Spin Wave Theory

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1 Magnons in Heisenberg Model

The Heisenberg interaction is:

$$\mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) + S_i^z S_j^z \tag{1.1}$$

The Hamiltonian is:

$$H = -\sum_{i,j} J_{ij}\left(S_i^+ S_j^- + S_i^z S_j^z\right) - B\sum_i S_i^z \tag{1.2}$$

where $J_{ij} = J_{ji};\quad J_{ii} = 0$, and $B = \frac{1}{\hbar} g_J \mu_B B_0$. Now we move to momentum space by F.T. defined as:

$$\begin{aligned} S^\alpha(k) &= \sum_i e^{-ikR_i} S_i^\alpha \\ S_i^\alpha &= \frac{1}{N}\sum_k e^{ikR_i} S^\alpha(k) \end{aligned} \tag{1.3}$$

we did not use the symmetric Fourier coefficient since we want a clean commutation in momentum space, as derived below:

$$\begin{aligned} [S^+(k_1), S^-(k_2)] &= \sum_{ij} e^{-ik_1R_i - ik_2R_j}[S_i^+, S_j^-] = 2\sum_{ij} e^{-ik_1R_i - ik_2R_j}\delta_{ij} S_i^z \\ &= 2\sum_j e^{-i(k_1+k_2)R_j} S_j^z = 2S^z(k_1+k_2) \end{aligned} \tag{1.4}$$

where we have set $\hbar = 1$. Similarly:

$$\begin{aligned} [S^z(k_1), S^\pm(k_2)] &= \sum_{ij} e^{-ik_1R_i - ik_2R_j}[S_i^z, S_j^\pm] = \pm\sum_{ij} e^{-ik_1R_i - ik_2R_j}\delta_{ij} S_i^\pm \\ &= \pm\sum_j e^{-i(k_1+k_2)R_j} S_j^\pm = \pm S^\pm(k_1+k_2) \end{aligned} \tag{1.5}$$

in short:

$$\boxed{[S^+(k_1), S^-(k_2)] = 2S^z(k_1+k_2), \quad [S^z(k_1), S^\pm(k_2)] = \pm S^\pm(k_1+k_2)} \tag{1.6}$$

and it's readily to see that:

$$\boxed{\left[S^\pm(k)\right]^\dagger = S^\mp(-k)} \tag{1.7}$$

Now we are going to transform the Hamiltonian to momentum space. Generically what we need is $\mathcal{F}\{\sum_{ij} J_{ij} S_i^\alpha S_j^\beta\}$. By translational symmetry we rewrite this term as:

$$\sum_{i,j} J_{ij} S_i^\alpha S_j^\beta = \sum_{i,r} J(r) S_i^\alpha S_{i+r}^\beta \tag{1.8}$$

expand spin operator in momentum space:

$$\begin{aligned} S_i^\alpha &= \frac{1}{N}\sum_k e^{ikR_i} S^\alpha(k) \\ S_{i+r}^\beta &= \frac{1}{N}\sum_k e^{ik(R_i+r)} S^\beta(k) \end{aligned} \tag{1.9}$$

Then we have:

$$\begin{aligned} \sum_{i,r} J(r) S_i^\alpha S_j^\beta &= \frac{1}{N^2}\sum_r J(r) \sum_{k,k'} e^{ik'r}\left(\sum_i e^{i(k+k')R_i}\right) S^\alpha(k) S^\beta(k') \\ &= \frac{1}{N}\sum_r J(r)\sum_k e^{-ikr} S^\alpha(k) S^\beta(-k) \\ &= \frac{1}{N}\sum_k \left(\sum_r J(r) e^{-ikr}\right) S^\alpha(k) S^\beta(-k) \\ &\equiv \frac{1}{N}\sum_k J(k) S^\alpha(k) S^\beta(-k) \end{aligned} \tag{1.10}$$

where we have defined $J(k) = \sum_r J(r)\exp(-ikr)$, which satisfies $J(k) = J(-k)$ if it is symmetric under reflection. Note that another equivalent form is sometimes useful:

$$J(k) = \frac{1}{N}\sum_{i,j} J_{ij} e^{-ik(R_j - R_i)} \tag{1.11}$$

there is an additional factor of $\frac{1}{N}$ due to the repeated counting of identical bonds.

The on-site operator in momentum space is:

$$\sum_i S_i^\alpha = \sum_i \frac{1}{N}\sum_k S^\alpha(k) e^{ikR_i} = S^\alpha(0) \tag{1.12}$$

Therefore the full Hamiltonian in momentum space is:

$$\boxed{H = -\frac{1}{N}\sum_k J(k)\left\{S^+(k)S^-(-k) + S^z(k)S^z(-k)\right\} - BS^z(0)} \tag{1.13}$$

Let the ground state be $|S\rangle$ that corresponds to an overall parallel orientation of all the spins, i.e. a product state with local magnetization S. Hence:

$$S_i^z|S\rangle = S|S\rangle, \quad S^z(k) = \sum_i e^{ikR_i} S_i^z|S\rangle = NS|S\rangle\,\delta_{k,0} \tag{1.14}$$

$$S_i^+|S\rangle = 0, \quad \boxed{S^+(k)|S\rangle = \sum_i e^{ikR_i} S_i^+|S\rangle = 0} \tag{1.15}$$

Now let's calculate the eigen energy. By Eq.(1.6) the first term in Hamiltonian gives:

$$\begin{aligned} -\frac{1}{N}\sum_k J(k) S^+(k) S^-(k)|S\rangle &= -\frac{1}{N}\sum_k J(k)\left[S^-(-k)S^+(k) + 2S^z(0)\right]|S\rangle \\ &= -\frac{1}{N}\left(\sum_k J(k)\right) 2NS|S\rangle \\ &= -\frac{1}{N} NJ(r=0)NS|S\rangle = 0 \end{aligned} \tag{1.16}$$

where at the 3rd row we used $\sum_k e^{-ikr} = N\delta_{r,0}$. While the 2nd term of Hamiltonian gives:

$$\begin{aligned} -\frac{1}{N}\sum_k J(k)S^z(k)S^z(-k)\left|S\right\rangle &= -\frac{1}{N}\sum_k J(k)S^z(-k)NS\delta_{k,0}\left|S\right\rangle \\ &= -SJ(0)S^z(0)\left|S\right\rangle \\ &= -NJ(0)S^2\left|S\right\rangle \end{aligned} \tag{1.17}$$

The zeeman term is trivial. Hence we have the eigen equation:

$$\begin{aligned} &H\left|S\right\rangle = E_0\left|S\right\rangle \\ &E_0 = -NJ(0)S^2 - NSB \end{aligned} \tag{1.18}$$

where E_0 is the ground state energy.

Next we show that

$$\left|k\right\rangle \equiv S^-(k)\left|S\right\rangle \tag{1.19}$$

is also an eigenstate of H. It's convenient to first look at the commutation $[H, S^-(k)]$:

$$\begin{aligned} [H,S^-(k)] =& -\frac{1}{N}\sum_p J(p)\Big\{[S^+(p),S^-(k)]S^-(-p) + S^z(p)[S^z(-p),S^-(k)] + [S^z(p),S^-(k)]S^z(-p)\Big\} \\ & - B[S^z(0),S^-(k)] \\ =& -\frac{1}{N}\sum_p J(p)\Big\{2S^z(k+p)S^-(-p) - S^z(p)S^-(k-p) - S^-(k+p)S^z(-p)\Big\} + BS^-(k) \end{aligned} \tag{1.20}$$

recall that:

$$\begin{aligned} &[S^z(k_1),S^\pm(k_2)] = \pm S^\pm(k_1+k_2) \\ \Rightarrow\ & 2S^z(k+p)S^-(-p) = -2S^-(k) + 2S^-(-p)S^z(k+p) \\ \&\ \ & S^z(p)S^-(k-p) = S^-(k-p)S^z(p) - S^-(k) \end{aligned} \tag{1.21}$$

we replace the 1st and 2nd term in Eq.(1.20) by the above, hence:

$$\begin{aligned} [H,S^-(k)] =& BS^-(k) - \frac{1}{N}\sum_p J(p)\Big\{-2S^-(k) + 2S^-(-p)S^z(k+p) + \\ & + S^-(k) - S^-(k-p)S^z(p) - S^-(k+p)S^z(-p))\Big\} \end{aligned} \tag{1.22}$$

Note that $\sum_p J(p) = NJ(r=0) = 0$, so the 1st and 3rd terms in the summation evaluate to zero. We finally find:

$$\boxed{\big[H,S^-(k)\big] = BS^-(k) - \frac{1}{N}\sum_p J(p)\Big\{2S^-(-p)S^z(k+p) - S^-(k-p)S^z(p) - S^-(k+p)S^z(-p)\Big\}} \tag{1.23}$$

Then it's readily to apply this commutator to $\left|S\right\rangle$ and extract dispersion:

$$[H,S^-(k)]\left|S\right\rangle = \omega(k)\left[S^-(k)\left|S\right\rangle\right] \tag{1.24}$$

$$\boxed{\omega(k) = B + 2S\left[J(0) - J(k)\right]} \tag{1.25}$$

in which we have used $J(k) = J(-k)$. Hence the eigen energy of state $S^-(k)\,|S\rangle$ is:

$$H\Big(S^-(k)\,|S\rangle\Big) = \Big(E_0 + \omega(k)\Big)\,|S\rangle \equiv E(k)\Big(S^-(k)\,|S\rangle\Big) \tag{1.26}$$

where we have defined the totol energy:

$$E(k) = E_0 + B + 2S[J(0) - J(k)] \tag{1.27}$$

Now we normalize the excitation:

$$\begin{aligned}\langle S|(S^-(k))^\dagger S^-(k)|S\rangle &= \langle S|S^+(-k)S^-(k)|S\rangle \\ &= \langle S|2S^z(0) + S^-(k)S^+(-k)|S\rangle \\ &= 2NS\end{aligned} \tag{1.28}$$

Therefore the Normalized single-magnon state is:

$$\boxed{|k\rangle = \frac{1}{\sqrt{2NS}}S^-(k)\,|S\rangle} \tag{1.29}$$

One can check [Wolfgang] which shows that magnons are bosons and carry spin-1 in a spin-1/2 system.

2 Holstein-Primakoff transformation

To arrive at an approximate solution that does not use unwieldy spin operators, we would like to a representation that uses creation and annihilation operators in the second quantization. The transformation read:

$$\begin{aligned}S_i^+ &= \sqrt{2S}\,\phi(n_i)\,a_i \\ S_i^- &= \sqrt{2S}\,a_i^\dagger\,\phi(n_i) \\ S_i^z &= S - n_i\end{aligned} \tag{2.1}$$

where we have defined:

$$\begin{aligned}n_i &= a_i^\dagger a_i \\ \phi(n_i) &= \sqrt{1 - \frac{n_i}{2S}}\end{aligned} \tag{2.2}$$

where $a, a^\dagger$ are bosonic operators. Before going to the implemetation, let us first have a review of its historical derivation. The building blocks of a spin Hamiltonian are:

$$S_j^+ = S_j^x + iS_j^y, \quad S_j^- = S_j^x - iS_j^y, \quad \hat{n}_j = S - S_j^z \tag{2.3}$$

with n_j the eigenvalue of $\hat{n}_j$, which is called the spin deviation of j-th site. For simplicity, let us consider the case in which S_j^z, thus n_l, is a good quantum number, such that the wavefunction can be labelled by local spin deviations:

$$|\psi\rangle = |n_1 \ldots n_l \ldots n_N\rangle \tag{2.4}$$

Now let us apply these operators to the state. The operator S_l^+ will raise S_l^z, thus lower n_l by 1. So we have:

$$S_l^+ |n_1 \dots n_l \dots n_N\rangle = c\,|n_1 \dots n_l - 1 \dots n_N\rangle \tag{2.5}$$

it has to satisfy normalization condition:

$$|c|^2 = \langle n_1 \dots n_l \dots n_N | S_l^- S_l^+ | n_1 \dots n_l \dots n_N \rangle \tag{2.6}$$

in order to work under n_l basis, we rewrite the $S_l^- S_l^+$ as:

$$\begin{aligned} S_l^- S_l^+ &= (S_l^x - iS_l^y)(S_l^x + iS_l^y) = S_l^x S_l^x + S_l^y S_l^y + iS_l^x S_l^y - iS_l^y S_l^x \\ &= \mathbf{S}^2 - S_l^z S_l^z + i[S_l^x, S_l^y] = S(S+1) - (S - n_l)^2 - (S - n_l) \\ &= 2Sn_l - n_l(n_l - 1) \\ &= (2S)\left(1 - \frac{n_l - 1}{2S}\right) n_l \end{aligned} \tag{2.7}$$

so that

$$c = \sqrt{2S}\sqrt{1 - \frac{n_l - 1}{2S}}\sqrt{n_l} \tag{2.8}$$

$$S_l^+ |n_1 \dots n_l \dots n_N\rangle = \sqrt{2S}\sqrt{1 - \frac{n_l - 1}{2S}}\sqrt{n_l}\,|n_1 \dots n_l - 1 \dots n_N\rangle \tag{2.9}$$

introducing the creation and annihilation operator $a^\dagger, a$, the above can be rewritten as:

$$S_l^+ |n_1 \dots n_l \dots n_N\rangle = \sqrt{2S}\sqrt{1 - \frac{\hat{n}_l}{2S}}\,\hat{a}_l\,|n_1 \dots n_l \dots n_N\rangle \equiv \sqrt{2S}\,\phi(\hat{n}_l)\,\hat{a}_l \tag{2.10}$$

where I have used $\hat{\bullet}$ to emphasize an operator. Hence we have the first Holstein-Primakoff transformation:

$$S_l^+ = \sqrt{2S}\,\phi(\hat{n}_l)\,\hat{a}_l \tag{2.11}$$

The mapping of S_l^- can be derived in the same way.

2.1 HP transformation of Heisenberg ferromagnet

In this section we will apply the symmetric Fourier transform to bosonic operators:

$$a_k = \frac{1}{\sqrt{N}}\sum_i e^{-ikR_i} a_i, \quad a_k^\dagger = \frac{1}{\sqrt{N}}\sum_i e^{ikR_i} a_i^\dagger \tag{2.12}$$

they can be interpreted as magnon annihilation or creation operators. Now we rewrite the Heisenberg Hamiltonian by bosons:

$$S_i^+ S_j^- = \left(\sqrt{2S}\phi(n_i) a_i\right)\left(\sqrt{2S} a_j^\dagger \phi(n_j)\right) = 2S\phi(n_i) a_i a_j^\dagger \phi(n_j) \tag{2.13}$$

$$S_i^z S_j^z = (S - n_i)(S - n_j) = S^2 + n_i n_j - S(n_i + n_j) \tag{2.14}$$

Note that:

$$\sum_{ij} J_{ij} S(n_i + n_j) = 2S\sum_{ij} J_{ij} n_j = 2S\sum_i J_{ij}\sum_j n_j = 2SJ(0)\sum_j n_j \tag{2.15}$$

$$S^2 \sum_{ij} J_{ij} = S^2 \sum_i \left(\sum_j J_{ij} \right) = N J(0) S^2 \tag{2.16}$$

so the Hamiltonian in boson representation is:

$$H = E_0 + 2SJ(0) \sum_i n_i - 2S \sum_{ij} J_{ij} \phi(n_i) a_i a_j^\dagger \phi(n_j) - \sum_{ij} J_{ij} n_i n_j \tag{2.17}$$

To work explicitly with H we have to carry out an expansion of the square root in $\phi(n_i)$:

$$\phi(n_i) = \sqrt{1 - \frac{n_i}{2S}} = 1 - \frac{n_i}{4S} - \frac{n_i^2}{32S^2} - O(S^{-3}) \tag{2.18}$$

The transformation is thus only reasonable when there is a physical justification for terminating the infinite series. The simplest approximation is the spin-wave approximation, where we only keep n_i to its lowest (linear) power. This can be justified at low temperatures, at which only a few magnons are excited. To show this, we first approximate:

$$\phi(n_i) \simeq 1 - \frac{n_i}{2S}.$$

and plug into Hamiltonian and keep the linear only.

$$\begin{aligned}
H &= E_0 + 2SJ(0) \sum_i n_i - 2S \sum_{ij} J_{ij} \left(1 - \frac{n_i}{2S}\right) a_i a_j^\dagger \left(1 - \frac{n_i}{2S}\right) - \sum_{ij} J_{ij} n_i n_j \\
&= E_0 + 2SJ(0) \sum_i n_i - \sum_{ij} J_{ij} \left(2S a_i a_j^\dagger - \frac{n_i}{2} a_i a_j^\dagger - \frac{a_i a_j^\dagger}{2} n_j + \frac{1}{8S} n_i a_i a_j^\dagger n_j \right) - \sum_{ij} J_{ij} n_i n_j \\
&\simeq E_0 + 2SJ(0) \sum_{ij} n_i \delta_{ij} - 2S \sum_{ij} J_{ij} a_i a_j^\dagger \\
&= E_0 + 2S \sum_{ij} \left(J(0)\delta_{ij} - J_{ij} \right) a_i^\dagger a_j
\end{aligned} \tag{2.19}$$

where in the last step we have switch the order of a_i and $a_j^\dagger$ and swapped their indices. This will not introduce the $1 = [a_i, a_i^\dagger]$ since it is mutiplied by $J_{ii} = 0$. Then it is readily to diagonalize by a F.T.

$$H = E_0 + \sum_k \omega(k) a_k^\dagger a_k \tag{2.20}$$

with

$$\omega(k) = 2S \left(J(0) - J(k) \right) \tag{2.21}$$