Linearly polarized spin waves in the antiferromagnetic Heisenberg model with exchange anisotropy toward the Ising limit

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(Received 8 June 1993)

We examine the nature of the singlet excitations introduced recently to describe the spin dynamics of the antiferromagnetic Heisenberg model with anisotropic coupling. It is shown that they excite spin waves polarized linearly, as opposed to the usual magnons, that are triplet excitations and correspond to circularly polarized waves. The approach yielding the singlet excitations give more accuracy than ordinary spin-wave theory, which shows that the absence of linearly polarized modes is an important flaw of the latter.

We present here insight into a formalism developed in recent years for dealing with the antiferromagnetic Heisenberg model with anisotropic coupling between the spins.[1-8] This approach provides a more accurate description of the ground state than common spin-wave theory[6,8] and shows that a class of excitations, additional to magnons, may be important in the spin dynamics of antiferromagnetic materials. The development we are reporting now clarifies the physical meaning of these excitations and makes apparent the essential difference with magnons.

The lattice is separated into spin-up and spin-down sublattices.[6] The one associated to spin up is characterized by a set of $N/2$ vectors denoted $\mathbf{R}$. The other one is described by the vectors $\mathbf{R}+\boldsymbol{\delta}_0$, where $\boldsymbol{\delta}_0$ is any of the vectors $\boldsymbol{\delta}$ which connect a lattice site with their z nearest neighbors. A translation in $\boldsymbol{\delta}$ always implies a change of sublattice. With this notation the anisotropic Heisenberg Hamiltonian becomes

$$H=J\sum_{\mathbf{R}\boldsymbol{\delta}}\left[s_z(\mathbf{R}+\boldsymbol{\delta})s_z(\mathbf{R})+\frac{\alpha}{2}[s_+(\mathbf{R}+\boldsymbol{\delta})s_-(\mathbf{R})+s_+(\mathbf{R})s_-(\mathbf{R}+\boldsymbol{\delta})]\right], \tag{1}$$

where J is a constant, s_i $(i=x,y,z)$ is a component of the spin assigned to the lattice site stated in the argument, α is the anisotropy parameter, and $s_\pm=s_x\pm is_y$.

The method starts with the observation that the operators[4,6,8]

$$\phi^\dagger_{\boldsymbol{\delta}}(\mathbf{k})=\frac{1}{\sqrt{2S^2N}}\sum_{\mathbf{R}}e^{i\mathbf{k}\cdot\mathbf{R}}s_+(\mathbf{R}+\boldsymbol{\delta})s_-(\mathbf{R})+\frac{\alpha S}{2zS-1}\sqrt{N/2}\,\delta_{\mathbf{k},0}\,, \tag{2}$$

where the vector $\mathbf{k}$ runs over the Brillouin zone associated to one of the two sublattices determined by the antiferromagnetic spin alignment, become good Bose excitations of the Hamiltonian (1) if high antiferromagnetic order is assumed. More precisely, in the asymptotic limit $\alpha\to 0$ one can write[4,6,8]

$$[\phi_{\boldsymbol{\delta}}(\mathbf{k}),\phi^\dagger_{\boldsymbol{\delta}'}(\mathbf{k}')]=\delta_{\boldsymbol{\delta},\boldsymbol{\delta}'}\delta_{\mathbf{k},\mathbf{k}'},\quad [\phi_{\boldsymbol{\delta}}(\mathbf{k}),\phi_{\boldsymbol{\delta}'}(\mathbf{k}')]=0 \tag{3}$$

and

$$[H,\phi^\dagger_{\boldsymbol{\delta}}(\mathbf{k})]=(2zS-1)J\phi^\dagger_{\boldsymbol{\delta}}(\mathbf{k})\,. \tag{4}$$

Hence the ϕ excitations allow us to write H in diagonal form, with the ground-state energy E_g as an additive constant. Within the limitations posed by the approximation of the theory the ground state $|g\rangle$ and its energy can be determined explicitly yielding[4,6,8]

$$|g\rangle=\exp\left[-\frac{\alpha S}{2zS-1}\sqrt{N/2}\sum_{\boldsymbol{\delta}}[\phi^\dagger_{\boldsymbol{\delta}}(0)-\phi_{\boldsymbol{\delta}}(0)]\right]|\mathcal{N}\rangle \tag{5}$$

and

$$\frac{E_g}{NJS^2}=-\frac{z}{2}\left[1+\frac{\alpha^2}{2zS-1}\right], \tag{6}$$

where $|\mathcal{N}\rangle$ is the Néel state assigning the spins up to the sublattice $\{\mathbf{R}\}$.

The procedure is shown to be valid for $0\le\alpha<1$. In one dimension and $S=\frac{1}{2}$ the theory proved to be highly reliable and accurate for $0\le\alpha\le 0.5$ in all calculations.[3] The validity range is expected to increase with S. The precision of the theory proves to improve rapidly with the lattice dimensionality. Equation (6) for the two-dimensional square lattice ($z=4$) and $S=\frac{1}{2}$ turns out to be accurate to better than 0.5% over the whole range $0\le\alpha\le 1$.[4,6]

The theory outlined above was subsequently generalized[8] to the range $1<\alpha<\infty$. The parametric phase transition conjectured by Barnes, Kotchan, and Swanson[9] for the square lattice at $\alpha=1$ on the basis of numerical calculations was clearly obtained. The expression for the ground-state energy given by the extended theory reads[8]

$$\frac{E_g(\alpha)}{NJ}=\begin{cases}-\frac{z}{8}\left[1+\frac{\alpha^2}{z-1}\right], & 0\le\alpha<1\\ -\frac{z}{8}\alpha\left[1+\frac{(1+\alpha)^2}{4(z-1)\alpha^2}\right], & 1<\alpha<\infty\ .\end{cases}\tag{7}$$

Table I compares the ground-state energies given by Eq. (7) with the quantum Monte Carlo (MC) results obtained by Barnes, Kotchan, and Swanson[9] which, to our knowledge, are the state of the art in the numerical computation of the anisotropic $S=\frac{1}{2}$ Heisenberg model in two dimensions. The agreement is better than 0.5% for any α in the interval $0.4\le\alpha\le1.4$. As spin order increases with the lattice dimension one can presume that the agreement is even better in three dimensions. The results of spin-wave theory are also given in Table I. The advantages of the present approach over linear spin-wave theory to describe the ground state of the Heisenberg model become apparent.

The new excitations are essentially different from the antiferromagnetic magnons of spin-wave theory. An important distinction is the spin of the quasiparticles. The ϕ excitations are associated to operators which are sums of terms of the form $s_+(i)s_-(j)$, where i and j denote neighboring sites. Thus they cannot modify the total spin when operating on a state and, consequently, create spinless quasiparticles. On the contrary, the excitations of spin-wave theory follow from a Holstein-Primakoff transformation yielding Bose operators which are sums of odd products of the ladder operators s_+ and s_-. Thus the magnon operators change the total spin in one unit when operating on any state and can be thought of as spin-one excitations.

The ground-state energy given by linear spin-wave theory (that considers no magnon interaction) departs significantly from the exact one-dimensional results of Orbach,[10] or those of reliable numerical computations in two dimensions,[9] as α goes to zero. Though reaching the right value at the Ising limit $\alpha=0$ the asymptotic behavior for $\alpha\approx0$ is clearly wrong. On the other hand, the present method gives, within a scheme of free bosons, the right asymptotic behavior of any physical magnitude when approaching the Ising limit. This strongly suggests that the problem with spin-wave theory is the lack of spin-zero excitations, which become more relevant when approaching the Ising limit.

TABLE I. Ground-state energy $E_g(\alpha)/(NJ)$. The square lattice $z=4$.

α	MC results[a]	Eq. (7)	Spin wave
0.40	−0.528	−0.527	−0.521
0.60	−0.562	−0.560	−0.548
0.80	−0.607	−0.607	−0.590
0.85	−0.620	−0.620	−0.603
0.90	−0.634	−0.635	−0.619
0.95	−0.653	−0.650	−0.636
1.00	−0.669	−0.667	−0.658
1.05	−0.694	−0.691	
1.10	−0.717	−0.717	
1.20	−0.769	−0.768	
1.40	−0.873	−0.871	

[a]Data from Ref. 9.

The Holstein-Primakoff transformation is exact provided the additional restriction is imposed that no more than $2S+1$ spin deviations can occur on any particular lattice site. Hence the failure of linear spin-wave theory in giving the right asymptotic behavior when going to the Ising limit is a consequence of the drop of magnon interactions. Manousakis has shown that interactions yielding magnon pairing are of paramount importance in the ground state.[11] This is quite intuitive since the action of a single magnon operator always changes the state to a subspace of different total spin. To keep within a subspace of given spin one has to add magnons in pairs. Although the results of our method applied to the square lattice are somewhat better than those of Manousakis the two approaches are in the same spirit.

In this paper we demonstrate that the ϕ excitations are associated with spin waves polarized linearly. This provides a physical meaning to the excitations and insight into the structure of the ground state and spin dynamics of the Heisenberg antiferromagnet. Common magnons excite spin waves constituted by coherent motions of the different spins precessing circularly, which shows that the two kinds of excitations are complementary. It follows a physical explanation of why linear spin-wave theory works better for isotropic, or very close to isotropic, spin-spin interactions ($\alpha\approx1$) and rapidly breaks down as α departs from unity. It is expected that the circular polarization of the spin projections on the XY plane be enhanced for isotropic exchange.

Turning to the Heisenberg picture the equations of motion of the z components of the spins

$$\dot{s}_z(\mathbf{R})=\frac{i}{\hbar}[H,s_z(\mathbf{R})],\quad \dot{s}_z(\mathbf{R}+\boldsymbol{\delta})=\frac{i}{\hbar}[H,s_z(\mathbf{R}+\boldsymbol{\delta})]\tag{8}$$

become

$$\dot{s}_z(\mathbf{R})=\frac{i}{\hbar}J\frac{\alpha}{2}\sum_{\boldsymbol{\delta}}[s_+(\mathbf{R}+\boldsymbol{\delta})s_-(\mathbf{R})-s_+(\mathbf{R})s_-(\mathbf{R}+\boldsymbol{\delta})]\tag{9}$$

and

$$\dot{s}_z(\mathbf{R}+\boldsymbol{\delta})=-\frac{i}{\hbar}J\frac{\alpha}{2}\sum_{\boldsymbol{\delta}'}[s_+(\mathbf{R}+\boldsymbol{\delta})s_-(\mathbf{R}+\boldsymbol{\delta}-\boldsymbol{\delta}')-s_+(\mathbf{R}+\boldsymbol{\delta}-\boldsymbol{\delta}')s_-(\mathbf{R}+\boldsymbol{\delta})]\tag{10}$$

after replacing the Hamiltonian (1).

On the other hand, inverting the lattice Fourier transform appearing in the definition (2) of the ϕ operators gives

$$s_+(\mathbf{R}+\boldsymbol{\delta})s_-(\mathbf{R})=2S\sqrt{2/N}\sum_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{R}}\phi_{\boldsymbol{\delta}}^{\dagger}(\mathbf{k})-\frac{2S^2}{2zS-1}\alpha\ .\tag{11}$$

On replacing this in Eqs. (9) and (10) the equations of motion become

$$\dot{s}_z(\mathbf{R})=-i\frac{S\alpha J}{\hbar}\sqrt{2/N}\sum_{\mathbf{k}\delta'}[e^{i\mathbf{k}\cdot\mathbf{R}}\phi_{\delta'}(\mathbf{k})-e^{-i\mathbf{k}\cdot\mathbf{R}}\phi^\dagger_{\delta'}(\mathbf{k})]\ , \tag{12}$$

and

$$\dot{s}_z(\mathbf{R}+\boldsymbol{\delta})=i\frac{S\alpha J}{\hbar}\sqrt{2/N}\sum_{\mathbf{k}\delta'}[e^{i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\delta}-\boldsymbol{\delta}')}\phi_{\delta'}(\mathbf{k})-e^{-i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\delta}-\boldsymbol{\delta}')}\phi^\dagger_{\delta'}(\mathbf{k})]\ . \tag{13}$$

The equations written above are exact. Introducing now the exponential time dependence

$$\phi^\dagger_\delta(\mathbf{k},t)=\phi^\dagger_\delta(\mathbf{k},0)e^{i\omega t}\ , \tag{14}$$

with

$$\omega=\frac{2zS-1}{\hbar}J\ , \tag{15}$$

of the ϕ operators, which rests on the approximation that they represent good excitations of H, Eqs. (12) and (13) can be integrated. The procedure yields

$$s_z(\mathbf{R},t)=\bar{s}_z(\mathbf{R})+\frac{S\alpha J}{2zS-1}\sqrt{2/N}\times\sum_{\mathbf{k}\delta'}[e^{i(\mathbf{k}\cdot\mathbf{R}-\omega t)}\phi_{\delta'}(\mathbf{k},0)+e^{-i(\mathbf{k}\cdot\mathbf{R}-\omega t)}\phi^\dagger_{\delta'}(\mathbf{k},0)]\ , \tag{16}$$

and

$$s_z(\mathbf{R}+\boldsymbol{\delta},t)=\bar{s}_z(\mathbf{R}+\boldsymbol{\delta})-\frac{S\alpha J}{2zS-1}\sqrt{2/N}\sum_{\mathbf{k}\delta'}[e^{i(\mathbf{k}\cdot\mathbf{R}-\omega t)}e^{i\mathbf{k}\cdot(\boldsymbol{\delta}-\boldsymbol{\delta}')}\phi_{\delta'}(\mathbf{k},0)+e^{-i(\mathbf{k}\cdot\mathbf{R}-\omega t)}e^{-i\mathbf{k}\cdot(\boldsymbol{\delta}-\boldsymbol{\delta}')}\phi^\dagger_{\delta'}(\mathbf{k},0)]\ . \tag{17}$$

The time-independent operators $\bar{s}_z(\mathbf{R})$ and $\bar{s}_z(\mathbf{R}+\boldsymbol{\delta})$ are integration constants that represent the time average of the projection of the spins.

Equations (16) and (17) make apparent the nature of the excitations as propagating spin waves in which s_z varies periodically through the lattice. Since the modulus of the spins is fixed this implies that the angle they subtend with the z axis varies the same way. Thus the waves are polarized linearly. The zero-point amplitude of oscillation is

$$\delta s_z=\sqrt{\langle(s_z-\bar{s}_z)^2\rangle}=\frac{\sqrt{z}S}{2zS-1}\alpha\ . \tag{18}$$

The calculation of mean values with respect to the ground state (5), and the excited states obtained from it by the action of the operators (2), deserves a word of caution. The exponent appearing in the expression of the ground state is proportional to $\alpha\sqrt{N}$. Then the parameter α is multiplied by a very large number and, unless $\alpha\ll 1/\sqrt{N}$, the exponent is always significant. This way the ground state has a discontinuity of width $1/\sqrt{N}$ at $\alpha=0$ and the Néel state $|\mathcal{N}\rangle$ does not connect adiabatically with the ground state for finite values of the parameter. Calculations involving the ground state cannot be accomplished by simply expanding the exponential in a Taylor series and retaining only terms with small powers of α. A procedure for deriving power expansions of mean values to finite order in α is given in Ref. 6.

The operators (2) do not change the total spin. Then they are not sufficient to generate the whole Hilbert space of states of the system starting from the ground state. As the ground state has spin zero the set of the ϕ operators spans just the subspace of states with vanishing total spin. In this sense it is not complete and additional spin-one excitations, like magnons, are needed to leave the spin-zero subspace and generate the rest of the Hilbert space. In any event the results displayed in Table I indicate that the ϕ excitations have the main role in the construction of the ground state starting from the Néel state.

The authors acknowledge financial support from FONDECYT.

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