Holstein-Primakov transformation

The usual spin operators: $S_x, S_y,\ S_z$ do not commute (for instance $[S_x, S_y] = i\hbar S_z$), and are therefore not conserved quantities. In a system where one can define a symmetry axis (for instance a ferromagnet) the eigenstates of S_z are $m_s\hbar$, with $m_s = -S \dots S$. It is convenient to introduce "ladder" operators $S^{\pm} = S_x \pm S_y$ so that for instance $[S_z, S^+] = \hbar S^+$, and $[S_z, S^-] = -\hbar S^-$. These ladder operators are reminiscent of the bosonic ladder operators, be it that they now act on the finite ladder $-m_s \dots m_s$. One can use this property to define operators $a, a^\dagger$, which do have bosonic commutation rules (bosonisation) through the Holstein-Primakov transformation:

$$\begin{aligned} S^+ &= \hbar(2S-n)^{1/2}a, \\ S^- &= \hbar a^\dagger(2S-n)^{1/2}, \\ S_z &= \hbar(S-n), \end{aligned}$$

where $n = a^\dagger a$ is the "number" operator. The commutation rules are $[a, a^\dagger] = 1$ and all others 0. In general these operators are quite cumbersome to work with. For small deviations from the ground state, one can however linearize them by taking $\langle n \rangle \approx 0$ in the first two equations. This leads to the linearized form:

$$\begin{aligned} S^+ &= \hbar\sqrt{2S}a, \\ S^- &= \hbar\sqrt{2S}a^\dagger, \\ S_z &= \hbar(S-a^\dagger a), \end{aligned}$$

Ordered magnetism[1]

As a generic model for a magnetic material with localized spins one could define a system consisting of antiferromagnetic two sublattices. The positions of the first one will be labeled by i, the second one by j. The distances between sites within a single lattice are denoted by k, the distances between two sites on different sublattices by l.
The interactions can now be split into two parts: one between spins on the same sublattice (anisotropic ferro- or antiferromagnetic), and one between spins of different lattice (anisotropic antiferromagnetic). The total hamiltonian now is $H = H_1 + H_2$ with:

$$H_2 = \sum_{i,k} S_i J'(k) S_{i+k} + \sum_{j,k} S_j J'(k) S_{j+k}$$

for spins on the same sublattice ($J'(k)$ is a diagonal tensor here with elements $J_x(k)$, $J_y(k)$, and $J_z(k)$), and

$$H_1 = \sum_{i,l} S_i J(l) S_{i+l} + \sum_{j,l} S_j J(l) S_{j+l}$$

for spins on different sublattices (again a diagonal $J(l)$). In order to make the most efficient use of the linearized Holstein-Primakov transformation, we start out with sublattices with

[1] treatment following A. Zheludev

rotated spin quantization axes by redefining our spin operators:

$$\begin{aligned} s_i^x &= S_i^x \\ s_i^y &= S_i^y \\ s_i^z &= S_i^z \end{aligned}$$

For the second:

$$\begin{aligned} s_j^x &= S_j^x \\ s_j^y &= -S_j^y \\ s_j^z &= -S_j^z \end{aligned}$$

The new operators still commute like the usual spin operators. The hamiltonian now becomes:

$$\begin{aligned} H_1 &= \sum_{i,l} J_x(l) s_i^x s_{i+l}^x - J_y(l) s_i^y s_{i+l}^y - J_z(l) s_i^z s_{i+l}^z \\ &\quad + \sum_{j,l} J_x(l) s_j^x s_{j+l}^x - J_y(l) s_j^y s_{j+l}^y - J_z(l) s_j^z s_{j+l}^z \end{aligned}$$

$$\begin{aligned} H_2 &= \sum_{i,k} J'_x(k) s_i^x s_{i+k}^x + J'_y(k) s_i^y s_{i+k}^y + J'_z(k) s_i^z s_{i+k}^z \\ &\quad + \sum_{j,k} J'_x(k) s_j^x s_{j+k}^x + J'_y(k) s_j^y s_{j+k}^y + J'_z(k) s_j^z s_{j+k}^z \end{aligned}$$

We can now use the linearized HP transformation to express our hamiltonian in terms of the bosonic $a^\dagger$ and a operators. We have $s^x = (s^+ + s^-)/2 = \sqrt{(S/2)}\left(a + a^\dagger\right)$, $s^y = -i(s^+ - s^-)/2 = -i\sqrt{(S/2)}\left(a - a^\dagger\right)$, and $s^z = s - a^\dagger a$, which is by the choice of a staggered coordinate system the same on both sublattices. For the terms in the Hamiltonian we now get for instance:

$$\begin{aligned} s_i^x s_{i+l}^x &= \frac{S}{2}\left(a_i^\dagger a_{i+l} + a_i^\dagger a_{i+l}^\dagger + a_i a_{i+l}^\dagger + a_i a_{i+l}\right) \\ s_i^y s_{i+l}^y &= \frac{S}{2}\left(a_i^\dagger a_{i+l} - a_i^\dagger a_{i+l}^\dagger + a_i a_{i+l}^\dagger - a_i a_{i+l}\right) \\ s_i^z s_{i+l}^z &= -S\left(a_i^\dagger a_i + a_{i+l}^\dagger a_{i+l}\right) \end{aligned}$$

To save a bit of writing, we will assume from here on that the exchange interactions are isotropic. T he full Hamiltonian now reads:

$$H_1 = S\sum_{i,l} J(l)\left(a_i^\dagger a_i + a_{i+l}^\dagger a_{i+l} + a_i^\dagger a_{i+l}^\dagger + a_i a_{i+l}\right) + S\sum_{j,l}\ldots$$

$$H_2 = S\sum_{i,k} J'(k)\left(-a_i^\dagger a_i - a_{i+k}^\dagger a_{i+k} + a_i a_{i+k}^\dagger + a_i^\dagger a_{i+k}\right) + S\sum_{j,k}\ldots$$

This is of course a monster of a hamiltonian, even after leaving out the possible anisotropy in J and J'. Luckily, the situation becomes a lot simpler by fourier transforming the hamiltonian using:

$$\begin{aligned} a_{\vec{i}} &= \frac{1}{\sqrt{(N)}} \sum_{\vec{q}} a_{\vec{q}} e^{i\vec{q}\cdot\vec{i}} \\ a^{\dagger}_{\vec{i}} &= \frac{1}{\sqrt{(N)}} \sum_{\vec{q}} a^{\dagger}_{\vec{q}} e^{-i\vec{q}\cdot\vec{i}} \end{aligned}$$

For instance, both parts of the Hamiltonian contain the following form:

$$\begin{aligned} \sum_{j,l} J(l) \left(a^{\dagger}_j a_j + a^{\dagger}_{j+l} a_{j+l} \right) &= \frac{1}{N} \sum_{j,l} J(l) \left[\sum_{q,q'} a^{\dagger}_q a_{q'} e^{-i\ (q-q')\cdot j} \left(1 + e^{-i\ (q-q')\cdot l} \right) \right] \\ &= \sum_{l} J(l) \sum_{q} a^{\dagger}_q a_q \\ &= \sum_{q} a^{\dagger}_q a_q J_0 \end{aligned}$$

Here we used that $\sum_j e^{-i\ (q-q')\cdot j} = \delta_{q,q'} N/2$, and defined the fourier transform of the exchange interaction as:

$$J_q = \sum_l J(l) e^{-i\ q\cdot l}$$

Since J is a real function, one has $J_q = J_{-q}$. Other types of terms appearing in the Hamiltonian are in H_1:

$$\sum_{j,l} J(l)(a_j a_{j+l} + a^{\dagger}_j a^{\dagger}_{j+l}) = \frac{1}{2} \sum_q J_q \left(a_q a_{-q} + a^{\dagger}_{-q} a^{\dagger}_q \right)$$

and in H_2

$$\sum_{j,k} J'(k)(a_j a^{\dagger}_{j+k} + a^{\dagger}_j a_{j+k}) = \sum_q J'_q a^{\dagger}_q a_q$$

Using the above relations the Hamiltonian can now be written in a more convenient form:

$$H = S \sum_q 2A_q a^{\dagger}_q a_q + B_q \left(a^{\dagger}_q a^{\dagger}_{-q} + a_q a_{-q} \right)$$

Where $A_q = J_0 - J'_0 + J'_q$, and $B_q = J_q$. The last term is only non-zero in the presence of antiferromagnetic coupling between the sublattices. If $B_q = 0$, the hamiltonian is diagonalized by the above procedure! This is for instance the case in a simple ferromagnet. The magnon dispersion is then given by:

$$\hbar\omega_q = 2SA_q = 2S \left(J'_q - J'_0 \right)$$

For nearest neighbor interaction $J(\pm a) = -J$ one has

$$J_q = -J \left(e^{i\ qa} + e^{-i\ qa} \right) = -2J \cos(qa),$$

so that $\hbar\omega_q = 4JS(1 - cos(qa))$. For small q one has $\hbar\omega_q \sim q^2$ leading to a magnetization which decreases with increasing temperature as $T^{3/2}$. The low temperature heat capacity increases with temperature as $T^{3/2}$.

Bogoliubov transformation for AF interactions

When $B_q \neq 0$ the second term introduces off-diagonal terms in the Hamiltonian, which have a form similar as found for the He problem. Therefore, we should be able to diagonalize the Hamiltonian using a Bogoliubov transformation:

$$\begin{aligned} a_q &= u_q b_q + v_q b_{-q}^\dagger \\ a_q^\dagger &= u_q b_q^\dagger + v_q b_{-q}, \end{aligned}$$

again with $u_q = u_{-q};\ v_q = v_{-q}$, and $u_q^2 - v_q^2 = 1$. The Hamiltonian can now be written as

$$H = S \sum_q \hbar\omega_q b_q^\dagger b_q$$

provided that

$$2A_q u_q v_q + B_q \left(u_q^2 + v_q^2)\right) = 0$$

The eigenvalues are $\hbar^2\omega_q^2 = 4S^2(A_q^2 - B_q^2)$. Since we have a two sublattice problem, $\hbar^2\omega_q^2 = 4S^2(A_{q+Q}^2 - B_{q+Q}^2)$ will also be a solution of the problem, where Q is the magnetic propagation vector. As an example we take the isotropic Heisenberg antiferromagnet with nearest neighbor interaction, which has $J' = 0;\ A_q = J_0;\ B_q = J_q$ and $J(l) = J$ for $l = \pm a$ so that $J_q = 2J\cos(qa)$. The dispersion is then

$$\hbar\omega_q = 2JS\sqrt{1 - \cos^2(qa)} = 2JS\,|sin(qa)|$$

For $Q = \pi/a$ we find the same solution. At small q this may be approximated as $\omega_q \sim q$, so that the low temperature heat capacity is expected to increase with increasing T as T^3.

The formalism described here is easily extendable to a variety of realistic situations such as anisotropic exchange, single ion anisotropy, helimagnetism, Ising magnets, presence of an external field, etc. For the case of non-ordered systems, one has to take higher order terms in the HP transformation into account ($\sqrt{(}S-n) = \sqrt{S}\left[1 - (1/2S)a^\dagger a - \ldots\right]$), leading to the appearence of 4-spin operator terms in the hamiltonian. The effective Hamiltonian can then be interpreted as a magnon Hamiltonian which includes magnon-magnon interactions.