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1994 J. Phys. A: Math. Gen. 27 3621

(http://iopscience.iop.org/0305-4470/27/11/012)

J. Phys. A: Math. Gen. 27 (1994) 3621–3634. Printed in the UK

A complete Bose transformation in magnetic systems

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Received 6 September 1993, in final form 25 January 1994

Abstract. A method is developed to treat the constraints in the spin wave theory and a new Hermitian Bose transformation decorated by all constraints is found which is different from those of Holstein–Primakoff or the Dyson–Maleev. The transformed Hamiltonian includes both dynamic and kinematic interaction and it has been confined in physical proper space automatically. A model Hamiltonian which has completely same eigenvalues is presented and a scheme of approximation is described.

1. Introduction

The spin wave theory (SWT) has had a long history. Some Bose transformations have been introduced, such as the Holstein–Primakoff (HP) [1], Dyson–Maleev (DM) [2, 3] and, recently, the Schwinger boson (SB) [4, 5] transformation. The most difficult problem is the constraints in Bose transformations which are not included in the transformed Hamiltonian. In principle, the transformed Hamiltonian is not equivalent to the original one so that it must be confined in physical proper space (PS). In HP and DM theory, PS means that the number of bosons at each lattice site must not be greater than $2S$ where S is the spin quantum number. Such additional constraints make the SWT very complicated and have been overlooked in many published papers. In the case of large S and a three-dimensional (3D) system, the excitation of the boson in non-physical space (so-called improper physical space (IPS)), relates to the large fluctuation of spin and is small at low temperature for ferromagnetic system. However, it may become large for low-dimensional systems, especially for the antiferromagnetic system. Therefore, the additional interactions induced by those constraints in HP or DM theory must be considered carefully and it may be significant in some properties of the system. The SB theory has become more popular recently in the study of the strongly correlated electronic system and two-dimensional (2D) antiferromagnetic systems. The constraints of Bose transformation in SB theory require that the total number of Bosons with both spin up and spin down at each site must be 1. Lagrange multipliers μ_i have been introduced to incorporate the constraints into the transformed Hamiltonian, then a mean-field approximation is taken to substitute all $\{\mu_i\}$ with an average value μ. However, the mean-field approximation for the constraints may not be valid for low-dimensional systems since the fluctuation is large. In many cases, calculation beyond the mean-field approximation may be necessary. In some previous works, we developed a method of step operator (ST) [6, 7] to treat the constraints for 3D ferromagnetic and antiferromagnetic systems. In our method, the constraint of Bose excitations was transformed to some additional interactions in the Hamiltonian. It gave us a way to consider both dynamic and kinematic interactions completely. Recently, Wrobel and Barentzen have presented a unique boson expansion

0305-4470/94/113621+14$19.50

for a spin system [8]. In fact, their transformation in total Bose space is exactly equal to our previous results [6] cited by the authors. Although the transformed Hamiltonian is exactly equivalent to the original one, it is too complicated due to the existence of globe constraints. Reference paper [8] gave an example for the 1D isotropic Heisenberg system and only considered the second term in the interactions that include both the dynamical and kinematics. It is necessary to study a more general scheme of approximation to treat such a complex Hamiltonian. In this paper, a much simpler model Hamiltonian has been presented and proved to have exactly the same eigenvalues as the original one. Therefore it could be possible to do the calculations in considering the kinematic interactions. We will give an example to show how we renormalize the total interactions including both the dynamics and statistics for the 3D antiferromagnetic isotropic Heisenberg model. More applications will be presented in separate papers.

One of the purposes of this work is to reformulate our previous method in a more systematic manner for treating the constraints in the transformations of angular momentum to Bose operator. In section 2, an introduction to the representation of the step operator which was published in a Chinese journal [6] will be given. Meanwhile, we will present some new considerations. In section 3, a new Hermitian Bose transformation of spin operators is presented. The Hamiltonian of magnetic systems is transformed by means of our new Hermitian transformation and their equivalence is proved in section 4. Additionally, an equivalent model Hamiltonian which is simpler and has exactly the same eigenvalues as the original ones is presented and a new scheme of approximation based on the correlation functions is also described. An extension of our transformation to the SB theory is given in section 5. An example to show how we can renormalize the interactions in the transformed Hamiltonian is given in section 6 for the isotropic antiferromagnetic Heisenberg model.

2. Introduction of the step operators

According to [6], the step operator in Bose space is defined by

$$\begin{aligned} \theta_i|n\rangle_i &= |n\rangle_i \qquad 0 \leqslant n \leqslant 2S \\ &= 0 \qquad n \geqslant 2S+1 \end{aligned} \tag{1}$$

where $|n\rangle_i$ denotes the excited state with n bosons at the ith site. In general, any state in Bose space related to the ith site can be written

$$|\Psi\rangle_i = |P\rangle_i + |I\rangle_i \tag{2}$$

where $|P\rangle_i$ is the component in proper space and $|I\rangle_i$ the component in improper space in which the number of bosons is greater than $2S$. θ_i has the properties:

$$\begin{cases} \theta_i|P\rangle_i = |P\rangle_i \\ \theta_i|I\rangle_i = 0 \\ \theta_i|\Psi\rangle_i = |P\rangle_i \\ \theta_i^2 = \theta_i. \end{cases} \tag{3}$$

Therefore, θ_i is a projection operator to the proper space and can be generally represented by

$$\theta_i = \sum_{l=0}^{\infty} B_l a_i^{\dagger l} a_i^l \tag{4}$$

where $a_i^\dagger$ (or a_i) is the creation (or annihilation) operator of bosons at the ith site. $\{B_l\}$ are some coefficients. We have

$$a_i^{\dagger l} a_i^l = n_i(n_i - 1)(n_i - 2)\cdots(n_i - l + 1). \tag{5}$$

where $n_i = a_i^\dagger a_i$. If we put equation (5) in (4) and use the conditions (1), then B_l can be found [6] as the following

$$B_l = \begin{cases} 1 & l = 0 \\ 0 & 1 \leqslant l \leqslant 2S \\ \dfrac{(-1)^{(l-2S)}(l-1)(l-2)\cdots(l-2S)}{l!(2S)!} & l \geqslant 2S+1. \end{cases} \tag{6}$$

Expression (6) of B_l can easily be checked. If we put (4), (5) and (6) into (1), then it can be found that

$$\begin{aligned} \theta_i|2S+n\rangle &= \left[1 + \sum_{k=1}^{n} \frac{(-1)^k (n+2S)!}{(n-k)!(k-1)!(k+2S)(2S!)}\right]|2S+n\rangle_i \\ &= [1 + M(n+2S)!/(2S)!]|2S+n\rangle_i \qquad n = 1, 2, \cdots \end{aligned} \tag{7}$$

where

$$\begin{aligned} M &= \sum_{k=1}^{n} (-1)^k/[(n-k)!(k-1)!(k+2S)] \\ &= (2S/n!)\sum_{k=0}^{n}(-1)^{k+1} C_k^n/(k+2S) \\ &= -(2S)!/(n+2S)!\,. \end{aligned} \tag{8}$$

Therefore,

$$\theta_i|2S+n\rangle = 0 \qquad n \geqslant 1. \tag{9}$$

It is easy to obtain the following equations:

$$[\theta_i, n_i]_- = 0 \tag{10}$$

$$a_i\theta_i = \sum_{l=1}^{\infty} C_l a_i^{\dagger l-1} a_i^l \tag{11}$$

$$a_i^\dagger a_i \theta_i = \sum_{l=1}^{\infty} C_l a_i^{\dagger l} a_i^l \tag{12}$$

where

$$C_l = \begin{cases} 1 & l = 1 \\ 0 & 2 \leqslant l \leqslant 2S \\ \dfrac{(-1)^{(l-2S)} 2S}{(2S)!(l-1)(l-2S-1)!} & l \geqslant 2S+1. \end{cases} \tag{13}$$

For example, for $S = \frac{1}{2}$,

$$B_l = (-1)^{l-1}(l-1)/l! \qquad l \geqslant 0 \tag{14}$$

$$C_l = (-1)^{l-1} l/l! \qquad l \geqslant 1. \tag{15}$$

For a more general S, expressions (6) and (13) can be rewritten into a simpler form:

$$B_l = (-1)^{l-1}(l-1)(l-2)\cdots(l-2S)/[(2S)!l!] \qquad l \geqslant 0 \tag{16}$$

$$C_l = (-1)^{l-1} l(l-2)(l-3)\cdots(l-2S)/[(2S-1)!l!] \qquad l \geqslant 1. \tag{17}$$

3. Bose transformation of spin operators

There are three spin operators $\{S_i^-, S_i^+, S_i^z\}$ for each lattice and they satisfy following commutation relations:

$$\begin{cases} [S_i^-, S_i^+]_- = -2S_i^z \\ [S_i^-, S_i^z]_- = S_i^- \\ [S_i^+, S_i^z]_- = -S_i^+. \end{cases} \tag{18}$$

If we apply the transformation $\{T_i\}$ from the Hilbert space of the spin Hamiltonian to the Bose one:

$$\begin{cases} T_i S_i^- T_i^{-1} \to f(a_i, a_i^\dagger) \\ T_i S_i^+ T_i^{-1} \to f(a_i^\dagger, a_i) \end{cases} \tag{19}$$

then the general form of the mapping can be represented by

$$\begin{cases} T_i S_i^- T_i^{-1} = \tilde{a}_i \\ \qquad = \sum_{k=1}^{2S} F_k a_i^{\dagger k-1} a_i^k \theta_i \\ T_i S_i^+ T_i^{-1} = \tilde{a}_i^\dagger \\ \qquad = \theta_i \sum_{k=1}^{2S} F_k a_i^{\dagger k} a_i^{k-1}. \end{cases} \tag{20}$$

The position of θ_i in expressions (20) ensures that the space we work on is PS. Let us further define the mapping of S^z:

$$T_i S_i^z T_i^{-1} = [-S + a_i^\dagger a_i]\theta_i = \sum_{k=0}^{\infty} D_k a_i^{\dagger k} a_i^k \tag{21}$$

where $\{D_k\}$ has been derived and is

$$D_k = -S \cdot B_k + C_k. \tag{22}$$

It can be found that

$$D_k = \begin{cases} -S & \text{if } k = 0 \\ 1 & \text{if } k = 1 \\ 0 & \text{if } 2 \leqslant l \leqslant 2S \\ (-1)^{k-2S} \dfrac{(k+1)(k-2)(k-3)\cdots(k-2S)}{(2S-1)!k!} & \text{if } k \geqslant 2S+1. \end{cases}$$

From the definitions of (20) and (21), all coefficients $\{F_k\}$ can be determined by means of the conditions of commutation (18). As an example, we discuss the most interesting case of $S = \frac{1}{2}$ and we have

$$[a_i\theta_i, \theta_i a_i^\dagger]_- = -2[-\tfrac{1}{2} + a_i^\dagger a_i]. \tag{23}$$

Therefore, F_1 must be 1 and all others $\{F_k\}$ zero. In this case, the transformation is

$$\begin{cases} T_i S_i^- T_i^{-1} = \tilde{a}_i \\ \qquad\qquad = a_i \theta_i \\ \qquad\qquad = \sum_{k=1}^{\infty} C_k a_i^{\dagger k-1} a_i^k \\ T_i S_i^+ T_i^{-1} = \tilde{a}_i^\dagger \\ \qquad\qquad = \theta_i a_i^\dagger \\ \qquad\qquad = \sum_{k=1}^{\infty} C_k a_i^{\dagger k} a_i^{k-1} \\ T_i S_i^z T_i^{-1} = [-1/2 + a_i^\dagger a_i]\theta_i \\ \qquad\qquad = \sum_{k=0}^{\infty} D_k a_i^{\dagger k} a_i^k \end{cases} \tag{24}$$

where $\{C_k\}$ is defined by (15) and

$$D_k = (-1)^{k-1}(k+1)/2(k!) \qquad k \geqslant 0. \tag{25}$$

It can also be checked that all commutators of spin operators $\{S_i^-, S_i^+, S_i^z\}$ are satisfied and the transformation (24) is Hermitian.

The physical system has N sites; any physical state in Bose space must be in PS for each site. Therefore we must introduce a total projection operator Θ to the Hilbert space of N sites. It is defined by

$$\begin{cases} \Theta \quad = \prod_{i=1}^{N} \theta_i \\ \qquad = P_i \theta_i \\ P_i \quad = \prod_{j\neq i}^{N} \theta_j. \end{cases} \tag{26}$$

The following general transformation T must be done in the generalized spin wave theory:

$$\begin{cases} T S_i^- T^{-1} = P_i \tilde{a}_i \\ \qquad\qquad = P_i \sqrt{2S} \sum_{k=1}^{2S} F_k a_i^{\dagger k-1} a_i^k \theta_i \\ T S_i^+ T^{-1} = P_i \tilde{a}_i^\dagger \\ \qquad\qquad = P_i \theta_i \sqrt{2S} \sum_{k=1}^{2S} F_k a_i^{\dagger k-1} a_i^k \\ T S_i^z T^{-1} = P_i \sum_{k=0}^{\infty} D_k a_i^{\dagger k} a_i^k. \end{cases} \tag{27}$$

The projection operator P_i must commutate with any operator at the ith lattice so that

$$\begin{cases} [P_i, \tilde{a}_i] \quad = 0 \\ [P_i, \tilde{a}_i^\dagger] \quad = 0. \end{cases} \tag{28}$$

In fact, we can use the following algebra to find the coefficients $\{F_k\}$ in (20)

$$\begin{aligned} T S_i^- T^{-1} &= \sqrt{2S} \left[1 - \frac{1}{2s} a_i^\dagger a_i\right]^{1/2} a_i \Theta \\ &= P_i \sqrt{2S} \sum_{k=1}^{2S} F_k a_i^{\dagger k-1} a_i^k \theta_i \end{aligned} \tag{29}$$

where

$$\begin{cases} F_1 = 1 \\ F_2 = \sum_{k=1}^{\infty} C_{1/2}^k[-1/(2S)]^k \\ \quad = \sqrt{1-1/(2S)} - 1, \cdots \\ F_l = \sum_{k=l-1}^{\infty} C_{1/2}^k[-1/(2S)]^k(l-1)^{k-2} \qquad l \leqslant 2S \\ F_l = 0 \qquad l \geqslant 2S+1. \end{cases} \tag{30}$$

For example, for $S = 1$:

$$\begin{cases} F_1 = 1 \qquad F_2 = 1/\sqrt{2} - 1, \cdots \qquad F_k = 0 \ (k \geqslant 2) \\ C_l = (-1)^l l[l - (\sqrt{2}+1)]/l! \qquad l \geqslant 1. \end{cases} \tag{31}$$

It is not too difficult to find the $\{C_k\}$ for the case of larger S.

4. Transformed Hamiltonian and approximation

We have introduced the Bose transformation T, which is Hermitian, in the previous section. In general, the Hamiltonian for a magnetic system has the form:

$$H = \sum_{i \neq j}^{\infty} H_{ij} \tag{32}$$

where H_{ij} is the Hamiltonian of a pair of sites $\{i, j\}$. After our new transformation, the Hamiltonian becomes

$$\begin{aligned} H' &= THT^{-1} \\ &= \sum_{i \neq j}^{\infty} P_{ij} \tilde{H}_{ij} \end{aligned} \tag{33}$$

where

$$P_{ij} = \prod_{k \neq \{i,j\}}^{N} \theta_k \tag{34}$$

$$\tilde{H}_{ij} = T_i T_j H_{ij} T_j^{-1} T_i^{-1}. \tag{35}$$

As we know from the last section, the transformed Hamiltonian H' is now exactly the same as H.

From the definition of equation (38), we have

$$[P_{ij}, \tilde{H}_{ij}]_- = 0. \tag{36}$$

Let us now define a model Hamiltonian $\tilde{H}$ as follows:

$$\tilde{H} = \sum_{i \neq j}^{N} \tilde{H}_{ij}. \tag{37}$$

If E is an eigenvalue of the model Hamiltonian $\tilde{H}$ and the eigenstate $|\psi\rangle$, then

$$\begin{aligned} P\tilde{H}|\psi\rangle &= EP|\psi\rangle \\ H'P|\psi\rangle &= EP|\psi\rangle. \end{aligned} \tag{38}$$

If $P|\psi\rangle \neq 0$, E is also an eigenvalue of the transformed Hamiltonian H' with the eigenfunction $P|\psi\rangle$. Meanwhile, if E is an eigenvalue of the Hamiltonian H' with the eigenfunction $|\psi\rangle$, then we must have

$$\begin{aligned} PH'|\psi\rangle &= EP|\psi\rangle \\ \tilde{H}P|\psi\rangle &= EP|\psi\rangle \\ \tilde{H}|\psi\rangle &= E|\psi\rangle. \end{aligned} \tag{39}$$

Therefore, the eigenvalues of H' can be found from those of the model Hamiltonian $\tilde{H}$. The relative eigenstates can be obtained from the projection to PS. Hence, we can study the model Hamiltonian $\tilde{H}$ instead of H'. Our transformation seems a little more complicated than HP and much more so than DM since there are more terms in our Hamiltonian. However, those additional terms just describe the kinematic interaction which has been missing in HP and DM and may have a significant effect on the system in some cases. In which case, our transformation may have the advantage of studying both the dynamic and kinematic effects on the spin-wave properties. Meanwhile, our transformation is Hermitian, as is HP, but not DM. Therefore, we have found a complete and exact Bose transformation for magnetic systems.

Let us divide the Hamiltonian $\tilde{H}$ into two parts:

$$\begin{cases} \tilde{H} = \tilde{H}_0 + \tilde{H}_\mathrm{I} \\ \tilde{H}_\mathrm{I} = \tilde{H} - \tilde{H}_0. \end{cases} \tag{40}$$

$\tilde{H}_0$ is selected as an unperturbed part and the remainder one, $\tilde{H}_\mathrm{I}$, is considered as perturbation. $\tilde{H}_0$ has solution:

$$\tilde{H}_0|0\rangle = E_0|0\rangle. \tag{41}$$

According to perturbation theory, the eigenvalue E and eigenfunction $|\psi\rangle$ can be written as follows

$$\begin{cases} E = E_0 + E_1 + E_2 + \cdots + E_n + \cdots \\ |\psi\rangle = |0\rangle + |1\rangle + \cdots + |n\rangle + \cdots \end{cases} \tag{42}$$

where E_n and $|n\rangle$ are the nth order corrections from the perturbation $\tilde{H}_\mathrm{I}$. In general, the eigenstate $|0\rangle$ of H_0 may not be a vector in PS and has some component in the improper space. However, the eigenstate of $\tilde{H}$ should be in PS so that the eigenfunction of $\tilde{H}$ with energy E must be

$$\begin{aligned} |\Psi\rangle &= P|\psi\rangle \\ &= P|0\rangle + P|1\rangle + \cdots + P|n\rangle + \cdots \\ &= |\tilde{0}\rangle + |\tilde{1}\rangle + \cdots + |\tilde{n}\rangle + \cdots \end{aligned} \tag{43}$$

$$|\tilde{n}\rangle = P|n\rangle. \tag{44}$$

In the first-order approximation, we assume the wavefunction to be

$$|\Psi\rangle = |\tilde{0}\rangle = P|0\rangle \tag{45}$$

then the energy

$$\begin{aligned} E &\approx \langle\tilde{0}|\tilde{H}|\tilde{0}\rangle / \langle\tilde{0} \mid \tilde{0}\rangle \\ &= \langle 0|\tilde{H}P|0\rangle / \langle 0|P|0\rangle \\ &= \sum_{i\neq j}^{N} \langle 0|P_{ij}\tilde{H}_{ij}|0\rangle \Big/ \sum_{i\neq j}^{N} \langle 0|P_{ij}\theta_i\theta_j|0\rangle \\ &\approx \sum_{i\neq j}^{N} \langle 0|\tilde{H}_{ij}|0\rangle / \langle 0|\theta_i\theta_j|0\rangle + \sum_{i\neq j;k=n.n.}^{N} \langle 0|\theta_k\tilde{H}_{ij}|0\rangle_C / \langle 0|\theta_i\theta_j\theta_k|0\rangle \\ &\quad + \cdots \end{aligned} \tag{46}$$

where $k = n.n.$, represents the sum of k taken through all of nearest neighbours of sites i and j, and $\langle 0|\cdots|0\rangle_C$ denotes an average only for linked terms where the diagram should include one link at least between the k site and i or j. Hence, we have a scheme of approximation based on the correlation of sites. It is believed the terms with higher-order correlation will give higher-order contribution. If one did a higher-order approximation, then the term $P|1\rangle$ may be necessary in some cases. It is a way of doing some calculations beyond the mean-field approximation for the constraint in transformation. An application to the ground state of the 2D isotropic antiferromagnetic Heisenberg system will be given in separated letters.

5. Bose representation of constraint in the Schwinger boson transformation

The spin operators are represented by two Schwinger bosons [4, 5] ($m = \uparrow, \downarrow$), namely $[b_{i,m}, b^{\dagger}_{i',m'}] = \delta_{ii'}\delta_{mm'}$, with the constraint:

$$b^{\dagger}_{i\uparrow}b_{i\uparrow} + b^{\dagger}_{i\downarrow}b_{i\downarrow} = 2S. \tag{47}$$

The transformation is

$$\begin{cases} S_i^{+} = b^{\dagger}_{i\uparrow}b_{i\downarrow} \\ S_i^{-} = b^{\dagger}_{i\downarrow}b_{i\uparrow} \\ S_i^{z} = \frac{1}{2}[b^{\dagger}_{i\uparrow}b_{i\uparrow} - b^{\dagger}_{i\downarrow}b_{i\downarrow}]. \end{cases} \tag{48}$$

If we discuss the most interesting case with $S = \frac{1}{2}$, the projection operator P_i to describe the constraint (47) can be represented as follows:

$$P_i = (n_{i\uparrow} + n_{i\downarrow} - 2n_{i\uparrow}\cdot n_{i\downarrow})\theta_{i\uparrow}\theta_{i\downarrow} \tag{49}$$

where θ_{im} is the step operator defined in section 2. Using equation (12), we have

$$n_{im}\theta_{im} = \sum_{k=1}^{\infty} C_k b_{im}^{\dagger k} b_{im}^k \tag{50}$$

where $\{C_k\}$ is defined by (15). If we define $C_0 = 0$, then the operator P_i can be written as

$$\begin{aligned} P_i &= \sum_{k,k'=0}^{\infty} [C_k B_{k'} + B_k C_{k'} - 2C_k C_{k'}] b_{i\uparrow}^{\dagger k} b_{i\uparrow}^k b_{i\downarrow}^{\dagger k'} b_{i\downarrow}^{k'} \\ &= \sum_{k,k'=0}^{\infty} G_{k,k'} b_{i\uparrow}^{\dagger k} b_{i\uparrow}^k b_{i\downarrow}^{\dagger k'} b_{i\downarrow}^{k'}. \end{aligned} \tag{51}$$

The coefficient $G_{k,k'}$ is defined by

$$G_{k,k'} = C_k B_{k'} + B_k C_{k'} - 2C_k C_{k'} \tag{52}$$

whre C_k and $B_{k'}$ have been defined by (6) and (13). Let us define

$$\begin{aligned} P_{i\uparrow} &= (n_{i\uparrow} - n_{i\uparrow} \cdot n_{i\downarrow})\theta_{i\uparrow}\theta_{i\downarrow} \\ &= \sum_{k,k'=0}^{\infty} G_{k,k',\uparrow} b_{i\uparrow}^{\dagger k} b_{i\uparrow}^k b_{i\downarrow}^{\dagger k'} b_{i\downarrow}^{k'} \end{aligned} \tag{53}$$

$$\begin{aligned} P_{i\downarrow} &= (n_{i\downarrow} - n_{i\uparrow} \cdot n_{i\downarrow})\theta_{i\uparrow}\theta_{i\downarrow} \\ &= \sum_{k,k'=0}^{\infty} G_{k,k',\downarrow} b_{i\uparrow}^{\dagger k} b_{i\uparrow}^k b_{i\downarrow}^{\dagger k'} b_{i\downarrow}^{k'} \end{aligned} \tag{54}$$

$$P_i = P_{i\uparrow} + P_{i\downarrow} \tag{55}$$

where

$$\begin{cases} G_{k,k',\uparrow} = C_k B_{k'} - C_k C_{k'} \\ G_{k,k',\downarrow} = B_k C_{k'} - C_k C_{k'} \\ G_{k,k'} = G_{k,k',\uparrow} + G_{k,k',\downarrow}. \end{cases} \tag{56}$$

For the same reason as in section 3, we should introduce the total projection operator Q:

$$\begin{cases} Q = \prod_{i=1}^{N} P_i \\ Q_i = \prod_{k\neq i}^{N} P_k. \end{cases} \tag{57}$$

Finally, the spin-boson transformation in SB theory should be replaced by

$$\begin{cases} S_i^+ = Q_i P_{i\uparrow} b_{i\uparrow}^\dagger b_{i\downarrow} P_{i\downarrow} \\ S_i^- = Q_i P_{i\downarrow} b_{i\downarrow}^\dagger b_{i\uparrow} P_{i\uparrow} \\ S_i^z = \frac{1}{2} Q_i \{ b_{i\uparrow}^\dagger b_{i\uparrow} P_{i\uparrow} - b_{i\downarrow}^\dagger b_{i\downarrow} P_{i\downarrow} \}. \end{cases} \tag{58}$$

6. An example for a 3D antiferromagnetic system

The three-dimensional (3D) isotropic antiferromagnetic Heisenberg (IAFH) model has been studied many years ago [9]. Its problems seemed to have been resolved. However, in most papers, only the dynamic interaction of the spin wave was considered. The kinematic interaction induced by the constraints in Bose transformation was generally neglected. In the antiferromagnetic case, particularly for the case $S = \frac{1}{2}$, there are large quantum fluctuations which will induce a certain amount of the excitations of the spin wave even at zero temperature. The probability that the number of bosons at each site is larger than $2S + 1$ will not be negligible, so we must consider the constraints for Bose excitations. Our complete Bose transformation has given an exact equivalent model Hamiltonian. It may provide a method of calculating the total contribution from both the dynamic and kinematic interactions. As an example, we will give the calculation of ground-state energy for the 3D IAFH model for the case $S = \frac{1}{2}$. The application to the case of the 2D IAFH model with a square lattice may be more interesting and will be presented in a separate paper.

The Hamiltonian of AFHM is

$$H = \sum_{f,g} J(f-g)S_f^z S_g^z + \frac{1}{2}\sum_{f,g} J(f-g)[S_f^+ S_g^- + S_f^- S_g^+] \tag{59}$$

where the coupling, $J(f-g)$, is positive and nearest neighbour. Let us divide square lattices into two sublattices F and G and do local Bose transformation:

$$S_f^- = \tilde{a}_f^\dagger = \sum_{l=0}^{\infty} C_{l+1} a_f^{\dagger(l+1)} a_f^l \tag{60}$$

$$S_f^z = \frac{1}{2}\left(1 - \sum_{l=1}^{\infty} D_l a_f^{\dagger l} a_f^l\right) \tag{61}$$

$$C_{l+1} = (-1)^l/l! \qquad D_l = (-1)^{l+1}(l+1)/l!. \tag{62}$$

The transformation of S_f^+ is the conjugate of S_f^-. Similarly, we can also find the transformation for the sublattices G.

$$S_g^- = -\tilde{b}_g^\dagger = -\sum_{l=0}^{\infty} C_{l+1} b_g^{\dagger(l+1)} b_g^l \tag{63}$$

$$S_g^z = -\frac{1}{2}\left(1 - \sum_{l=1}^{\infty} D_l b_g^{\dagger l} b_g^l\right). \tag{64}$$

The local constraint on the excitation of the spin wave in the transformation has been included automatically. The transformed model is

$$H = \sum_{f,g} J(f-g)S_f^z S_g^z - \frac{1}{2}\sum_{f,g} J(f-g)(\tilde{a}_f\tilde{b}_g + \tilde{a}_f^\dagger\tilde{b}_g^\dagger) \tag{65}$$

where S_f^z and S_g^z are defined by (61) and (63). The Hamiltonian H can be expressed as

$$H = U_0 + H_2 + H_I \tag{66}$$

$$H_2 = \frac{1}{2}\left[\sum_{f,g} J(f-g)(a_f^\dagger a_f + b_g^\dagger b_g) - \sum_{f,g} J(f-g)(a_f b_g + a_f^\dagger b_g^\dagger)\right] \tag{67}$$

where $U_0 = -\frac{NJ(0)}{8}$ and H_1 describes the interaction of spin waves. H_2 can be diagonalized by means of the Bogolubov transformation. The excitation energy of the free spin wave in the representation of H_2 is

$$\varepsilon_k = \frac{J(0)}{2}\sqrt{1-\gamma_k^2} \tag{68}$$

$$\gamma_k = (\cos k_x d + \cos k_y d)/2 \tag{69}$$

where d is the distance between the nearest-neighbour sites. In the representation of the free spin wave, the averages $\langle a_f^\dagger b_g\rangle$, $\langle a_f b_g^\dagger\rangle$, $\langle a_f^\dagger a_{f'}^\dagger\rangle$, $\langle a_f a_{f'}\rangle$, $\langle b_g^\dagger b_{g'}^\dagger\rangle$ and $\langle b_g b_{g'}\rangle$ must be zero and

$$\langle a_f^\dagger a_{f'}\rangle = f(f-f') - \tfrac{1}{2}\delta_{f,f'} \tag{70}$$

$$\langle b_g^\dagger b_{g'}\rangle = f(g-g') - \tfrac{1}{2}\delta_{g,g'} \tag{71}$$

$$n = \langle a_f^\dagger a_f\rangle = \langle b_g^\dagger a_g\rangle \tag{72}$$

$$\langle a_f^\dagger b_g^\dagger\rangle = \langle a_f b_g\rangle = g(f-g) \tag{73}$$

$$f(r) = \frac{1}{N}\sum_k \frac{1}{\sqrt{1-\gamma_k^2}}\exp(-k\cdot r) \tag{74}$$

$$g = g(d) = \frac{1}{N}\sum_k \frac{\gamma_k}{\sqrt{1-\gamma_k^2}}\exp(-k\cdot d). \tag{75}$$

We can calculate the average $\langle H\rangle$ in the representation of the free spin wave by means of the Wick expansion theorem without any approximation. For example,

$$\langle a_f^{\dagger k} a_f^k\rangle = k!\langle a_f^\dagger a_f\rangle = k!n \tag{76}$$

$$\langle a_f^k b_g^k\rangle = k!g. \tag{77}$$

From the Bose representation (61) and (64) of S^z, we have

$$\begin{aligned}\langle S_f^z S_g^z\rangle = {} & \frac{1}{4} - \frac{1}{2}\sum_{k=1}^{\infty} D_k k! n^k + \frac{1}{4}\left\{\sum_{k=1}^{\infty} D_k(k)! n^k\right\}^2 + \frac{1}{4}\left\{\sum_{k=1}^{\infty} D_k(k-1)! k^2 n^k\right\}^2 X \\ & + \frac{1}{4}\left\{\frac{1}{2!}\sum_{k=1}^{\infty} D_k(k-2)! k^2(k-1)^2 n^k\right\}^2 X^2 + \cdots \end{aligned} \tag{78}$$

where $X = g^2/n^2$. If we define

$$\begin{aligned} f(n) &= \sum_{k=1}^{\infty} D_k k! n^k \\ &= \sum_{k=1}^{\infty} (-1)^{k+1}(k+1)n^k = (n^2+2n)/(1+n)^2 \end{aligned} \tag{79}$$

$$
\begin{aligned}
nf'(n) &= \sum_{k=1}^{\infty} D_k (k-1)! k^2 n^k \\
&= \sum_{k=1}^{\infty} (-1)^{k+1} (k+1) k n^k
\end{aligned} \tag{80}
$$

$$
\begin{aligned}
n^2 f^{(2)}(n) &= \sum_{k=1}^{\infty} D_k (k-2)! k^2 (k-1)^2 n^k \\
&= \sum_{k=1}^{\infty} (-1)^{k+1} (k+1) k (k-1) n^k
\end{aligned} \tag{81}
$$

$$\vdots$$

where we have denoted the $f^{(k)}(n)$ as the kth-order differential of functions $f(n)$ with n. Therefore, we can obtain

$$
\begin{aligned}
\langle S_f^z S_g^z \rangle &= \tfrac{1}{4} - \tfrac{1}{2} f(n) + \tfrac{1}{4} f(n)^2 + \tfrac{1}{4} \{ (n^2 X) f'(n)^2 + \frac{1}{(2!)^2} (n^2 X)^2 f^{(2)}(n)^2 \\
&\quad + \frac{1}{(3!)^2} (n^2 X)^3 f^{(3)}(n)^2 + \cdots .
\end{aligned} \tag{82}
$$

Because

$$f^{(k)}(n) = (-1)^{k+1} (k+1)! / (1+n)^{k+2} \qquad k = 1, 2, \cdots \tag{83}$$

we have

$$W = (n^2 X) f'(n)^2 + \frac{1}{(2!)^2} [f^{(2)} n)]^2 (n^2 X)^2 + \cdots + \frac{1}{(k!)^2} [f^{(k)}(n)]^2 (n^2 X)^k + \cdots . \tag{84}$$

Since

$$
\begin{aligned}
\frac{1}{(k!)^2} [f^{(k)}(n)]^2 (n^2 X)^k &= \frac{[(k+1)!(-1)^{k-1}]^2 [n^2 X]^k}{(k!)^2 (1+n)^{2(k+2)}} \\
&= \frac{(k+1)^2 (n^2 X)^k}{(1+n)^{2(k+2)}} \\
&= (k+1)^2 \left[\frac{n^2 X}{(1+n)^2} \right]^k \frac{1}{(1+n)^4}
\end{aligned} \tag{85}
$$

we have

$$W = \sum_{k=1} (k+1)^2 \left[\frac{n^2 X}{(1+n)^2} \right]^k \frac{1}{(1+n)^4}. \tag{86}$$

Let us define

$$Z = \frac{n^2 X}{(1+n)^2} = \frac{g^2}{(1+n)^2}. \tag{87}$$

The result of $\langle S_f^z S_g^z \rangle$ is

$$\begin{aligned}\langle S_f^z S_g^z \rangle &= \tfrac{1}{4} - \tfrac{1}{2} f(n) + \tfrac{1}{4} f(n)^2 + \tfrac{1}{4} W \\ &= \tfrac{1}{4}[1 - f(n)]^2 + \frac{Z(4 - 3Z + Z^2)}{4(1+n)^4(1-Z)^3} \\ &= \frac{1}{4(1+n)^4} + \frac{Z(4-3Z+Z^2)}{4(1+n)^4(1-Z)^3} \\ &= \frac{1+Z}{4(1+n)^4(1-Z)^3}.\end{aligned} \tag{88}$$

Similarly, we can obtain

$$\tfrac{1}{2}\langle \tilde{a}_f \tilde{b}_g + \tilde{a}_f^\dagger \tilde{b}_g^\dagger \rangle = \frac{g}{(1+n)^4(1-Z)^2}. \tag{89}$$

Finally, we obtain

$$\langle H \rangle = -\frac{NJ(0)}{8(1+n)^4}\left[\frac{1+Z}{(1-Z)^3} + 4\frac{g}{(1-Z)^2}\right] \tag{90}$$

where

$$Z = \frac{g^2}{(1+n)^2}. \tag{91}$$

In the 3D case, we have

$$n = \begin{cases} 0.078 & \text{for NaCl type} \\ 0.059 & \text{for CsCl type} \end{cases}$$

and

$$g = \begin{cases} 0.1265 & \text{for NaCl type} \\ 0.0958 & \text{for CsCl type.} \end{cases}$$

Therefore, the ground-state energy is

$$\frac{4\langle H \rangle}{NJ(0)} = \begin{cases} -\frac{1}{2} - (0.097 - 0.0131) & \text{for NaCl type} \\ -\frac{1}{2} - (0.073 - 0.0080) & \text{for CsCl type.} \end{cases}$$

In the approximation of the free spin wave, the ground-state energy is

$$\frac{4\langle U_0 + H_2 \rangle}{NJ(0)} = \begin{cases} -\frac{1}{2} - 0.097 & \text{for NaCl type} \\ -\frac{1}{2} - 0.073 & \text{for CsCl type.} \end{cases}$$

The total correction of interaction in the first-order approximation is 0.0131 for NaCl-type and 0.008 for CsCl-type systems. However, according to the results obtained by Oguchi [9], where they considered a part of the dynamic interactions only, the values are −0.0047 for NaCl-type and −0.0027 for CsCl-type systems, where we can find that the kinematic interaction seems very important and could not be neglected. Our calculation is only in the first-order approximation; it might change significantly for a higher-order approximation. However, the cancellation of the total kinematic interactions might not be expected.

In conclusion, we have developed a complete Bose transformation for a spin system with any value of S based on the step operator representation. A model Hamiltonian has been found which is simpler and has exactly the same eigenvalues as the original Hamiltonian. The method has been extended to the Schwinger boson transformation. An example of an application our method has been shown for an isotropic antiferromagnetic Heisenberg model. The calculation shows that the constraints in the transformation could be treated as part of a total interaction including both the dynamic and kinematic interactions, and the kinematic interaction is important as well as dynamic interaction for quantum antiferromagnetic systems. The method can be extended to any magnetic system in studying the ground-state and low-temperature properties, such as the system including the uniaxial crystal-field anisotropy term $(D\sum_i (S_i^z)^2)$, biquadratic anisotropic exchange interaction between nearest-neighbour spin S_i and S_j $(\sum_{i,j} I(i-j)(S_i^z \cdot S_j^z)^2)$, and perhaps other interesting systems including spin operators. The method could be considered as an extension of conventional spin wave theory. More applications should be investigated in the future.

Acknowledgments

This research is supported by the National Science Foundation of China and the National Education Commission under the grant for trainee doctors.

References

[1] Holstein T and Primakoff H 1940 *Phys. Rev.* **59** 1098
[2] Dyson F J 1956 *Phys. Rev.* **102** 1217
[3] Maleev S V 1957 *Zh. Eksp. Teor. Fiz.* **30** 1010 (Engl. Transl. 1958 *Sov. Phys.–JETP* **6** 776)
[4] Auerbach A and Arovas D P 1988 *Phys. Rev. Lett.* **61** 617
[5] Arovas D P and Auerbach A 1988 *Phys. Rev.* B **38** 316
[6] Tao Yung (present name Ruibao Tao) 1966 *Acta Physica Sinica* **22** 449; 1966 *Chin. J. Phys.* **22** 357
[7] Tao R and Pu F 1980 *Acta Physica Sinica* **29** 635; 1981 *Chin. Phys.* **1** 557
[8] Wrobel P and Barentzen H 1992 *Phys. Lett.* **162A** 282
[9] Oguchi T 1960 *Phys. Rev.* **117** 117