Quantization of spin waves: the Holstein-Primakoff transformation; quantum fluctuations in the Neél state

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We have already performed 'quantization' before, namely in the context of lattice dynamics in crystals. Now we are going to quantize spin waves in antiferromagnets using what become known as the Holstein-Primakoff transformation. This transformation leans heavily on the following observation: harmonic oscillators (bosons) and spins both have a ladder-like spectrum!

$$S^{+}|S, M_s\rangle \propto |S, M_s+1\rangle$$

$$b^{+}|n\rangle \propto |n+1\rangle$$

There is one fundamental difference, though; the oscillator spectrum is not bounded from above, while the spin spectrum is bounded (the largest M_s is S!). Thus the dimensionality of the Hilbert space for harmonic oscillators and spins is totally different. On a formal level, this can be accounted for by the introduction of a projection operator which removes all the harmonic-oscillator states with $n > 2S$ from the boson Hilbert space:

$$P = 1 - \sum_{n=2S+1}^{\infty} |n\rangle\langle n| \ .$$

The correspondence between the bosonic and spin spectra is based on the following relation:

$$\boxed{S_i^z = S - b_i^\dagger b_i} \qquad (\#)$$

$$S_i^z |0\rangle = S|0\rangle \quad \left(\begin{array}{c}\text{absence of} \\ \text{bosons}\end{array}\right)$$

$$S_i^z |1\rangle = (S-1)|1\rangle \quad \left(\begin{array}{c}\text{one boson} \\ \text{present}\end{array}\right)$$

$$\cdots$$

The central question at this point is which operators (expressed in terms of the bosonic ones) form an su(2) spin algebra together with the S_i^z defined by the relation (#) above?

The answer was found by Holstein and Primakoff.
[T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940)]
The desired operators are given by

$$S_i^+ = (2S)^{1/2} \sqrt{1 - \frac{b_i^\dagger b_i}{2S}}\, b_i$$

$$S_i^- = (2S)^{1/2}\, b_i^\dagger \sqrt{1 - \frac{b_i^\dagger b_i}{2S}}$$

It is relatively straightforward to show that the last two operators and S_i^z indeed satisfy the commutation relations of a su(2) algebra (Problem 3 in Blatt 11)!

Now we are going to apply the Holstein-Primakoff transformation to the antiferromagnetic Heisenberg model.

On the A sublattice we take $|S,S\rangle$ states as the vacuum. However, on the B sublattice $\langle S_z \rangle = -S$ and we cannot use the Holstein-Primakoff transformation directly. On the B sublattice, we have to rotate all the spins by $180°$ with respect to the x-axis so that $M_s = -S \rightarrow S$ and, more generally,

$$\boxed{\begin{array}{l} S^z_{i\in B} \rightarrow -S^z_{i\in B} \\ S^{\pm}_{i\in B} \rightarrow S^{\mp}_{i\in B} \end{array}}.$$

Then the Heisenberg Hamiltonian becomes

$$H_{spin} = J\sum_{i,\delta}\left[-S_i^z S_{i+\delta}^z + \frac{1}{2}\left(S_i^+ S_{i+\delta}^+ + S_i^- S_{i+\delta}^-\right)\right].$$

We substitute in the last Hamiltonian the relations $S_i^z = S_i^z(b_i, b_i^+)$, $S_i^{\pm} = S_i^{\pm}(b_i, b_i^+)$. By so doing we obtain a Hamiltonian which contains both terms <u>bilinear in bosonic operators</u> and those <u>quartic in bosons</u> (describing <u>boson-boson interaction</u>). We will here be interested <u>only in bilinear terms</u> (the quartic ones are covered in Problem 3 of Blatt <u>11</u>).

So the Hamiltonian of linear spin waves (LSW) reads:

$$H_{spin}^{LSW} = J \sum_{i,\delta} \Big[-S^2 + S\big(b_i^+ b_i + b_{i+\delta}^+ b_{i+\delta} + b_i^+ b_{i+\delta}^+ + b_i b_{i+\delta}\big)\Big]$$

$$H_{spin}^{LSW} = -\frac{z}{2} NJS^2 + SJ \sum_{i,\delta} \big(b_i^+ b_i + b_{i+\delta}^+ b_{i+\delta} + b_i^+ b_{i+\delta}^+ + b_i b_{i+\delta}\big)$$

To diagonalize the last Hamiltonian, we first apply a Fourier transformation (to momentum space)

$$b_i^+ = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} b_{\vec{k}}^+$$

$$b_i = \frac{1}{\sqrt{N}} \sum_i e^{-i\vec{k}\cdot\vec{R}_i} b_{\vec{k}}$$

to obtain the same Hamiltonian in momentum space

$$H_{spin}^{LSW} = -\frac{z}{2} NJS^2 + \frac{z}{2} SJ \sum_{k>0} \Big[b_{\vec{k}}^+ b_{\vec{k}} + b_{-\vec{k}}^+ b_{-\vec{k}} + \gamma_{\vec{k}} \big(b_{\vec{k}}^+ b_{-\vec{k}}^+ + b_{-\vec{k}} b_{\vec{k}} \big)\Big].$$

The second term is diagonalized by the boson version of the Bogoliubov transformation

$$a_{\vec{k}} = \cosh(u_{\vec{k}})\, b_{\vec{k}} + \sinh(u_{\vec{k}})\, b_{-\vec{k}}^+ ,$$

$$a_{-\vec{k}}^+ = \sinh(u_{\vec{k}})\, b_{\vec{k}} + \cosh(u_{\vec{k}})\, b_{-\vec{k}}^+ .$$

The inverse transformation reads

$$b_{\vec{k}} = \cosh(u_{\vec{k}})\, a_{\vec{k}} - \sinh(u_{\vec{k}})\, a_{-\vec{k}}^+ ,$$

$$b_{-\vec{k}}^+ = -\sinh(u_{\vec{k}})\, a_{\vec{k}} + \cosh(u_{\vec{k}})\, a_{-\vec{k}}^+ .$$

$\boxed{\text{note that also } u_{\vec{k}} = u_{-\vec{k}}}$

When H_{spin}^{LSW} is recast using the last two relations, it is rather simple to establish that this Hamiltonian becomes diagonal in operators $a_{\vec{k}}$ if we choose $u_{\vec{k}}$ such that

$$(*) \quad \boxed{\tanh(2u_{\vec{k}}) \equiv \gamma_{\vec{k}}}$$

Then we have
$$H_{spin}^{LSW} = -\frac{z}{2} NJS(S+1) + \sum_{\vec{k}>0}' \hbar\omega_k \left(a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{1}{2}\right),$$
with $\boxed{\hbar\omega_{\vec{k}} = zJS\sqrt{1-\gamma_{\vec{k}}^2}}$.

This is exactly the same dispersion relation as what we previously found semi-classically!

Let us now consider quantum fluctuations of the Neél-ordered state. To this end, we first rewrite the Neél order parameter in terms of Holstein-Primakoff bosons:

$$O_{AFM} \equiv \frac{1}{N}\left\langle \sum_{i\in A} S_i^z + \sum_{i\in B} S_i^z \right\rangle,$$

"+" because of the rotation we performed!

that is:

$$O_{AFM} = \langle S_i^z \rangle = S - \langle b_i^\dagger b_i \rangle$$

The fluctuation of the order parameter is then

$$\delta S = \frac{\langle b_i^+ b_i \rangle}{S} = \frac{1}{NS} \sum_{\vec{k}} \langle b_{\vec{k}}^+ b_{\vec{k}} \rangle .$$

Using the Bogolubov transformation performed above and condition (*) for diagonalization, one obtains

$$\delta S = \frac{1}{NS} \sum_{\vec{k}} \sinh^2(u_{\vec{k}}) = \frac{1}{2NS} \sum_{\vec{k}} \left(\frac{1}{\sqrt{1-\gamma_{\vec{k}}^2}} - 1 \right)$$

The quantum fluctuations of the Néel order parameter vanish if the size of the spin S becomes infinite!

You can also phrase this by saying that the Néel state becomes more classical for larger spin!

There is, however, a more direct way to understand physically the relation between the size of the spin (S) and the quantum fluctuations:

We want to understand what precisely causes these quantum fluctuations.

The Neél state (with the z-axis being the spin-quantization axis) is the <u>exact ground state</u> of the <u>antiferromagnetic Ising model</u>

$$H_{\text{Ising}} \propto \sum_{i,\delta} S_i^z S_{i+\delta}^z$$

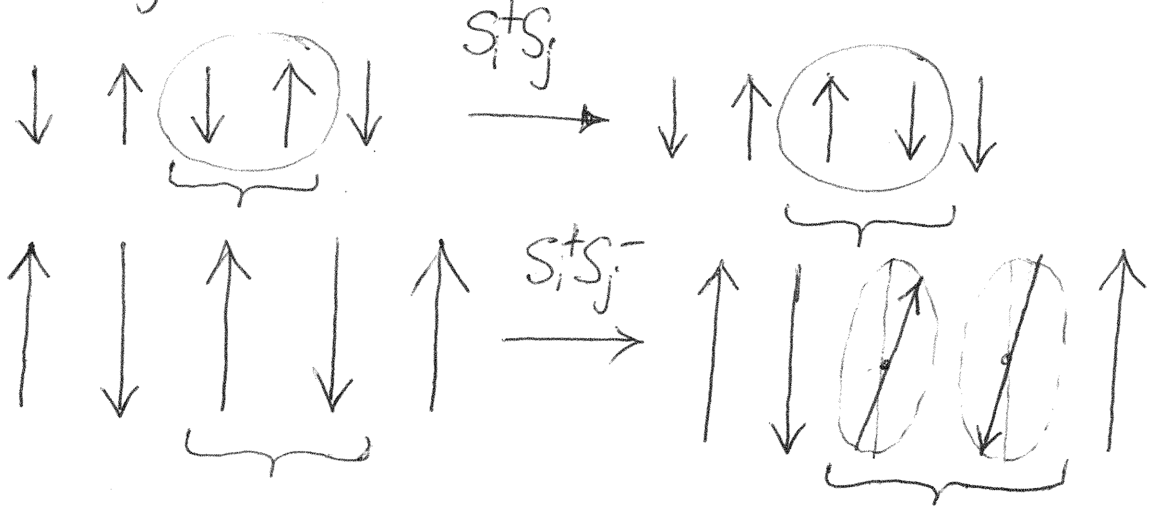
but <u>not of the Heisenberg model</u>!

Thus the <u>spin-flip terms</u> $\propto \left(S_i^+ S_j^- + h.c.\right)$ are those responsible for the quantum-spin fluctuations in the Heisenberg model!

The relation between the size of the spin (S) and the effect of the spin-flip terms can be illustrated as follows

$\boxed{S = \frac{1}{2}}$

$\boxed{S \gg \frac{1}{2}}$



Thus for spin-$\frac{1}{2}$ $S_i^+ S_j^-$ <u>reverses order parameter locally</u>, while for $S \gg \frac{1}{2}$ these flip terms only cause small displacements from the Neél configuration!

Let us now look at the <u>order-parameter fluctuations</u> in more detail; we want to see <u>the role of dimensionality (d).</u>

$$\delta S = \frac{1}{2S}\frac{1}{N}\sum_{\vec{k}}\left(\frac{1}{\sqrt{1-\gamma_{\vec{k}}^{2}}}-1\right) =$$

$$= \frac{1}{2S}\left(\frac{1}{N}\sum_{\vec{k}}\frac{1}{\sqrt{1-\gamma_{\vec{k}}^{2}}}-1\right) =$$

$$= \frac{1}{2S}\left(\int d^d\vec{k}\,\frac{1}{\sqrt{1-\gamma_{\vec{k}}^{2}}}-1\right),$$

where we switched <u>from the $\vec{k}$ sum to a $\vec{k}$ integral in the thermodynamic limit.</u>

We have already established that $\sqrt{1-\gamma_{\vec{k}}^{2}} \sim k$ at small $\vec{k}$, thus the relevant integral becomes

$$\int \frac{d^d\vec{k}}{k}$$

Note that for $d=1$ (one-dimensional system) the last integral diverges! Thus <u>the Néel order cannot exist in $d=1$!</u>

Does this sound familiar? Crystals and Fermi liquids also do not exist in 1d!

The study of <u>1d spin systems</u> ("quantum spin liquids") is one of the frontiers in condensed