Analytical results for a hole in an antiferromagnet

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Abstract

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 $t/J \exp[-c(t/J)^2] \ (c$ is a constant). The connection of the long-wavelength approximation to the first-order approximation in the cumulant expansion is also clarified.

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It has been recognised for some time \[1\] that understanding the motion of a hole in a 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 non-trivial 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 \[6–10\], the restricted basis method \[11\], the Bogoliubov-de Gennes (BdeG) equation \[12\], and classical descriptions \[13,14\] (see \[1\] 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. Firstly, in the small $J/t$ limit the SCBA yielded a power law dependence for the hole band width $\sim t(J/t)^{\alpha}$ \[4\]. 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 BdeG equation \[12\] and another variational approach \[1\] 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 behaviour 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 quasi-particle 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 \[6,7\]

\[
\tilde{H}_1 = H_0 + V,
\]
\[
H_0 = \sum_q \omega_q \beta_q^\dagger \beta_q, \tag{1}
\]
\[
V = \frac{tz}{\sqrt{N}} \sum_{kq} h_{k-q} h_k \{ u_q \gamma_{k-q} + v_q \gamma_k \} \beta_q^\dagger + \{ u_q \gamma_k + v_q \gamma_{k-q} \} \beta_{-q}. \]

Here $h_k$ and $\beta_q$ are the annihilation operators of the hole and the spin wave, $z$ is the
coordination number ($z = 4$ for a 2D square lattice), $\gamma_q = \sum_\delta e^{i\delta \cdot q}/z$ with $\delta$ 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:

\[
G(k, \bar{t}) = -i \langle Th_k^H(\bar{t}) h_k^H(0) \rangle, \tag{2}
\]

where $\bar{t}$ denotes time throughout the paper. $h_k^H(\bar{t})$ 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
\[ G(k, \bar{t}) = -i\theta(\bar{t}) \langle Te^{iH_0\bar{t}}h_k e^{-iH_0\bar{t}} e^{-i \int_0^\bar{t} d\bar{t}_1 V(\bar{t}_1)} h_k^\dagger \rangle, \]
\[ \equiv -i\theta(\bar{t}) \sum_{m=0}^\infty G_m(k, \bar{t}), \quad (3) \]

where
\[ G_m(k, \bar{t}) = \frac{(iz)^{2m}}{(2m)!} \int_0^{\bar{t}} d\bar{t}_1 \ldots \int_0^{\bar{t}} d\bar{t}_{2m} \langle Th_k(\bar{t})V(\bar{t}_1) \ldots V(\bar{t}_{2m})h_k^\dagger \rangle. \]
\[ = \frac{(iz)^{2m}}{(2m)! N^m} \sum_{k_1 q_1, \ldots, k_{2m} q_{2m}} \int_0^{\bar{t}} d\bar{t}_1 \ldots \int_0^{\bar{t}} d\bar{t}_{2m} \langle TM_{k_{2m}, q_{2m}}(\bar{t}_{2m}) \ldots TM_{k_1 q_1}(\bar{t}_1) \rangle \]
\[ \langle 0| Th_k(\bar{t}) \rho_{k_{2m}, q_{2m}}(\bar{t}_{2m}) \ldots \rho_{k_1 q_1}(\bar{t}_1) h_k^\dagger(0)|0 \rangle. \quad (4) \]

Here \( \rho_{k,q}(\bar{t}) = h_k^\dagger(\bar{t})h_k(\bar{t}) \), and
\[ M_{k,q}(\bar{t}) = (u_q \gamma_{k-q} + v_q \gamma_k) \beta^\dagger_{q}(\bar{t}) + (u_q \gamma_k + v_q \gamma_{k-q}) \beta^{}_{q}(\bar{t}). \quad (5) \]

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

The hole part in (4), \( \langle 0| h_k(\bar{t}) \rho_{k_{2m}, q_{2m}}(\bar{t}_{2m}) \ldots \rho_{k_1 q_1}(\bar{t}_1) h_k^\dagger(0)|0 \rangle \), equals \( \langle 0| h_k(\bar{t}) h_k^\dagger(0)|0 \rangle \) when \( k_i = k - \sum_{i=1}^{l-1} q_i \), and is zero otherwise. We can therefore trace out the hole part and write (4) into
\[ G_m(k, \bar{t}) = \frac{(iz)^{2m}}{N^m (2m)!} \int_0^{\bar{t}} d\bar{t}_2 \ldots \int_0^{\bar{t}} d\bar{t}_1 \sum_{q_1 \ldots q_{2m}} \langle M_{k_1} \sum_{q_{1}, q_{2m}} (\bar{t}_{2m}) \ldots M_{k_{2m} q_{2m}}(\bar{t}_1) \rangle \].
\[ \quad (6) \]

In general, it is impossible to obtain an analytical expression for (4) for large \( m \) since the momentum \( k_i \) in \( M_{k_i q_i}(\bar{t}_i) \) varies with time \( \bar{t}_i \), reflecting the “history” of the distortion of the spin background induced by the hole.

Here we derive an analytical expression for the Green’s function treating spin waves in the long wavelength or continuum limit. Based on Wick’s theorem, the expectation value (see (4)), \( \langle M_{k_{2m}, q_{2m}}(\bar{t}_{2m}) \ldots M_{k_1 q_1}(\bar{t}_1) \rangle \), is composed of contractions like
\[ B_{k,k_j q_j}(\bar{t}_i, \bar{t}_j) = \langle M_{k_i q_i}(\bar{t}_i) M_{k_j q_j}(\bar{t}_j) \rangle \]
\[ = C_{k,k_j q_j} \delta_{q, -q_j} [\langle \beta^\dagger_{q_j}(\bar{t}_i) \beta_{q_j}(\bar{t}_j) \rangle + \langle \beta^\dagger_{q_j}(\bar{t}_j) \beta_{q_j}(\bar{t}_i) \rangle], \quad (7) \]
where
\[ C_{k_{i}q_{i}k_{j}q_{j}} = (u_{q_{i}}\gamma_{k_{i}} + v_{q_{i}}\gamma_{k_{i}+q_{i}})(u_{q_{j}}\gamma_{k_{j}-q_{i}} + v_{q_{j}}\gamma_{k_{j}}), \] (8)

We find that
\[ C_{k_{i}q_{i}k_{j}q_{j}} = \frac{1}{8\nu_{q_{i}}} \left[ (q_{ix}\sin k_{x} + q_{iy}\sin k_{y})^2 + O(q^2, q^2\cos^2 k) \right], \] (9)

for \( k \) near the band minimum \( k_{0} \) and for small momentum transfers \( q \). The important feature of Eq (9) is that \( C_{k_{i}q_{i}k_{j}q_{j}} \) 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 \( G_{m}(k, \bar{t}) \) in (6) as
\[ G_{m}(k, \bar{t}) = \frac{(itz)^{2m}}{(2m)!N^{m}} \sum_{q_{1}...q_{2m}} \int_{\bar{t}_{0}}^{\bar{t}} \int_{\bar{t}_{0}}^{\bar{t}} d\bar{t}_{1}...d\bar{t}_{2m} \langle T\bar{M}_{k,q_{2m}}(\bar{t}_{2m})...\bar{M}_{k,q_{1}}(\bar{t}_{1}) \rangle, \] (10)

where
\[ \bar{M}_{k,q}(\bar{t}) = \frac{1}{\sqrt{8\nu_{q}}} |q_{x}\sin k_{x} + q_{y}\sin k_{y}|[\beta_{q}(\bar{t}) + \beta_{q}^{\dagger}(\bar{t})]. \] (11)

Using (8), we have
\[ G(k, \bar{t}) = -i\theta(\bar{t})\langle T e^{-itz} \int_{\bar{t}_{0}}^{\bar{t}} d\bar{t}_{1} \sum_{q} \bar{M}_{k,q}(\bar{t}_{1}) \rangle \] (12)

and hence [16]
\[ G(k, \bar{t}) = -i\theta(\bar{t})e^{-\epsilon_{k}\bar{t}} - \phi_{k}(\bar{t}), \] (13)

with
\[ \epsilon_{k} = -t^2 \frac{1}{JN} \sum_{q} \frac{q_{x}^2\sin^2 k_{x} + q_{y}^2\sin^2 k_{y}}{\nu_{q}^2}, \]
\[ \phi_{k}(\bar{t}) = -\frac{1}{2} \left( \frac{t}{J} \right)^2 \frac{1}{N} \sum_{q} \frac{q_{x}^2\sin^2 k_{x} + q_{y}^2\sin^2 k_{y}}{\nu_{q}^3} \left[(e^{-i\omega_{q}\bar{t}} - 1)(N_{q} + 1) + (e^{i\omega_{q}\bar{t}} - 1)N_{q} \right]. \] (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 \( \phi_k(\tilde{t})|_{k=\pi/2} \sim \ln(1 + i\xi\tilde{t}) \) here \( \tilde{t} = \tilde{t}/Jzs \) and the momentum cut-off \( \xi \sim O(1) \). 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 \( \phi_{k_0}(\tilde{t}) \sim i\tilde{t}^{-1}(e^{-i\xi\tilde{t}} - 1) - \xi \). For large \( \tilde{t} \) (or \( \tilde{t} \)), since the first term is irrelevant, there is no logarithmic term. The constant term left in \( \phi_{k_0}(\tilde{t}) \) at the large \( \tilde{t} \) limit contributes a finite quasiparticle weight and the spectral function \( A(k, \omega) \) is then of the form

\[
A(k, \omega) = 2\pi Z_k \delta(\omega - \epsilon_k) + A_{inc}(k, \omega),
\]

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 a 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

\[
A(k_0, \omega) = 2\pi Z_k \delta(\omega - \epsilon_k) + \text{Re} \int_0^\infty d\tilde{t} e^{i(\omega - \epsilon_{k_0})\tilde{t}} Z \left[ e^{i\alpha(e^{-i\xi\tilde{t}} - 1)/\tilde{t}} - 1 \right],
\]

where \( \alpha = (t/J)^2/(4\pi c) \). The second term in (16), i.e. the incoherent part, is well-behaved. \( A(k, \omega) \) 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) [12,21], many secondary peaks in \( A(k, \omega) \) 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 and, 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

\[ G(k, \bar{t}) = -i\theta(\bar{t}) \exp\{ \sum_{n=1}^{\infty} F_n(k, \bar{t}) \}, \tag{17} \]

where

\[ F_1(k, \bar{t}) = G_1(k, \bar{t}), \]
\[ F_2(k, \bar{t}) = G_2(k, \bar{t}) - \frac{1}{2!} F_1^2, \]
\[ F_3(k, \bar{t}) = G_3(k, \bar{t}) - F_1 F_2 - \frac{1}{3!} F_1^3, \ldots \]

Here \( G_i \) is defined in (8). The first order term is given by

\[ F_1(k, \bar{t}) = (t_2)^2 \sum_q \frac{(u_q \gamma_{k-q} + v_q \gamma_{k})^2}{\omega_q} \left\{ i\bar{t} + \left[ (e^{-i\omega_q \bar{t}} - 1)(N_q + 1) + (e^{i\omega_q \bar{t}} - 1)N_q \right] / \omega_q \right\}. \tag{19} \]

Since in the long-wavelength limit the spin waves are uncorrelated for the hole at the band minimum, \( F_i(k, \bar{t}) = 0 \) for \( i \geq 2 \) and \( F_1(k, \bar{t}) = -i\epsilon_k \bar{t} - \phi_k(\bar{t}) \). So the result of the first-order approximation in the cumulant expansion is exact in the long-wavelength limit for the hole momentum \( k = k_0 \). For the usual polaron problem [13,20], 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 establish a connection between the first order approximation in the cumulant expansion and the long-wavelength approximation for the boson excitations.

The LWA gives that the energy of the hole scales as \( t^2/J \), as seen in (14), which should be correct only in the large \( J/t \) case. In the intermediate and strong coupling regions, the BdeG study [12] suggests that the energy should be multiplied by the Huang-Rhys factor, in which case the bandwidth should be represented by
\[ W/t = a \frac{t}{J} e^{-c(t/J)^2}, \]  

where \( a \) and \( c \) are independent of \( t \) and \( J \). To see how well this universal functional 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 “⋆” correspond to results obtained using the variational approach by Sachdev \cite{22} and ED on clusters of 20 sites by Poilblanc et al \cite{4}. The variational approach is reliable in the large \( J/t \) case, while most ED’s are only available for small \( J/t \). 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 very close to the variational results for large \( J/t \) and to the ED results for small \( J/t \), especially \( J/t \geq 0.4 \). 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 \cite{2,3,1}. The form (20) 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. For comparison, the results of SCBA (open circles) are also shown in Fig. 1. The SCBA seems to substantially underestimate values of the bandwidth in the intermediate and the large \( J/t \) cases \cite{8}.

We would like to mention that although the energy of the hole \( \epsilon_k \) in (14), which is proportional to \( \sin^2 k_x + \sin^2 k_y \), gives rise to the hole pockets at \( k_0 \) correctly, the other terms like \( \cos k_x \cos k_y \), which lead to anisotropy of the effective mass, are of higher order in LWA. So the LWA cannot be expected to give the anisotropy quantitatively. To discuss the anisotropy of the effective mass qualitatively, one could use the result of the first order approximation of the cumulant expansion, i.e., Eq. (19).

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

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FIGURES

FIG. 1. The hole spectral function \( A(k_0, \omega) \) as a function of \( \omega \). We take \( \xi = \pi \) and \( J/t = 1.0 \). \( \omega \) is in unit of \( Jzs \).

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 \( W/t = 2.87e^{-0.5(t/J)^2} \) (see the text) is shown by the solid curve, along with the results from the exact diagonalization calculations on 20 sites (“⋆”) [2], from the self-consistent Born approximation on a cluster of 16 × 16 (open circles), [9] and using a variational approach. [22] The dashed curve, which is proportional to \( (J/t)^{0.677} \), is the best fit to the solid curve for small \( J/t \).