An accurate mapping of quantum Heisenberg magnetic models of spin ***s*** to strong-coupling magnon systems

1997 J. Phys.: Condens. Matter 9 5449

(http://iopscience.iop.org/0953-8984/9/25/012)

J. Phys.: Condens. Matter **9** (1997) 5449–5459. Printed in the UK PII: S0953-8984(97)80817-X

An accurate mapping of quantum Heisenberg magnetic models of spin s to strong-coupling magnon systems

Bang-Gui Liu† and Gerd Czycholl
Institute for Theoretical Physics, Universität Bremen, D-28334 Bremen, Germany

Received 10 January 1997

Abstract. An infinite-U term is introduced into the Holstein–Primakoff-transformed magnon Hamiltonian of quantum Heisenberg magnetic models of spin s. This term removes the unphysical spin-wave states at every site, and automatically truncates the expansion in powers of the magnon occupation operator. The resultant strong-coupling magnon Hamiltonians are accurately equivalent to the original spin Hamiltonians. The on-site U-levels and their implications are studied. Within a simple decoupling approximation for our strong-coupling magnon models, we can easily reproduce the results for the (sublattice) magnetizations obtained previously for the original spin model. But our bosonic Hamiltonians without any unphysical states allow substantially improved values to be obtained for the spectral weight in the ground state, and for ground-state energies lower than those obtained within previous approximations.

1. Introduction

Quantum Heisenberg magnetic models, including ferromagnetic (FM) and antiferromagnetic (AFM) ones, are well accepted models for insulating ferromagnets and antiferromagnets. The exact analytical solution is limited to one dimension and FM ground states. For general parameters, one has to turn to approximation methods or to numerical work. As for analytical methods, one can work directly with the original Heisenberg model, i.e. using spin operators and their algebra. In this category are the decoupling approaches [1, 2], the spherical approach [3], the projection method [4], and an isotropic decoupling approach [5]. The first of these is a mean-field approximation in the context of Green functions, the second one is for paramagnetic states, the third one investigates the ground states only, and the last one is for short-range magnetic correlation. In any case, 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 Heisenberg model onto a spin-wave model, using the well known Holstein–Primakoff [6] or the Dyson [7] transformation. In fact, many experimental physicists tend to describe their experimental results in terms of spin-wave theory [10, 11]. But if one chooses the Holstein–Primakoff transformation, a series expansion of a square-root term in powers of magnon occupation operators is necessary [6, 8]; and one has to violate the spin-operator relation $(S^+)^\dagger = S^-$ if one chooses Dyson's spin-wave transformation [7, 9].

The simplest spin-wave theory is linear spin-wave theory [12, 13]. Some nonlinear effects, namely, essentially the next terms in the expansion of the square root, are taken into

† Permanent address: Institute of Physics, Chinese Academy of Sciences, PO Box 603, Beijing 100080, People's Republic of China.

0953-8984/97/255449+11$19.50

account in nonlinear spin-wave theories [12, 6, 7, 14, 15]. But the Hilbert space on which the spin-wave (magnon) operators are defined is much larger than the physical Hilbert space. For spin s, the Hilbert space for a single site has the dimension $2s+1$. But the Hilbert space on which the magnon operators operate is infinite dimensional. In 3D ferromagnets there should be only few spin-wave excitations at low temperature. As for antiferromagnets, there should be a substantial number of magnons even at zero temperature, as the sublattice magnetization is less than s. The effect of the unphysical magnon states on the physical quantities becomes more serious with increasing temperature, because then a thermal occupation of the unphysical states becomes possible. In the paramagnetic (PM) phase, the unphysical states lead to serious problems. Lindgård and Danielsen [16] proposed the matching-of-matrix-elements (MME) method, in which operators with a complicated algebra (like spin operators) are expressed in terms of Bose operators, so that not only the commutation rules, but also certain matrix elements of the original operators remain unchanged, and the matrix elements connecting unphysical states vanish. This MME method can be considered to be a generalization of the Holstein–Primakoff transformation. Spin Hamiltonians like the Heisenberg model are mapped onto an interacting Bose model containing on-site interaction terms, but they operate on a Hilbert space, which has a still much larger dimension than the physical Hilbert space. In Mattis's books [12], a similarity transformation is used to eliminate partly the unphysical states in the FM phase. In Takahashi's modified spin-wave theory, the total number of magnons is fixed in the PM phase [17, 18]. But on a single site, the dimension of the magnon Hilbert space is still much larger than $2s+1$. Friedberg, Lee and Ren [19] introduced an on-site interaction term into a lattice Bose Hamiltonian, and proved the equivalence of this Bose model to a spin-wave model which is equivalent to a spin-$\frac{1}{2}$ Heisenberg model; they applied the theorem to the anisotropic ferromagnetic Heisenberg model in a magnetic field [19].

In this paper we shall introduce a large-U term into the Holstein–Primakoff-transformed magnon Hamiltonian of quantum Heisenberg magnetic models of any spin s. In the $U \to \infty$ limit, this term rigorously removes the unphysical magnon states at every site, so the magnon Hilbert space is mapped accurately onto the original spin-state space. At the same time, it automatically truncates the high-power terms of the magnon operators arising in the series expansion. This approach has some connections with earlier attempts [16, 19], but we present a formulation that is valid for arbitrary spin s, and apply it to the calculation of physical quantities like the order parameter. We shall study the hierarchy of the on-site U-levels, and its implication as regards the spin physics. Within a simple decoupling approximation, we can easily reproduce results for the FM magnetization and AFM sublattice magnetization which were obtained previously only in theories working with the original spin operators, and were better than the results from conventional spin-wave theories. Furthermore, our bosonic Hamiltonians without unphysical states allow us to obtain improved values for the renormalization of the spectral factor at zero temperature, and ground-state energies lower than those of the existing approximations.

2. Bosonic Hamiltonians without unphysical states

Our FM and AFM Heisenberg Hamiltonians are defined by

$$H = \pm \sum_{\langle ij \rangle} J_{ij} \left(\frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z \right) \tag{1}$$

where J_{ij} is positive, and the summation is over the nearest-neighbour sites. Here the negative sign corresponds to the ferromagnetic case, and the positive sign to the antiferromagnetic case. For the AFM case, it is better to make a π spin rotation for the operators in one of the two sublattices. The rotated AFM Hamiltonian reads

$$H = \sum_{\langle ij\rangle} J_{ij}\left(\frac{1}{2}(S_i^+S_j^+ + S_i^-S_j^-) - S_i^zS_j^z\right). \qquad (2)$$

We choose Holstein–Primakoff (HP) transformation to transform the spin operators into the magnon operators:

$$S_i^- = a_i^\dagger\sqrt{2s-n_i} \qquad S_i^+ = \sqrt{2s-n_i}\,a_i \qquad S_i^z = s - n_i \qquad n_i = a_i^\dagger a_i. \qquad (3)$$

The magnon operators a_i are standard bosonic operators. We prefer HP transformation, because Dyson transformation violates the conjugate relation of the spin operators. When substituting the transformation (3) into the Hamiltonians, one obtains the following FM Hamiltonian:

$$H = \sum_i \epsilon a_i^\dagger a_i - \sum_{\langle ij\rangle} J_{ij}\left[\frac{1}{2}(a_i^\dagger\sqrt{2s-n_i}\sqrt{2s-n_j}\,a_j + \text{HC}) + a_i^\dagger a_i a_j^\dagger a_j\right] - \frac{1}{4}\epsilon N \qquad (4)$$

and the following AFM Hamiltonian:

$$H = \sum_i \epsilon a_i^\dagger a_i + \sum_{\langle ij\rangle} J_{ij}\left[\frac{1}{2}(a_i^\dagger a_j^\dagger\sqrt{2s-n_i}\sqrt{2s-n_j} + \text{HC}) - a_i^\dagger a_i a_j^\dagger a_j\right] - \frac{1}{4}\epsilon N. \qquad (5)$$

Here N is the total number of the sites, $\epsilon = JZ/2$, and J is the exchange constant in the isotropic case or the largest of the J_{ij} in the anisotropic case, and Z is the coordination number. Since the operator a_i is a standard Bose operator, it operates on an infinite-dimensional Hilbert space. But the physical Hilbert space corresponding to a single site is spanned by only $2s+1$ states. The extra states are unphysical. The magnon Hamiltonians (4) and (5) are not equivalent to the original spin Hamiltonians (1) and (2) if the unphysical states are not removed. For the exact FM ground state, it is expected that there is no bosonic excitation, so the unphysical states remain unoccupied at zero temperature. The higher the temperature, the more serious the problems that may arise, if the thermal occupation of the unphysical states becomes possible. In the AFM case, even the ground state has some substantial bosonic excitations. The largest discrepancy appears in the paramagnetic (PM) phase, where the average spin in conventional magnon theory becomes very unreasonable if one tries to calculate it without introducing some constraints.

To remove completely the effect of the unphysical magnon states at every site, we can make their energy levels infinitely higher than those of the physical spin states. We introduce a large-U term into the HP-transformed Hamiltonians. This U-term resembles the strong-coupling positive U-term in the Hubbard model of electronic systems. But it is not dynamical; it is introduced only as a constraint to raise the energies of the unphysical states so that they are infinitely high as compared with those of the physical states. This means that our new Hamiltonians H' are composed of the original Hamiltonians H and the following U-terms:

$$H_U = \frac{1}{(2s+1)!}Ua_i^{\dagger(2s+1)}a_i^{(2s+1)}.$$

In fact, U should be considered to be infinite. Therefore, the energies of the unphysical states should be pushed infinitely high compared to those of the physical states by the U-term. For the half-spin case, the resultant FM Hamiltonian reads

$$H' = \sum_i\left(\epsilon a_i^\dagger a_i + \frac{1}{2}Ua_i^{\dagger 2}a_i^2\right) - \sum_{\langle ij\rangle} J_{ij}\left[\frac{1}{2}(a_i^\dagger a_j + a_i a_j^\dagger) + a_i^\dagger a_i a_j^\dagger a_j\right] - \frac{1}{4}\epsilon N \qquad (6)$$

and the AFM Hamiltonian reads

$$H' = \sum_i \left(\epsilon a_i^\dagger a_i + \frac{1}{2} U a_i^{\dagger 2} a_i^2 \right) + \sum_{\langle ij \rangle} J_{ij} \left[\frac{1}{2}(a_i^\dagger a_j^\dagger + a_i a_j) - a_i^\dagger a_i a_j^\dagger a_j \right] - \frac{1}{4}\epsilon N. \tag{7}$$

Here we need no chemical potential, since the unphysical magnon states have been removed rigorously by the infinite-U term. Furthermore, the square-root terms $\sqrt{2s - a^\dagger a}$ in the Hamiltonians (4), (5) have been expanded as

$$\sqrt{2s - a^\dagger a} = \sqrt{2s} - (\sqrt{2s} - \sqrt{2s-1}) a^\dagger a + (\sqrt{2s} - 2\sqrt{2s-1} + \sqrt{2s-2}) \frac{a^{\dagger 2} a^2}{2!}$$
$$+ \text{ (terms in } a^{\dagger n} a^n, \ n \geqslant 3) \tag{8}$$

and all terms $a^{\dagger n} a^n$ with $n \geqslant 2s$ can be neglected after introduction of the U-terms, because their energy is already shifted to infinity by the U-term. In the cases where $s = \frac{1}{2}$, all operator product terms, including $a_j^{\dagger n} a_i^m$ ($m > 1$ and/or $n > 1$), disappear automatically, so the Hamiltonians (6) and (7) are very simple. For larger spin s, there are more terms resulting from the expansion of the square root, because the terms including $a_i^{\dagger n} a_j^m$ ($m \leqslant 2s$ and $n \leqslant 2s$) are allowed. This expansion is different from the $1/s$ expansion in the spin-wave theories. We make no approximation in the expansion (8). The U-term not only pushes the unphysical states infinitely high above the physical states, but also automatically truncates the expansion of the square root. Our expansions of S_i^+ and S_i^- are composed of only $2s$ terms, and S_i^z is $s - a_i^\dagger a_i$, and so are different from the infinite sums of the three spin operators in reference [16]. Our mapping works for ferromagnetic and antiferromagnetic Heisenberg models of any spin s, and so is in contrast to the equivalence theorem, which works only for half-spin systems [19].

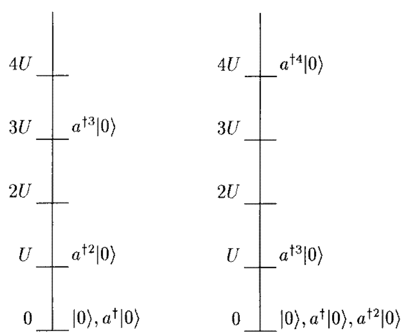

Figure 1. Left: on-site U-levels in the case of the half-spin. At the ground level there are only $|0\rangle$ and $a_i^\dagger|0\rangle$. Right: on-site U-levels in the case of the unit spin. At the ground level there are only $|0\rangle$, $a_i^\dagger|0\rangle$, and $a_i^{\dagger 2}|0\rangle$.

3. On-site U-levels

To study the effect of the U-term, we first study the on-site U-levels. In the half-spin case, we have the following commutation relations:

$$[a^{\dagger 2} a^2, a^{\dagger p} a^q]_- = [p(p-1) - q(q-1)] a^{\dagger p} a^q + 2(p-q) a^{\dagger (p+1)} a^{(q+1)}. \tag{9}$$

For $q = 0$ and $p = n$, we obtain by application of this expression to the magnon vacuum

$$H_U^{1/2}|n\rangle = \frac{n(n-1)U}{2}|n\rangle \tag{10}$$

where

$$H_U^{1/2} = \frac{U}{2}a^{\dagger 2}a^2$$

and $|n\rangle = a^{\dagger n}|0\rangle$. $|n\rangle$ is an eigenstate of $H_U^{1/2}$. The magnon states for the lowest five U-levels are shown in the left-hand part of figure 1. The magnon vacuum state $|0\rangle$ and the single-magnon state $a_i^\dagger|0\rangle$ correspond to the two physical spin states. The multiple-magnon states $a_i^{\dagger n}|0\rangle$ $(n > 1)$ are separated from these physical states by an energy of the magnitude of U, and are thus projected out from the Hilbert space in the limit $U \to \infty$. Therefore, we expect $\langle a_i^{\dagger n}a_i^n\rangle = 0$ $(n \geqslant 2)$ when U tends to ∞.

As for the case of spin 1, we have the following operator equality:

$$[a^{\dagger 3}a^3, a^{\dagger p}a^q]_- = [p(p-1)(p-2) - q(q-1)(q-2)]a^{\dagger p}a^q + 3[p(p-1) - q(q-1)]a^{\dagger(p+1)}a^{(q+1)} + 3(p-q)a^{\dagger(p+2)}a^{(q+2)}. \tag{11}$$

The on-site U-part of the Hamiltonian is

$$H_U^1 = \frac{U}{6}a^{\dagger 3}a^3.$$

We obtain the following eigenstate equation:

$$H_U^1|n\rangle = \frac{n(n-1)(n-2)U}{6}|n\rangle. \tag{12}$$

The states within the first five on-site levels are shown in the right-hand part of figure 1. At the ground level are the magnon vacuum $|0\rangle$, the single-magnon state $a_i^\dagger|0\rangle$, and the double-magnon state $a_i^{\dagger 2}|0\rangle$. They correspond to the three physical states of the spin operator: $-1, 0, 1$. Other states are separated from the physical states by energies of at least U. Therefore, we expect $\langle a_i^{\dagger n}a_i^n\rangle = 0$ $(n \geqslant 3)$ when U tends to ∞.

For higher spins s, we can derive some operator equations similar to (9) and (11). We always have $2s + 1$ magnon states on the ground level, corresponding to all of the physical spin states, and the unphysical states are separated from the physical states by energies of order U. We expect $\langle a_i^{\dagger n}a_i^n\rangle = 0$ $(n \geqslant 2s + 1)$ when U tends to ∞.

4. The first-order decoupling approximation

Since the U is very large, we cannot apply Hartree–Fock approximation to the magnon Hamiltonians. Now we study the FM and AFM systems of half-spin in a first-level decoupling approach to their equations of motion. We choose a_i as our dynamical variable.

4.1. The FM case

Using the Zubarev notation for the commutator Green function

$$\langle\langle A; B\rangle\rangle_z = -\mathrm{i}\int_{-\infty}^{+\infty} \theta(t)\langle[A(t), B]\rangle \mathrm{e}^{\mathrm{i}zt}\, \mathrm{d}t \tag{13}$$

we get the equation of motion

$$(z-\epsilon)\langle\langle a_i; a_j^\dagger\rangle\rangle_z = \delta_{ij} - \frac{1}{2}\sum_l J_{il}\langle\langle a_l; a_j^\dagger\rangle\rangle_z - \sum_l J_{il}\langle\langle a_i n_l; a_j^\dagger\rangle\rangle_z + U\langle\langle a_i^\dagger a_i^2; a_j^\dagger]\rangle\rangle_z. \tag{14}$$

In the above equation, the third term comes from the inter-site interaction, and the fourth term comes from the on-site large-U interaction. Without these two terms, one recovers the conventional FM linear spin-wave theory. Since U is very large, the fourth term cannot be neglected. We have to write down its equation of motion to get closed equations:

$$(z-\epsilon-U-JZn)\langle\langle a_i^\dagger a_i^2; a_j^\dagger\rangle\rangle_z = 2n\delta_{ij} - n\sum_l J_{il}\langle\langle a_l; a_j^\dagger\rangle\rangle_z. \tag{15}$$

Here $n_l = a_l^\dagger a_l$ denotes the magnon occupation operator, and $n = \langle n_l\rangle$ its thermal expectation value. In the latter equation, other higher-order Green functions have been neglected because they involve an even higher multiple-magnon occupation of a single site, and, therefore, vanish for infinite U. Furthermore, a decoupling approximation for the magnon and occupation operators for different sites has been made, but operators operating on the same site are not decoupled. Since U tends to infinity, and z is of the order of J, the prefactor on the left-hand side can be simplified to $-U$. Substituting it into (14), and using once more the above-mentioned decoupling approximation, we get

$$(z-(1-2n)\epsilon)\langle\langle a_i; a_j^\dagger\rangle\rangle_z = (1-2n)\delta_{ij} - \frac{1}{2}(1-2n)\sum_l J_{il}\langle\langle a_i; a_j^\dagger\rangle\rangle_z. \tag{16}$$

By Fourier transformation, we obtain for the $\boldsymbol{k}$-dependent Green function

$$G_{\boldsymbol{k}}(z) = \frac{1}{N}\sum_{i,j}\langle\langle a_i; a_j^\dagger\rangle\rangle_z \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i-\boldsymbol{R}_j)} = \frac{1-2n}{z-(1-2n)\epsilon(1-r_k)} \tag{17}$$

where

$$r_k = \frac{1}{Z}\sum_{\boldsymbol{\Delta}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\Delta}} \tag{18}$$

denotes the (dimensionless) magnon dispersion characteristic for the lattice under consideration; $\boldsymbol{\Delta}$ denotes the nearest-neighbour vectors. For a d-dimensional simple cubic lattice, we have

$$r_k = \frac{1}{d}\sum_{i=1}^{d}\cos k_i.$$

The self-consistency equation for determining n reads

$$n = (1-2n)\frac{1}{N}\sum_{\boldsymbol{k}} 1\Bigg/\left[\exp\frac{JZ(1-2n)(1-r_k)}{2T} - 1\right]. \tag{19}$$

This equation is equivalent to that expressed in terms of the spin-operator average, $\langle S_i^z\rangle$, obtained by Bogoliubov [1]. In the limit $T \to 0$, we obtain $n = 0$ or 1 as solutions of the above equation. These two solutions correspond to $\langle S_i^z\rangle = \frac{1}{2}$ or $-\frac{1}{2}$, respectively , since $S_i^z = \frac{1}{2} - n_i$. When the temperature increases to the Curie temperature T_c, the two branches converge to $n = \frac{1}{2}$, or $\langle S_i^z\rangle = 0$. For finite but small T, we obtain $\langle S_i^z\rangle = \frac{1}{2} - \alpha(T/J)^{3/2}$, where α is a positive constant. When $T \to T_c$, $(1-2n)$ tends to zero, so we can derive an asymptotic expression for $\langle S_i^z\rangle$ as follows:

$$\langle S_i^z\rangle \propto \sqrt{1-T/T_c} \qquad T_c = JZ/4P \qquad P = \frac{1}{N}\sum_{\boldsymbol{k}} 1/(1-r_k). \tag{20}$$

In two or one dimensions, the $\boldsymbol{k}$-integration diverges, i.e. $P = \infty$, so $T_c = 0$ in accordance with the Mermin–Wagner theorem [24].

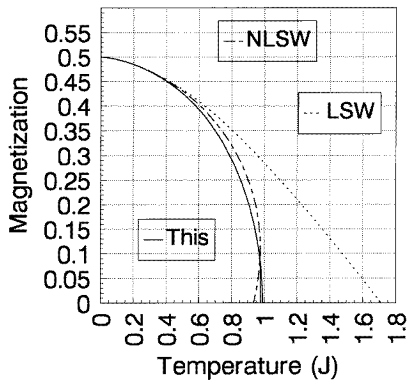

Figure 2. The 3D magnetization of the FM model as a function of the temperature. The solid line is for the approximation in this paper; the dashed line is for nonlinear spin-wave theories; and the dotted line is for linear spin-wave theory. The values of T_c are $0.989J$, $0.98J$, and $1.71J$, respectively. But the high-temperature expansion result is $0.889J$. The transition for the nonlinear spin-wave theory is of first order.

For $T \leqslant T_c$ in three dimensions, we obtain two solutions. These two solutions correspond to the two degenerate ferromagnetic solutions. The resulting order parameter, i.e. the magnetization, is shown in figure 2. The 3D results from the conventional nonlinear and linear spin-wave theories are also presented for comparison [12]. The nonlinear spin-wave theory produces an unphysical first-order transition at $T = 0.98J$ [12]. The magnetization obtained within our strong-coupling magnon theory according to (19) is obviously a substantial improvement over the whole temperature regime; we obtain as the critical (Curie) temperature $T_c = 0.989J$, whereas the series expansion result for T_c is $T_c = 0.889J$ [20]. It is interesting to compare this result for T_c to the spherical approximation for the paramagnetic phase [3]. The spherical approximation result, $T_c = 0.82J$, is slightly smaller than the numerical results, whereas our result $T_c = 0.989J$ is on the higher-temperature side of the numerical results. Our ground-state energy is $-0.25Jd$ per site in two and three dimensions, as it should be.

4.2. The AFM case

In this case, the Green function $G_{ij}(z) = \langle\langle a_i; a_j^\dagger\rangle\rangle_z$ alone is not sufficient, and we have to consider also the 'anomalous' one-particle Green function $F_{ij}(z) = \langle\langle a_i^\dagger; a_j^\dagger\rangle\rangle_z$. We obtain the following equation of motion for the Green function $G_{ij}(z)$:

$$(z-\epsilon)G_{ij} = \delta_{ij} + \frac{1}{2}\sum_l J_{il}F_{lj} - \sum_l J_{il}\langle\langle a_i n_l; a_j^\dagger\rangle\rangle_z + U\langle\langle a_i^\dagger a_i^2; a_j^\dagger\rangle\rangle_z. \tag{21}$$

In the above equation, the third term comes from the inter-site interaction, and the fourth term comes from the on-site large-U interaction. Without these two terms, one obtains the existing AFM linear spin-wave theory. In the same way as in the FM case, we have to write down a further equation of motion for the U-term. This reads

$$(z-\epsilon-U-JZn)\langle\langle a_i^\dagger a_i^2; a_j^\dagger\rangle\rangle_z = 2n\delta_{ij} + n\sum_l J_{il}F_{lj}(z) \tag{22}$$

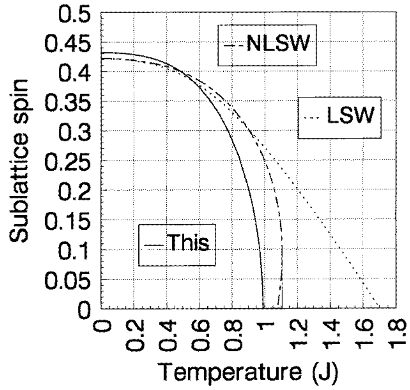

Figure 3. The 3D sublattice magnetization of the AFM model as a function of temperature. The solid line is for the approximation in this paper; the dashed line is for nonlinear spin-wave theories; and the dotted line is for linear spin-wave theory. The values of T_N are $0.989J$, $1.107J$, and $1.70J$, respectively. But the high-temperature expansion result is $0.951J$. The transition for the nonlinear spin-wave theories is of first order.

where we have again decoupled magnon occupation number operators and single-magnon operators at different lattice sites. Inserting this into (14), and using the decoupling approximation once more, we get

$$(z-(1-2n)\epsilon)G_{ij}=(1-2n)\delta_{ij}+\frac{1}{2}(1-2n)\sum_l J_{il}F_{lj}. \tag{23}$$

In the same way, we obtain

$$(z-(1-2n)\epsilon)F_{ij}=-\frac{1}{2}(1-2n)\sum_l J_{il}G_{lj}. \tag{24}$$

These two equations are closed, and yield the Green functions. This approximation is similar to the first-order Hubbard approximation of the electronic Hubbard model. Since $S_i^z=1/2-n_i$, it is clear that the above result is equivalent to results obtained previously for the spin model [1, 2]. The Green functions are given by

$$\begin{aligned}G_k&=(1-2n)[z+(1-2n)\epsilon]/[z^2-\epsilon^2(1-2n)^2(1-r_k^2)]\\F_k&=-(1-2n)^2\epsilon r_k/[z^2-\epsilon^2(1-2n)^2(1-r_k^2)].\end{aligned} \tag{25}$$

The self-consistent equation for determining n is given by

$$\frac{1}{2}=\left(\frac{1}{2}-n\right)\frac{1}{N}\sum_k\frac{1}{\sqrt{1-r_k^2}}\coth\frac{\omega_k}{2T} \tag{26}$$

where $\omega_k=(\frac{1}{2}-n)JZ\sqrt{1-r_k^2}$. In three dimensions we get for the zero-temperature sublattice magnetization $S_0=0.4325$, and the Néel temperature is $T_N=0.989J$. The sublattice magnetization as a function of T is shown in figure 3. The Néel temperature is better than that of the conventional spin-wave theories, because the high-temperature expansion result is $0.951J$ [20]. For low temperature T, we obtain $\langle S^z\rangle=S_0-\eta(T/J)^2$. When the temperature tends to T_N, the sublattice magnetization has the following asymptotic expression:

$$\langle S^z\rangle\propto\sqrt{1-T/T_N}\qquad T_N=JZ/4P. \tag{27}$$

The sublattice magnetization as a function of temperature is shown in figure 3. The results from the linear spin-wave theory and a nonlinear spin-wave theory are also presented for comparison. The nonlinear theories produce an unphysical first-order transition at $T = 1.11J$ in three dimensions [25], which is similar to the FM case. The result from (26) is best over the whole temperature region. In two dimensions, $T_N = 0$, and the zero-temperature sublattice magnetization is equivalent to 0.3587, which is larger than the results from the spin-wave theories and a series expansion result [21], in which the spin-wave behaviour was used in the extrapolation; but it is consistent with a Monte Carlo result 0.34 ± 0.01 [22]. The Green function Monte Carlo result is 0.31 ± 0.02 [23]. In one dimension, the average sublattice magnetization is zero even at zero temperature. This is consistent with the Mermin–Wagner theorem [24]. It is clear that the inter-site coupling modifies the spectra, and the U-term reduces the spectral weight. Without these two terms, we should get the linear spin-wave theory. But the U-term is necessary for removing the unphysical states. The linear spin-wave theory overestimated the spectral weight by about thirty per cent in a study on the sum rules and spin excitations of the quantum AFM Heisenberg models [26].

The U-term does not contribute to the ground-state energy. Our ground-state energies in two and three dimensions are $E_0^{AFM}/\epsilon N = -0.327$ and -0.297, respectively. The ground-state energies are a little higher than the existing results from spin-wave theories [13, 14, 17, 18]. On the other hand, the spectral factor $f = 1 - 2n$ is less than 1. Therefore, some improvement to the ground state is desirable.

Table 1. The AFM ground-state energy and sublattice spin available in various approximations of quantum Heisenberg models of half-spins. The values of E_0 are in units of Jd. 'LSW': the linear spin-wave theory; 'NLSW': the nonlinear spin-wave theory; 'Series + SW': the series expansion method in which some spin-wave behaviour was used in the extrapolation; 'MC': the Monte Carlo method; 'GFMC': the Green function Monte Carlo method; 'Projection': the method of projection using spin operators; 'SGFMF': the spin Green function mean-field method; and 'This work': the results obtained in this paper.

Approximation	2D S_0^3	2D E_0	3D S_0^3	3D E_0
LSW [13]	0.303	−0.329	0.422	−0.2985
NLSW^1 [8, 9]	0.3069			
NLSW^2 [18, 25]	0.303	−0.335	0.422	−0.301
Series + SW [21]	0.3025	−0.3348		
MC [22]	0.34±0.01	−0.335		
GFMC [23]	0.31±0.02	−0.3346		
Projection [4]	0.359	−0.132		
SGFMF [2]	0.3587	−0.327	0.4325	−0.297
This work	0.3587	−0.327	0.4325	−0.297
This work (improved)	0.3587	−0.365	0.4325	−0.309

4.3. The AFM ground states in a relaxed decoupling

To improve our approximation, we relax the constraint of the decoupling by permitting the decoupling of the operators on a site without changing the position of the operator product in the on-site U-level hierarchy. In this approximation, the inter-site correlation functions enter the spectral renormalization factor f, so we obtain the following nonlinear equation set with two variables at zero temperature:

$$\begin{aligned}\frac{1}{2} &= \left(\frac{1}{2}-n\right)\frac{1}{N}\sum_k \frac{1}{\sqrt{1-r_k^2}} \\ \xi &= -\left(\frac{1}{2}-n\right)\frac{1}{N}\sum_k \frac{r_k^2}{\sqrt{1-r_k^2}}.\end{aligned} \tag{28}$$

Now our magnon spectrum is defined by $\omega_k = \frac{1}{2}JZf\sqrt{1-r_k^2}$, and our spectral factor is defined by $f = 1 - 2n - 2\xi$. For the ground state, we obtain the same n and ξ as above. Therefore we obtain $(E_0^{AFM}/\epsilon N, S_0^z, f) = (-0.3106, 0.4325, 1.084)$ in three dimensions and $(-0.345, 0.3587, 1.113)$ in two dimensions. The renormalization factors are acceptable, and the ground-state energies are lower than those of the spin-wave theories [13, 14, 18, 8, 9] and other available results [22, 23, 21, 4, 2]. The details are summarized in table 1. The ground-state energies, E_0, in table 1 are given in units of Jd, where d is the dimension.

5. Discussion and summary

We have studied the half-spin strong-coupling magnon Hamiltonians without any unphysical states in a simple Hubbard-like decoupling approximation. For higher spins, the strong-coupling Hamiltonians can be treated similarly. Following the routine described by Fulde [27], we can also treat our magnon Hamiltonians by means of the projection method. In the above simple decoupling approximation, we obtain the same sublattice spins as were obtained directly from the original spin Hamiltonians, but our spectral renormalization factors at zero temperature are improved substantially, and our ground-state energies are lower than those of existing approximations. From figure 2 and figure 3, it is clear that our strong-coupling magnon Hamiltonians in the simple decoupling approximation improve on those from the conventional spin-wave theories. The nonlinear spin-wave theories produce unphysical first-order transitions. There have been many versions of the nonlinear spin-wave theory, but the main features and drawbacks are similar in all of these versions. But our strong-coupling magnon theories do not lead to such unphysical behaviour, because all of the unphysical states in the Hilbert space have been removed, and are, therefore, advantageous as compared with the original spin model and the conventional magnon Hamiltonian. Unlike in reference [19], where the introduction of a similar strong-coupling U-term was suggested, here we have presented a formulation which works for ferromagnetic and antiferromagnetic Heisenberg models of any spin s, and we have applied a Green function decoupling approximation to this model for the first time, and were able to calculate quantities like the order parameter (magnetization), and the critical temperature T_c.

In summary, we introduce an infinite-U term into the Holstein–Primakoff magnon Hamiltonian of quantum Heisenberg magnetic models of any spin s. This term rigorously removes the unphysical magnon states at every site, and at the same time automatically truncates the expansion of the square root $\sqrt{1-n_i/s}$. The resultant magnon Hamiltonians are accurately equivalent to the original spin Hamiltonians. We have studied the on-site U-levels, and their implications as regards the spin physics. Within a simple decoupling approximation, we obtain physically reasonable results for the FM magnetization and AFM sublattice magnetization, in agreement with existing results obtained for the original spin model. But we obtain lower ground-state energies than those from the previous theories, because our Hamiltonians are composed of the bosonic magnon operators, and are free of unphysical states.

Acknowledgments

BGL gratefully acknowledges financial support from the Alexander von Humboldt foundation (Jean-Paul-Strasse 12, 53173 Bonn, Germany). The authors are grateful to the referees for supplying the references [3, 16, 19].

References

[1] Bogoliubov N N and Tyablikov S V 1959 *Dokl. Akad. Nauk.* **126** 53
[2] Pu F-C 1960 *Sov. Phys.–Dokl.* **5** 128
[3] Hubbard J 1971 *J. Phys. C: Solid State Phys.* **4** 53
Lindgård P 1983 *Phys. Rev.* B **27** 2980
[4] Krüger P and Schuck P 1994 *Europhys. Lett.* **27** 395
Kleine B, Uhrig G S and Müller-Hartmann E 1995 *Europhys. Lett.* **31** 37
[5] Sokol A, Singh R R P and Elstner N 1996 *Phys. Rev. Lett.* **76** 4416
[6] Holstein T and Primakoff H 1940 *Phys. Rev.* **58** 1098
[7] Dyson F J 1956 *Phys. Rev.* **102** 1217
[8] Igarashi J 1992 *Phys. Rev.* B **46** 10 763
[9] Canali C M, Girvin S M and Wallin M 1992 *Phys. Rev.* B **45** 10 131
[10] See, e.g.,
Heyden S M, Aeppli G, Mook H A, Perring T G, Mason T E, Cheong S-W and Fisk Z 1996 *Phys. Rev. Lett.* **76** 1344
[11] Kampf A P 1994 *Phys. Rep.* **249** 219
Keimer B *et al* 1992 *Phys. Rev.* B **46** 14 034
[12] Mattis D C 1988 *The Theory of Magnetism I (Statics and Dynamics)* (2nd corrected printing) (Berlin: Springer)
Mattis D C 1985 *The Theory of Magnetism II (Thermodynamics and Statistical Mechanics)* (Berlin: Springer)
[13] Anderson P W 1952 *Phys. Rev.* **86** 694
Callaway J 1976 *Quantum Theory of the Solid State* (New York: Academic)
[14] Marshall M and Lovesey S W 1971 *Theory of Thermal Neutron Scattering* (Oxford: Clarendon)
[15] Kubo R 1952 *Phys. Rev.* **87** 568
Oguchi T 1960 *Phys. Rev.* **117** 117
[16] Lindgård and Danielsen O 1974 *J. Phys. C: Solid State Phys.* **7** 1523
[17] Takahashi M 1989 *Phys. Rev.* B **40** 2494
[18] Liu B-G 1992 *Phys. Lett.* **165A** 83
Liu B-G 1992 *J. Phys.: Condens. Matter* **4** 8339
[19] Friedberg R, Lee T D and Ren H C 1993 *Ann. Phys., NY* **228** 52
[20] Jou D and Chen H 1973 *Phys. Lett.* **45A** 239
Baker G 1967 *Phys. Rev.* **164** 800
[21] Singh R R P 1989 *Phys. Rev.* B **39** 9760
Singh R R P and Huse D A 1989 *Phys. Rev.* B **40** 7247
[22] Carlson J 1989 *Phys. Rev.* B **40** 846
Dagotto E 1994 *Rev. Mod. Phys.* **66** 763
Kampf A 1994 *Phys. Rep.* **249** 219
[23] Trivedi N and Ceperley D M 1989 *Phys. Rev.* B **40** 2737
[24] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
[25] See [17, 18]. But those two papers were on two-dimensional and quasi-two-dimensional cases. Extension of these to three dimensions is performed for comparison with the current result.
[26] Stringari S 1994 *Phys. Rev.* B **49** 6710
[27] Fulde P 1995 *Electronic Correlations in Molecules and Solids* 3rd enlarged edn (Berlin: Springer)