Quasiparticle band structure of a hole in a quantum Heisenberg antiferromagnet

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The problem of the single-hole motion in a two-dimensional quantum Heisenberg antiferromagnet is examined in the t-J model. By introducing a kind of slave-fermion representation for Hubbard operators a hole is treated as a spinless fermion strongly interacting with spin-$\frac{1}{2}$ degrees of freedom. We suggest an analytic approach based on a decoupling procedure for two-time fermionic Green functions that allows us to describe a hole as a magnetic polaron of a minimal size (i.e., involving one-step "string" spin excitations) and reproduce the main features characteristic of a one-hole band in a quantum antiferromagnet. A generalization of the procedure in the spirit of the Lanczos approach to extend the internal structure of the magnetic polaron is discussed.

It is now widely believed that the most essential physics of a CuO_2 plane in oxide superconductors is described by the t-J model.[1,2] In the framework of this model a particular problem of a single-hole motion in a quantum antiferromagnetic background has been examined recently in analytical[3–6] and numerical (see the review by Dagotto[7] and references therein) studies. In particular, Kane, Lee, and Read[4] have developed a perturbation theory for a hole motion both for the Néel state and the resonating-valence-bond (RVB) state of a spin background. In the former case a spin wave expansion was performed in the large-S limit and a hole was treated as a spinless fermion (holon) strongly interaction with spin waves. By summing the "noncrossing" diagrams, Kane, Lee, and Read have derived a self-consistent integral equation for the hole propagator. To get qualitative information about the low-energy structure of a hole spectrum in the Heisenberg limit, they evaluated this equation in the "dominant pole approximation" and obtained a well-defined quasiparticle (QP) description for a coherent hole propagation with the band minima at the momenta $(\pi/2;\pi/2)$ and the bandwidth $W\sim J$. Recently Martinez and Horsch[5] have evaluated numerically the same integral equation for the hole propagator as in Ref. 4 and obtained the spectral function $A(k,w)$ of a hole in the Heisenberg atomic force microscope (AFM) for different ratio J/t. They found a narrow QP peak at the bottom of the spectrum, which is well separated from the incoherent part for a large enough J value. Like in Ref. 4, the characteristics of the QP state obtained in Ref. 5 are in good agreement with previous numerical diagonalization studies for small systems.[7] In this paper we follow a different line of thought in treating the problem of a hole motion in a quantum background. Namely, a QP state of a hole may be considered as a sort of a magnetic polaron in terms of the "string picture."[8–11] Coming initially from the Ising limit for a spin-$\frac{1}{2}$ magnetic background this picture involves the local spin excitations (overturned spins along a hole track). Considering the Heisenberg limit for spin-$\frac{1}{2}$ background along this way we avoid a spin wave expansion and use only some general properties for spin-spin correlation functions for a singlet ground state. The analytical approach suggested here is rather simple and is based on the decoupling scheme for two-time Green functions. We developed here a minimal version of the scheme, i.e., considered a polaron structure of a minimal size involving only one-step "string" excitations. It is remarkable that even this minimal version allows us to reproduce, at least qualitatively, the main features for a QP behavior of a hole. An extension of this scheme to the case of a polaron of a larger size seems to be straightforward.

Let us recall that the t-J Hamiltonian can be written as

$$H_{t\text{-}J}=\sum_{i,j,\sigma} t_{ij}X_i^{\sigma 0}X_j^{0\sigma}+\tfrac{1}{2}\sum_{i,j}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{1}$$

where the Hubbard operators X_i^{pq} are related to the canonical fermion operators $C_{i\sigma},C_{i\sigma}^{\dagger}$ by

$$X_i^{\sigma 0}=(1-n_{i-\sigma})C_{i\sigma}^{+} \tag{2}$$

while the spin operators $\mathbf{S}_i$ are given by

$$\mathbf{S}_i=\tfrac{1}{2}X_i^{\sigma 0}\tau_{\sigma\sigma'}X_i^{0\sigma'}\ , \tag{3}$$

where τ are the Pauli matrices. In this representation, spin and charge degrees of freedom are tightly bound. To distinguish between them we propose as a first step a new kind of slave fermion representation for Hubbard operators in (1) which is different from the widely used slave fermion factorization.[3–6] Actually, this factorization requires some additional constraints to avoid unphysical states with a hole and a spin deviation present at the same site simultaneously. It is clear that being not so important in the case of large spin value S this constraint becomes much more pronounced in the realistic case of one-half spin. In the representation suggested here charge and spin degrees of freedom are independently introduced without requiring any additional constraint.

The local fermion Hilbert space at site i, say, consists of three states, namely, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|0\rangle$. The action of

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Hubbard operators is then given by

$$X_i^{\sigma 0}|0\rangle=|\sigma\rangle\ ,\qquad X_i^{\sigma 0}|\sigma'\rangle=0\ . \tag{4}$$

Let us introduce another local Hilbert space as the tensor produce $|\text{hole}\rangle\otimes|\text{spin}\rangle$ with four states, namely, $|0,\uparrow\rangle$, $|0,\downarrow\rangle$, $|1,\uparrow\rangle$, and $|1,\downarrow\rangle$ as it is explicitly defined in Ref. 6, where "1" denotes the presence of one hole. In that space, we introduce the canonical spinless fermion operators $f_i, f_i^\dagger$ and the usual spin-$\frac{1}{2}$ operators $\mathbf{s}_i$ acting on the hole and spin spaces, respectively. Let us then define the one-to-one correspondence

$$|\uparrow\rangle\rightarrow|0,\uparrow\rangle\ ,\qquad |\downarrow\rangle\rightarrow|0,\downarrow\rangle\ ,\qquad |0\rangle\rightarrow|1,\uparrow\rangle\ , \tag{5}$$

which we shall call "canonical" for convenience and the following representation for the Hubbard operators:

$$X_i^{\uparrow 0}=f_i(\tfrac{1}{2}+s_i^z)\ ,\quad X_i^{\downarrow 0}=f_i s_i^-$$
$$X_i^{0\uparrow}=f_i^+(\tfrac{1}{2}+s_i^z)\ ,\quad X_i^{0\downarrow}=f_i^+ s_i^+\ . \tag{6}$$

Clearly, these operators identically vanish on the $|1,\downarrow\rangle$ state. Then it is easy to check that the Hubbard operators have the same action as in (4) within the subspace generated by the states $|0,\uparrow\rangle$, $|0,\downarrow\rangle$, and $|1,\uparrow\rangle$. It is also clear that the correct anticommutation relations at different sites are preserved due to the fermionic nature of the hole operators f_i and f_i^+. And the spin operators (3) then become

$$\mathbf{S}_i=(1-n_i)\mathbf{s}_i\ , \tag{7}$$

where $n_i=f_i^+ f_i$ is the number of holes at site i.

In the above representation (6), the t-J Hamiltonian then reads

$$H_{t\text{-}J}=\sum_{i,j}t_{ij}f_i f_j^+[(\tfrac{1}{2}+s_i^z)(\tfrac{1}{2}+s_j^z)+s_i^- s_j^+]+\tfrac{1}{2}\sum_{i,j}J_{ij}(1-n_i)(1-n_j)\mathbf{s}_i\cdot\mathbf{s}_j\ . \tag{8}$$

The interpretation of the t and J terms is quite easy. The magnetic energy is the standard one except at a site where a hole is present, in which case the magnetic energy vanishes as expected. Of course, at half-filling the Hamiltonian (8) is just the AFM Heisenberg Hamiltonian.

Let us emphasize also that this representation is quite independent of any assumption about the nature of the spin background.

However the "canonical" mapping (5) we have introduced is in some way arbitrary. Indeed, in the one-hole sector the identification of the state $|0\rangle$ with the state $|1,\uparrow\rangle$ has no physical meaning and we may identify the state $|0\rangle$ with any linear combination of the states $|1,\uparrow\rangle$ and $|1,\downarrow\rangle$. In the zero hole sector the identification can be made up to a canonical transformation too. More precisely, at each site we can perform a unitary transformation U_i given by

$$U_i=(1-n_i)U_i^{(0)}+n_i U_i^{(1)}\ , \tag{9}$$

where $U_i^{(0)}$ and $U_i^{(1)}$ are unitary transformations acting on the spin space. Under the transformation $U=\prod_i U_i$, the t-J Hamiltonian (8) becomes

$$H_{t\text{-}J}=\sum_{i,j}t_{ij}f_i f_j^\dagger[U_i^{(0)}(\tfrac{1}{2}+s_i^z)U_i^{(1)\dagger}U_j^{(1)}(\tfrac{1}{2}+s_j^z)U_j^{(0)\dagger}+U_i^{(0)}s_i^- U_i^{(1)\dagger}U_j^{(1)}s_j^\dagger U_j^{(0)\dagger}]$$
$$+\tfrac{1}{2}\sum_{i,j}J_{ij}(1-n_i)(1-n_j)U_i^{(0)}\mathbf{s}_i U_i^{(0)\dagger}U_j^{(0)}\mathbf{s}_j U_i^{(0)\dagger}\ . \tag{10}$$

The choice of a suitable form for the U transformation may provide a more convenient basis in treating the particular magnetic background. For example, let us assume a square lattice with the long-range antiferromagnetic background. Then we may choose for U the following definition:

$$U_i=\begin{cases}1 & \text{if } +i\in A\\ (1-n_i)(s_i^+ +s_i^-)+n_i & \text{if } i\in B\ ,\end{cases} \tag{11}$$

where A and B are the sublattices with up and down spins, respectively. This unitary transformation changes the Néel state into a ferromagnetic one and, hence, from now on one does not need to distinguish between sublattices. The transformed Hamiltonian is written as

$$\tilde{H}=\sum_{i,j}t_{ij}f_i f_j^\dagger[(\tfrac{1}{2}+s_i^z)s_j^+ +(\tfrac{1}{2}+s_j^z)s_i^-]+\tfrac{1}{2}\sum_{i,j}J_{ij}(1-n_i)(1-n_j)\times[-s_i^z s_j^z+\tfrac{1}{2}(s_i^+ s_j^+ +s_i^- s_j^-)] \tag{12}$$

which is nothing more than the exact expression of the Hamiltonian for the model proposed in Refs. 4–7. To get a closer connection, we introduce the Holstein-Primakoff representation for the spin operators, namely,

$$s_i^z=\tfrac{1}{2}-a_i^\dagger a_i\ ,\qquad s_i^+=\sqrt{1-a_i^\dagger a_i}\,a_i\ ,\qquad s_i^-=a_i^\dagger\sqrt{1-a_i^\dagger a_i}\ , \tag{13}$$

where a_i and $a_i^\dagger$ are boson operators. If now we consistently linearize the spin dynamics to the lowest order one gets the model used in Refs. 6 and 7. In particular, the hopping term $\tilde{H}_t$ reads

$$\tilde{H}_t\simeq\sum_{i,j}t_{ij}f_i f_j^\dagger[a_j+a_i^\dagger]\ . \tag{14}$$

However, now the hopping term generates unphysical states (a hole with a spin deviation at a given site) and an additional constraint must be involved to reject these states.[6]

More important is the fact that some gauge invariance

is hidden in our representation. Indeed, let us consider the unitary transformation (9) which leaves the Hamiltonian (8) invariant up to a gauge transformation on the hole operators. One gets the following result:

$$U_i=(1-n_i)U^{(0)}+n_i[e^{-i\varphi_i}(\tfrac{1}{2}+s_i^z)+e^{-i\theta_i}(\tfrac{1}{2}-s_i^z)] \quad (15)$$

together with the gauge transformation

$$f_i\rightarrow e^{-i\varphi_i}f_i\ , \qquad f_i^+\rightarrow e^{i\varphi_i}f_i^+\ . \quad (16)$$

In Eq. (15), $U^{(0)}$ is an SU_2 matrix and corresponds to total spin conservation. Clearly, the phase transformations $e^{-i\varphi_i}$ and $e^{-i\theta_i}$ correspond to the fact that in the one-hole sector we can define the one-hole states up to a phase. This property can be exploited when evaluating expectation values. To illustrate this point and in connection with the hole motion problem, let us consider the following two-time Green function:

$$G_{ij}^{\sigma\sigma}(t)=\langle\langle X_i^{0\sigma}(t)|X_j^{\sigma 0}\rangle\rangle\ . \quad (17)$$

Since the Hamiltonian (8) is invariant under the simultaneous transformation (15) and (16) and assuming total spin conservation, one has

$$\langle\langle f_i^\dagger(t)|f_j\rangle\rangle=\langle\langle e^{\dagger i\varphi_i}[U_i f_i^\dagger U_i^\dagger](t)|e^{-i\varphi_j}U_j f_j U_j^\dagger\rangle\rangle\ . \quad (18)$$

A simple computation leads to the following result:

$$\langle\langle f_i^\dagger(t)|f_j\rangle\rangle=G_{ij}^{\sigma\sigma}(t)\ , \quad (19)$$

owing to the fact that the phases φ_i and θ_i and the SU_2 rotation $U^{(0)}$ defining the transformation U_i, Eq. (15), are arbitrary.

It is then clearly established that the physical Green function to be evaluated is just the Green function for the hole fermion operators. Due to this gauge invariance other relations between correlation functions can be established.

On the basis of our representation we examine properties of a polaron of minimal size. It is expected that this polaron can provide good quasiparticle state of a hole in the system.[9]

We start with the one-hole Green function at $T=0$,

$$G_{ij}(t)=\langle\langle f_i^\dagger(5)|f_j\rangle\rangle =-i\theta(t)\langle\psi_0,\{f_i^\dagger(t),f_j\}\psi_0\rangle\ , \quad (20)$$

where i,j belong to the same sublattice A, say, and ψ_0 is the wave function of a state with no holes (half-filled case) and hence it is a background wave vector of the two-dimensional Heisenberg Hamiltonian.

The Fourier-transformed Green function (20) obeys the following equation:

$$[\omega-E^{(0)}]G_\omega(\mathbf{p})=1+F_\omega(\mathbf{p})\ , \quad (21)$$

where $E^{(0)}=\sum_l J_{il}\langle\mathbf{s}_i\cdot\mathbf{s}_l\rangle=J\sum_\tau\langle\mathbf{s}_0\cdot\mathbf{s}_\tau\rangle$, with τ being the unit vectors of the square lattice, and $F_\omega(\mathbf{p})$ denotes the Fourier transform of the new Green function

$$F_{ij}(t)=\sum_l\langle\langle(f_l^\dagger T_{li})(t)|f_j\rangle\rangle \quad (22)$$

that describes a hole dressed with a "string" excitation of length 1.[9] According to Eq. (8), we use the following notation:

$$T_{li}=t_{li}[(1/2+s_i^z)(1/2+s_l^z)+s_i^-s_l^+]\ ;i\in A,l\in B$$

and $T_{il}=T_{li}^\dagger$. The Green function $F_{ij}(t)$ obeys the equation

$$i\frac{\partial}{\partial t}F_{ij}(t)=\sum_l\langle\langle[f_l^\dagger T_{li},H_t+H_J](t)|f_j\rangle\rangle\ . \quad (23)$$

To make the system of equations closed we apply the following decoupling procedure:

$$\langle\langle[f_l^\dagger T_{li},H_t](t)|f_j\rangle\rangle=\sum_{i'}\langle\langle(f_{i'}^\dagger T_{i'l}T_{li})(t)|f_j\rangle\rangle \simeq\sum_{i'}\langle T_{i'l}T_{li}\rangle\langle\langle f_{i'}^\dagger(t)|f_j\rangle\rangle\ , \quad (24)$$

$$\langle\langle[f_l^\dagger T_{li},H_J](t)|f_j\rangle\rangle=\sum_{i'\neq i}\sum_{l'\neq l}J_{i'l'}\langle\langle(f_l^\dagger T_{li}\mathbf{s}_{i'}\cdot\mathbf{s}_{l'})(t)|f_j\rangle\rangle+\sum_{l'\neq l}J_{il}\langle\langle(f_l^\dagger T_l[1/2+s_i^z]\mathbf{s}_{l'}\cdot\mathbf{s}_l)(t)|f_j\rangle\rangle$$
$$\simeq\left\{\sum_{i'\neq i}\sum_{l'\neq l}J_{i'l'}\langle\mathbf{s}_{i'}\cdot\mathbf{s}_{l'}\rangle+\sum_{l'\neq l}J_{il'}\langle(1/2+s_i^z)\mathbf{s}_{l'}\cdot\mathbf{s}_l\rangle\right\}\langle\langle(f_l^\dagger T_{li})(t)|f_j\rangle\rangle\ . \quad (25)$$

In our notations this procedure just corresponds to the construction of the quasiparticle hole operator describing a polaron of minimal size. The final form of the equation for $F_\omega(\mathbf{p})$ is

$$(\omega-E^{(1)})F_\omega(\mathbf{p})=M(\mathbf{p})G_\omega(\mathbf{p})\ , \quad (26)$$

where

$$E^{(1)}=\tfrac{1}{4}J\left[(2z-1)\sum_\tau\langle\mathbf{s}_0\cdot\mathbf{s}_\tau\rangle-\sum_\tau\sum_{\tau'\neq\tau}\langle(1/2+s_0^z)\mathbf{s}_{\tau'}\cdot\mathbf{s}_\tau\rangle\right] \quad (27)$$

and

$$M(\mathbf{p})=t^2[z\langle 1/2+s_0^z\rangle-4K_2+4K_2(\cos p_x+\cos p_y)^2+2(K_3-K_2)(\cos 2p_x+\cos 2p_y)] \quad (28)$$

with z being the number of nearest neighbors ($z=4$ in our case). The quantities K_2 and K_3, which are spin correlation functions, are given by

$$t^2K_2=\tfrac{1}{8}\sum_\tau\sum_{\tau'\neq\pm\tau}\langle T_{\tau+\tau',\tau}T_{\tau,0}\rangle\ , \quad (29)$$

$$t^2K_3=\tfrac{1}{4}\sum_\tau\langle T_{2\tau,\tau}T_{\tau,0}\rangle\ . \quad (30)$$

Hence according to Eqs. (21) and (26), the possible quasiparticle energies are given by

$$E^{(\pm)}(\mathbf{p})=-\tfrac{1}{2}(E^{(0)}+E^{(1)})\pm\sqrt{\tfrac{1}{4}(E^{(0)}-E^{(1)})^2+M(\mathbf{p})}\ . \tag{31}$$

At this stage it is necessary to emphasize that the spin correlation functions K_2 and K_3 are both negative for any reasonable antiferromagnetic ground state ψ_0 and vanish for the pure Ising case. Excluding this particular case, one can easily check that the low-lying branch $E^{(-)}(\mathbf{p})$ possesses extrema at $\mathbf{p}=(0,0)$; $(\pm\pi,0)$, $(0,\pm\pi)$, and $(\pm\pi/2,\pm\pi/2)$. The point (0,0) is the absolute maximum while $(\pm\pi/2,\pm\pi/2)$ are isolated minima when $K_2>K_3$. If $K_2<K_3$, the position of the minima are shifted to $(0,\pm\pi)$ and $(\pm\pi,0)$. For $K_2=K_3$ the minimum energy is degenerate and coincides with the Fermi "surface" of the Hubbard model in the noninteracting case ($U=0$).

We now restrict our discussion to the pure $2d$ case for which the ground state ψ_0 is known to be a singlet state.[12] Then the spin correlation functions K_2 and K_3 read

$$K_2=\tfrac{1}{8}+\tfrac{1}{4}\sum_{\tau}\langle\mathbf{s}_0\cdot\mathbf{s}_\tau\rangle+\tfrac{1}{16}\sum_{\tau}\sum_{\tau'\neq\pm\tau}\langle\mathbf{s}_0\cdot\mathbf{s}_{\tau+\tau'}\rangle\ , \tag{32}$$

$$K_3=\tfrac{1}{8}+\tfrac{1}{4}\sum_{\tau}\langle\mathbf{s}_0\cdot\mathbf{s}_\tau\rangle+\tfrac{1}{8}\sum_{\tau}\langle\mathbf{s}_0\cdot\mathbf{s}_{2\tau}\rangle\ . \tag{33}$$

The value of the energy per bond $\varepsilon_0=-\langle\mathbf{s}_0\cdot\mathbf{s}_\tau\rangle$ is by now well established numerically,[13] $\varepsilon_0\simeq\frac{1}{3}$. Moreover,

$$\langle\mathbf{s}_0\cdot\mathbf{s}_{2\tau}\rangle<|\langle\mathbf{s}_0\cdot\mathbf{s}_\tau\rangle| \tag{34}$$

and we expect

$$\langle\mathbf{s}_0\cdot\mathbf{s}_{2\tau}\rangle<\langle\mathbf{s}_0\cdot\mathbf{s}_{\tau+\tau'}\rangle\ , \tag{35}$$

where τ' and τ are orthogonal to each other so that K_2 is strictly larger than K_3 and the ground-state energy of a hole is located at $\mathbf{p}=(\pm\pi/2,\pm\pi/2)$. If the two expectation values in (35) are equal, then $K_2=K_3$ and we are in the case of a degenerate minimal hole energy.

In any case, it is easy to check that $|K_2|$ and $|K_3|$ are larger than $\frac{1}{24}$. According to Ref. 13 for nonzero "staggered" magnetization, one sees that $\langle\mathbf{s}_0\cdot\mathbf{s}_{2\tau}\rangle>0.2$. Hence $|K_2|$ and $|K_3|$ are between 0.04 and 0.11, and $|E^{(1)}|$ in between 2.78 and 2.63. Then it is clear that the hole energy near its minimum takes the familiar form ($t=1$)

$$E^{(-)}(\mathbf{p})=E^{(-)}_{\min}+\lambda_1(\cos p_x+\cos p_y)^2+\lambda_2(2+\cos 2p_x+\cos 2p_y)\ , \tag{36}$$

where λ_1 is proportional to $|K_2|$ and positive and λ_2 is proportional to (K_2-K_3) and either positive ($|K_2|<|K_3|$) or zero ($K_2=K_3$). The minimum energy is given by

$$E^{(-)}_{\min}=-\sqrt{2+4|K_3|+0.56J^2}+2.08J \tag{37}$$

and the bandwidth reads

$$W=E^{(-)}(0,0)-E^{(-)}\left(\frac{\pi}{2},\frac{\pi}{2}\right)=\sqrt{2+4|K_3|}-\sqrt{2-8|K_2|-6|K_3|} \tag{38}$$

when J is small. Then the bandwidth is estimated as

$$0.26<W<0.88\ ,$$

that is, $J\lesssim W\lesssim 4J$ for physical values of $J\sim 0.2$.

To summarize, we have set up a representation for strongly correlated electronic systems in which charge and spin degrees of freedom are independently introduced and can be treated without any additional constraint between them. We have shown that the model presented in Refs. 4, 6, and 7 can be easily derived when linearizing self-consistently the spin excitations. Moreover, some gauge invariance allowed us to show that for a hole motion only one Green function is relevant, namely, the Green function for the spinless fermionic operators. Finally, we have shown that the basic properties for the one hole motion can be derived in the framework of a simple decoupling procedure for this Green function. This decoupling procedure can be generalized by incorporating into our scheme higher order in T_{il} Green functions corresponding to "string" excitations of two or more steps. A proper decoupling step by step of these higher order Green functions in the same way as is done in (24) and (25) would provide a more complete set of equations that is similar in spirit to the Lanczos approach. Of course, such an extension of the internal structure of the QP state would improve our results and make them closer to the numerical ones.[7] However, it is remarkable that even the minimal version of the procedure developed here gives, at least qualitatively, a correct description.

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