Spectral Function of Holes in a Quantum Antiferromagnet

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By use of an effective Hamiltonian which takes into account the constraints on the motion of a hole in a quantum antiferromagnet, the spectral function of the hole is calculated. For small exchange and away from the antiferromagnetic zone boundary, it is found to be dominated by incoherent multiple-spin-wave processes. The dispersion of the quasiparticle part and the possible implications for disordering of the quantum antiferromagnet are discussed.

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It is becoming increasingly clear that the new oxide superconductors are insulating antiferromagnets for compositions corresponding to one electron per Cu site.[1] The magnetic correlations are strongly two-dimensional (2D) and the three-dimensional ordering at quite high temperatures T is a parasitic effect. The observed temperature dependence of the correlation length is now well understood in terms of the fluctuations of a spin-$\frac{1}{2}$ 2D Heisenberg model with a Néel-type order as $T \rightarrow 0$.[2]

These discoveries have revived the classic problem of the transition from the Mott insulating antiferromagnetic state to the conducting nonmagnetic state as the density of electrons is varied away from one electron per (Cu) site. An essential first step in the solution of this problem is to understand the motion of a hole in the quantum antiferromagnetic (QAFM) Heisenberg model.[3,4]

In the case of highly anisotropic, Ising spin interactions, the motion of the hole always leaves behind a "string" of overturned spins which can be healed only by retracing of the original path, thus leading to self-trapped states centered at the original hole position. These effects were discussed in detail by Nagaev and coworkers,[3,5] and rediscovered by Hirsch,[6] Shraiman and Siggia,[7] and Trugman,[8] in their work on hole pairing in AFM insulators. As recognized by most of these authors, the physics is qualitatively different when the quantum fluctuations associated with the transverse exchange interactions are included from the start. In that case, in a QAFM with a hole, the ground-state wave function is a linear combination of the Néel state and other basis states with different multiple spin deviations. As the hole hops to a neighboring site, it also creates spin deviations, so that the new state is a different linear combination of the Néel state and spin-deviated states—with finite overlap with the earlier state, thus allowing for a Bloch-wave-type solution. Using wave functions which bear close resemblance to that of liquid ^{4}He,[9] we show that the corresponding hole spectral function can easily be calculated.

The Hamiltonian H_t, which describes the hopping of holes from site to site, takes on a relatively simple form if we consider the Néel state $|N\rangle$ as the vacuum state. We define hole operators h_i (that obey Fermi statistics) so that $h_i = c_{i\uparrow}^\dagger$ on the $\uparrow$ sublattice and $c_{i\downarrow}^\dagger$ on the $\downarrow$ sublattice. Furthermore, we define hard-core boson operators b_i, such that $b_i|N\rangle = 0$, $b_i^\dagger = S_i^-$ on the $\uparrow$ sublattice and S_i^+ on the $\downarrow$ sublattice. With these, it may be seen that the hopping part of the Hamiltonian

$$H_t = t \sum_{\langle i,j \rangle} h_i^\dagger h_j [b_j^\dagger (1 - b_i^\dagger b_i) + (1 - b_j^\dagger b_j) b_i] \qquad (1)$$

satisfies all the constraints on the motion of a hole. In particular, it commutes with the number of doubly occupied sites, $\sum_i h_i^\dagger h_i b_i^\dagger b_i$, i.e., it conserves the constraint of no double occupancy, $h_i b_i = 0$. It also properly describes the alteration of spin configurations as the hole moves. The Heisenberg Hamiltonian H_J may similarly be written in terms of b's and projection operators $1 - h_i^\dagger h_i$.

A good ground-state wave function for QAFM's, which includes the zero-point spin deviations, is the Bogolyubov wave function

$$\phi_0 \sim \exp\left(-\sum_{i<j} \lambda_{ij} b_i^\dagger b_j^\dagger\right)|N\rangle. \qquad (2)$$

In linear spin-wave theory (i.e., treating the b's as ideal bosons) ϕ_0 gives results identical to those obtained from the leading term of the Holstein-Primakoff transformation. In the same framework, the Hamiltonian (1) can be rewritten as

$$H_t \simeq \frac{tz}{N^{1/2}} \sum_{\mathbf{k},\mathbf{q}} h_\mathbf{k}^\dagger h_{\mathbf{k}-\mathbf{q}} [a_\mathbf{q}(u_\mathbf{q}\gamma_{\mathbf{k}-\mathbf{q}} + v_\mathbf{q}\gamma_\mathbf{k}) + a_{-\mathbf{q}}^\dagger (v_\mathbf{q}\gamma_{\mathbf{k}-\mathbf{q}} + u_\mathbf{q}\gamma_\mathbf{k})], \qquad (3)$$

where

$$u_{\mathbf{k}}=\{\tfrac{1}{2}[(1-\gamma_{\mathbf{k}}^2)^{-1/2}+1]\}^{1/2}, \tag{4a}$$

$$v_{\mathbf{k}}=-\operatorname{sgn}(\gamma_{\mathbf{k}})\{\tfrac{1}{2}[(1-\gamma_{\mathbf{k}}^2)^{-1/2}-1]\}^{1/2}. \tag{4b}$$

Here, $\lambda_{\mathbf{k}}=-v_{\mathbf{k}}/u_{\mathbf{k}}$ and $\gamma_{\mathbf{k}}=\sum_\delta \exp(i\mathbf{k}\cdot\delta)/z$, where z is the coordination number. The a's are spin-wave operators, $b_{\mathbf{k}}=u_{\mathbf{k}}a_{\mathbf{k}}+v_{\mathbf{k}}a_{-\mathbf{k}}^\dagger$, with dispersion $\omega_{\mathbf{q}}=Jz(1-\gamma_{\mathbf{q}}^2)^{1/2}$.

With (3), a self-consistent diagrammatic approach can be used to evaluate the self-energy of a hole. The leading term in such a series is given by the self-consistent Born approximation

$$\Sigma(\mathbf{k},\omega)=\frac{t^2z^2}{N}\sum_{\mathbf{q}}(u_{\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{q}}+v_{\mathbf{q}}\gamma_{\mathbf{k}})^2G(\mathbf{k}-\mathbf{q},\omega-\omega_{\mathbf{q}}), \tag{5}$$

where

$$G(\mathbf{k},\omega)=[\omega+i0-\Sigma(\mathbf{k},\omega)]^{-1} \tag{6}$$

is the hole Green's function. Here, the limit $T=0$ has been adopted. By inspection, $G(\mathbf{k},\omega)=G(\mathbf{k}+\mathbf{Q},\omega)$, where $\mathbf{Q}=(\pi,\ldots,\pi)$; i.e., the dispersion along $\mathbf{Q}$ is that for next-nearest-neighbor hopping, as it should be if there is a sublattice magnetization.

For $J\gg t$, perturbation theory has been used by Huse and Elser.[10] In this case, Eqs. (5) and (6) can be solved analytically. Most of the spectral weight, $1-O(t^2/J^2)$, appears in the "quasiparticle" (i.e., zero spin-wave) part of $G(\mathbf{k},\omega)$ which has a dispersion

$$\epsilon_{\mathbf{k}}=-\frac{t^2z^2}{N}\sum_{\mathbf{q}}\frac{(u_{\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{q}}+v_{\mathbf{q}}\gamma_{\mathbf{k}})^2}{\omega_{\mathbf{q}}}. \tag{7}$$

The bandwidth of the hole is thus small, $O(t^2/J)$. For frequencies $\omega>\epsilon_{\mathbf{k}}$, the hole spectral function $A(\mathbf{k},\omega)=-\operatorname{Im}G(\mathbf{k},\omega)$ also shows multiple-spin-wave incoherent excitations of weight $O(t^2/J^2)$ (see Fig. 1).

The limit $J\ll t$ is more interesting and relevant to experiments. Unfortunately, it requires a numerical solution of Eqs. (5) and (6). But the general nature of the solution of Eqs. (5) and (6) is well known and has been obtained many times in, for example, electron-phonon problems.[11] At any given $\mathbf{k}$, there is in general a relatively narrow "quasiparticle" peak and a broad, incoherent, multiple-spin-wave background extending to the full free-electron bandwidth. (Strictly speaking, the narrow peak is not a quasiparticle since, except at the AFM zone boundary, it has a width due to scattering with spin waves. This width increases away from $\mathbf{k}=\mathbf{Q}/2$.)

For purpose of illustration, we have evaluated $A(\mathbf{k},\omega)$ in one dimension and for ease of computation inserted a hole lifetime of $10^{-1}t$. [One dimension does have the special property that the quasiparticle peak acquires a finite (asymmetric) width even at $k=Q/2$.] The resulting spectral function is shown in Fig. 2, for various J's and k's, with $t=1$. First of all, the overall picture of Fig. 1 persists. For small but finite J and $k=\pi/2$, $A(\mathbf{k},\omega)$ has a well-defined quasiparticle part situated near the bottom of the *free* hole band, i.e., near $-2t$ [consistent with $-(12t)^{1/2}$ in 2D[4,7]], and a broad, multiple-spin-wave incoherent part. As k is varied away from $\pi/2$, the quasiparticle part follows a dispersion

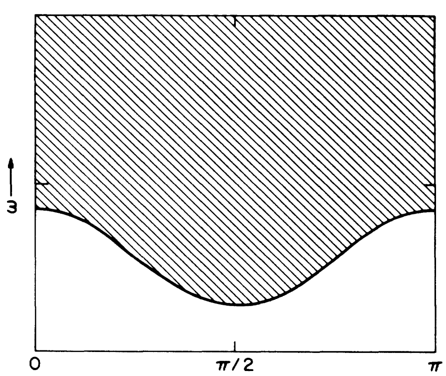

FIG. 1. Sketch of the one-hole excitation spectrum in a QAFM for $\mathbf{k}$ along $\mathbf{Q}=(\pi,\ldots,\pi)$. The full line gives the position of the "quasiparticle" (zero spin-wave) peak, the shaded area the multiple-spin-wave incoherent excitations.

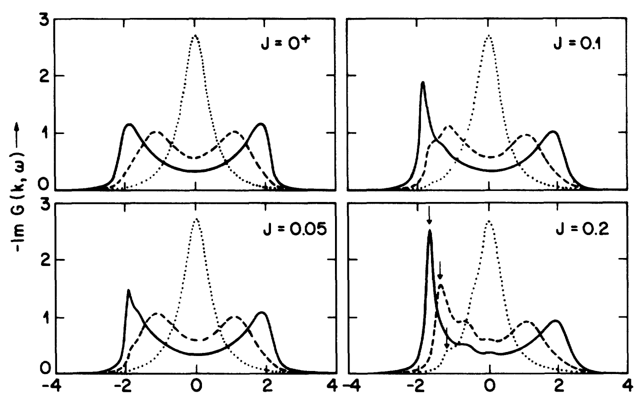

FIG. 2. Hole spectral function as a function of frequency for various exchange interactions J and wave vectors k (full lines, $k=\pi/2$; dashed lines, $k=\pi/4$; dotted lines, $k=0$). The true spectral function has been convoluted with a Lorentzian of half width $10^{-1}t$. The arrows in the $J=0.2$ figure mark the position of the "quasiparticle" peak, which follows a dispersion similar to that sketched in Fig. 1.

similar to that sketched in Fig. 1, but now with a bandwidth of order J.[12] At the same time, the quasiparticle peak decreases in intensity, while the area under the incoherent part grows (the total area is of course conserved and equal to π). As J decreases, the scattering becomes more and more quasielastic and both the quasiparticle spectral weight and bandwidth decrease, until at $J=0^+$ the whole spectrum is incoherent, extending from $-2t$ to $2t$ [$-(12t)^{1/2}$ to $(12t)^{1/2}$ in 2D]. We note that our results for the quasiparticle part are in good agreement with recent exact diagonalization studies of Huse and Elser[10] which yield the lowest energy at a given $\mathbf{k}$. We have verified, for $J=0^+$, where computations are not very complicated, that a spectral function similar to but more slowly varying than in Fig. 2 is obtained in 2D.

Given (3), the only approximation made is the neglect of vertex corrections. These are absent for a Cayley tree. More generally, for $t \ll J$, they are always negligible. In the opposite limit, $J=0^+$, the spectral function $A(\mathbf{k},\omega)$ is all incoherent and weakly dependent on $\mathbf{k}$. This is more so for more dimensions. The vertex corrections are then also nearly momentum independent and do not change the results by more than numerical factors which themselves are small since vertex corrections can be shown to be zero if $A(\mathbf{k},\omega)$ is $\mathbf{k}$ independent.

The major approximation is that (3) neglects the various hard-core constraints and the distortion in the spins due to a static hole. Guided by (2), the former can be included by our writing

$$\phi_0 \sim \prod_{i<j} (1-\lambda_{ij} b_i^\dagger b_j^\dagger)\,|N\rangle. \tag{8}$$

The Fourier transform of λ_{ij} can, as in ^{4}He, be related to the susceptibility.[13] Additionally, in analogy with the wave function for liquid ^{4}He with a defect,[13] which changes the structure factor, we can construct basis states $\phi_0^{(n)}$ which are modifications of (8); the corresponding distortions of the spin orientation and zero-point deviations decay asymptotically as power laws from the position of the hole, n, as may be seen in linear response by use of spin-wave theory. (Similar wave functions are being considered by Shraiman and Siggia.[14]) Once the wave functions ϕ_0 and $\phi_0^{(n)}$ are known, excited states $\psi_i \sim b_i^\dagger \phi_0$ and $\psi_1^{(n)} \sim b_i^\dagger \phi_0^{(n)}$ can be defined, in analogy with Feynman's work on ^{4}He and the related discussion of the motion of a ^{3}He impurity in ^{4}He by McMillan.[9,13] Following the latter, the resulting complete set of wave functions can be used to calculate matrix elements of H_t, thus generating a Hamiltonian of the same form as (3) but with renormalized coefficients. Qualitatively, the results above remain unchanged —quantitatively, the incoherent part is expected to increase somewhat over the results presented.

The hole generates real spin waves while moving and for $J \ll t$, according to Fig. 2, its spectral function is dominated by such incoherent processes, especially for $\mathbf{k}$ away from $\mathbf{Q}/2$. This leads to disordering of the AFM when the number of extra spin deviations per spin is ~ 1. As can be seen from a Lehmann representation in terms of exact eigenstates with $0,1,\ldots,n$ spin waves, the average number of spin waves created can be estimated from the first moment of the incoherent part of $A(\mathbf{k},\omega)$ divided by J. According to our results, Fig. 2, it diverges in the limit $J \to 0$, suggesting that in this limit a hole completely disorders the AFM. This is consistent with Nagaoka's theorem, which states that the ground state for $J=0$ is a saturated ferromagnet (FM).[15] For small J, if we start from the latter and note that the AFM is nothing but a $\mathbf{q}=\mathbf{Q}$ Bose condensate of FM spin flips, the disordered state can be thought of as a vortex created by the hole. (Such states appear to be similar to those postulated in Ref. 14.) In fact, recent *exact* solutions of the problem of a hole interacting with multiple spin flips in a FM yield bound states *above* the free-hole continuum, showing that Néel-type order is pushed away from the hole to large distances.[16] For small J, as more holes are added, the disordering from every additional hole becomes very rapid, since disordering increases with hole momentum away from $\mathbf{Q}/2$. In addition, at a finite hole concentration, if we know the Green's function (6), the holes can be eliminated in Eq. (1), generating additional, frustrating spin-spin interactions, which compete with the original AFM Heisenberg interaction.

Given the spectral function, transport properties like mobility and optical absorption can be directly calculated. Also given H_t, the interaction between two holes can be easily evaluated, much like McMillan's calculation of the interaction of two ^{3}He atoms in ^{4}He.[13] We hope to present these results in the future using wave functions (8).

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[1]D. Vaknin *et al.*, Phys. Rev. Lett. **58**, 2802 (1987); G. Shirane *et al.*, Phys. Rev. Lett. **59**, 1613 (1987); J. M. Tranquada *et al.*, to be published.

[2]S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988).

[3]E. L. Nagaev, *Physics of Magnetic Semiconductors* (MIR, Moscow, 1979).

[4]W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).

[5]L. N. Bulaevskii, E. L. Nagaev, and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **54**, 1562 (1968) [Sov. Phys. JETP **27**, 836 (1968)].

[6]J. E. Hirsch, Phys. Rev. Lett. **59**, 228 (1987).

[7]B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **60**, 740 (1988).

[8]S. A. Trugman, Phys. Rev. B **37**, 1597 (1988).

[9]R. P. Feynman, Phys. Rev. **94**, 262 (1954).

[10]D. A. Huse and V. Elser, private communication.

[11]See, for example, S. Engelsberg and J. R. Schrieffer, Phys. Rev. **131**, 993 (1963); D. Dunn, Phys. Rev. **174**, 855 (1968), and **166**, 822 (1968).

[12]The first suggestion that the "quasiparticle" bandwidth is of order J (rather than t) appears in E. L. Nagaev, Zh. Eksp. Teor. Fiz. **58**, 1269 (1970) [Sov. Phys. JETP **31**, 682 (1970)]. More recently, it was also conjectured by B. I. Shraiman and E. D. Siggia (to be published and private communication), who also obtained the shift in the minimum of the dispersion curve to $\mathbf{k}=(\pi/2,\ldots,\pi/2)$ on the basis of perturbation theory in t/J. The latter result had been discussed independently by Trugman (Ref. 8). An analogous narrowing of the hole bandwidth was also found in a "slave boson" calculation of the hole self-energy in the resonating valence-bond state by C. L. Kane, P. A. Lee, and N. Read (private communication). Finally, we note that both results are also implied by the pair hopping terms in the mean-field treatment of A. E. Ruckenstein, P. J. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1987).

[13]W. L. McMillan, Phys. Rev. **175**, 266 (1968).

[14]Shraiman and Siggia, Ref. 12.

[15]Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[16]Y. Fang, A. E. Ruckenstein, and S. Schmitt-Rink, to be published.