TFY4210, Quantum theory of many-particle systems, 2016: Solution to tutorial 6

1. The Holstein-Primakoff representation.

(a) With

$$S^{\pm} \equiv S^x \pm iS^y \tag{1}$$

we get[1]

$$\begin{aligned}
[S^+, S^-] &= [S^x + iS^y, S^x - iS^y] = -2i[S^x, S^y] = -2i \cdot iS^z = 2S^z, &(2)\\
[S^z, S^{\pm}] &= [S^z, S^x] \pm i[S^z, S^y] = iS^y \pm i(-i)S^x = \pm(S^x \pm iS^y) = \pm S^{\pm}. &(3)
\end{aligned}$$

(b) We have

$$[S^+, S^-] = \underbrace{\sqrt{2S-\hat{n}}\,aa^\dagger\sqrt{2S-\hat{n}}}_{\text{(i)}} - \underbrace{a^\dagger\sqrt{2S-\hat{n}}\sqrt{2S-\hat{n}}\,a}_{\text{(ii)}}. \tag{4}$$

To simplify (i) and (ii) we use $[a, a^\dagger] = 1$, $[\hat{n}, a] = -a$, and the fact that $[f(\hat{n}), g(\hat{n})] = 0$. This gives

$$\begin{aligned}
\text{(i)} &= \sqrt{2S-\hat{n}}(1+\hat{n})\sqrt{2S-\hat{n}} = (2S-\hat{n})(1+\hat{n}) = 2S + 2S\hat{n} - \hat{n} - \hat{n}^2, &(5)\\
\text{(ii)} &= a^\dagger(2S-\hat{n})a = 2S\hat{n} - a^\dagger\hat{n}a = 2S\hat{n} - a^\dagger(a\hat{n} - a) = 2S\hat{n} - \hat{n}^2 + \hat{n}. &(6)
\end{aligned}$$

Thus

$$[S^+, S^-] = \text{(i) - (ii)} = 2S - 2\hat{n} = 2S^z. \quad \text{QED.} \tag{7}$$

Furthermore,

$$[S^z, S^+] = (S-\hat{n})\sqrt{2S-\hat{n}}\,a - \sqrt{2S-\hat{n}}\,a(S-\hat{n}) \tag{8}$$

In the second term we rewrite as follows: $a(S-\hat{n}) = Sa - a\hat{n} = Sa - a - \hat{n}a = (S-\hat{n})a - a$. This gives

$$[S^z, S^+] = \sqrt{2S-\hat{n}}\,a = S^+. \quad \text{QED.} \tag{9}$$

Also, since the HP representations of S^+ and S^- are adjoints of each other it follows from the footnote that $[S^z, S^-] = -S^-$ is reproduced as well. Finally,

$$\begin{aligned}
\boldsymbol{S}\cdot\boldsymbol{S} &= S^xS^x + S^yS^y + S^zS^z = \frac{1}{2}(S^+S^- + S^-S^+) + S^zS^z\\
&= \frac{1}{2}\left[\sqrt{2S-\hat{n}}\,aa^\dagger\sqrt{2S-\hat{n}} + a^\dagger\sqrt{2S-\hat{n}}\sqrt{2S-\hat{n}}\,a\right] + (S-\hat{n})(S-\hat{n})\\
&= \frac{1}{2}\left[(2S-\hat{n})(1+\hat{n}) + a^\dagger(2S-\hat{n})a\right] + (S-\hat{n})(S-\hat{n})\\
&= \frac{1}{2}\left[2S + 2S\hat{n} - \hat{n} - \hat{n}^2 + 2S\hat{n} - \hat{n}^2 + \hat{n}\right] + S^2 - 2S\hat{n} + \hat{n}^2\\
&= S + S^2 = S(S+1). \quad \text{QED.} &(10)
\end{aligned}$$

[1] Note that

$$[S^z, S^-] = S^zS^- - S^-S^z = (S^+S^z - S^zS^+)^\dagger = -[S^z, S^+]^\dagger,$$

where we used that S^+ and S^- are adjoint operators of each other, S^z is hermitian, and $(AB)^\dagger = B^\dagger A^\dagger$.

2. Ferromagnetic Heisenberg model with a spin anisotropy.

The Hamiltonian H can be written

$$H = H_{\text{Heis}} + H_D \tag{11}$$

where H_{Heis} is the Hamiltonian of the Heisenberg model that we have discussed in the lectures and

$$H_D = -D\sum_i (S_i^z)^2. \tag{12}$$

(a) Since $J < 0$, H_{Heis} is a ferromagnetic Heisenberg model. It wants a ground state in which the spins order ferromagnetically along some arbitrary direction. On the other hand, with $D > 0$, H_D wants a ground state in which the absolute value of the z-component of each spin is maximized, i.e. it wants each spin to be in an eigenstate with eigenvalue $S_i^z = +S$ or $S_i^z = -S$ (the sign of the eigenvalue may vary between lattice sites). While most ground states of H_{Heis} are not ground states of H_D and vice versa, it is possible to find some ground states that are, and which therefore are ground states of H too: those states which have ferromagnetic order in the $+z$ direction or in the $-z$ direction. QED.

(b) The Heisenberg Hamiltonian can be written as

$$H_{\text{Heis}} = J\sum_{i,\boldsymbol{\delta}}\left[\frac{1}{2}(S_i^+S_{i+\boldsymbol{\delta}}^- + S_i^-S_{i+\boldsymbol{\delta}}^+) + S_i^zS_{i+\boldsymbol{\delta}}^z\right]. \tag{13}$$

Let us assume ordering along the $+z$ direction. Using the Holstein-Primakoff expansion, expanding the square roots, and only keeping terms in H_{Heis} of order S^2 and S, gives

$$\begin{aligned} H_{\text{Heis}} &= J\sum_{i,\boldsymbol{\delta}}\left[\frac{1}{2}(\sqrt{2S})^2(a_ia_{i+\boldsymbol{\delta}}^\dagger + a_i^\dagger a_{i+\boldsymbol{\delta}} + \underbrace{(S-n_i)(S-n_{i+\boldsymbol{\delta}})}_{\text{neglect } n_in_{i+\boldsymbol{\delta}} = O(S^0)}\right] \\ &= J\sum_{i,\boldsymbol{\delta}}[S(a_{i+\boldsymbol{\delta}}^\dagger a_i + a_i^\dagger a_{i+\boldsymbol{\delta}}) + S^2 - S(n_i + n_{i+\boldsymbol{\delta}})]. \end{aligned} \tag{14}$$

Note that

$$\sum_{i,\boldsymbol{\delta}} 1 = \sum_i \cdot \sum_{\boldsymbol{\delta}} 1 = N\cdot(z/2) \tag{15}$$

where z is the coordination number of the lattice (i.e. the number of nearest neighbours; $z = 2d$ for a d-dimensional hypercubic lattice). Also, since $J < 0$ we write $J = -|J|$. Thus

$$H_{\text{Heis}} = -|J|NS^2z/2 - |J|S\sum_{i,\boldsymbol{\delta}}[a_{i+\boldsymbol{\delta}}^\dagger a_i + a_i^\dagger a_{i+\boldsymbol{\delta}} - a_i^\dagger a_i - a_{i+\boldsymbol{\delta}}a_{i+\boldsymbol{\delta}}]. \tag{16}$$

This can be simplified a little further by noting that

$$\sum_i a_{i+\boldsymbol{\delta}}^\dagger a_{i+\boldsymbol{\delta}} \overset{i'\equiv i+\boldsymbol{\delta}}{=} \sum_{i'} a_{i'}^\dagger a_{i'} = \sum_i a_i^\dagger a_i \tag{17}$$

and so

$$H_{\text{Heis}} = -|J|NS^2z/2 - |J|S\sum_{i,\boldsymbol{\delta}}[a^\dagger_{i+\boldsymbol{\delta}}a_i + a^\dagger_i a_{i+\boldsymbol{\delta}} - 2a^\dagger_i a_i]. \tag{18}$$

Now we do a Fourier transformation:

$$a_i = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i}a_{\boldsymbol{k}} \tag{19}$$

where the $\boldsymbol{k}$-sum goes over the 1st Brillouin zone. This gives (using $\boldsymbol{r}_{i+\boldsymbol{\delta}} = \boldsymbol{r}_i + \boldsymbol{\delta}$ in the 2nd line)

$$\begin{aligned}
\sum_i (a^\dagger_{i+\boldsymbol{\delta}}a_i + a^\dagger_i a_{i+\boldsymbol{\delta}}) &= \sum_i (a^\dagger_{i+\boldsymbol{\delta}}a_i + \text{h.c.}) \\
&= \sum_i \frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_i+\boldsymbol{\delta})}e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_i}a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}'} + \text{h.c.}) \\
&= \sum_{\boldsymbol{k},\boldsymbol{k}'} a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}'}e^{-i\boldsymbol{k}\cdot\boldsymbol{\delta}}\underbrace{\frac{1}{N}\sum_i e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_i}}_{\delta_{\boldsymbol{k},\boldsymbol{k}'}} + \text{h.c.} \\
&= \sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}e^{-i\boldsymbol{k}\cdot\boldsymbol{\delta}} + \text{h.c.} = \sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}(e^{-i\boldsymbol{k}\cdot\boldsymbol{\delta}} + e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}}) \\
&= \sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}} \cdot 2\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}).
\end{aligned} \tag{20}$$

Similarly,

$$\begin{aligned}
\sum_i a^\dagger_i a_i &= \sum_i \frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_i}a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}'} \\
&= \sum_{\boldsymbol{k},\boldsymbol{k}'} a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}'}\underbrace{\frac{1}{N}\sum_i e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_i)}}_{\delta_{\boldsymbol{k},\boldsymbol{k}'}} \\
&= \sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}.
\end{aligned} \tag{21}$$

This gives

$$H_{\text{Heis}} = -|J|NS^2z/2 + \sum_{\boldsymbol{k}}\left[2|J|S\sum_{\boldsymbol{\delta}}(1-\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}))\right]a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}. \tag{22}$$

Next we consider H_D. We have

$$(S^z_i)^2 = (S-n_i)^2 = S^2 - 2Sa^\dagger_i a_i + O(S^0), \tag{23}$$

and thus

$$H_D = -D\sum_i (S_i^z)^2 = -DNS^2 + 2DS\sum_i a_i^\dagger a_i = -DNS^2 + 2DS\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}. \tag{24}$$

So the total Hamiltonian becomes

$$H = -NS^2(|J|z/2 + D) + \sum_{\boldsymbol{k}} 2S\left\{|J|\sum_{\boldsymbol{\delta}}(1-\cos(\boldsymbol{k}\cdot\boldsymbol{\delta})) + D\right\} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} \tag{25}$$

Since the quantity in curly brackets is > 0, magnons (created by the operators $a_{\boldsymbol{k}}^\dagger$) cost a finite positive energy. Thus the ground state (eigenstate with lowest energy) has no magnons. Therefore only the first term contributes to the ground state energy E_0. Thus

$$E_0 = -NS^2(|J|z/2 + D), \tag{26}$$

$$\omega_{\boldsymbol{k}} = 2S\left\{D + |J|\sum_{\boldsymbol{\delta}}(1-\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}))\right\}. \tag{27}$$

(c) The lowest excited state will have one magnon, whose wavevector $\boldsymbol{k}$ minimizes $\omega_{\boldsymbol{k}}$. It is easy to see that the minimum of $\omega_{\boldsymbol{k}}$ occurs for $\boldsymbol{k} = 0$, with $\omega_{\boldsymbol{k}=0} = 2SD$. Thus $E_1 = E_0 + 2SD$, giving

$$\Delta = E_1 - E_0 = 2SD. \tag{28}$$

(d) If $D < 0$, H_D wants a ground state with $S_i^z = 0$. This can be reconciled with the ferromagnetic ordering that H_{Heis} wants by ordering the spins in the xy plane. Thus we can predict that the spins will order ferromagnetically along some direction lying in the xy plane.

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Some final remarks about Problem 2: Since we have used spin-wave theory to analyze the problem, neglecting terms of order S^0 or higher in the $1/S$ expansion, we expect as usual for this approach that the analysis is most accurate for large values of S. For the particular value $S = 1/2$ (i.e. the smallest possible nonzero value of S, and thus also the value of S for which one would naively expect a spin-wave analysis to be least reliable) one can see that the analysis given here is not valid, since in that case the anisotropy term H_D is just a constant[2] and thus the magnon dispersion $\omega_{\boldsymbol{k}}$ should be the same as for $D = 0$. But for general values of S, H_D is not a constant.

[2] For $S = 1/2$, the only possible eigenvalues of S_i^z are $\pm 1/2$, and thus $(S_i^z)^2|\Phi\rangle = (1/4)|\Phi\rangle$ for any state $|\Phi\rangle$.

3. Physical picture of ferromagnetic spin waves.

$$\vec{S}_i^{\perp} \cdot \vec{S}_j^{\perp} = S_i^x S_j^x + S_i^y S_j^y$$

$$= \frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right)$$

We assume $i \neq j$ in the following.

Using the HP representation we have

$$\left.\begin{aligned} S_i^+ &= \sqrt{2S - n_i}\, a_i \approx \sqrt{2S}\, a_i \\ S_i^- &\approx \sqrt{2S}\, a_i^+ \end{aligned}\right\} \text{ to lowest order in the spin-wave expansion}$$

and similarly for S_j^+, S_j^-.

$$\Rightarrow \vec{S}_i^\perp \cdot \vec{S}_j^\perp = \frac{1}{2}\left(\sqrt{2S}\right)^2 \left[a_i a_j^+ + a_i^+ a_j \right]$$

$$= S\left(a_j^+ a_i + a_i^+ a_j \right) \qquad (i \neq j)$$

$$= \frac{S}{N} \sum_{\vec{k}_1 \vec{k}_2} a^+_{\vec{k}_1} a_{\vec{k}_2}$$

$$\cdot \left[e^{-i\vec{k}_1 \cdot \vec{r}_j} e^{i\vec{k}_2 \cdot \vec{r}_i} + e^{-i\vec{k}_1 \cdot \vec{r}_i} \cdot e^{i\vec{k}_2 \cdot \vec{r}_j} \right]$$

where we used $a_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}'} e^{i\vec{k}' \cdot \vec{r}_i} a_{\vec{k}'}$

$$\Rightarrow \langle \vec{k} | \vec{S}_i^\perp \cdot \vec{S}_j^\perp | \vec{k} \rangle$$

$$= \frac{S}{N} \sum_{\vec{k}_1 \vec{k}_2} \left[e^{-i\vec{k}_1 \cdot \vec{r}_j} e^{i\vec{k}_2 \cdot \vec{r}_i} + e^{-i\vec{k}_1 \cdot \vec{r}_i} e^{i\vec{k}_2 \cdot \vec{r}_j} \right]$$

$$\cdot \langle 0 | \underbrace{a_{\vec{k}} a^+_{\vec{k}_1}}_{a^+_{\vec{k}_1} a_{\vec{k}} + \delta_{\vec{k}_1 k}} \underbrace{a_{\vec{k}_2} a^+_{\vec{k}}}_{a^+_{\vec{k}} a_{\vec{k}_2} + \delta_{\vec{k}\vec{k}_2}} | 0 \rangle$$

Since there are no magnons in the ferromagnetic ground state, we get zero if we try to annihilate a magnon in the ground state, i.e.

$$a_{\vec{k}'} |0\rangle = 0 \quad \text{for any } \vec{k}'$$

$$\Rightarrow \quad \langle 0 | a^{\dagger}_{\vec{k}'} = 0 \quad \text{as well}$$

$$\Rightarrow \quad \langle 0 | a_{\vec{k}} \, a^{\dagger}_{\vec{k}_1} \, a_{\vec{k}_2} \, a^{\dagger}_{\vec{k}} |0\rangle = \delta_{\vec{k}\vec{k}_1} \delta_{\vec{k}\vec{k}_2}$$

$$\Rightarrow \langle \vec{k} | \vec{S}^{\perp}_i \cdot \vec{S}^{\perp}_j | \vec{k} \rangle$$

$$= \frac{S}{N} \left[e^{-i\vec{k}\cdot(\vec{r}_j - \vec{r}_i)} + e^{-i\vec{k}\cdot(\vec{r}_i - \vec{r}_j)} \right]$$

$$= \frac{2S}{N} \cos \vec{k}\cdot(\vec{r}_i - \vec{r}_j)$$

This shows that in the state $|\vec{k}\rangle \equiv a^{\dagger}_{\vec{k}} |0\rangle$, on average each spin has a small transverse component of magnitude $\sqrt{2S/N}$ and the orientations of the transverse components of two spins i and j differ by an angle $\vec{k}\cdot(\vec{r}_i - \vec{r}_j)$.