Infinite coupling magnon theory of quantum Heisenberg magnetic models of spin $s$

Bang-Gui Liu$^a$ and Gerd Czycholl$^b$

$^a$Institute of Physics, Chinese Academy of Sciences, P O Box 603, Beijing 100080, P R China

$^b$Institute for Theoretical Physics, University of Bremen, D–28334 Bremen, Germany

An infinity magnon coupling term is introduced into the Holstein-Primakoff transformed forms of the Heisenberg ferromagnetic and antiferromagnetic models of any spin $s$ to rigorously remove the unphysical magnon states. This term makes the series expansion of the square root of the magnon operators become a finite series of magnon operator products. Under a simple Hubbard-like approximation our infinite coupling theory yields much better result than the existing spin wave theories, especially near transition temperatures.

**Introduction:** Quantum Heisenberg ferromagnetic (FM) and antiferromagnetic (AFM) models are well-accepted models for insulating ferromagnets and antiferromagnets. For general parameters one has to turn to some approximation methods or to numerical work. As for analytical methods, someone worked directly with the spin operators and their spin algebra. Anyway, a treatment in terms of the bosonic magnon operators should be advantageous because of the simpler commutation rules and the Bose statistics. For this purpose one has to map the spin Heisenberg models on spin wave (or magnon) models using the well known Holstein-Primakoff (HP) or the Dyson transformation. But, on one hand, the Dyson’s transformation one breaks the conjugate relation of spin operators; and in the Holstein-Primakoff transformation one has to treat the square root terms of magnon occupation operators. On the other hand, the magnon Hilbert space is much larger than the physical Hilbert space. For spin $s$, the spin Hilbert space on a single site consists of $2s + 1$ states but the magnon Hilbert space on a single site is infinite dimensional. In 3D ferromagnets there should be only few magnon excitations at low temperature. But in antiferromagnets, there should be a substantial number of magnons even at zero temperature because the sublattice magnetization is less than $s$. The effect of the extra unphysical magnon states on the physical quantities becomes more serious with increasing temperature.

We introduced an infinite magnon coupling terms into the Holstein-Primakoff transformed hamiltonians and thereby, for the first time, completely removed the effect of the extra unphysical states for any spin $s$. At the same time this infinite coupling term made the resultant magnon hamiltonians automatically truncated into finite series of the magnon operator products without any approximation. Under a simple nonperturbation approximation our hamiltonians yielded much better results than the existing spin wave theories.

**Infinite coupling magnon term:** We began with the standard isotropic Heisenberg FM and AFM hamiltonians of any spin $s$. Since Dyson transformation breaks the conjugate relation of spin operators, we chose HP transformation to transform the spin operators into the magnon operators.

\begin{equation}
S_i^- = a_i^\dagger \sqrt{2s - n_i}, \quad S_i^+ = \sqrt{2s - n_i} a_i,
\end{equation}

\begin{equation}
S_i^z = s - n_i; \quad n_i = a_i^\dagger a_i
\end{equation}

The HP transformed FM hamiltonian read:

\begin{equation}
H = \sum_i e a_i^\dagger a_i - \sum_{\langle ij \rangle} J_{ij} [\frac{1}{2} (a_i^\dagger A_{ij} a_j + h.c.) + a_i^\dagger a_j^\dagger a_j] - \frac{1}{4} \epsilon N
\end{equation}
and the AFM one read:

$$H = \sum_i \epsilon a_i^\dagger a_i + \sum_{\langle ij \rangle} J_{ij} [\frac{1}{2} a_i^\dagger a_j A_{ij} + \text{h.c.}] - a_i^\dagger a_i a_j^\dagger a_j - \frac{1}{4} \epsilon N$$  \hspace{1cm} (3)

Here \( N \) was the total number of the sites, \( \epsilon = JZ/2 \), and \( A_{ij} = \sqrt{2} (s - n_i) \sqrt{2} (s - n_j) \). To completely remove the effect of the extra unphysical states defined by \( |m\rangle_i = a_i^m |0\rangle \) \((m > 2s)\), we introduced the following infinite coupling term into the hamiltonians.

$$H_U = \sum_i \frac{U}{(2s+1)!} a_i^{(2s+1)} a_j^{(2s+1)}, \quad U \to \infty \quad (4)$$

so that our total hamiltonians were defined by \( H' = H + H_U \). The extra unphysical states were raised infinitely high in energy so that they actually decoupled from the 2s + 1 physical states. The hamiltonians included the square roots of the operators: \( \sqrt{2s - n_i} \) which was able to be expanded in terms of \( a_i^m a_j^m \). The \( U \) term makes the expansion automatically truncated into a finite series accurately.

$$\sqrt{2s - n_i} = \sum_{m=0}^{2s} (-1)^m C_m \frac{1}{m!} a_i^m a_j^m$$

$$C_m = \sum_i (-1)^i \frac{m!}{i!(m-i)!} \sqrt{2s - i} \quad (5)$$

Therefore the hamiltonians only consisted of finite number of operator product terms.

**Hubbard approximation:** Since we had the infinite coupling terms in our hamiltonians, an unperturbation method was needed to treat them properly. Our approximation was that the on-site \( U \) energy hierarchy was conserved during decoupling process. This meant that we made the decoupling \( n_i a_j = \langle n_i \rangle a_j \) only if \( i \neq j \) and instead we made further equations of motion for \( n_i a_i \). For half spin the resultant 3D FM magnetization and AFM sublattice magnetization are demonstrated in Figure 1 and Figure 2, respectively. Our results are much better than the existing spin wave theories, especially near the transition temperatures. At transition temperatures our magnetization and sublattice spin tend to zero with an exponent of 1/2 but those of nonlinear spin wave theories (NLSW) are uncontinuous and unreasonable. We can obtain lower ground state energy than any existing theories in the AFM case.

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