gamma_k = \frac{1}{z} \sum_{\vec{\lambda}} e^{i\vec{k}\cdot\vec{\lambda}}$

To find the eigenmodes need to solve:

$$\det \begin{pmatrix} -i\omega & JSz(\gamma_k - 1) \\ JSz(\gamma_k - 1) & i\omega \end{pmatrix} = 0$$

We obtain:

$$\omega^2 - J^2 S^2 z^2 (1-\gamma_k)^2 = 0$$

Thus:

$$\omega_k = JSz(1-\gamma_k).$$