Analytical results for a hole in an antiferromagnet

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The Green's function for a hole moving in an antiferromagnet is derived analytically in the long-wavelength limit. We find that the infrared divergence is eliminated in two and higher dimensions so that the quasiparticle weight is finite. Our results also suggest that the hole motion is polaronic in nature with a bandwidth proportional to $t^2/J \exp[-c(t/J)^2]$ (c is a constant) for $J/t \gtrsim 0.5$. The connection of the long-wavelength approximation to the first-order approximation in the cumulant expansion is also clarified. [S0163-1829(96)50522-9]

It has been recognized for some time[1] that understanding the motion of a hole in a two-dimensional (2D) antiferromagnet (AF) would be an important first step towards a complete understanding of the effect of doping on the CuO_2 planes of high-T_c cuprates, which are known to show antiferromagnetism in the undoped case. The AF with one hole is also a highly nontrivial correlated electron system, and is therefore of fundamental interest from a purely theoretical point of view. There have already been many studies of the one-hole problem including those based on exact diagonalizations (ED) of small clusters,[1–5] the self-consistent Born approximation (SCBA),[6–10] the restricted basis method,[11] the Bogoliubov–de Gennes (BdG) equation,[12] and classical descriptions[13,14] (see Ref. 1 for further references).

The few analytical results which do exist have proved very valuable. However, most of the previous studies have involved numerical calculations (even the studies using the SCBA have to solve Dyson's equation numerically for small clusters). This has left a few points which still need clarification. We mention two of these. First, in the small J/t limit the SCBA yielded a power law dependence for the hole bandwidth [$\sim t(J/t)^\alpha$].[7] This is consistent with the results of ED's on small clusters and gives support to the ''string'' picture.[1] Numerical calculations based on the BdG equation[12] and another variational approach[4] have suggested that the motion of the hole is polaronic in nature in a wide parameter region. However, both of the approaches use a Born-Oppenheimer type approximation, which explicitly breaks translational invariance, and it is not clear how much this may have affected the conclusions. Secondly, although numerical calculations on clusters show that the hole has a finite quasiparticle weight, there is still some uncertainty as to whether the quasiparticle weight vanishes or not in the thermodynamic limit.[15]

Here, by treating spin waves in the long-wavelength (continuum) limit, we derive an analytical expression for the hole Green's function for the hole momentum close to the band minimum $(\pi/2, \pi/2)$. As we work directly in momentum space, translational invariance is *not* broken. This allows us to confirm explicitly the polaronic behavior of the hole. The analytical expression we obtain for the hole Green's function can also be used to directly examine the hole quasiparticle weight. Our expression for the Green's function shows that the infrared catastrophe, which leads to the vanishing of the quasiparticle weight in the 1D case, is eliminated in 2D (and higher dimensions), so that there is a finite quasiparticle weight in 2D. This is consistent with many other studies. We also show that our approach is equivalent to a cumulant expansion and is suitable for large and intermediate J/t, as for the usual polaronic problem. Our approach is therefore complementary to the SCBA, which is better in the small J/t limit.

Our study is based on the t-J model. Treating the spin waves as the collective excitations of the Heisenberg antiferromagnet, the following effective Hamiltonian for the t-J model has been obtained by previous authors:[6,7]

$$\widetilde{H}_1 = H_0 + V, \quad H_0 = \sum_q \omega_q \beta_q^\dagger \beta_q, \tag{1}$$

$$V = \frac{tz}{\sqrt{N}} \sum_{kq} h_{k-q}^\dagger h_k [(u_q \gamma_{k-q} + v_q \gamma_k)\beta_q^\dagger$$

$$+ (u_q \gamma_k + v_q \gamma_{k-q})\beta_{-q}].$$

Here h_k and β_q are the annihilation operators of the hole and the spin wave, z is the coordination number ($z=4$ for a 2D square lattice), $\gamma_q = \sum_\delta e^{iq\cdot\delta}/z$ with δ the unit vectors to nearest neighbors, and N is the number of the lattice

sites. The spin wave excitation spectrum $\omega_q = Jzs\nu_q$ with $\nu_q = \sqrt{1-\gamma_q^2}$ and $s = 1/2$. The Bogoliubov transformation coefficients are $u_q = [(1+\nu_q)/(2\nu_q)]^{1/2}$ and $v_q = -\text{sgn}(\gamma_q)(u_q^2-1)^{1/2}$. Although (1) is not an exact mapping of the t-J model, very good agreement between the results obtained from the effective Hamiltonian and those from the original t-J model have been demonstrated for small clusters by many authors.[8–10] We take the Hamiltonian (1) as our starting point.

The hole Green's function is defined as

$$G(k,\overline{t}) = -i\langle Th_k^H(\overline{t})h_k^{H\dagger}(0)\rangle, \qquad (2)$$

where $\overline{t}$ denotes time throughout the paper. $h_k^H(\overline{t})$ is the Heisenberg operator with respect to H. The thermal average $\langle\cdots\rangle$ is for the spin subsystem. Since there is no hole for the spin subsystem, we can write

$$G(k,\overline{t}) = -i\theta(\overline{t})\langle Te^{iH_0\overline{t}}h_k e^{-iH_0\overline{t}}e^{-i\int_0^{\overline{t}}d\overline{t}_1 V(\overline{t}_1)}h_k^\dagger\rangle,$$

$$\equiv -i\theta(\overline{t})\sum_{m=0}^{\infty} G_m(k,\overline{t}), \qquad (3)$$

where

$$G_m(k,\overline{t}) = \frac{i^{2m}}{(2m)!}\int_0^{\overline{t}}d\overline{t}_1\cdots\int_0^{\overline{t}}d\overline{t}_{2m}$$

$$\times\langle Th_k(\overline{t})V(\overline{t}_1)\cdots V(\overline{t}_{2m})h_k^\dagger\rangle$$

$$= \frac{(itz)^{2m}}{(2m)!N^m}\sum_{k_1q_1,\ldots,k_{2m}q_{2m}}\int_0^{\overline{t}}d\overline{t}_1\cdots\int_0^{\overline{t}}d\overline{t}_{2m}$$

$$\times\langle TM_{k_{2m},q_{2m}}(\overline{t}_{2m})\cdots M_{k_1,q_1}(\overline{t}_1)\rangle$$

$$\times\langle 0|Th_k(\overline{t})\rho_{k_{2m},q_{2m}}(\overline{t}_{2m})\cdots\rho_{k_1,q_1}(\overline{t}_1)$$

$$\times h_k^\dagger(0)|0\rangle. \qquad (4)$$

Here $\rho_{k,q}(\overline{t}) = h_{k-q}^\dagger(\overline{t})h_k(\overline{t})$, and

$$M_{k,q}(\overline{t}) = (u_q\gamma_{k-q}+v_q\gamma_k)\beta_q^\dagger(\overline{t})$$

$$+ (u_q\gamma_k+v_q\gamma_{k-q})\beta_{-q}(\overline{t}). \qquad (5)$$

Formally we are treating V as a perturbation. The operators $O(\overline{t})$ are now defined in an interaction picture with $O(\overline{t}) = \exp(iH_0\overline{t})O\exp(-iH_0\overline{t})$.

The hole part in (4), $\langle 0|h_k(\overline{t})\rho_{k_{2m},q_{2m}}(\overline{t}_{2m})\cdots\rho_{k_1,q_1}(\overline{t}_1)h_k^\dagger(0)|0\rangle$, equals $\langle 0|h_k(\overline{t})h_k^\dagger(0)|0\rangle$ when $k_i = k-\sum_{l=1}^{i-1}q_l$, and is zero otherwise. We can therefore trace out the hole part and write (4) as

$$G_m(k,\overline{t}) = \frac{(itz)^{2m}}{N^m(2m)!}(2m)!\int_0^{\overline{t}}d\overline{t}_{2m}\cdots\int_0^{\overline{t}_3}d\overline{t}_2\int_0^{\overline{t}_2}d\overline{t}_1$$

$$\times\sum_{q_1\cdots q_{2m}}\langle M_{k-\sum_{i=1}^{2m-1}q_i,q_{2m}}(\overline{t}_{2m})\cdots M_{k-q_1,q_2}$$

$$\times(\overline{t}_2)M_{k,q_1}(\overline{t}_1)\rangle. \qquad (6)$$

In general, it is impossible to obtain an analytical expression for (6) for large m since the momentum k_i in $M_{k_i,q_i}(\overline{t}_i)$

varies with time $\overline{t}_i$, reflecting the "history" of the distortion of the spin background induced by the hole.

Based on Wick's theorem, the expectation value [see (6)], $\langle M_{k_{2m},q_{2m}}(\overline{t}_{2m})\cdots M_{k,q_1}(\overline{t}_1)\rangle$, is composed of contractions like

$$B_{k_ik_jq_iq_j}(\overline{t}_i,\overline{t}_j) = \langle M_{k_i,q_i}(\overline{t}_i)M_{k_j,q_j}(\overline{t}_j)\rangle$$

$$= C_{k_ik_jq_iq_j}\delta_{q_i,-q_j}[\langle\beta_{q_i}(\overline{t}_i)\beta_{q_i}^\dagger(\overline{t}_j)\rangle$$

$$+ \langle\beta_{q_i}^\dagger(\overline{t}_i)\beta_{q_i}(\overline{t}_j)\rangle], \qquad (7)$$

where

$$C_{k_ik_jq_iq_j} = (u_{q_i}\gamma_{k_i}+v_{q_i}\gamma_{k_i+q_i})(u_{q_i}\gamma_{k_j-q_i}+v_{q_i}\gamma_{k_j}). \qquad (8)$$

We find that

$$C_{k_ik_jq_iq_j} = \frac{1}{8\nu_{q_i}}[(q_{ix}\sin k_x+q_{iy}\sin k_y)^2+O(q^3,q^2\cos^2 k)], \qquad (9)$$

for k near the band minimum k_0 and for small momentum transfers $\{q_i\}$. The important feature of Eq. (9) is that $C_{k_ik_jq_iq_j}$ does not depend on the exact value of the hole momenta, k_i and k_j, but only on the momentum transfer q_i and the initial momentum k. This result requires only that $\gamma_q = 1+O(q^2)$ for small q and, for $k = k_0+(\delta k_x,\delta k_y)$, $\gamma_k = (\delta k_x+\delta k_y)+O(\delta k^3)$. We can then formally rewrite $G_m(k,\overline{t})$ in (6) as

$$G_m(k,\overline{t}) = \frac{(itz)^{2m}}{(2m)!N^m}\sum_{q_1}\cdots\sum_{q_{2m}}\int_0^{\overline{t}}d\overline{t}_1\cdots\int_0^{\overline{t}}d\overline{t}_{2m}$$

$$\times\langle T\overline{M}_{k,q_{2m}}(\overline{t}_{2m})\cdots\overline{M}_{k,q_1}(\overline{t}_1)\rangle, \qquad (10)$$

where

$$\overline{M}_{k,q}(\overline{t}) = \frac{1}{\sqrt{8\nu_q}}|q_x\sin k_x+q_y\sin k_y|[\beta_q(\overline{t})+\beta_{-q}^\dagger(\overline{t})]. \qquad (11)$$

Using (3), we have

$$G(k,\overline{t}) = -i\theta(\overline{t})\langle Te^{-itz\int_0^{\overline{t}}d\overline{t}_1\Sigma_q\overline{M}_{k,q}(\overline{t}_1)}\rangle \qquad (12)$$

and hence[16]

$$G(k,\overline{t}) = -i\theta(\overline{t})e^{-i\epsilon_k\overline{t}-\phi_k(\overline{t})}, \qquad (13)$$

with

$$\epsilon_k = -\frac{t^2}{J}\frac{1}{N}\sum_q\frac{q_x^2\sin^2 k_x+q_y^2\sin^2 k_y}{\nu_q^2},$$

$$\phi_k(\overline{t}) = -\frac{1}{2}\left(\frac{t}{J}\right)^2\frac{1}{N}\sum_q\frac{q_x^2\sin^2 k_x+q_y^2\sin^2 k_y}{\nu_q^3}$$

$$\times[(e^{-i\omega_q\overline{t}}-1)(N_q+1)+(e^{i\omega_q\overline{t}}-1)N_q]. \qquad (14)$$

Here we will only discuss properties of the hole at zero temperature. At $T = 0$, $N_q \to 0$. In 1D, after performing the sum (integration for an infinite system) over q in (14), we find that the function $\phi_k(\overline{t})|_{k=\pi/2} \sim \ln(1+i\xi\overline{t})$,
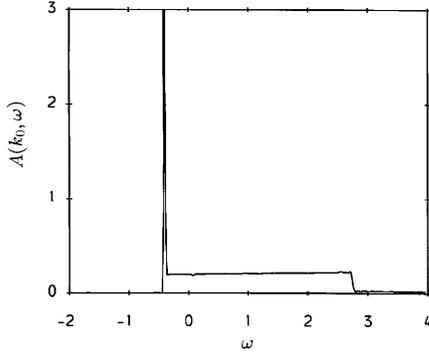
FIG. 1. The hole spectral function $A(k_0,\omega)$ as a function of ω. We take $\xi=\pi$ and $J/t=1.0$. ω is in unit of Jzs.

where $\tilde{t}=\overline{t}Jzs$ and the momentum cutoff $\xi\sim O(1)$. We have approximated the spin spectrum by linear dispersion. The logarithmic divergence at large times leads to the so-called orthogonality catastrophe. The corresponding spectral function $A(k_0,\omega)\sim\theta(\omega-\epsilon_{k_0})(\omega-\epsilon_{k_0})^{g-1}$, with $g=(t/J)^2/2\pi$, and there is no quasiparticle behavior in this case. In 2D, however, we obtain that $\phi_{k_0}(\overline{t})\sim i\tilde{t}^{-1}(e^{-i\xi\tilde{t}}-1)-\xi$. For large $\overline{t}$ (or $\tilde{t}$), since the first term is irrelevant, there is no logarithmic term. The constant term left in $\phi_{k_0}(\overline{t})$ at the large $\overline{t}$ limit contributes a finite quasiparticle weight and the spectral function $A(k,\omega)$ is then of the form

$$A(k,\omega)=2\pi Z_k\delta(\omega-\epsilon_k)+A_{\text{inc}}(k,\omega),\qquad(15)$$

where the quasiparticle weight $Z_k=\exp[-c_k(t/J)^2]$ (c_k are constants). This exponential factor is reminiscent of the Huang-Rhys factor[17,18] in the usual electron-phonon problem, indicating polaronic behavior. This Huang-Rhys factor is in agreement with that obtained using the BdG equation.[12]

Using (13) and linear dispersion as the spin wave spectrum, we obtain that in two dimensions the hole spectral function at k_0 is given by

$$A(k_0,\omega)=2\pi Z_{k_0}\delta(\omega-\epsilon_{k_0})$$
$$+\text{Re}\int_0^\infty d\overline{t}e^{i(\omega-\epsilon_{k_0})\overline{t}}Z_{k_0}[e^{i\alpha(e^{-i\xi c\overline{t}}-1)/\overline{t}}-1],$$
$$(16)$$

where $c=Jzs$ and $\alpha=(t/J)^2/(4\pi c)$. The second term in (16), i.e., the incoherent part, is well behaved. $A(k_0,\omega)$ is shown in Fig. 1. The incoherent part is almost constant over a broad energy region. In the results of very small cluster calculations (both exact and SCBA),[1,21] many secondary peaks in $A(k_0,\omega)$ were found above the lowest quasiparticle one. These secondary peaks were attributed to "string" resonances. However, the cluster calculations also show that, when the size of the system increases, these peaks become less pronounced. Recently, Leung and Gooding[3] found in exact diagonalizations that the secondary peaks which are well defined for a 16-site lattice disappear in a 32-site system and that the secondary peaks are a finite size effect. Our results are consistent with this suggestion. If the secondary peaks were smeared out the spectral function obtained from

the small-cluster calculations would have the same broad feature as that shown in Fig. 1.

We note that the hole Green's function (13) has the same form as that of the first-order approximation in the cumulant expansion. In fact, in the cumulant expansion[17]

$$G(k,\overline{t})=-i\theta(\overline{t})\exp\left\{\sum_{n=1}^\infty F_n(k,\overline{t})\right\},\qquad(17)$$

where $F_1(k,\overline{t})=G_1(k,\overline{t})$, $F_2(k,\overline{t})=G_2(k,\overline{t})-\frac{1}{2!}F_1^2$, $F_3(k,\overline{t})=G_3(k,\overline{t})-F_1F_2-\frac{1}{3!}F_1^3$, $\ldots$. Here G_i is defined in (6). The first order term is given by

$$F_1(k,\overline{t})=(tz)^2\sum_q\frac{(u_q\gamma_{k-q}+v_q\gamma_k)^2}{\omega_q}\{i\overline{t}+[(e^{-i\omega_q\overline{t}}-1)$$
$$\times(N_q+1)+(e^{i\omega_q\overline{t}}-1)N_q]/\omega_q\}.\qquad(18)$$

Since in the long-wavelength limit the spin waves are uncorrelated for the hole at the band minimum, $F_i(k,\overline{t})=0$ for $i\geq2$ and $F_1(k,\overline{t})=-i\epsilon_k\overline{t}-\phi_k(\overline{t})$. So the result of the first-order approximation in the cumulant expansion is exact in the long-wavelength limit for the hole momemtum $k=k_0$. For the usual polaron problem,[19,20] numerical calculations have indicated that the cumulant expansion converges rapidly for weak and intermediate couplings.[20] But quite why the resummation into the exponential like the cumulant expansion is a proper choice for the problem has not been understood clearly. Here for the spin polaron problem, we have established a connection between the first order approximation in the cumulant expansion and the long-wavelength approximation (LWA) for the boson excitations.

The LWA gives a hole energy proportional to t^2/J (14). This is just the first term in an expansion in t/J. We expect that the higher order terms would contribute the usual polaron (band-narrowing) effect, which is described by the Huang-Rhys factor (the quasiparticle weight Z_k). The polaron bandwidth, W, would then scale as[22]

$$W/t=a(t/J)e^{-c(t/J)^2},\qquad(19)$$

with a and c constants. We can justify this expression, at least for small t/J, using Brillouin-Wigner perturbation theory (the usual Rayleigh-Schrodinger expansion is divergent). Since the contribution of the second-order vertex correction in the Brillouin-Wigner expansion vanishes and that of the third-order vertex is small,[8] the lowest order diagrams are given by those of the SCBA. The hole energy is then given by[6–10]

$$E_k=\sum_q\frac{(tz)^2(u_q\gamma_{k-q}+v_q\gamma_k)^2}{E_k-\omega_q-\Sigma(k-q,E_k-\omega_q)},\qquad(20)$$

where $\Sigma(k,\omega)$ is the self-energy of the hole and $E_k=\Sigma(k,E_k)$ for a self-consistent solution. We expand

$$\Sigma(k-q,E_k-\omega_q)=E_{k-q}+\frac{\partial\Sigma(k-q,\omega)}{\partial\omega}\bigg|_{\omega=E_{k-q}}$$
$$\times(E_k-\omega_q-E_{k-q})+O(q^2),\quad(21)$$

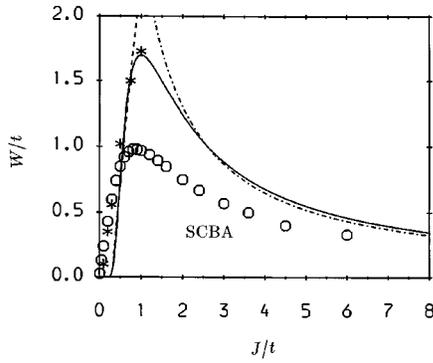for small q and, using the LWA, we obtain

FIG. 2. The hole bandwidth W/t as a function of J/t for a hole moving in a 2D antiferromagnetic background. The functional dependence $W/t = 2.8 (t/J) e^{-0.5(t/J)^2}$ (see the text) is shown by the solid curve, along with the results from the exact diagonalization calculations on 20 sites ("$*$") (Ref. 2), from the self-consistent Born approximation on a cluster of 16×16 (open circles) (Ref. 9), and using a variational approach (Ref. 23). The dashed curve, which is proportional to $(J/t)^{0.677}$, is the best fit to the solid curve for small J/t.

$$E_k = \sum_q (tz)^2 \frac{(u_q \gamma_{k-q} + v_q \gamma_k)^2}{E_k - \omega_q - E_{k-q}} Z_{k-q}, \qquad (22)$$

where $Z_{k-q} = (1 - \partial\Sigma(k-q,\omega)/\partial\omega|_{\omega=E_{k-q}})^{-1}$. From (14), we have $Z_{k-q} = Z_k + O(q^2)$ near $k = k_0$, and Eq. (22) reduces to $E_k = Z_k \epsilon_k$ in LWA [note that $E_k - E_{k-q} = O(q^2)$ near $k = k_0$]. This is the result we expected and justifies in part the assumption that the bandwidth scales as given in (19).

To see how well the universal functional (19) can represent the hole bandwidth, we compare it with numerical results of other studies. We show various estimates for the hole bandwidth in Fig. 2. The dashed-dotted line and "$*$" corre-

spond to results obtained using the variational approach by Sachdev[23] and ED on clusters of 20 sites by Poilblanc et al.[2] The variational approach is reliable in the large J/t case, while most ED's are only available for small J/t. For comparison, the results of SCBA (open circles) are also shown in Fig. 1. We choose $a = 2.8$ and $c = 0.5$ for the functional dependence to fit results of other studies. The functional dependence is shown by the solid curve in Fig. 2. It is close to the variational results for large J/t and to the ED results for small J/t, especially $J/t \gtrsim 0.5$. For small J/t, a power law fit to the functional dependence gives $b + d(J/t)^{0.667}$ (the dashed curve). The coefficients b and d are different from those obtained from the numerical calculations.[2,3,1] The form (19) is thus only qualitatively correct in the small J/t limit. In the region of J/t between 1.0 and 2.0, the functional dependence describes a smooth crossover from t/J behavior in the J/t limit to roughly J/t behavior in the small J/t limit.

In conclusion, we have derived an analytical expression for the Green's function of the hole moving in an antiferromagnet near the band mimimum in the long-wavelength limit. The Green's function clearly indicates that the infrared divergence is eliminated in two dimensions so that the quasiparticle weight is finite. It also suggests that the hole motion has a polaronic nature for intermediate and large J/t. We have shown that the cumulant expansion is a good choice for studying the hole motion in the weak and intermediate coupling cases, with the first-order approximation equivalent to the long-wavelength approximation at the band minimum of the hole. This should be complementary to the self-consistent Born approximation which is better for small J/t limit.

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[16] In deriving Eq. (13) we use the relation $\langle T\exp\{\int_0^t dt \overline{M}(t)\}\rangle = \exp\{\frac{1}{2}\int_0^t dt_1 \int_0^t dt_2 \langle T\overline{M}(t_1)\overline{M}(t_2)\rangle\}$, where $\overline{M}$ is a linear combination of boson operators $\beta_q^\dagger$ and β_q. Equation (13) can also be obtained from the cumulant expansion from the usual polaron problem; see Ref. 17.

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