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Self-consistent wave function for magnetic polarons in the t-J model

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We derive a wave function for a single hole in the t-J model that is an approximate solution to the Schrödinger equation to all orders in the number of excited spin waves in the quasiparticle, for arbitrary values of t/J. The self-consistent Green-function equation used by Schmitt-Rink, Varma, and Ruckenstein and Kane, Lee, and Read arises as a consistency condition for the existence of a solution to the Schrödinger equation. The approximation provides a wave function for the strong-polaron problem due to electron-phonon coupling as well. The wave function predicts the same dipolar variation of the average staggered spin deviation at large distances, at the band minimum, as does the semiclassical wave function of Shraiman and Siggia, but the quasiparticle state is not orthogonal to the bare-hole state ($z_k \neq 0$).

The problem of a single hole in an antiferromagnetic background has been studied extensively within the t-J model. Excellent agreement is found between analytic results for the Green function obtained by a lowest-order self-consistent approximation (LSCA) introduced by Kane, Lee, and Read,[1] and Schmitt-Rink, Varma, and Ruckenstein,[2] and the Green function obtained by exact diagonalization of small systems.[3] There has been no theory for the wave function associated with the energies calculated through the LSCA. It is shown here that an approximation analogous to the retraceable path approximation[4] allows one to solve the infinite dimensional set of equations that are the Schrödinger equation to all orders in the number of excited spin waves in the quasiparticle. This leads to the LSCA for the Green function as a self-consistency requirement for the solution for the wave function to exist. The wave function permits a detailed calculation at long and short distances of the structure of the magnetic polaron formed around the hole. We find that the long-distance behavior at the band minimum is identical to that predicted by Shraiman and Siggia[5] (SS) from a semiclassical treatment, although the behavior at the band maximum is different. The same method is applicable to the electron-phonon interaction. The wave function also permits a resolution of an apparent contradiction in the literature between the prediction of the LSCA and the semiclassical wave function of Shraiman and Siggia[5] (SS). The spin deviations of the background at large distances from the hole are predicted to be dipolar in their theory, and as Anderson has pointed out,[6,7] if this is true, then the quasiparticle wave function used by SS is orthogonal to the bare hole in the antiferromagnet. There would then be a vanishing strength for the quasiparticle pole in the Green function, $z_k=0$, in contradiction to the result of the LSCA, where the pole at the band minimum has a finite strength. Sorella[7] has investigated this question numerically for the large U Hubbard model and gives results that tend to support the vanishing of the strength of the pole while the work of Song and Annett on the t-J model,[8] also numerical, suggests that it is not zero.

Malshukov and Mahan[9] have discussed the problem of a static vacancy in the Heisenberg model, obtaining a finite pole strength. Their results do not bear directly on the problem with a finite hopping, since the dipolar pattern is due to the hopping, and they make no argument that the pole strength is continuous as $t \to 0$. The question is central to discussions of the many-particle state, since it is difficult to see how a Fermi liquid would arise at finite densities if the pole strength was zero for a single particle. We show here that the apparent contradiction between the two lines of approach can be resolved by the present fully quantum mechanical calculation of the wave function for the hole.

The Hamiltonian we begin with is the approximation to the t-J Hamiltonian obtained by treating the copper spins with a spin-wave approximation, as derived in different fashions in Refs. 1 and 2

$$H_{t\text{-}J} \cong 4tN^{-1/2}\sum_{k,q} U(k,q)[f^\dagger_{k-q}f_k\alpha^\dagger_q + f^\dagger_k f_{k-q}\alpha_q] + \sum \omega_q \alpha^\dagger_q \alpha_q \ , \tag{1}$$

where $U(k,q)=\mu_q\gamma_{k-q}+\nu_q\gamma_k$, $\gamma_k=\frac{1}{2}(\cos k_x+\cos k_y)$, $\omega_q=4JS(1-\gamma_k^2)^{1/2}$, and μ_q and ν_q are the Bogolyubov coefficients satisfying $\mu_q+\nu_q=[(1-\gamma_k)/(1+\gamma_k)]^{1/4}$, $\mu_q^2-\nu_q^2=1$. The f_k are spinless fermion operators and the α_q the boson spin wave operators. Let

$$|\Psi\rangle = a^0(k)f^\dagger_k|0\rangle + N^{-1/2}\sum_q a^1(k,q)f^\dagger_{k-q}\alpha^\dagger_q|0\rangle + N^{-1}\sum_{q_1q_2} a^2(k,q_1,q_2)f^\dagger_{k-q_1-q_1}\alpha^\dagger_{q_2}\alpha^\dagger_{q_1}|0 + \cdots \ , \tag{2}$$

where $a^n(k,q_1,\ldots,q_n)$ are coefficients to be determined, and the vacuum is the product of the hole vacuum and the spin-wave vacuum.

Then the Schrödinger equation $(\lambda-H)|\Psi\rangle=0$ corresponds to an infinite set of equations, the first two of which are

$$\mathbf{a}^0(k)\lambda - \frac{1}{N}\sum_q \mathbf{a}^1(k,q)\mathbf{U}(k,q)=0 \ , \tag{3}$$

$$\mathbf{a}^1(k,q)(\lambda-\omega_q) - \frac{1}{N}\sum_{q_2}\mathbf{a}^2(k,q,q_2)\mathbf{U}(k-q,q_2) - \frac{1}{N}\sum_{q_1}\mathbf{a}^2(k,q_1,q)\mathbf{U}(k-q,q_1)=\mathbf{a}^0(k)\mathbf{U}(k,q) \ . \tag{4}$$

Let us assume that

$$a^2(k,q_1,q_2)=a^1(k,q_1)U(k-q_1,q_2)\times G(k-q_1-q_2,\lambda-\omega_{q_1}-\omega_{q_2}) , \quad (5)$$

where

$$G(k,\lambda)=[\lambda-\Sigma(k,\lambda)]^{-1} \quad (6)$$

and Σ and G are related by the LSCA

$$\Sigma(k,\lambda)=N^{-1}\sum_q U(k,q)^2 G(k-q,\lambda-\omega_q) . \quad (7)$$

Then, neglecting the second sum appearing in Eq. (4), we have

$$a^1(k,q)=a^0(k)U(k,q)G(k-q,\lambda-\omega_q) \quad (8)$$

and λ is determined by

$$a^0(k)[\lambda-\Sigma(k,\lambda)]=0 . \quad (9)$$

If λ is a pole of G, then $a^0(k)$, which can be chosen to be 1, $a^1(k,q), a^2(k,q_1,q_2)$ will be the wave function of the quasiparticle in this approximation. The procedure outlined above can be extended to all orders and we will obtain the solution

$$a^n(k,q_1,\ldots,q_n)=a^{n-1}(k,q_1,\ldots,q_{n-1})\times U(k-q_1-q_2\ldots-q_{n-1})\times G(k-q_1-q_2\ldots-q_n,\omega-\omega_{q_1}-\omega_{q_2}\ldots-\omega_{q_n}) . \quad (10)$$

The right-hand side of the equation for $a^n(k,q_1,\ldots,q_n)$ will be $a^{n-1}(k,q_1,\ldots,q_{n-1})U(k-q_1-q_2\ldots-q_{n-1},q_n)$. Of the $n+1$ terms that arise from annihilating one of the $n+1$ magnons in the $n+1$st term in the wave function, only the term corresponding to annihilation of the $n+1$st magnon, or in other words, the last one created as we have written the wave function, is retained. It is easy to see that (10) is then always a solution at any order. The neglect of the annihilation of all but the last spin deviation created is the essence of the Brinkman and Rice retraceable path approximation for the Green function,[4] and the present work extends that approximation to the calculation of the wave function. In fact, Rice and Brinkman[10] have given a derivation for the Green function for a related model that is similar in spirit to the derivation given here for the wave function. The wave function obtained here is evidently on the same level of approximation as the Green function of the LSCA. It is also obvious that the approximation is valid for any Hamiltonian with the same structure as (1), such as the electron-phonon interaction. Having obtained the wave function, we can examine the spin pattern around the hole.

The average value of the spin on the copper at site j due to the presence of a hole at site i is $\langle\Psi|n_i\mathbf{S}_j|\Psi\rangle/\langle\Psi|\Psi\rangle$, where $n_i=f_i^\dagger f_j$. $S_q^\pm$ in terms of the spin-wave creation and annihilation operators is $S_q^\pm=\frac{1}{2}(\mu_q+\nu_q)[(a_{-q}^\dagger+\alpha_q)\pm(\alpha_{-\bar{q}}^\dagger-\alpha_q^-)]$. Then

$$N\langle\Psi|n_iS_j^\pm|\Psi\rangle=N^{-1}\sum_q e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\tfrac{1}{2}(\mu_1+\nu_q)\times\sum_{n=0}^{\infty}N^{-n}\sum_{P,q_1,\ldots,q_n}[a_{n+1}^*(k,P(q_1,\ldots,q_n-q))a_n(k,q_1,\ldots,q_n)+a_n^*(q_1,\ldots,q_n)a_{n+1}(k,P(q_1,\ldots,q_nq))]\pm a_{n+1}^*(k,P(q_1,\ldots,q_n-\bar{q}))a_n(k,q_1,\ldots,q_n)-a_n^*(q_1,\ldots,q_n)a_{n+1}(k,P(q_1,\ldots,q_n\bar{q}))e^{i\mathbf{q}_0\cdot\mathbf{r}_i} \quad (11)$$

where $P(q_1,\ldots,q_n,q)$ is a permutation of the arguments, and all permutations are summed over. $\bar{q}=\mathbf{q}-\mathbf{q}_0, \mathbf{q}_0=(\pi,\pi)$.

The leading term, setting $a_0=1$, is

$$N^{-1}\sum_q e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\tfrac{1}{2}(\mu_q+\nu_q)[U(k,-q)G^*(k+q,\lambda-\omega_q)+U(k,q)G(k-q,\lambda-\omega_q)]\pm[U(k,-\bar{q})G^*(k+\bar{q},\lambda-\omega_{\bar{q}})-U(k,\bar{q})G(k-\bar{q},\lambda-\omega_q)]e^{i\mathbf{q}_0\cdot\mathbf{r}_i} . \quad (12)$$

We want to evaluate this for large values of $(\mathbf{r}_i-\mathbf{r}_j)$, that is, small $\mathbf{q}$, or $\bar{q}$. We will choose k to be at the band minimum $(\pi/2,\pi/2)$ and $\lambda=\lambda_k$. We have then

$$G^{-1}(k-q,\lambda_k-\omega_q)=\lambda_k-\Sigma(k-q,\lambda_k-\omega_q)-\omega_q \quad (13)$$

Since $\lambda_k=\Sigma(k,\lambda_k)$ is the energy at the band minimum,

$$\frac{\partial\Sigma}{\partial k}(k,\lambda_k)=\frac{\partial\lambda_k}{\partial k}=0 , \quad (14)$$

and hence

$$G(k-q,\lambda_k-\omega_q)\underset{q=0}{\rightarrow}\frac{1}{-\omega_q}\left[1-\frac{\partial\Sigma}{\partial\omega}(k,\lambda_k)\right]^{-1} . \quad (15)$$

The Green functions are real for the values of the arguments we are interested in. Since $U(k+q_0,q)=-U(k,q)$ it follows that $G(k+q_0,q)=G(k,q)$. Then (15) holds as well when $\bar{q}\rightarrow 0$. At $k=(\pi/2,\pi/2)$, the band minimum, $U(k,q)=\frac{1}{2}\mu_q[\sin q_x+\sin q_y]$, and is odd under $q\rightarrow -q$, so that only the second bracketed term in (12) contributes. The spin deviation is entirely in the y direction and has the value

$$N\langle\Psi|n_iS_j^y|\Psi\rangle=\pm N^{-1}\frac{4t}{1-\partial\Sigma/\partial\omega}\sum_q\sin\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)\times\left[\frac{(\mu_q+\nu_q)\mu_q[\sin q_x+\sin q_y]}{\omega_q}\right] \quad (16)$$

which approaches, at large distances,

$$\pm e^{i\mathbf{q}^0\cdot(\mathbf{r}_i-\mathbf{r}_j)}\frac{\sqrt{2T}}{J(1-\partial\Sigma/\partial\omega)}N^{-1}\times\sum_q\sin\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)\frac{q_x+q_y}{q^2} , \quad (17)$$

where the $\pm$ sign depends upon the sublattice the hole is on. $\mu_q+\nu_q\propto q^{1/2}$ for small q, and $\bar{q}^{-1/2}$ for small $\bar{q}$. There is thus no long-range component for the magneti-

zation, but the staggered magnetization is the Fourier transform of $(\bar{q}_x+\bar{q}_y)/\bar{q}^2$, the small $\bar{q}$ limit of the term in brackets in (16). This is the asymptotic form predicted by SS on the basis of a variational calculation, and corresponds to a dipolar pattern in real space.

At $k=0$, $U(k,q)=\mu_q\gamma_q+\nu_q$ and the functional form $G(k-q,\lambda_k-\omega_q)$ given by (15) still holds for sufficiently small q, since λ_k is now a maximum. $U(k,q)$ is even under $q\rightarrow -q$, so that only the first bracketed term in (12) contributes.

$$N\langle\Psi|n_i S_j^x|\Psi\rangle = N^{-1}\frac{4t}{1-\partial\Sigma/\partial\omega} \times\sum\cos q(r_i-r_j) \times\frac{(\mu_q+\nu_q)(\mu_q\gamma_q+\nu_q)}{\omega_q} . \quad (18)$$

The magnetization is in the x direction and short ranged as SS predict, but there is also a long-ranged isotropic component of the staggered magnetization varying as $1/r$ that they have not treated. We would not expect a dipolar contribution at this wave vector as there is no particle current to produce it.

When higher-order terms in (11) are considered, the only terms that contribute to the long-distance behavior are the permutations in Eq. (11) in which the wave vector q is the first, for these are the only terms that are singular as $\mathbf{q}\rightarrow\mathbf{q}_0$. Then

$$a^{n+1}(k,q,q_1,\ldots,q_n) =U(k,q)G(k-q,\lambda_k-\omega_q)U(k-q,q_1) \times G(k-q-q_1,\lambda_k-\omega_q-\omega_{q_1})\cdots . \quad (19)$$

The first factor of G is singular at $\mathbf{q}=\bar{\mathbf{q}}$. The remainder are not. When the singularity due to the first Green's function is factored out of $a^{n+1}(k,q_1,\ldots,q_n)$, and the limit $q=(\pi,\pi)$ is taken in the remaining sums, we see that the integrals are identical to those that would appear in the nth term of the normalization factor $\langle\Psi|\Psi\rangle$ except that half of the vertices and Green's function are evaluated at $\bar{k}$, rather than k. The vertex $U(\bar{k},q)=-U(k,q)$ while $G(\bar{k},\omega)=G(k,\omega)$. Thus, if $\langle\Psi|\Psi\rangle=\sum_{n=0}^{\infty}I_n$, where $2n$ is the number of vertices appearing in the integrals, then the right-hand side of Eqs. (16) and (18) is simply multiplied by a factor of $\sum_{n=0}^{\infty}(-1)^n I_n$ when we include the higher-order terms in Eq. (11).

The factor $[1-\partial\Sigma/\partial\omega]^{-1}$ in Eqs. (16) and (18) is just the quasiparticle amplitude, z_k, giving the overlap of a bare hole with the quasiparticle. z_k may be defined directly from the wave function

$$z_k=|\langle 0|f_k|\Psi\rangle|^2/\langle\Psi|\Psi\rangle=\langle\Psi|\Psi\rangle^{-1} \quad (20)$$

with $a_0=1$ in Eq. (2). The two expressions for z_k are not obviously equivalent, and in fact, are not equal if one includes all possible permutations of the boson indices in (2) when one calculates $\langle\Psi|\Psi\rangle$. However, if only those permutations corresponding to what would be noncrossing diagrams for a self-energy are considered, it may be shown that the two expressions are identical.[11] In this case, the terms I_n in the expression for the normalization factor and the form factor $\sum_{n=0}^{\infty}(-1)^n I_n$ can be obtained by iterating the equation

$$\langle\Psi|\Psi\rangle=\left[1-\frac{\partial\Sigma(k,\lambda_k)}{\partial\omega}\right] =1+\sum_q U(k,q)^2|G(k-q,\lambda_k-\omega_q)|^2 \times\left[1-\frac{\partial\Sigma}{\partial\omega}(k-q,\lambda_k-\omega_q)\right] . \quad (21)$$

Anderson has shown,[6] using the SS wave function, that $z_k\neq 0$ if the spin deviations are dipolar at large distances. It is clear from the numerical work on the Green function[2,3] that $z_k\neq 0$, when calculated from the definition $[1-\partial\Sigma/\partial\omega]$, within the LSCA, even though, as we have just shown, the average spin deviations at large distances *are* dipolar, when $\mathbf{k}=(\pi/2,\pi/2)$.

The vanishing of z_k is equivalent to $|\Psi\rangle$ being unnormalizable. From the above it is evident that $z_k\neq 0$ when calculated directly from the wave function we have constructed, since it agrees with the value obtained from the Green function. A comparison of the semiclassical wave function of SS with the expression we have obtained will make clear what the difficulty is with Anderson's argument.

In order to bring out the difference between the two wave functions, we will rewrite the SS wave function in a form similar to (2).

$$|\Psi\rangle_{SS}=\prod_{i\neq 0}(1+e^{i\mathbf{q}_0\cdot\mathbf{r}_i}2iS_i^x\tan\theta_{i/2})|0\rangle_N , \quad (22)$$

where $|0\rangle_N$ is the Néel state, and the hole is at $i=0$. Then z_k, for this wave function is again ${}_{SS}\langle\Psi|\Psi\rangle_{SS}^{-1}$, where

$${}_{SS}\langle\Psi|\Psi\rangle_{SS}^{-1}=\prod_{i\neq 0}[\cos\theta_i/2]^2 \quad (23)$$

If we take for θ_i the dipolar form $\mathbf{p}\cdot\mathbf{r}_i/r_i^2$, or any other form that is not square integrable, ${}_{SS}\langle\Psi|\Psi\rangle_{SS}$ will diverge, and z_k will be 0. This is Anderson's argument, and it is valid even if one keeps only the leading terms involving a single spin deviation, which are in any case, the dominant terms at large distances. Nothing is lost by making a spin-wave approximation for small values of θ_i, so we have

$$|\Psi\rangle_{SS}\cong\left[1+N^{-1/2}\sum\theta_q a_{\bar{q}}^{\dagger}\right]|0\rangle_N , \quad (24)$$

where the $a_q^{\dagger}$ are related to the spin-wave operator $\alpha_q^{\dagger}$ by a Bogolyubov transformation. In particular $S_q^x=\frac{1}{2}(a_{-q}^{\dagger}+a_q)=\frac{1}{2}(\mu_q+\nu_q)(\alpha_{-q}^{\dagger}+\alpha_q)$, $S_q^y=i/2(a_{-\bar{q}}^{\dagger}-a_{\bar{q}})=i/2(\mu_q+\nu_q)(\alpha_{-\bar{q}}^{\dagger}-\alpha_{\bar{q}})$.

The wave function (22) remains unnormalizeable, for a dipolar pattern, for which

$$\theta_q\propto(\bar{q}_x+\bar{q}_y)/\bar{q}^2 \quad (25)$$

for small $\bar{q}$ since ${}_{SS}\langle\Psi|\Psi\rangle_{SS}=1+N^{-1}\Sigma|\theta_q|^2$. In the state (24), assuming θ_q is real and $\theta_{-q}=-\theta_q$, as it is for the dipolar pattern, $\langle S_q^y\rangle=-i\theta_q$. By contrast, the state we have constructed in Eqs. (2 and 10) is to lowest order, leaving out the fermion,

$$|\Psi\rangle=|0\rangle_{SW}+N^{-1/2}\sum_q B_q\alpha_{\bar{q}}^{\dagger}|0\rangle_{SW} , \quad (26)$$

where $|0\rangle_{SW}$ is the spin-wave ground state.

With the same value for $\langle S_q^y \rangle$ as calculated from (24), $B_q = (\mu_q + \nu_q)^{-1}\theta_q$. For small values of $\bar{q}$, since $\mu_q + \nu_q \propto \bar{q}^{-1/2}$

$$B_q \propto (\bar{q}_x + \bar{q}_y)/q^{3/2} \tag{27}$$

and $\langle \Psi|\Psi\rangle = 1 + N^{-1}\Sigma|B_q|^2$ is finite.

Inclusion of higher-order terms in (26) will not affect the normalizability since the hole can only excite a finite number of spin waves, and the series for the normalization of $|\Psi\rangle$ will effectively terminate after a finite number of terms. (The simplest estimate for I_n, where $nJ \gg t$, would be $I_n \propto 1/n^2$.)

The dipolar behavior of the spin pattern, as pointed out by SS, arises from the symmetry of the terms coupling the hopping of the hole to the background spins. This is a general feature of the t-J model that is preserved by the Hamiltonian (1) and the LSCA. The nonnormalizability arising from the use of the SS wave function as a variational ansatz is, however, an artifact of the ansatz, and is not inherent in the dipolar long-distance behavior of the spin deviation on the quasiparticle. As to which wave function is a better choice, it seems clear that the SS wave function ignores correlations that are actually present in the physical ground state, which will be rather close to the spin-wave vacuum,[12] and it is the ignoring of these correlations that leads to $z_k = 0$.

It might be thought that if the wave function was obtained exactly, z_k would be zero, and that the LSCA result is an artifact of *that* approximation. But for any wave function, at sufficiently large distances, the amplitude of the spin deviation would be small, and the wave function would be describable by (26). The only effect of solving for $|\Psi\rangle$ more accurately would be to change the coefficient in front of B_q, which would change the value of z_k but not the fact that it was nonzero. This is corroborated to some extent by the work of Liu and Manousakis,[13] in which they have included the leading vertex correction to Eq. (7), with very small effects, suggesting that z_k would not be far from the value predicted by the LSCA. As $t \to 0$, the value of z_k should go continuously to that calculated by Malshukov and Mahan. It will not do so in the present calculation because we have left out the terms corresponding to the vacancy in the Heisenberg part of the model. There is then no reason to doubt that z_k is finite for a single hole in the t-J model and the possibility remains that the many-hole state is a Fermi liquid.

If that is the case, then for a density of holes sufficiently low that antiferromagnetic order is not destroyed, the properties of the system may be treated as a noninteracting gas of the quasiparticles we have described. The wave function can also be used in a variational calculation of the interaction between quasiparticles.

In conclusion, we have presented a completely quantum mechanical solution for the wave function of a hole in the t-J model based on an extension of the retraceable path approximation. The lowest-order self-consistent approximation for the Green function arises as a consistency condition for the existence of a solution. The method can be applied directly to the electron-phonon interaction to provide a wave function in the strong polaron limit. The long-distance behavior of the spin deviations around the hole reproduce the form predicted by Shraiman and Siggia from a semiclassical theory, at the band minimum, with a prediction for the absolute amplitude of the deviations. At the band maximum, there is a long-ranged isotropic distortion described by the quantum wave function not treated in the semiclassical theory. There is no orthogonality catastrophe for the quantum solution ($z_k \neq 0$), as the correlations due to the zero point motion make it possible for the overlap between the bare hole and the quasiparticle to be finite even though the spin pattern is long ranged.

Ramsak and Horsch[11] have recently published a comparison of the predictions of the wave function derived here with the results of exact diagonalizations on finite size systems. The agreement is excellent at the physical value of t/J, where three terms in the series for the wave function [Eq. (2)], are sufficient for an accurate representation.

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