Sublattice-symmetric spin-wave theory for the Heisenberg antiferromagnet

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(Received 12 May 1989)

We apply the sublattice-symmetric spin-wave theory (SSSW) for Heisenberg antiferromagnets to obtain excited states at zero temperature. We identify a set of spin-wave states that have the correct total spin and correspond to the states with lowest energy in a given sector where S_z, the z component of the total spin, is fixed. This approximation gives results in good agreement with the results of exact diagonalization. We also discuss results of SSSW for finite-temperature and dynamical correlations. We recover the same equations as those obtained in the mean-field Schwinger boson theory of Arovas and Auerbach, except for a factor of 3/2. From comparison with exact results obtained by exact diagonalization, we assess the accuracy of the theory when the temperature is finite.

I. INTRODUCTION

Recently two-dimensional quantum antiferromagnets have attracted tremendous theoretical interest[1-8] due to their possible relevance to high-T_c superconductivity. The current numerical work has conclusively established that the ground state of the $S=\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice with nearest-neighbor coupling possesses long-range order,[4-7,1] the actual value of the staggered magnetization being slightly higher than that predicted by linear spin-wave theory.[1] Thus the spin-wave approximation is quite successful even in the $S=\frac{1}{2}$ case, for which it is supposed to be least accurate.

The spin-wave calculation for the Heisenberg model has a long history. Andersen first performed a semiclassical spin-wave calculation for the antiferromagnetic Heisenberg model, and obtained the ground-state energy and the staggered magnetization.[9] Later Kubo elaborated Anderson's method and developed a full quantum approach.[10] Oguchi showed that the next-order correction to their results is negligibly small.[11] A modified spin-wave theory was introduced by Takahashi for the Heisenberg ferromagnet.[12] Imposing a constraint that the total magnetization be zero, he obtained results which agree very well with the thermodynamic Bethe ansatz integral equations in one dimension. Recently, Arovas and Auerbach (AA) have developed an approach for this model based on a Schwinger boson representation.[13] In their formula for the spin-correlation function, there is a cutoff parameter η which removes the singularity for finite lattices; thus one can use their formula on finite lattices and directly compare with exact results. Hirsch and Tang then pointed out that AA's expressions yielded the same long-range order in the thermodynamic limit as obtained from linear spin-wave theory, and that the cutoff parameter η could be introduced within spin-wave theory by adding the constraint that the total staggered magnetization be zero.[1,14] Under this constraint, they obtained the same results as AA's at zero temperature and compared the sublattice-symmetric spin-wave (SSSW) results with the results of exact diagonalization for the ground state on square lattices of 4 to 26 sites. In the present paper, we show that, besides the ground state, SSSW also gives good results for some excited states. We also extend the previous work to finite-temperature and dynamical properties, and compare the results with finite-lattice calculations as well as with AA's theory. We have recently received unpublished work by Takahashi[15] and by Ohara and Yosida,[16] who reported results in agreement with Ref. 1 and with some of the results discussed here.

The paper is organized as follows: in Sec. II we define our notation and summarize the results obtained in the previous paper; Sec. III gives new results at zero temperature; Sec. IV deals with thermodynamic properties and dynamical correlations. We end in Sec. V with a discussion and conclusions.

II. SUBLATTICE-SYMMETRIC SPIN WAVE THEORY

The Hamiltonian of interest is the conventional Heisenberg Hamiltonian

$$H=J\sum_{\langle i,j\rangle} \mathbf{S}_i\cdot\mathbf{S}_j \ , \tag{1}$$

where $J>0$ for antiferromagnetism, and $\langle i,j\rangle$ runs over nearest neighbors. This Hamiltonian can be rewritten as

$$H=J\sum_{\langle i,j\rangle}[S_i^zS_j^z+\tfrac{1}{2}(S_i^+S_j^-+S_i^-S_j^+)] \ . \tag{2}$$

We consider the Hamiltonian on a bipartite lattice with sublattices A and B. The Holstein-Primakoff transformation[17] for A and B sublattices is defined as

$$S_i^+=(2S)^{1/2}(1-a_i^\dagger a_i/2S)^{1/2}a_i \ , \quad S_i^-=(2S)^{1/2}a_i^\dagger(1-a_i^\dagger a_i/2S)^{1/2} \ , \tag{3a}$$

$$S_j^\dagger=(2S)^{1/2}b_j^\dagger(1-b_j^\dagger b_j/2S)^{1/2} \ , \quad S_j^-=(2S)^{1/2}(1-b_j^\dagger b_j/2S)^{1/2}b_j \ , \tag{3b}$$

$$S_i^z=S-a_i^\dagger a_i, \quad S_j^z=-S+b_j^\dagger b_j \ , \tag{3c}$$

where $i \in A$ and $j \in B$. The boson operator $a_i^\dagger$ lowers the spin on site i of sublattice A, while $b_j^\dagger$ raises the spin on site j of sublattice B. The boson commutation relation is imposed on these operators.

In the thermodynamic limit, the up-down symmetry, as well as the sublattice symmetry, can be broken in various states. However, this will not happen on a finite lattice of N sites. To preserve these symmetries, we impose the constraint that *the total staggered magnetization be zero:*

$$\sum_{i \in A} S_i^z - \sum_{i \in B} S_i^z = 0 \tag{4a}$$

or

$$\sum_{i \in A} a_i^\dagger a_i + \sum_{i \in B} b_j^\dagger b_j = NS \ . \tag{4b}$$

Now, if we only keep the bilinear terms in spin-wave operators, the Hamiltonian (1) can be approximated by

$$H = -\tfrac{1}{2} NzJS^2 + JS \sum_{\langle i,j \rangle} (a_i b_j + a_i^\dagger b_j^\dagger + a_i^\dagger a_i + b_j^\dagger b_j) \ , \tag{5}$$

where z is the coordinate number of the lattice. We can diagonalize the spin-wave Hamiltonian Eq. (5) under the additional constraint that the sublattice magnetization be zero, i.e., Eq. (4b). First we introduce the Fourier transformation

$$a_k = \frac{1}{\sqrt{N_A}} \sum_{i \in A} e^{i\mathbf{k}\cdot\mathbf{R}_i}, \quad b_k = \frac{1}{\sqrt{N_a}} \sum_{j \in B} e^{-i\mathbf{k}\cdot\mathbf{R}_j} \ , \tag{6}$$

where k runs on the half-Brillouin zone of the lattice, and N_A is the number of sites on each sublattice. Then we apply a Bogoliubov transformation

$$\begin{aligned} a_k &= (\cosh\theta_k) c_k + (\sinh\theta_k) d_k^\dagger \ , \\ b_k &= (\sinh\theta_k) c_k^\dagger + (\cosh\theta_k) d_k \end{aligned} \tag{7}$$

to make the spin-wave Hamiltonian diagonal. The resultant Hamiltonian is given by

$$H = -\tfrac{1}{2} NzJS^2 + \frac{zJS}{\eta} \sum_k (\epsilon_k - 1) + \frac{zJS}{\eta} \sum_k \epsilon_k (c_k^\dagger c_k + d_k^\dagger d_k) \ , \tag{8}$$

where

$$\epsilon_k = (1 - \eta^2 \gamma_k^2)^{1/2} \ ,$$

and

$$\gamma_k = \frac{1}{D} \sum_i^D \cos k_{x_i} \ .$$

D is the dimension of the lattice. The constraint (4b) becomes

$$\frac{1}{N_A} \sum_k \frac{1 + n_k + n_k'}{(1 - \eta^2 \gamma_k^2)^{1/2}} = 2S + 1 \ , \tag{9}$$

where n_k and n_k' is the occupation number of magnons of c type and d type. The parameter η is determined by Eq. (9).

If we restrict η to be real, then there is an upper bound for the total number of magnons we can have. Setting η to its lowest allowable value zero, we find that this number cannot exceed NS. Also, we find

$$S_z = \frac{N}{2} (-\langle a_i^\dagger a_i \rangle + \langle b_j^\dagger b_j \rangle) = \sum_k (-n_k + n_k') \ . \tag{10}$$

Thus the z component of the total spin total S_z is determined by the difference between the total occupation numbers of the magnons of c type and d type.

III. ZERO-TEMPERATURE RESULTS

The energy spectrum given in Eq. (8), however, does not yield accurate results in comparison with exact results for finite lattices. More accurate estimates can be achieved through calculation of the spin-correlation functions. In doing so, we include the terms up to order $1/S$. We find that the spin-correlation functions are given by

$$\mathbf{S}_i \cdot \mathbf{S}_j = \left| \sum_k (n_k - n_k') \right|^2 - \left| \frac{1}{2N_A} \sum_k e^{ikR} \frac{\eta \gamma_k}{(1 - \eta^2 \gamma_k^2)^{1/2}} (1 + n_k + n_k') \right|^2 \ , \tag{11a}$$

for i,j on the different sublattice, where $R = R_i - R_j$ and

$$\mathbf{S}_i \cdot \mathbf{S}_j = -\tfrac{1}{4}\delta_{i,j} + \left| \sum_k (1 - e^{ikR})(n_k - n_k') \right|^2 + \left| \frac{1}{2N_A} \sum_k e^{ikR} \frac{1}{(1 - \eta^2 \gamma_k^2)^{1/2}} (1 + n_k + n_k') \right|^2 \ , \tag{11b}$$

for i,j on the same sublattice, after we take an average over the two sublattices. For the ground state, all occupation numbers are zero. The SSSW results for this special case were already discussed in our previous paper.[1,14] Spin correlations are exact for lattices of $N=2$, 4, and 8 sites, and accurate to a fraction of percent up to the largest N studied, $N=26$.

One wave vector, $k_0 = (0,0)$, has special importance. Because we only consider wave vectors in half the Brillouin zone, we will not take $k_{\pi,\pi}$ into account. If we put l magnons on, say, d_{k_0}, the z component of the total spin $S_z = l$. In addition, as can be verified by direction evaluation, the total spin is exactly

$$\mathbf{S} \cdot \mathbf{S} = NS(0) = l(l+1) \ ,$$

where $S(0)$ is the spin structure factor for wave vector 0, i.e., the sum of all the spin-spin correlation functions. The staggered magnetization is given by the relation between the structure factor $S(\pi,\pi)$ and the mean-squared staggered magnetization

$$Nm^2 = S(\pi,\pi) \ ,$$

where the order parameter

$$m^2=\left\langle \left[\sum_R \epsilon_R S_R \right]^2 \right\rangle$$

and $\epsilon_R=\pm 1$. Now we can use the foregoing results to calculate the magnetization in the thermodynamic limit. When N approaches infinity, for $l \ll N$, the parameter η reaches its limit 1, and the summation on k in (9), (11a), and (11b) become integrals. We separate the divergent terms from the integral in a fashion similar to the case of Bose-Einstein condensation.[14] For sufficiently large N, we have

$$m^2=\frac{(l+1)^2}{N^2}\frac{1}{1-\eta^2}+\frac{1}{4N}\int\frac{d^Dk}{(2\pi)^D}\frac{1+\eta^2\gamma_k^2}{1-\eta^2\gamma_k^2}\ , \qquad (12)$$

after discarding negligible terms. However, the integral in (12) is only proportional to $\ln N$ in two dimensions; thus only the first term needs to be considered. Meanwhile, the constraint Eq. (11) now becomes

$$\frac{1}{N}\frac{2(l+1)}{(-\eta^2)^{1/2}}+\int\frac{d^Dk}{(2\pi)^D}\frac{1}{(1-\eta^2\gamma_k^2)^{1/2}}=2S+1\ . \qquad (13)$$

That is, the constraint parameter η depends on the number of magnons in the state. Combining (12) and (13), we find that the staggered magnetization is

$$m=\tfrac{1}{2}\left[(2S+1)-\int\frac{d^Dk}{(2\pi)^D}\frac{1}{(1-\eta^2\gamma_k^2)^{1/2}}\right]\ . \qquad (14)$$

Thus, the dependence on l drops out for $l \ll N$, and all those states have equal staggered magnetization. Equation (14) is the same as the old spin-wave result of Anderson.[9] For two dimensions, the case we are especially interested in, Eq. (14) gives a staggered magnetization $m=0.3034$.

Because those states, with occupation number l on d_{k_0} (or on c_{k_0}), would have the same staggered magnetization for the ground state in the thermodynamic limit, we expect them to have the lowest energy in their corresponding $S_z=1$ sectors on a finite lattice. We calculated the exact spin structure factors for the lowest states in different S_z sections for the 4×4 lattice. A comparison of the exact spin structure factors with the SSSW results is presented in Fig. 1. The sublattice-symmetric spin-wave approximation gives very accurate results for low l. The errors for the singlet ground state and the lowest triplet state are less than 1%. The error increases for the higher S_z states, as interactions of higher order between magnons become more significant. However, when $S_z=NS$, i.e., the trivial ferromagnetic case, SSSW becomes exact. In Table I, we present the SSSW results for energy and staggered magnetization for the singlet ground state and the lowest triplet, together with the results obtained by exact diagonalization, on square lattices from 10 sites to 26 sites. The agreement is excellent. SSSW is exact for four-site and eight-site square lattices. An interesting observation is that the SSSW approximation systematically underestimates the staggered magnetization for all lattices we studied and for all S_z values.

IV. THERMODYNAMICS

At finite temperatures we introduce the occupation probabilities $P_k(n)$ and $P'_k(n')$ representing the probabili-

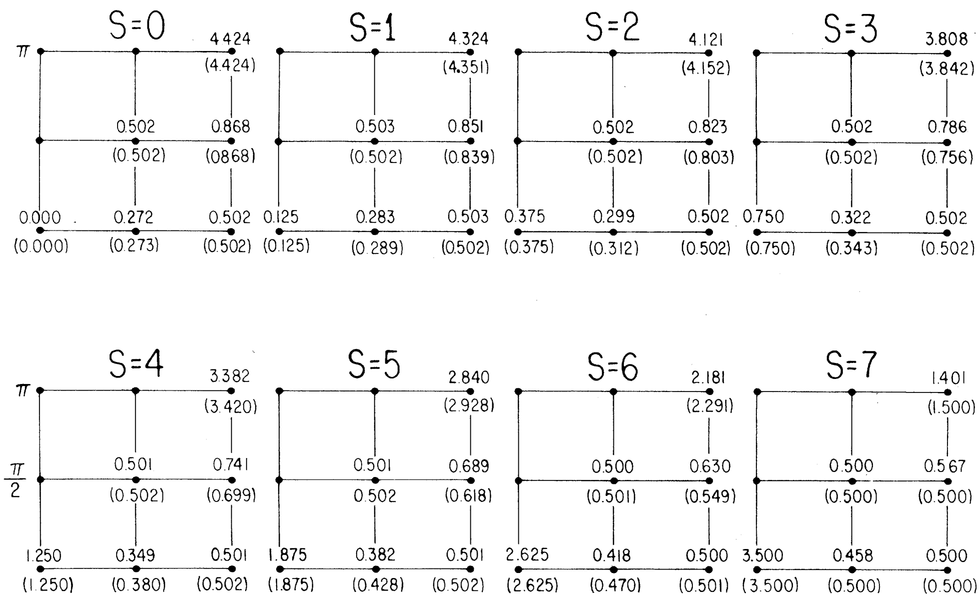

FIG. 1. SSSW results for the spin structure factors from $S_z=0$ to $S_z=7$ on the 4×4 lattice. SSSW is exact if $S_z=8$, i.e., when all spins align ferromagnetically. The values in parentheses are the results of exact diagonalization.

TABLE I. The SSSW values of the energy and mean squared staggered magnetization for the ground state (singlet, $S=0$) and the lowest excitation state (triplet, $S=1$) for the two-dimensional $S=\frac{1}{2}$ antiferromagnetic Heisenberg model. The values in parentheses are the results of exact diagonalization.

	Ground state		Lowest excited state	
Lattice	Energy E_0	Stag. mag.	Energy E_1	Stag. mag.
4	−2.0000	0.500	−1.000	0.3750
	(−2.0000)	(0.5000)	(−1.0000)	(0.3750)
8	−1.5000	0.3750	−1.2500	0.3438
	(−1.5000)	(0.3750)	(−1.2500)	(0.3438)
10	−1.4599	0.3375	−1.2946	0.3186
	(−1.4600)	(0.3380)	(−1.2928)	(0.3242)
16	−1.4031	0.2763	−1.3342	0.2703
	(−1.4036)	(0.2765)	(−1.3312)	(0.2720)
18	−1.3994	0.2665	−1.3344	0.2619
	(−1.3880)	(0.2686)	(−1.3315)	(0.2637)
20	−1.3831	0.2555	−1.3379	0.2521
	(−1.3816)	(0.2577)	(−1.3349)	(0.2541)
26	−1.3704	0.2315	−1.3426	0.2301
	(−1.3689)	(0.2339)	(−1.3399)	(0.2326)

ty that n (n') c-type (d-type) bosons occupy the state with momentum k; we have then

$$c_k^\dagger c_k = n_k = \sum_n n P_k(n) \; , \tag{15a}$$

$$d_k^\dagger d_k = n_k' = \sum_{n'} n' P_k'(n') \; , \tag{15b}$$

with

$$\sum_n P_k(n) = 1 \; , \tag{16a}$$

$$\sum_{n'} P_k'(n') = 1 \; , \tag{16b}$$

for all k. To order $1/S$ the constraint of zero staggered magnetization still takes the form (9). The Hamiltonian (2) can be written as

$$\langle H\rangle = -\frac{JN}{2\eta^2}\sum_\delta \left| (S+\tfrac{1}{2}) - \frac{1}{2N_A}\sum_k \frac{1-\eta^2\gamma_k e^{ik\delta}}{(1-\eta^2\gamma_k^2)^{1/2}}(n_k+n_k'+1)\right|^2 , \tag{17}$$

where δ is a vector connecting a site to a nearest neighbor, and the constraint (9) has been used. The entropy and the free energy are given by

$$\mathcal{S} = -\sum_k\sum_n P_k(n)\ln[P_k(n)] - \sum_k\sum_{n'} P_k' n'\ln[P_k'(n')] \; , \tag{18}$$

$$\mathcal{F} = \langle H\rangle - T\mathcal{S} \; . \tag{19}$$

We minimize the quantity

$$W = \mathcal{F} - \sum_k \mu_k \sum_n P_k(n) - \sum_k \mu_k' \sum_{n'} P_k'(n') \; , \tag{20}$$

with respect to $P_k(n)$ and $P_k'(n')$ to derive expressions for n_k and n_k'. μ_k and μ_k' are Lagrange multipliers determined from conditions (16a) and (16b), respectively. We find

$$n_k = n_k' = \frac{1}{e^{\beta\omega_k}-1} \; , \tag{21}$$

where

$$\omega_k = \Lambda\epsilon_k \; , \tag{22}$$

and

$$\frac{\eta^2\Lambda}{Jz} = \frac{1}{2N}\sum_k \frac{\eta^2\gamma_k^2}{(1-\eta^2\gamma_k^2)^{1/2}}\coth(\tfrac{1}{2}\beta\omega_k) \; , \tag{23}$$

where the wave vector k now has its conventional meaning, i.e., it now runs over the full Brillouin zone. The equations (17), (22), and (23) are the same as the mean-field equations of AA.[13]

The preceding formulas are consistent with our zero-temperature results. Due to the symmetry between c-type and d-type magnons, the terms involving $(n_k - n_k')$ in (11a) and (11b) will vanish. We rewrite $(n_k + n_k')$ as n_k, the occupation number of magnon of wave vector k, and substitute its expectation value (21) into (11a) and (11b); the spin-correlation function is now

$$\mathbf{S}_i \cdot \mathbf{S}_j = -\tfrac{1}{4}\delta_{i,j} + |f(R)|^2 - |g(R)|^2 \;, \tag{24}$$

where

$$f(R) = \frac{1}{2N} \sum_k e^{ikR} \frac{1}{(1-\eta^2\gamma_k^2)^{1/2}} \coth(\tfrac{1}{2}\beta\omega) \;,$$

$$g(R) = \frac{1}{2N} \sum_k e^{ikR} \frac{\eta\gamma_k}{(1-\eta^2\gamma_k^2)^{1/2}} \coth(\tfrac{1}{2}\beta\omega) \;.$$

Assuming $n_k = n_{-k}$, $g(R)$ will be zero if i and j are on the same sublattice, while $f(R)$ will be zero if they are on different sublattices. The constraint, which was introduced with some arbitrariness, now becomes an explicit requirement that $S_i \cdot S_i$ should be $S(S+1)$, i.e.,

$$f(0) = S + \tfrac{1}{2} \;. \tag{25}$$

Equation (25) determines η from the energy spectrum ω_k. Takahashi has recently obtained the same expressions for

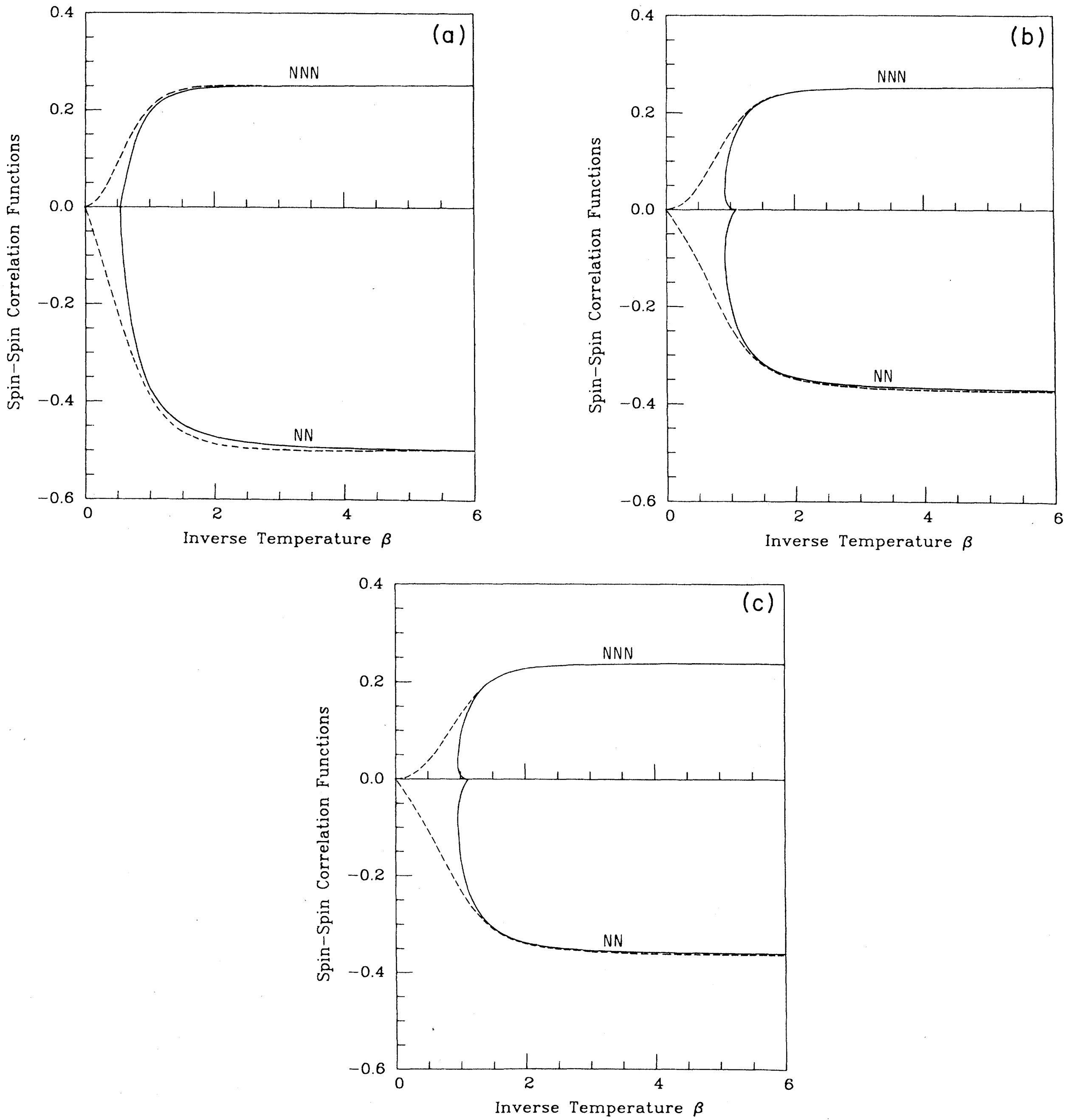

FIG. 2. (a) Spin-spin correlation functions for 2×2 lattice, (b) spin-spin correlation functions for eight-site lattice; (c) spin-spin correlation functions for ten-site lattice. The solid lines are results of SSSW; the dashed lines are the exact results. Nearest-neighbor (NN) and next-nearest-neighbor (NNN) correlations are plotted. The agreement between SSSW and the exact result is very good at temperatures lower than the interaction strength, except for the 2×2 lattice, the smallest one.

the spin-spin function and ω_k using an antiferromagnetic Dyson-Maleev (ADM) transformation.[15]

In Fig. 2 we compare the exact correlation functions to the ones obtained from this theory for square lattices of four, eight, and ten sites. Up to temperature T around J, the agreement is excellent, particularly for the larger lattices, but as the temperature is increased the correlation functions diverge from the exact values due to the contribution of the unphysical states present in this approximation. Because the average number of magnons cannot exceed NS, the product of $\beta\Lambda$ cannot be less than ln3. This value yields an upper bound of Λ given by Eq. (23), and hence a highest temperature one can reach in this spin-wave approximation. In Fig. 3 we show spin structure factors for the square lattice of ten sites. The agreement with exact results is again very good at low temperatures.

The dynamical spin-spin structure factor is defined by

$$S(q,\omega)=\sum_{l}\int dt\, e^{iql-i\omega t}\langle S_0^z(t)\cdot S_l^z(0)\rangle \ . \qquad (26)$$

We calculate the last expression to order $1/S$ and find

$$\begin{aligned} S(q,\omega)=&\frac{1}{N}\frac{\pi}{3}\sum_{k}\{\cosh[2(\theta_k-\theta_{k+\tilde{q}})]+1\} \\ &\times n_k(n_{k+\tilde{q}}+1)\delta(\omega_{k+\tilde{q}}-\omega_k-\omega) \\ &+\frac{1}{N}\frac{\pi}{6}\sum_{k}\{\cosh[2(\theta_k+\theta_{k+\tilde{q}})]-1\} \\ &\times[n_k+\Theta(\omega)][n_{k+\tilde{q}}+\Theta(\omega)] \\ &\times\delta(\omega_{k+\tilde{q}}+\omega_k-|\omega|) \ , \end{aligned} \qquad (27)$$

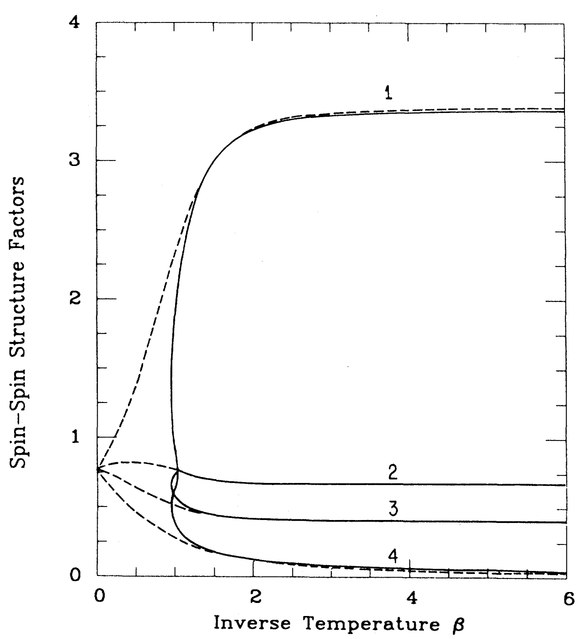

FIG. 3. Spin structure factors for the 10-site lattice. The solid lines are results of SSSW; the dashed lines are the exact results. Lines labeled 1 are for $q=(\pi,\pi)$; 2 for $q=(0.8\pi,0.4\pi)$; 3 for $q=(0.2\pi,0.3\pi)$; 4 for $q=(0,0)$. The agreement between SSSW and the exact result is very good at temperatures lower than the interaction strength.

where

$$\cosh(2\theta_k)=1(1-\eta^2\gamma_k^2)^{1/2} \ .$$

We have used the same notation as in AA,[18] $\tilde{q}$ is measured from the antiferromagnetic vector (π,π). We have used the Heisenberg equation of motion for the operators c_k, d_k and their conjugates. As pointed out by AA, the first term corresponds to the scattering of spin waves, whereas the second corresponds to the creation or annihilation of two spin waves. This expression is in agreement with the mean-field Schwinger boson formulation except for a factor of $\frac{3}{2}$. However, (27) is derived by expanding (26) to the order $1/S$, which indicates that as S goes to infinity, it becomes exact; this point is not evident in AA's derivation.

By using (27), we calculate the energy gap for the lowest triplet state. As expected, on 2×2 and eight-site lattices, the results are exact. The accuracy of formula (27) is also confirmed by the numerical results of Chen and Schüttler.[8]

V. CONCLUSIONS AND DISCUSSION

We have examined various aspects of the sublattice-symmetric spin-wave approach of the Heisenberg model, and compared the analytical results with exact results for finite lattices. For the ground state, the SSSW does not preserve the rotational invariance. In fact, the expectation value of $\langle S_i^+S_j^-+S_i^-S_j^+\rangle$ is zero, only $\langle S_i^zS_j^z\rangle$ contributes to the spin-correlation functions.

At zero temperature, we identified a set of spin-wave states, i.e., the lowest-energy states in a given S_z sector. For the spin-correlation functions, the agreement with the exact diagonalization results is very good, especially in the small S_z case. The exact staggered magnetization is always slightly higher than the spin-wave value for all the lattices and S_z we calculated.

For finite temperatures, the results calculated by using (24) to (25) are in good agreement with the exact results at low temperature. However, when the temperature becomes comparable to the strength of the interaction, SSSW begins to deviate from the exact results, even on the 2×2 lattice, even though SSSW reproduces exactly the spin-spin correlations of a few states at zero temperature. Within SSSW, we can have a maximum of NS magnons for N wave vectors, $N/2$ for c-type magnon, and $N/2$ for d type. This means that we can have C_{NS+N-1}^{NS} spin-wave states, a number usually much larger than $(2S+1)^N$, the number of physically meaningful states for the original Heisenberg Hamiltonian. On the other hand, SSSW fails to reproduce the spin-wave counterpart for some physically meaninful states even in the case of 2×2 lattice. For example, in SSSW, there are only two lowest triplet states, i.e., one has a magnon d_{k_0} and the other c_{k_0}, but there are three lowest triplet states for the original Heisenberg Hamiltonian (1). SSSW fails to reproduce the lowest triplet state of $S_z=0$. Thus, it is not surprising that the finite-temperature results are not as good as those at zero temperature. Nevertheless, results for spin structure factors at finite temperature are in reasonable agreement with exact results.

ACKNOWLEDGMENTS

This work is supported by National Science Foundation Grant No. DMR 85-17756 as well as contributions from AT&T Bell Laboratory and Cray Corporation. Parts of the calculations were done on the Cray at the San Diego Supercomputer Center.

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