Hole motion in an arbitrary spin background: Beyond the minimal spin-polaron approximation

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The motion of a single hole in an arbitrary magnetic background is investigated for the 2D $t$-$J$ model. The wavefunction of the hole is described within a generalized string picture which leads to a modified concept of spin polarons. We calculate the one-hole spectral function using a large string basis for the limits of a Néel ordered and a completely disordered background. In addition we use a simple approximation to interpolate between these cases. For the antiferromagnetic background we reproduce the well-known quasiparticle band. In the disordered case the shape of the spectral function is found to be strongly momentum-dependent, the quasiparticle weight vanishes for all hole momenta. Finally, we discuss the relevance of results for the lowest energy eigenvalue and its dispersion obtained from calculations using a polaron of minimal size as found in the literature.

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I. INTRODUCTION

Since the discovery of the high-temperature superconductivity the hole motion in strongly correlated electronic systems has attracted much interest. It is widely accepted that many properties of the superconducting cuprates are determined by the hole-doped CuO$_2$ planes. Angle-resolved photoemission (ARPES) experiments at zero or small doping indicate a quasiparticle band with a small bandwidth providing evidence for strong electronic correlations in the high-$T_c$ compounds.

The undoped materials are known to be antiferromagnetic Mott–Hubbard insulators. Neutron scattering experiments show that their magnetic behavior can be well described by a spin $S = \frac{1}{2}$ Heisenberg model on a square lattice. The doped materials exhibit a strong dependence of magnetic properties on the hole concentration $\delta$ in the CuO$_2$ planes. With increasing hole concentration both the Néel temperature and the staggered magnetization decrease and vanish at a critical hole concentration $\delta_c$ of a few percent before the system becomes paramagnetic and metallic (or superconducting at sufficiently low temperatures). Antiferromagnetic correlations are present also beyond the magnetic phase transition, e.g., in La$_{2-x}$Sr$_x$CuO$_4$ at $\delta = 4\%$ ($\delta_c \approx 2\%$) the magnetic correlation length is about 20 Å.

The magnetic long-range order is already destroyed at a rather small hole concentration $\delta$. Therefore exists a parameter regime where a small number of holes move in a spin background which is only short-range ordered. Here hole-hole correlations play no dominant role. This motivates the investigation of a single hole moving in an arbitrary spin background. It is assumed that the holes move independently, i.e., that there is no phase separation or hole-binding.

The motion of a hole in a paramagnetic background is also relevant for the study of the copper-oxide compound Ba$_2$Cu$_3$O$_4$Cl$_3$. Its Cu$_3$O$_4$ planes consist of two copper subsystems with different Néel temperatures. Therefore one finds a temperature range where one subsystem exhibits antiferromagnetic order whereas the other one shows paramagnetic behavior.

The low-energetic degrees of freedom of the copper-oxide planes are believed to be well described by the two-dimensional $t$-$J$ model:

$$H = -t \sum_{\langle ij \rangle \sigma} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma}) + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}).$$

(1)

Here, $\mathbf{S}_i$ is the electronic spin operator and $n_i$ the electron number operator at site $i$. The symbol $\langle ij \rangle$ refers to a summation over pairs of nearest neighbors. At half-filling the $t$-$J$ Hamiltonian reduces to the antiferromagnetic Heisenberg model. The electronic creation operators $\hat{c}^\dagger_{i\sigma}$ exclude double occupancies:

$$\hat{c}_{i\sigma}^\dagger = c_{i\sigma}^\dagger (1 - n_{i,-\sigma}).$$

(2)

The hole motion within the $t-J$ and related models has been subject of numerous investigations, see e.g. review articles. Special attention has been payed to the undoped case, i.e., to the case where the spin background is given...
by the ground-state of the 2D Heisenberg antiferromagnet. The main contribution to the hole motion in such an antiferromagnetic background can be understood as follows: the hopping hole locally destroys the antiferromagnetic spin order leaving behind a string of spin defects. Quantum spin fluctuations can repair pairs of frustrated spins. These processes lead to a coherent motion of the hole in each of the two sublattices. For $t/J > 1$ the bandwidth of this coherent hole motion is of order $J$ because the spin-flip part of the Hamiltonian is necessary to remove the spin defects caused by hopping.

However, a spin background with more ground-state fluctuations allows for additional hole motion processes with an energy scale $t$. With increasing spin disorder one expects the hopping term to become the dominant contribution to the hole motion. The special cases we consider are the completely disordered or random background (R) with $\langle S_i \cdot S_j \rangle = \frac{3}{4} \delta_{ij}$ and the ferromagnetic background (F) $\langle S_i \cdot S_j \rangle = \frac{1}{2} + \frac{1}{2} \delta_{ij}$. Note that the hole motion in a random background is a non-trivial situation even in the case $J \to 0$ since we are still dealing with strongly correlated electrons, i.e., with the restriction of no doubly occupied sites. The ferromagnetic background is easily discussed: A hole (with appropriate spin) can hop like a free particle through the lattice without changing the ferromagnetic background. The only difference to a free electron is a negative phase for the hopping term, i.e., $t \to -t$, since the object is a hole rather than a particle. The bandwidth for the hole motion is $8t$ (in two dimensions).

Up to now, the hole motion in weakly ordered or disordered spin backgrounds has been studied analytically only in a few papers. Brinkman and Rice used the retracable path approximation to discuss Néel-type (AF), random (R) and ferromagnetic (F) backgrounds. This approach only includes hole walks being completely background-restoring which is only a good approximation for systems with strong antiferromagnetic order. Metzner, Schmit, and Vollhardt employed a different method to discuss these three types of magnetic backgrounds within the Hubbard model for $U \to \infty$. They considered a hypercubic lattice in $d$ dimensions and determined the one-hole Green’s function exactly in the limit $d \to \infty$. These calculations were extended in refs.\cite{12,13} for generalized spin backgrounds in infinite dimensions.

One possibility for the analytical treatment of the one-hole problem in an arbitrary background is a variational ansatz for the hole wavefunction using strings of local spin deviations. The resulting object is a hole surrounded by a cloud of spin deviations. It is usually referred to as spin-bag quasiparticle or magnetic polaron. This approach was reduced to a “polaron of minimal size” where the basis set includes only the bare hole and strings of length 1. Usually the calculation is then restricted to the lowest energy eigenvalue only. In this paper we use a generalized string picture to discuss the hole motion in an arbitrary magnetic background. We go beyond the minimal polaron ansatz mentioned above and include strings with large lengths in the wavefunction. Using Mori-Zwanzig projection technique for these strings one can calculate the one-hole spectral function providing much more information about the hole states than the lowest eigenvalue alone. We have evaluated the arising expectation values for some special cases. Based on these results we discuss the quality of the minimal polaron approximation.

Besides these analytical approaches numerical studies have been carried out for the Hubbard and $t$–$J$ models at larger hole concentrations or finite temperatures. There one expects a spin background with larger fluctuations compared to the undoped system. However, the system sizes accessible to numerical methods leave many problems unresolved. Furthermore, the consideration of a given arbitrary magnetic background is difficult to realize within exact diagonalization or Lanczos methods.

The paper is organized as follows: In Sec. II we briefly sketch the variational ansatz for the one-hole wavefunction in an arbitrary spin background. We show how to calculate the one-hole spectral function using projection technique and discuss approximations used within the polaron approach. In Sec. III we consider two cases which can be treated exactly within the polaron ansatz: A Néel ordered background for arbitrary $t/J$ and a completely disordered background for $J = 0$. Based on these results we present in Sec. IV a simple interpolation between the cases of an antiferromagnetic, a random and a ferromagnetic background. The discussion of the lowest energy eigenvalue within the minimal polaron approximation is subject of Sec. V. We evaluate the dispersion of the lowest energy eigenvalue for different maximum polaron sizes and discuss the spectral weight of the lowest energy eigenvalue depending on the spin background. A short conclusion will close the paper.

**II. SPIN POLARON APPROACH AND ONE-HOLE SPECTRAL FUNCTION**

In this section we outline the idea of generalized spin polarons. We consider the ground state $|\Phi\rangle$ of a two-dimensional half-filled system of $S = \frac{1}{2}$ fermions where double occupancies of sites are forbidden. We assume that the state $|\Phi\rangle$ has a given magnetic configuration and is an eigenstate of $S^2_{tot}$. This spin configuration can be either long-range ordered (AF or F), short-range ordered or completely disordered (R). The configuration depends on the model parameters, the hole concentration, possible additional frustrating interactions and finite temperature, see e.g. refs.\cite{13,14}. In this paper we are not going to investigate the magnetic properties of this state depending on this system.
parameters, we rather prefer to take the magnetic configuration as given.

Next we inject one hole (with fixed momentum) into the state $|\Phi\rangle$ and study its motion. Hopping processes will disturb the spin background in the vicinity of the hole. These spin deviations can be described by generalized string operators $A_{n,\xi}(i)$ which contain multiple hole hopping. $n$ denotes the path length, $\xi$ is the individual shape of the path and $i$ is the initial lattice site; $A_{n,\xi}(i)$ operating on a state with one hole at site $i$ moves the hole $n$ steps away by shifting the spins along the path with the shape $\xi$ by one lattice spacing. By $m_n$ we denote the number of paths with length $n$. For $n=1$ there are $m_1=4$ different path shapes, for $n=2$ there are $m_2=12$ paths and so on. Explicitly, the operators $A_{n,\xi}(i)$ are defined by:

$$
A_{0,1} = 1, \\
A_{1,\xi}(i) = \sum_{j \sigma} \hat{c}_{j \sigma} \hat{c}_{1 \sigma}^\dagger R_{i j}^\xi, \\
A_{2,\xi}(i) = \sum_{j l \sigma' \sigma''} \hat{c}_{l \sigma''} \hat{c}_{j \sigma'} \hat{c}_{1 \sigma} \hat{c}_{i \sigma}^\dagger R_{i j l}^\xi, \\
A_{3,\xi}(i) = \sum_{j l m \sigma' \sigma'' \sigma'''} \hat{c}_{m \sigma''} \hat{c}_{l \sigma''} \hat{c}_{j \sigma'} \hat{c}_{i \sigma} \hat{c}_{i \sigma}^\dagger R_{i j l m}^\xi.
$$

(3)

The matrices $R_{i_n \ldots i_1}^\xi$ allow the hole to jump along a path of shape $\xi$:

$$
R_{i_n \ldots i_1}^\xi = \begin{cases} 
1 & \text{if } i_1, \ldots, i_n \text{ are connected by path of shape } \xi \\
0 & \text{otherwise}
\end{cases}
$$

(4)

Note that we include only self-avoiding paths. Therefore so-called Trugman paths and other loops are not included in $[3]$. They only arise in expectations values like $\langle \Phi | \hat{c}_{k \sigma}^\dagger A_{n,\xi}^\dagger \hat{c}_{k \sigma} | \Phi \rangle$ and $\langle \Phi | \hat{c}_{k \sigma}^\dagger A_{n,\xi}^\dagger H A_{n,\xi} \hat{c}_{k \sigma} | \Phi \rangle$. Fig. 1 shows the first path shapes for $n=0,1,2$.

If the background state is a Néel state then the application of a path operator $A_{n,\xi}$ leads to a string of $n$ overturned (mismatched) spins attached to the hole. In a general spin background we generate a string of spin deviations since all spins along the path are shifted by one lattice spacing. For the limiting case of a ferromagnetic background the application of a path operator moves the hole without changing the background.

### A. Projection technique

To investigate the hole motion we consider a Green’s function for a single hole describing the creation of a hole with momentum $k$:

$$
G(k, \omega) = \sum_\sigma \langle \Phi | \hat{c}_{k \sigma}^\dagger \frac{1}{z - L} \hat{c}_{k \sigma} | \Phi \rangle
$$

(5)

where $z$ is the complex frequency variable, $z = \omega + i\eta$, $\eta \to 0$. The quantity $L$ denotes the Liouville operator defined by $LA = [H, A]$, for arbitrary operators $A$. The correlation function $[3]$ can be evaluated using Mori-Zwanzig projection technique $[4]$. In the following we briefly sketch this method. One considers a set of operators $\{B_{\nu}\}$ (which here contains the hole creation operator $\hat{c}_k$) and defines dynamical correlation functions

$$
G_{\nu \mu}(z) = \langle \Phi | B_{\nu}^\dagger \frac{1}{z - L} B_{\mu} | \Phi \rangle.
$$

(6)

Using projection technique one can derive the following set of equations of motion for the correlation functions $G_{\nu \mu}(z)$:

$$
\sum_{\nu} (z \delta_{\eta \nu} - \omega_{\eta \nu} - \Sigma_{\eta \nu}(z)) G_{\nu \mu}(z) = \chi_{\eta \mu}.
$$

(7)

Here, $\chi_{\eta \nu}$, $\omega_{\eta \nu}$, and $\Sigma_{\eta \nu}$ are so-called static correlation functions, frequency terms, and self-energies, respectively. They are given by the following expressions:
\[ \chi_{\nu \mu} = \langle \Phi | B_{\nu}^\dagger B_{\mu} | \Phi \rangle, \]
\[ \omega_{\nu \mu} = \sum_{\lambda} \langle \Phi | B_{\nu}^\dagger (LB_{\lambda}) | \Phi \rangle \chi_{\lambda \mu}^{-1}, \]
\[ \Sigma_{\nu \mu}(z) = \sum_{\lambda} \langle \Phi | B_{\nu}^\dagger \left( LQ \rho_{\nu \mu} \frac{1}{z - QLQ L B_{\lambda}} \right) | \Phi \rangle \chi_{\lambda \mu}^{-1}, \]

(8)

\( \chi_{\nu \mu}^{-1} \) is the inverse matrix of \( \chi_{\nu \mu} \), and \( Q \) is defined by
\[ Q = 1 - P, \quad P = \sum_{\nu \mu} |B_{\nu} \rangle \langle \Phi | \chi_{\nu \mu}^{-1} \langle \Phi | B_{\mu}^\dagger | \Phi \rangle. \]

(9)

\( P \) denotes a projection operator projecting onto the subspace of the Liouville space spanned by the operators \( \{ B_{\nu} \} \), whereas \( Q \) projects onto the complementary subspace.

Using as dynamical variables the path operators \( A_{n, \xi} \) defined above multiplied by \( \hat{c}_k \), i.e.,
\[ B_{n, \xi} = \sum_{\sigma} A_{n, \xi} \hat{c}_{k\sigma}, \]

(10)

the one-hole correlation function we are interested in is the diagonal correlation function \( G_{\nu \nu} \) with \( \nu = (0, 1) \). With these dynamical variables the static and frequency matrices are explicitly given by
\[ \chi_{\mu \nu, n \xi} = \sum_{\sigma} \langle \Phi | \hat{c}_{k\sigma}^\dagger A_{m, \nu}^\dagger A_{n, \xi} \hat{c}_{k\sigma} | \Phi \rangle, \]
\[ \omega_{\mu \nu, n \xi} = \sum_{\sigma} \langle \Phi | \hat{c}_{k\sigma}^\dagger A_{m, \nu}^\dagger (L A_{n, \xi} \hat{c}_{k\sigma}) | \Phi \rangle \]

(11)

Often one neglects the self-energy terms which describe processes outside the subspace spanned by the dynamical variables (which are here the path operators). This can be done if the set of relevant variables is chosen sufficiently large to cover the essential part of the dynamical behavior of the system.

The poles of the correlation function \( G_{\nu \nu} \) correspond to eigenstates of the object which is usually called "spin polaron". Using projection technique one obtains the energies and the spectral weight distribution for these poles. This means that all spectra calculated here are discrete spectra because the self-energy terms within projection technique are neglected. (In the figures presented below we have introduced an artificial Lorentzian broadening to plot the spectral functions.) Therefore the present approach cannot account for analytical features of the spectral functions as e.g. the nature of the spectra at the band edges.

When calculating expectation values containing path operators \( A_{n, \xi} \) as \( \chi_{\mu \nu, n \xi} \) and \( \omega_{\mu \nu, n \xi} \) the effect of hopping processes can be rewritten in terms of spin operators. The lowest matrix elements are:
\[ \sum_{\sigma} \langle \Phi | \hat{c}_{j\sigma}^\dagger A_{0,1} \hat{c}_{i\sigma} | \Phi \rangle = 1, \]
\[ \sum_{\sigma} \langle \Phi | \hat{c}_{j\sigma}^\dagger A_{1,1} \hat{c}_{i\sigma} | \Phi \rangle = 2 \langle \Phi | \left( S_j \cdot S_i + \frac{1}{4} \right) | \Phi \rangle R_{ji}^{(\xi)}, \]
\[ \sum_{\sigma} \langle \Phi | \hat{c}_{k\sigma}^\dagger A_{2,1} \hat{c}_{i\sigma} | \Phi \rangle = \langle \Phi | \left( -S_k \cdot (S_j \times S_i) + S_j \cdot S_i + S_k \cdot S_i + S_k \cdot S_j + \frac{1}{4} \right) | \Phi \rangle R_{kji}^{(\xi)}, \]

... (12)

In this way all matrix elements from (11) can be transformed into expectation values of multi-products of spin operators formed with the background state \( | \Phi \rangle \). Note that this is the only point where the properties of the magnetic background enter: For the investigation of the one-hole motion one has to know static multi-point spin correlation functions. For a general spin background the knowledge of all these many-point correlators is usually not available. One way to evaluate these functions could be factorizing them into two-point (or two-point and four-point) correlation functions, see e.g. refs. [12,13]. For the special backgrounds discussed below a factorization is not necessary.

Next we shall discuss some approximations which have to be done within the polaron scheme. In most practical calculations one can take into account only a finite number of path operators up to a certain length \( n_{\text{max}} \). This truncation should be possible if the weight of the path states decreases rapidly with increasing path length, i.e., if the polaron is localized in space and longer paths do not contribute to the wavefunction, see also next subsection. This
is certainly true only for low-lying polaron states in an antiferromagnetic background and for finite antiferromagnetic exchange $J > 0$. In this case the hopping hole creates frustrated spins in the antiferromagnetic background leading to an Ising potential which increases with increasing path length [1,2]. The question is whether this truncated polaron method gives reliable results also in different magnetic backgrounds. One purpose of the present paper is to illustrate that it does: We have calculated the one-hole spectral function for the random spin background and different maximum path lengths up to 256. With increasing path length we have found only minor changes in the shape of the spectral function, i.e., beyond a path length of about 30 the problem is almost converged. Furthermore, our results for the random background coincide with those from refs. [3,4] which have been obtained using a completely different analytical approach.

A second approximation within the polaron method concerns the individual paths. Especially when considering longer paths the number of individual path shapes increases rapidly ($m_n \approx 3^n$). Therefore we are usually forced to consider only one variable per path length which is the sum of all individual paths of this length, i.e., the set of dynamical variables reduces to

$$B_n = \sum_{\xi=1}^{m_n} \sum_{\sigma} A_{n,\xi} c_{k\sigma}.$$  \hspace{1cm} (13)

Here, all different paths with equal length have been given the same weight which is a variational restriction compared to (14). However, if the hole momentum does not favor a particular direction, i.e., if $k = (0,0)$ or $(\pi, \pi)$, and if one neglects geometrical differences between the paths of same length then the weights of these paths are in fact equal for the lowest polaron eigenstate. This results in an s-like ground state of the quasiparticle. For general momenta the symmetry of the ground state is only nearly s-like. This point will be discussed further in Sec. V. Higher polaron states can have angular nodes in the coefficients, these states are not covered by the approximation (13). However, we have found that for the one-particle dynamics these states give only minor contributions to the spectrum. Only the (nearly) s-like states contribute considerable spectral weight to the one-hole spectral function leading to $n_{max}$ poles with non-vanishing weight. The reason lies in the symmetry of the Hamiltonian: None of the four lattice directions are preferred, so hopping processes in all directions carry equal weight. We summarize that the reduced set of variables (13) gives almost the same result as (10), at least for momenta $(0,0)$ and $(\pi, \pi)$.

B. Ansatz wavefunction

An alternative approach to the polaron problem consists of an ansatz wavefunction using the generalized path operators defined above [3]. A variational wavefunction for one hole with momentum $k$ can be constructed as linear combination of path states:

$$|\psi\rangle = \sum_{n=0}^{n_{max}} \sum_{\xi=1}^{m_n} \sum_{\sigma} (\lambda_{n,\xi} A_{n,\xi}) \hat{c}_{k\sigma} |\Phi\rangle,$$

$$A_{n,\xi} = \sum_{i} A_{n,\xi}(i).$$  \hspace{1cm} (14)

Inserting this ansatz (14) into the Schrödinger equation we obtain a generalized eigenvalue problem:

$$\sum_{n\xi} \lambda_{n,\xi} \langle \Phi | \hat{c}^\dagger_{k\sigma} A_{m,\nu} H A_{n,\xi} \hat{c}_{k\sigma} |\Phi\rangle = E \sum_{n\xi} \sum_{\sigma} \lambda_{n,\xi} \langle \Phi | \hat{c}^\dagger_{k\sigma} A_{m,\nu} A_{n,\xi} \hat{c}_{k\sigma} |\Phi\rangle. $$  \hspace{1cm} (15)

The matrix elements in (14) are the same expressions as in the eigenvalue problem (13). So the physics covered by both methods is the same: All processes which can be described by local spin deviations near the hole are taken into account. The poles of the Green’s function (8) equal the energy eigenvalues of the variational problem (13) (besides an energy shift). The solutions of (13) are the eigenstates of the spin polaron. An important additional information obtained via projection technique is of course the spectral weight distribution among the poles of $G(k,\omega)$.

The approximation of using only one variable per path length, i.e., the reduced set of dynamical variables (13) as described above, corresponds to a restricted variational ansatz for the wavefunction:

$$|\psi^{red}\rangle = \sum_{n=0}^{n_{max}} \lambda_{n} \sum_{\xi=1}^{m_n} \sum_{\sigma} A_{n,\xi} \hat{c}_{k\sigma} |\Phi\rangle.$$  \hspace{1cm} (16)

The energy eigenvalues which are obtained using this wavefunction are the same as the poles of the one-hole Green’s function calculated with projection technique and the reduced set of operators (13).
III. DISORDERED AND NÉEL BACKGROUNDS

In this section we consider two cases where the expectation values (11) can be calculated for arbitrary long paths. One is the completely disordered or random background (R) without exchange interaction ($J = 0$) where the strong correlations are present only in the exclusion of double occupancies. The other one is a Néel ordered background (AF) (for any value of $J$). In the numerical calculations we have used the full set of variables (10) with paths up to length $n_{\text{max}} = 5$ and the reduced set (13) up to $n_{\text{max}} = 256$.

A. Disordered background

For the random background the expectation value of all spin correlation functions between different sites vanish. Therefore expectation values of path operators are easily evaluated. One finds (compare (12)):

$$\sum_\sigma \langle \Phi | \hat{c}^{\dagger}_{j\sigma} A_{n,\xi} \hat{c}_{i\sigma} | \Phi \rangle = \frac{1}{2^n} R_{j...i}^{(\xi)}.$$

This can be understood as follows: The expectation value of a path operator is non-zero only if the hopping process does not change the spin background, i.e., if all spins along the path are parallel aligned. In the random background the probability for each spin of pointing up or down is $\frac{1}{2}$. Therefore the probability of two neighboring spins being parallel aligned is $\frac{1}{2^n}$. For a path of length $n$ which includes $n + 1$ spins the probability of all spins being parallel is $\frac{1}{2^n}$.

For $J = 0$ all matrix elements in (11) reduce to expectation values of path operators since the hopping term $H_0$ only changes the length of a path by one. The remaining non-trivial terms to calculate are the phase factors $e^{i\mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_i)}$ arising from expectation values like $\langle \Phi | \hat{c}^{\dagger}_{i\sigma} A_{n,\xi} \hat{c}_{k\sigma} | \Phi \rangle$. In principle such a phase factor has to be calculated for every individual path. For long paths the number of terms is very large ($\approx 3^{n_{\text{max}}}$), so we have performed Monte-Carlo sampling over $10^5$ different paths (which is sufficient for statistical errors $< 1\%$).

Results for the spectral function for different momenta are displayed in Fig. 2. The shape of the spectral function is strongly momentum dependent. The spectral weight of the lowest pole vanishes which indicates the absence of a quasiparticle (QP) peak. Considerable spectral weight near the band minimum is present only at momenta near $(\pi, \pi)$. The energy difference between the maxima at $(0,0)$ and $(\pi, \pi)$ is about $6.4t$ which can be considered as a "bandwidth".

In a random spin background the probability of large ferromagnetically aligned spin clusters is non-zero (but goes to zero with increasing cluster size in the thermodynamic limit). In such a cluster the hole moves like a free particle. This should cause the density of states to have tails with exponentially small weight extending to the edges of the free-particle band, see also refs. 3,4. So we expect the one-hole spectral function e.g. at momentum $(\pi, \pi)$ to have a tail down to $\omega = -4t$ (being the energy of the free hole) with vanishing weight at $\omega = -4t$. However, such analytical features cannot be extracted from the results of the projection-technique calculations presented here, see discussion in Sec. II A. The tails at the band edges visible e.g. in Fig. 2 arise only from the artificial broadening of the lines and do not have a physical meaning.

Note that the results presented in Fig. 2 agree well with the ones obtained within $d \rightarrow \infty$ approaches3,4. From this agreement we conclude that the processes included in our calculation, i.e., local spin deviations caused by hole hopping, cover the essential part of the dynamics of the one-hole motion in a disordered background. This is a non-trivial fact since the hole motion processes are not as localized in real space as in the case of a Néel background (AF) with non-zero Ising interaction. In the R case paths with all lengths contribute to the hole states, but a truncation of the subspace of path operators (with $n_{\text{max}}$ being sufficiently large) causes no essential changes in the one-hole spectral function. The influence of the maximum path length $n_{\text{max}}$ included in the calculation is illustrated in Fig. 3. It can be seen that beyond a maximum path length of 30 there are practically no changes in the shape of the spectral function.

B. Néel background

The hole motion in a Néel ordered background using strings of spin defects has been discussed in a number of papers, see e.g. 5,6,7,8. Hole motion on a self-avoiding path in the AF background always creates spin defects, so the expectation value of a single path operator vanishes:

$$\sum_\sigma \langle \Phi | \hat{c}^{\dagger}_{j\sigma} A_{n,\xi} \hat{c}_{i\sigma} | \Phi \rangle = \delta_{n,0} \delta_{ij}.$$


Non-zero matrix elements arise only from paths returning to their origin, and from spin-flip terms present in the Hamiltonian. Important matrix elements are the Ising energies due to frustration

\[ \sum_{\sigma} \langle \Phi | c_{j\sigma}^\dagger A_{n,\xi} \left( L_{\text{Ising}} A_{n,\xi} \hat{c}_{i\sigma} \right) | \Phi \rangle = J/2 (2n + 3 - \delta_{n,0}) \]  

(19)

and the spin-flip contribution

\[ \sum_{\sigma} \langle \Phi | c_{j\sigma}^\dagger A_{n+2,\xi'} \left( L_{\perp} A_{n,\xi} \hat{c}_{i\sigma} \right) | \Phi \rangle = J/2 \delta_{\xi+2,\xi'} \delta_{R_j-R_i,\Delta_2}. \]  

(20)

Here, the symbol \( \delta_{\xi+2,\xi'} \) means that path \( \xi' \) has to be obtained from path \( \xi \) by two further hopping steps, and \( \Delta_2 \) is a lattice vector consisting of two hops. For details concerning the evaluation of the matrix elements we refer to former publications.

The spectral function obtained with the reduced set of variables \( m, \nu \) is showed in Fig. 4 for \( J/t = 0.4 \) and for different momenta. We observe a non-zero weight of the lowest pole for all momenta indicating a quasiparticle peak. As mentioned the present approach cannot give analytical information about the spectra at the band edges. So we cannot answer exactly the question for the quasiparticle weight. However, a non-zero QP weight in the quantum AF ordered state (as well as in the Néel state considered here) is in agreement with most finite-size scaling studies of numerical calculations and with some analytical investigations of the \( t-J \) model. Note that this is in variance with an argument by Anderson.

Fig. 5 shows the one-hole spectrum for \( J = 0 \). Here the hole is localized since we have no \( H_{\perp} \) terms destroying spin fluctuations caused by hole hopping. (The variable set does not cover loops like trugman paths.) Therefore the spectrum is momentum-independent. No quasiparticle peak is present because the coherent motion of the hole is suppressed.

**IV. INTERPOLATION BETWEEN ANTIFERROMAGNETIC AND FERROMAGNETIC BACKGROUND**

Up to now we have considered three background states: antiferromagnetic (AF), disordered (R) (and \( J = 0 \)) and ferromagnetic (F). For the cases AF and R we have calculated the spectral function using arbitrarily long paths, the ferromagnetic case F is trivial. To see how the crossover of the quasiparticle behavior between these cases occurs we try a simple interpolation between the results (2) and (8). We consider the following ansatz:

\[ \sum_{\sigma} \langle \Phi | c_{j\sigma}^\dagger A_{n,\xi} \hat{c}_{i\sigma} | \Phi \rangle = p^n R_{j...i}^{(\xi)}. \]  

(21)

As explained above, non-zero contributions to the expectation value of a path operator arise only from hopping process along paths of parallel aligned spins. Thus \( p \) can be seen as the probability for two neighboring spins to be parallel aligned. This interpolation covers the three limiting cases:

\[ p = \begin{cases} 
1 & \text{ferromagnetic background (F)} \\
\frac{1}{2} & \text{random background (R)} \\
0 & \text{antiferromagnetic background (AF)} 
\end{cases} \]  

(22)

In this way parameter values \( 0 < p < 0.5 \) can be interpreted as weak antiferromagnetic order, whereas \( 0.5 < p < 1 \) describe weak ferromagnetic order. Of course this simple ansatz does not distinguish between short-range and long-range order. Furthermore, it does not cover the ground state of the Heisenberg antiferromagnet, i.e., a Néel state with quantum fluctuations. There we have \( \langle \Phi | S_i S_j | \Phi \rangle \approx -0.303 \) with \( i \) and \( j \) being nearest neighbor sites. This leads to \( \sum_{\sigma} \langle \Phi | c_{j\sigma}^\dagger A_{1,\xi} \hat{c}_{i\sigma} | \Phi \rangle \approx -0.053 R_{ji}^{(\xi)} \), compare (12). Nevertheless, the ansatz (21) shows the main effect of the crossover between the antiferromagnetic and disordered spin backgrounds.

To include the exchange interaction \( J \) we employ a simple mean-field treatment. The following matrix elements are taken into account:

\[ \sum_{\sigma} \langle \Phi | c_{i\sigma}^\dagger A_{m,\mu}^\dagger \left( L_{\text{Ising}} A_{n,\xi} \hat{c}_{i\sigma} \right) | \Phi \rangle = J \left( p - \frac{1}{2} \right) (p - 1) (n + m + 2) \sum_{\sigma} \langle \Phi | c_{i\sigma}^\dagger A_{m,\mu}^\dagger A_{n,\xi} \hat{c}_{i\sigma} | \Phi \rangle \]  

(23)
These terms represent the change of the Ising energy due to spin deviations coming from hopping processes. They interpolate between the three limiting cases AF, R, and F: In the antiferromagnetic background (AF) the Ising energy increases linearly with the path length provided here by the term $J(n+m+2)$. For both the R and F cases the change of the Ising energy via hole hopping vanishes: For the R case the Ising energy does not change since the average Ising energy is zero whereas in the F background all spins remain parallel aligned. Furthermore, the dependence of the Ising energy on $p$ near $p = 0$ is quadratic. These two factors $p$ follow from the average Ising energy being linear in $p$ and the probability of creating a spin defect via hole hopping being also linear in $p$.

Results for the spectral function at momentum $(0,0)$, $J/t = 0.4$ and different values of $p$ are shown in Fig. 6. At the bottom of the spectrum quasiparticle weight develops with increasing antiferromagnetic order. However, these quasiparticle peak is dominant only for strong antiferromagnetism. So it is obvious that the position of this quasiparticle peak is not the only relevant quantity, especially when comparing with photoemission experiments done at underdoped high-$T_c$ superconductors. Fig. 7 shows the spectra for $J = 0$. In this case we have no quasiparticle peak even for the antiferromagnetic background since coherent motion of the hole due to the transverse part of the magnetic exchange is absent.

V. DISCUSSION OF THE LOWEST ENERGY EIGENVALUE

In this section we consider the lowest energy eigenvalue obtained within the polaron ansatz for the wavefunction. The lowest eigenvalue has been calculated before for a "polaron of minimal size". This ansatz includes only paths up to length 1 for an antiferromagnetic as well as for a disordered background. Two questions have to be answered: 1) Is the lowest energy eigenvalue relevant in the sense that it carries spectral weight? 2) Does the reduced ansatz provide enough basis states to give reliable results compared with the "full" ansatz, e.g., with paths up to length 256?

The first question has already been addressed in the last section. The spectral weight of the lowest energy eigenvalue decreases with decreasing antiferromagnetic correlations in the spin background state. It seems to be non-zero for all states with antiferromagnetic correlations in the case $J > 0$, but to resolve this subtle question clearly more work is necessary. However, the spectrum is dominated already for a weak antiferromagnetic background (or a disordered one) by structures which are not located at the band minimum. These dominant structures should be visible in ARPES experiments. Thus the lowest energy eigenvalue is only relevant for a background with strong AF correlations, i.e., at very small hole concentrations and low temperatures. It is completely irrelevant for a disordered background.

The second question concerns the truncation of the polaron wavefunction. For a Néel-ordered background the minimal polaron ansatz with paths up to length $n_{\text{max}} = 1$ fails completely because the dominant hole motion process caused by $H_\perp$ is not covered by paths with maximum length 1. But also a wavefunction with maximum path length of $n_{\text{max}} = 2$ gives a bandwidth ($E(0,0) - E(\pi/2,\pi/2)$) being a factor of 2 too small as compared with a full ansatz (for values of $J/t = 0.2 - 0.5$). Fig. 7 shows the quasiparticle dispersion of the hole motion in a Néel background for different maximum path lengths (calculated with the ansatz (14)).

Considering an antiferromagnetic background state with more ground-state spin fluctuations one expects that the results for the hole dispersion obtained using the minimal polaron ansatz (14) become better with increasing spin fluctuations since nearest-neighbor hopping processes of order $t$ become more important. However, the bandwidths obtained in these calculations are still not reliable. The reason lies in the small number of basis states which do not provide sufficient degrees of freedom for the variational wavefunction. For detailed investigations we refer to a forthcoming publication.

For a disordered background one can also evaluate the dispersion of the lowest energy eigenvalue although it does not carry spectral weight. With $n_{\text{max}} = 0$ (only the bare hole as trial state) one obtains $E(0,0) - E(\pi,\pi) = 4t$ ($J = 0$), using $n_{\text{max}} = 1$ one finds $E(0,0) - E(\pi,\pi) \approx 1.5t$, $n_{\text{max}} = 2$ leads to $E(0,0) - E(\pi,\pi) \approx 0.6t$, and the "converged" value within our calculations is $|E(0,0) - E(\pi,\pi)| < 10^{-2}t$.

VI. CONCLUSION

In this work we have studied the dynamics of a single hole moving in an arbitrary spin background within the framework of the two-dimensional $t$-$J$ model. The one-hole spectral function has been calculated using Mori-Zwanzig projection technique for a large set of path operators. These operators describe local spin deviations around the hole which lead to a generalized picture of spin-bag quasiparticles or spin polarons.

We have calculated the one-hole spectral function using three limiting cases for the spin background: antiferromagnetic (AF), disordered (R) (and $J = 0$) and ferromagnetic (F). The obtained results for the AF case shows the features well-known from numerical and analytical investigations on the one-hole problem, i.e. a quasiparticle-like peak with a
dispersion which has its minima at \((\pm \pi/2, \pm \pi/2)\) and a bandwidth of about 2.2\(J\). For the disordered background the spectral function is strongly momentum dependent but shows no quasiparticle peak. These results coincide with the ones of a \(d \to \infty\) approach for the \(U \to \infty\) Hubbard model. A hole in a ferromagnetic background behaves like a free particle. Using a simple interpolation we have studied the crossover between the AF, R and F situations. The present calculation neglects processes outside the subspace of path operators. These processes would provide lifetime effects due to the scattering of the polaron states with spin waves. However, we expect no essential changes in the spectral function.

Finally, we have discussed the quality of the "minimal polaron approximation" often used in the literature. This reduced description consists of truncating the ansatz for the polaron wavefunction to paths with maximum length 1 and calculating the lowest energy eigenvalue only. In most cases this approximation is not sufficient to cover essential properties of the hole motion process.

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FIG. 1. The first path shapes of lengths $n = 0, 1, \text{ and } 2$ created by the operators $A_n, \xi$ acting on a hole at site $i$.

FIG. 2. One-hole spectral function for the random spin background and $J = 0$. Curves are shown for different hole momenta. The reduced variable set including paths up to length 256 has been used. We have introduced an artificial broadening of $10^{-3}t$. 

$\phi_{\text{Néel}}$
FIG. 3. Effect of maximum path length $n_{\text{max}}$ on the spectral function. The curves are calculated for random background, $J = 0$ and momentum $(\pi, \pi)$. Note that the artificial linewidths are different for the three curves.

FIG. 4. One-hole spectral function for the Néel-type background, $J/t = 0.4$ and different hole momenta. We have used the reduced set (13) of dynamical variables with $n_{\text{max}} = 256$ and a linewidth of $0.1t$. The total bandwidth of the quasiparticle dispersion is $2J$ which is smaller than the correct value $2.2J$ which would be obtained with the full set of variables (10).
FIG. 5. One-hole spectral function for the Néel-type background and $J = 0$. Note that this spectrum does not depend on the hole momentum since the hole is localized.

FIG. 6. One-hole spectral function calculated using the interpolation ansatz (21), $J/t = 0.4$, the mean-field term (28), momentum $(0,0)$ and different values of $p$. The linewidth is $0.02t$. 
FIG. 7. Same as Fig. 6, but for $J = 0$.

FIG. 8. Dispersion of the lowest energy eigenvalue for $J/t = 0.4$, antiferromagnetic background and the full variable set \cite{10}. Curves are shown for maximum path lengths $n_{\text{max}} = 1, 2, 3, \text{and } 4$. The zero energy level has been set to the center of mass of the band.