ICFP M1 - Quantum Matter - TD n°6 - Solutions
Spinwaves in the antiferromagnetic Heisenberg model

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Consider the antiferromagnetic Heisenberg model for a cubic lattice of spin s, considering only nearest-neighbor exchange. De note N the number of sites in the lattice, d the dimension and put the lattice size $a = 1$.

1. Write down the Hamiltonian.

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \qquad J > 0 \tag{1}$$

2. What is the ground state (albeit not exact) of this model?

The cubic lattice is a bipartite lattice. The ground state has spin $S^z = -s$ on one "sublattice", and spin $S^z = s$ on the other, with the z direction in spin space chosen arbitrarily.

3. What is the ground state energy of this model?

We just need to plug in the above answer into the Hamiltonian: $E_0 = -Js^2 \times d \times N$.

Using Holstein-Primakoff bosons we want to calculate the spin wave spectrum above this ground state.

4. Rewrite the spin vectors using Holstein-Primakoff bosons. Recall that we have two sublattices.

$$i \in \mathrm{A}: \begin{cases} S_i^z = -s + a_i^\dagger a_i \\ S_i^+ \approx \sqrt{2s} a_i^\dagger \\ S_i^- \approx \sqrt{2s} a_i \end{cases}, \qquad i \in \mathrm{B}: \begin{cases} S_i^z = s - a_i^\dagger a_i \\ S_i^+ \approx \sqrt{2s} a_i \\ S_i^- \approx \sqrt{2s} a_i^\dagger \end{cases}. \tag{2}$$

where $S^+ = S^x + iS^y$ and $S^- = S^x - iS^y$.

5. Go to momentum space (we still have two sublattices) and rewrite the Hamiltonian neglecting 4-order terms.

$$a_{\mathrm{A},i} = \sqrt{\frac{2}{N}} \sum_{\mathbf{k}} a_{\mathrm{A}\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i}, \qquad a_{\mathrm{B},j} = \sqrt{\frac{2}{N}} \sum_{\mathbf{k}} a_{\mathrm{B}\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_j} \tag{3}$$

so, e.g.

$$\sum_{i\in \mathrm{A}, <i,j>} a_{\mathrm{A}i}^\dagger a_{\mathrm{B}j}^\dagger = \frac{2}{N} \sum_{\mathbf{k},\mathbf{k}'} a_{\mathrm{A}\mathbf{k}}^\dagger a_{\mathrm{B}\mathbf{k}'}^\dagger \sum_{i \in \mathrm{A}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} \sum_{\mathbf{u}_l = \pm \hat{\mathbf{x}}^\mu} e^{-i\mathbf{k}'\cdot(\mathbf{R}_i + \mathbf{u}_l)} \tag{4}$$

$$= \sum_{\mathbf{k}} \left(\sum_{\mu = x,y,z} 2\cos k^\mu \right) a_{\mathrm{A}\mathbf{k}}^\dagger a_{\mathrm{B}-\mathbf{k}}^\dagger \tag{5}$$

Then one gets

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s^2 + Js \sum_{\mathbf{k}} \left[2d \left(a_{\mathrm{A}\mathbf{k}}^\dagger a_{\mathrm{A}\mathbf{k}} + a_{\mathrm{B}\mathbf{k}}^\dagger a_{\mathrm{B}\mathbf{k}} \right) + 2\lambda_{\mathbf{k}} \left(a_{\mathrm{A}\mathbf{k}}^\dagger a_{\mathrm{B}-\mathbf{k}}^\dagger + a_{\mathrm{A}\mathbf{k}} a_{\mathrm{B}-\mathbf{k}} \right) \right], \tag{6}$$

with

$$\lambda_{\mathbf{k}} = \sum_{\mu} \cos k^\mu \tag{7}$$

(we took the lattice spacing $\mathfrak{a} = 1$).

Notice that what you obtained does not take the form of a simple harmonic oscillator Hamiltonian, but that it is quadratic and that fields with different **k** and −**k** are decoupled. In order to transform boson bilinears of the form $a^\dagger a^\dagger$ and aa into "normal" terms such as $a^\dagger a$ (or $aa^\dagger$), it is necessary to perform a Bogoliubov transformation, i.e. to define

$$\begin{cases} a_{\mathrm{A}\mathbf{k}} = (\cosh \eta_{\mathbf{k}}) b_{1\mathbf{k}} + (\sinh \eta_{\mathbf{k}}) b^\dagger_{2-\mathbf{k}} \\ a^\dagger_{\mathrm{B}-\mathbf{k}} = (\cosh \eta_{\mathbf{k}}) b^\dagger_{2-\mathbf{k}} + (\sinh \eta_{\mathbf{k}}) b_{1\mathbf{k}} \end{cases} \tag{8}$$

We will choose $\eta_{\mathbf{k}}$ to simplify H

6. check that b and $b^\dagger$ satisfy canonical bosonic commutation relations, $[b_{l\mathbf{k}}, b^\dagger_{l\mathbf{k}}] = 1$ $(l = 1, 2)$ etc.

Just use the definition and use that a fulfil these relations as well as $\cosh^2 - \sinh^2 = 1$.

7. Plug these expression into the Hamiltonian and find $\eta_{\mathbf{k}}$ such that all the "anormal" terms vanish. You can ignore constants.

We find

$$\mathcal{H} = \text{const} + Js \sum_k [2d \cosh(2\eta_k) + 2\lambda_k \sinh(2\eta_k)](b^\dagger_{1k} b_{1k} + b^\dagger_{2k} b_{2k}) + \mathcal{H}_{\text{out}} \tag{9}$$

where

$$\mathcal{H}_{\text{out}} = Js \sum_k [2d \sinh(2\eta_k) + 2\lambda_k \cosh(2\eta_k)](b^\dagger_{1k} b_{2-k} + b^\dagger_{2-k} b_{1k}) \tag{10}$$

should vanish. We then put:

$$\sinh 2\eta_{\mathbf{k}} = \frac{-\lambda_{\mathbf{k}}}{\sqrt{d^2 - \lambda^2_{\mathbf{k}}}}, \qquad \cosh 2\eta_{\mathbf{k}} = \frac{d}{\sqrt{d^2 - \lambda^2_{\mathbf{k}}}} \tag{11}$$

8. Now find the dispersion relation at small k and plot it.

$$\begin{aligned} \mathcal{H} &= \text{const} + 2Js \sum_{\mathbf{k}} \sqrt{d^2 - \lambda^2_{\mathbf{k}}} (b^\dagger_{1\mathbf{k}} b_{1\mathbf{k}} + b^\dagger_{2\mathbf{k}} b_{2\mathbf{k}}) & (12) \\ &= \text{const} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (b^\dagger_{1\mathbf{k}} b_{1\mathbf{k}} + b^\dagger_{2\mathbf{k}} b_{2\mathbf{k}}), & (13) \end{aligned}$$

with

$$\epsilon_{\mathbf{k}} = 2Js \sqrt{d^2 - \left(\sum_\mu \cos k^\mu\right)^2} \approx 2Js \sqrt{d^2 - \left(d - \frac{k^2}{2}\right)^2} = 2\sqrt{d} Js |\mathbf{k}| \tag{14}$$

9. What are the main differences with the ferromagnetic spectrum?

The dispersion is not quadratic but in $|k|$.

10. Compute $\langle S^z_{i\in\mathrm{B}} \rangle - s$. This is the correction to the staggered magnetization (due to quantum fluctuations at $T = 0$).

$$\langle S^z_{i\in\mathrm{B}} \rangle = s - \langle n_i \rangle = s - \langle a^\dagger_{i\in\mathrm{B}} a_{i\in\mathrm{B}} \rangle = s - \frac{2}{N} \sum_{\mathbf{k}} \langle a^\dagger_{\mathrm{B}\mathbf{k}} a_{\mathrm{B}\mathbf{k}} \rangle \tag{15}$$

so

$$\begin{aligned} \langle S^z_{i\in\mathrm{B}} \rangle - s &= -\frac{2}{N} \sum_{\mathbf{k}} \left[\cosh^2 \eta_{\mathbf{k}} \langle b^\dagger_{2\mathbf{k}} b_{2\mathbf{k}} \rangle + \sinh^2 \eta_{\mathbf{k}} \langle b_{1-\mathbf{k}} b^\dagger_{1-\mathbf{k}} \rangle \right] & (16) \\ &= -\frac{2}{N} \sum_{\mathbf{k}} \left[\frac{1}{2} \cosh 2\eta_{\mathbf{k}} \langle b^\dagger_{1-\mathbf{k}} b_{1-\mathbf{k}} + b^\dagger_{2\mathbf{k}} b_{2\mathbf{k}} \rangle + \sinh^2 \eta_{\mathbf{k}} \right] & (17) \\ &= -2 \int_{\mathrm{BZ}} \frac{d^d k}{(2\pi)^d} \left[\frac{d}{\sqrt{d^2 - \lambda^2_{\mathbf{k}}}} \frac{2}{e^{\beta \epsilon_{\mathbf{k}}} - 1} + \frac{1}{2} \left(\frac{d}{\sqrt{d^2 - \lambda^2_{\mathbf{k}}}} - 1 \right) \right] & (18) \end{aligned}$$

The first term represents thermally excited magnons, while the second captures zero-point fluctuations. At $T \to 0$, we have:

$$\langle S_i^z \rangle_{\mathrm{B}} - s \approx - \int_{\mathrm{BZ}} \frac{d^d k}{(2\pi)^d} \left(\frac{d}{\sqrt{d^2 - \lambda_{\mathbf{k}}^2}} - 1 \right) = \begin{cases} -0.197 & d = 2 \\ -0.078 & d = 3 \end{cases} \tag{19}$$