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Spin-wave theory of the quantum antiferromagnet with unbroken sublattice symmetry

J. E. Hirsch and Sanyee Tang
Department of Physics, University of California, San Diego, La Jolla, California 92093
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We discuss the properties of spin-wave theory of quantum antiferromagnets with an additional constraint that restores the sublattice symmetry. Our treatment is analogous to Takahashi's recent theory of low-dimensional ferromagnets, and closely related to the Schwinger boson theory of Arovas and Auerbach. We obtain *exact* results for spin-spin correlations of 2, 4, and 8 spins in a singlet state, and exceedingly close agreement with exact results for $S=\frac{1}{2}$ in a variety of other cases. The implication for the long-range order of the $d=2$, $S=\frac{1}{2}$ Heisenberg antiferromagnet is discussed.

There has recently been some progress in the theory of quantum magnetism. Takahashi[1] has formulated a generalized spin-wave theory for low-dimensional Heisenberg ferromagnets that yields excellent agreement with Bethe ansatz results for spin $S=\frac{1}{2}$ in one dimension. Takahashi's idea was to supplement the usual spin-wave theory of ferromagnets with the constraint that the total magnetization be zero, which enforces the condition that the total number of spin waves per site is S on the average. As the Heisenberg algebra only allows for $2S$ spin waves per site, the constraint eliminates a lot of unphysical states in low dimensions where the number of spin waves otherwise diverges in zero magnetic field.

In this paper we formulate, along the same lines, a theory for the quantum antiferromagnet. Our original motivation came from an attempt to compare results of finite-lattice calculations for antiferromagnets[2] with predictions of spin-wave theory in two dimensions. Because the conventional spin-wave theory[3] yields a broken-symmetry state with finite staggered magnetization (in more than one dimension) while the ground state of the Heisenberg antiferromagnet on a finite lattice with an even number of sites is a singlet, there is no natural way to do such a comparison; in fact, attempting to use the spin-wave expressions on a finite lattice leads to divergences. In the approach discussed here, the ground state on a finite lattice has no broken sublattice symmetry and all quantities are well behaved; in fact, the agreement with exact results is best on small lattices. As the lattice size diverges the disconnected part of the spin-spin correlation function yields the same long-range order as predicted by conventional spin-wave theory.

Arovas and Auerbach[4] (AA) have recently formulated in remakable detail a large-N theory of quantum Heisenberg models based on a Schwinger boson representation. For the ferromagnet they recover Takahashi's results except for an overall factor of $\frac{3}{2}$, and these authors suggest that their results should be multiplied by $\frac{2}{3}$ to take into account fluctuation effects. Although AA focus their discussion on the disordered state at finite temperature, we have recently shown[5] that their theory in fact describes a state with long-range order where it is expected, i.e., at $T=0$ in $d=2$ and for $T<T_c$ in $d=3$. The theory discussed here is in fact equivalent to the AA theory except again for an overall factor of $\frac{3}{2}$.

We consider the Hamiltonian for a Heisenberg antiferromagnet on a bipartite lattice, given by

$$H=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j =J\sum_{\langle i,j\rangle}[2(S_i^+S_j^-+S_i^-S_j^+)+S_i^zS_j^z]\ , \tag{1}$$

and define boson operators on each sublattice (A and B) through the usual Holstein-Primakoff transformation:

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

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

$$S_i^z=S-a_i^\dagger a_i,\quad S_j^z=-S+b_j^\dagger b_j\ , \tag{2c}$$

where $i\in A$, $j\in B$. The boson creation 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; they obey the usual boson commutation relations.

We now rewrite the Hamiltonian Eq. (1) in terms of spin-wave operators and keep only the leading terms in $1/S$; defining Fourier-transformed operators

$$a_k=\frac{1}{\sqrt{N_A}}\sum_{i\in A}e^{i\mathbf{k}\cdot\mathbf{R}_i}a_i\ , \tag{3a}$$

$$b_k=\frac{1}{\sqrt{N_A}}\sum_{j\in B}e^{-i\mathbf{k}\cdot\mathbf{R}_j}b_j\ , \tag{3b}$$

where k runs over $\frac{1}{2}$ of the original Brillouin zone, and N_A is the number of sites in a sublattice, the Hamiltonian becomes

$$H=2SzJ\sum_k[\gamma_k(a_kb_k+a_k^\dagger b_k^\dagger)+a_k^\dagger a_k+b_k^\dagger b_k]+\text{const}\ , \tag{4}$$

TABLE I. Comparison of the present "sublattice-symmetric spin-wave theory" (SSSW) with exact results for the structure factor and spin-spin correlations for one-dimensional chains of N sites, $S=\frac{1}{2}$. SSSW is exact for $N=2$ and 4.

N	$S(\pi)^{\text{ex}}$	$S(\pi)^{\text{SSSW}}$	$\langle\sigma_0\sigma_l\rangle^{\text{ex}}$	$\langle\sigma_0\sigma_l\rangle^{\text{SSSW}}$	η
2	2	2	1, −1	1, −1	0.8660
4	2.667	2.667	1, −0.667, 0.333	1, −0.667, 0.333	0.9428
6	3.109	2.984	1, −0.6228, 0.2774, −0.3090	1, −0.6317, 0.2459, −0.2282	0.9632
8	3.442	3.138	1, −0.6085, 0.2610, −0.2519, 0.1988	1, −0.6223, 0.2196, −0.1621, 0.1296	0.9719

with $\gamma_k=\sum_\delta e^{i\mathbf{k}\cdot\boldsymbol{\delta}}/z$, where $\boldsymbol{\delta}$ are the lattice vectors to the z nearest-neighbor sites of the origin.

Diagonalization of the Hamiltonian Eq. (4) yields the conventional spin-wave results. In the ground state, the up-down symmetry, as well as the sublattice symmetry, is broken: spins on sublattice A point predominantly up, and on sublattice B predominantly down. Here we wish to preserve these symmetries, and thus we diagonalize the Hamiltonian Eq. (4) subject to the constraint that the *total staggered magnetization be zero*

$$\sum_{i\in A} S_i^z-\sum_{j\in B} S_j^z=0 \tag{5a}$$

or

$$\frac{1}{N_A}\sum_k (a_k^\dagger a_k+b_k^\dagger b_k)=2S\ . \tag{5b}$$

To enforce the constraint Eq. (5), we introduce a Lagrange multiplier and diagonalize

$$H'=H-\lambda\sum_k (a_k^\dagger a_k+b_k^\dagger b_k)\ , \tag{6}$$

with λ to be determined by Eq. (5b). H' is diagonalized by a Bogoliubov transformation to yield

$$H'=\sum_{k'}\varepsilon_k(c_{1k}^\dagger c_{1k}+c_{2k}^\dagger c_{2k})+\text{const}\ , \tag{7}$$

$$\varepsilon_k=\frac{zJS}{\eta}(1-\eta^2\gamma_k^2)^{1/2}\ , \tag{8}$$

with $\eta[=1/(1+2SzJ\lambda)]$ determined by the condition

$$\frac{1}{N}\sum_k\frac{1}{1-\eta^2\gamma_k^2)^{1/2}}=2S+1\ . \tag{9}$$

The constraint Eq. (9) ensures that $\eta<1$ on a finite lattice and prevents divergences associated with the points $\mathbf{k}=0$ and $\mathbf{k}=\pi$ that would occur with conventional spin-wave theory. In one dimension ($d=1$), the sum on the left-hand side of Eq. (9) diverges in the thermodynamic limit as $\eta\to 1$, and thus $\eta<1$ as $N\to\infty$. In $d=2$ and 3, the sum is finite and less than 2 as $N\to\infty$. Thus, to satisfy the constraint (9) $\eta\to 1$ as $N\to\infty$. For a finite N, η differs from 1 by $O(1/N^2)$. Thus, the parameter η introduces a gap in the spin-wave spectrum for a finite lattice. Condition (9) ensures that the ground state has no staggered magnetization.

We compute spin-spin correlation functions, to order $1/S$,[1] by evaluating $\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle$ in the ground state of the Hamiltonian Eq. (6). Our theory, as Takahashi's, is *not* rotationally invariant; in fact $\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle=\langle S_i^zS_j^z\rangle$. The result is

$$\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle=|f(R)|^2-|g(R)|^2-\tfrac{1}{4}\delta_{R,0}\ , \tag{10a}$$

with

$$f(R)=\frac{1}{2N}\sum_k e^{i\mathbf{k}\cdot\mathbf{R}}\frac{1}{(1-\eta^2\gamma_k^2)^{1/2}}\ , \tag{10b}$$

$$g(R)=\frac{1}{2N}\sum_k e^{i\mathbf{k}\cdot\mathbf{R}}\frac{\eta\gamma_k}{(1-\eta^2\gamma_k^2)^{1/2}}\ . \tag{10c}$$

Equation (10) is in fact identical to that obtained in the Schwinger boson mean-field theory of Arovas and Auerbach[4] except for a factor of $\frac{3}{2}$.

Since $f(0)=S+\frac{1}{2}$ [from Eq. (9)] and $g(0)=0$ we get $\langle\mathbf{S}_i\cdot\mathbf{S}_i\rangle=S(S+1)$ as expected. For two spins in a singlet state, the spin correlation is $\mathbf{S}_1\cdot\mathbf{S}_2=-S(S+1)$; for four spins with nearest-neighbor couplings, the correlations are $\mathbf{S}_1\cdot\mathbf{S}_2=-S(S+\frac{1}{2})$ and $\mathbf{S}_1\cdot\mathbf{S}_3=S^2$, and for eight spins in a square arrangement, $\mathbf{S}_{i1}\cdot\mathbf{S}_2=-S(S+\frac{1}{4})$ and

TABLE II. Same as Table I for a two-dimensional 4×4 lattice.

4×4 lattice	Exact	SSSW ($\eta=0.992\,88$)
$\langle\sigma_0\sigma_{\hat{x}}\rangle=$	−0.467 85	−0.467 69
$\langle\sigma_0\sigma_{\hat{x}+\hat{y}}\rangle=\langle_0\sigma_{2\hat{x}}\rangle$	0.285 02	0.284 60
$\langle\sigma_0\sigma_{2\hat{x}+\hat{y}}\rangle$	−0.269 55	−0.269 14
$\langle\sigma_0\sigma_{2\hat{x}+2\hat{y}}\rangle$	0.239 50	0.239 71
$S(\pi)$	5.8996	5.8946

TABLE III. Same as Table I for a three-dimensional 2×2×2 lattice.

2×2×2	Exact	SSSW ($\eta=0.978\,30$)
$\langle\sigma_0\sigma_{\hat{x}}\rangle$	−0.5356	−0.5348
$\langle_0\sigma_{\hat{x}+\hat{y}}\rangle$	0.2956	0.2959
$\langle\sigma_0\sigma_{\hat{x}+\hat{y}+\hat{z}}\rangle$	−0.2800	−0.2832
$S(\pi)$	3.7734	3.7754

TABLE IV. Comparison with exact and Monte Carlo (Ref. 6) (MC) results for two-dimensional lattices of N sites. The statistical error in the Monte Carlo data is given in parentheses.

	Energy		$S(\pi)$		$C_{L/2,L/2}$	
Size (N)	Exact/MC	SSSW	Exact/MC	SSSW	Exact/MC	SSSW
4	−0.5000	−0.5000	2.667	2.667	0.333	0.333
8	−0.3750	−0.3750	4.000	4.000	0.333	0.333
10	−0.3650	−0.3650	4.507	4.500	−0.307	−0.303
16	−0.3509	−0.3508	5.899	5.895	0.240	0.240
18	−0.3470	−0.3474	6.447	6.395	−0.267	−0.260
20	−0.3456	−0.3458	6.873	6.813	0.239	0.234
26	−0.3421	−0.3426	8.104	8.026	−0.225	−0.221
36		−0.3398	10.1(4)	9.956	0.205(12)	0.200
64		−0.3372	15.3(6)	14.937	0.186(11)	0.180
144		−0.3358	28.7(1.3)	27.767	0.167(10)	0.160

$\mathbf{S}_1\cdot\mathbf{S}_3=S^2$. The reader can verify for him/herself that these relations are *exactly satisfied* by Eqs. (9) and (10).

The $\mathbf{q}=\pi$ structure factor is given by

$$S(\pi)=\sum_R(-1)^R\langle \mathbf{S}_0\cdot\mathbf{S}_R\rangle=\frac{1}{N}\sum_k\frac{1+\eta^2\gamma_k^2}{1-\eta^2\gamma_k^2}-\frac{1}{4}\,. \qquad (11)$$

We have recently shown[5] that Eqs. (9) and (10) predict a long-range order in the thermodynamic limit (in $d>1$) that is identical to the one obtained by conventional spin-wave theory.

We next solve Eqs. (9) to (11) on finite lattices and compare with exact results for the case $S=\frac{1}{2}$. Table I shows results in one dimension, compared with results of exact diagonalization. [$S(\pi)$ is defined as in Eq. (13).] The theory is exact for $N=2$ and 4, and increasingly inaccurate for larger N. It correctly yields no long-range order, but the correlation function decays exponentially because $\eta<1$ as $N\to\infty$, in contradiction with the known algebraic decay.

Table II shows comparison with exact results on a two-dimensional 4×4 lattice, and Table III on a three-dimensional 2×2×2 lattice. For both cases the agreement is remarkable, the error being of order 0.1% in most cases. Table IV shows comparison for the energy, the $\mathbf{q}=\pi$ structure factor and the spin-spin correlation function

$$C_{L/2,L/2}=\langle\sigma_0^z\sigma_{L/2}^z\rangle \qquad (12)$$

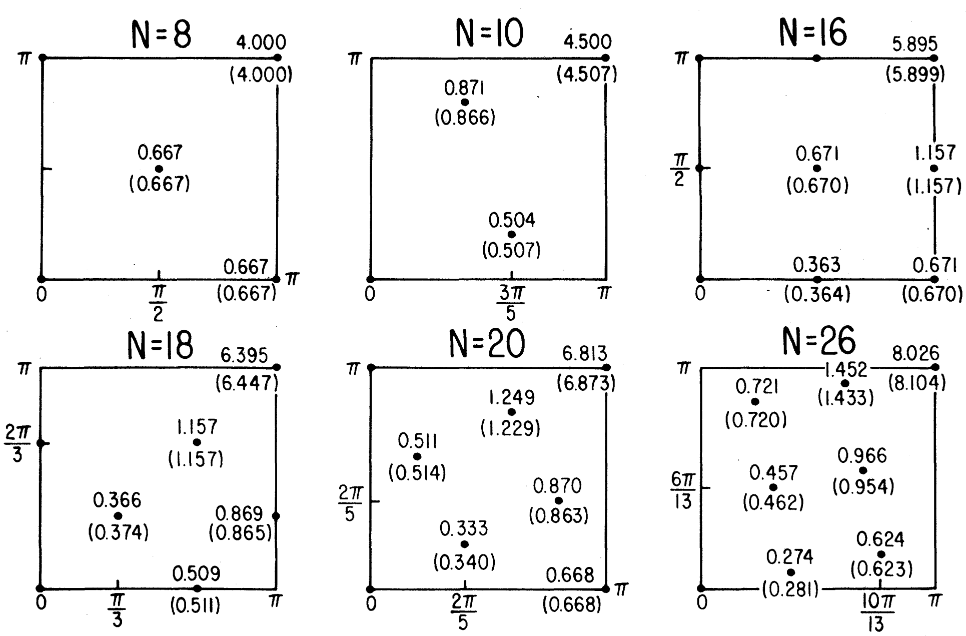

FIG. 1. Spin structure factor on six two-dimensional lattices of N sites. Upper numbers are results of the present sublattice-symmetric spin-wave theory, lower numbers (in parentheses) are exact diagonalization results. We show the first quadrant of the Brillouin zone in each case. The values of the wave vector are given by Eq. (14). For $N=4$ (not shown, see Table I) and $N=8$ the spin-wave results are exact.

on N-site lattices in two dimensions, from exact diagonalization up to $N=26$ and from Monte Carlo simulations by Reger and Young[6] for sizes up to 12×12. $C_{L/2,L/2}$ is the spin-spin correlation for the two spins farthest away on the finite lattice. The lattices of size $N=8$, 10, 18, 20, and 26 are tilted squares that can accommodate the Néel state with periodic boundary conditions, as discussed by Oitmaa and Betts.[7] $N=r^2+s^2$, with $r+s$ even. The agreement is again remarkable, especially for the energy. Note that the spin-wave results for $S(\pi)$ slightly *underestimate* the exact values.

Figure 1 shows comparison of the spin structure factor

$$S(\mathbf{q})=\frac{1}{N}\sum_{l} e^{i\mathbf{q}\cdot\mathbf{l}}\langle \sigma_0\cdot\sigma_1\rangle \ , \tag{13}$$

with exact results for up to $N=26$. The values of q for the tilted lattices of size $N=r^2+s^2$ are given by

$$q_x=\frac{2\pi}{N}(rm+sn) \ , \tag{14a}$$

$$q_y=\frac{2\pi}{N}(sm-rn) \ . \tag{14b}$$

For $N=8$ the spin-wave results are exact, as discussed. For larger N they start to deviate; still, for the entire q dependence the results agree to about 1% in almost all cases.

In summary, we have discussed an extension of conventional spin-wave theory for antiferromagnets that restores the sublattice symmetry in the ground state. The resulting theory is applicable to finite lattices, unlike conventional spin-wave theory, and yields remarkable agreement with exact calculations. For $N=2$, 4, and 8 spins, results for spin-spin correlations are exact. For $S=\frac{1}{2}$, we found the results to be remarkably accurate for a variety of other cases in more than one dimension. As this is a $1/S$ expansion, we expect the results to become even more accurate for larger S.

As $N\rightarrow\infty$, the long-range order m is obtained in the present theory from $S(\pi)=Nm^2+0(\sqrt{N})$. Solution of Eqs. (9) and (11) yields

$$m=\frac{1}{2}\left[2S+1-\int\frac{d^dk}{(2\pi)^d}\frac{1}{(1-\gamma_k^2)^{1/2}}\right] \ , \tag{15}$$

which is the same as conventional spin-wave theory,[5] and yields $m=0.303$ for the $d=2$, $S=\frac{1}{2}$ Heisenberg antiferromagnet. The fact the exact values of $S(\pi)$ on finite lattice are close but slightly above the spin-wave results indicates that the spin-wave result slightly underestimates the long-range order.

The theory discussed here is straightforwardly generalized to finite temperatures. It predicts no long-range order at finite temperatures in $d=2$, and a critical temperature $T_c>0$ in $d=3$. Comparison with exact and renormalization group[8] results at finite temperatures, as well as for dynamic spin-correlation functions, will be discussed in a future publication.

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