Spin polarons in the $t$-$t'$-$J$ model

Jan Bala and Andrzej M. Oleś
Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Kraków, Poland

Jan Zaanen
Lorentz Institute for Theoretical Physics, Leiden University, P.O.B. 9506, NL-2300 RA Leiden, The Netherlands
(Received 21 February 1995)

Treating the hole-magnon interaction within the self-consistent Born approximation, we demonstrate that the low-energy quasiparticles that occur in the $t$-$J$ model due to quantum fluctuations of the spin system survive in the models including free hole propagation on the sublattices. The quasiparticle dispersion and weight are found to be strongly dependent on the next-neighbor hopping parameter. The flat band observed near the X point in the high-temperature superconductors is reproduced, but not for the realistic parameters that correspond to the hole-doped system.

I. INTRODUCTION

It is widely accepted that the three-band model is a minimal model to describe the relevant part of the electronic structure of CuO$_2$ planes of high-temperature superconducting oxides (HTSO). However, soon after the discovery of the HTSO Anderson proposed that a single-band Hubbard model should suffice to describe qualitatively the low-energy physics of CuO$_2$ planes. Indeed, while the more realistic three-band (called also charge-transfer) model has been the subject of intense investigations, considerable evidence has been presented that it may in fact be reduced to an effective single-band model, either Hubbard or $t$-$J$. The mapping to the Hubbard model suffices, as it is well known that at large Coulomb interaction $U$ this model may be transformed to the strong-coupling (SC) model, being the $t$-$J$ model extended by the three-site hopping terms. Furthermore, it has been shown recently that the three-band model can be reduced to the single-band model even when the inter-site Coulomb interactions are significant. The antiferromagnetic (AF) superexchange at the filling of one hole per Cu atom has been derived from the three-band model, and is now well understood. Hole doping leads then to the formation of Zhang-Rice singlets, and the effective Hamiltonian is just the $t$-$J$ model. However, the parameters of the effective single-band model evaluated by using Cu$_2$O$_7$ and Cu$_2$O$_8$ clusters have shown that the $t$-$J$ model does not reproduce the low-energy states of the three-band model and has to be extended by the next-nearest-neighbor hopping, $t'$. The sign of $t'$ in the resulting $t$-$t'$-$J$ model changes between the hole and electron doping systems. In fact, $t > 0$ and $t' < 0$ ($t < 0$ and $t' > 0$) corresponds to the hole (electron) doping, respectively. This change of sign of the $t'$ element with respect to $t$ corresponds to the change from an s-like to a d-like lattice, realized in the $t$-$t'$-$J$ model for HTS. Accpeting the above mapping procedure to the single-band model, we end up with the problem of a hole propagation within an AF background which has been studied extensively within the $t$-$J$ model. It is well established that the kinetic energy of doped carriers in the $t$-$J$ model competes with the magnetic order and an added hole may propagate coherently in the AF background only by its coupling to local quantum fluctuations. The hole Green function calculated by exact diagonalization of small systems exhibits a quasiparticle (QP) peak at low energies for all k values in a two-dimensional (2D) lattice, having low dispersion $\sim J$. The QP states were also found from the analytic calculation of the Green function obtained in the lowest order self-consistent Born approximation (SCBA) introduced by Schmitt-Rink, Varma, and Ruckenstein, in excellent agreement with the above exact diagonalization results. Furthermore, it was demonstrated by Ramšák and Horsch that the self-consistent wave function for magnetic polarons in $t$-$J$ model predicts the same dipolar variation of the staggered spin deviation at large distances, as predicted in the semiclassical wave function of Shraiman and Siggia.

The nature of the hole propagation in a quantum antiferromagnet described by the $t$-$t$ model deviates from standard polaron physics. The fluctuations themselves cause an emerging kinetic scale for the coherent hopping of the renormalized hole, as was first discovered in exact diagonalization studies. The topology of the QP band is that of a particle hopping on a magnetic sublattice, while the QP bandwidth $\sim 2J$ is now set by the scale of the spin fluctuations. The total extent of the spectrum, $\sim 7t$, is determined by the hole hopping $t$ (i.e., the hole-magnon interaction scale). Below we use the analytic method based on the evaluation of the Green function using the SCBA to investigate whether these essential features of the hole propagation in the quantum antiferromagnet known from the $t$-$J$ model survive, provided the hole moves in addition over the sublattices of up and down spins by free hopping terms. In this respect the motivation of this paper is twofold. First, we study the effect of the three-site hopping terms ($\sim t'/U$) which follow from the canonical transformation of the
Hubbard model at large $U$. The latter terms are usually neglected, but recently were shown to be essential to reproduce the correct behavior of the optical conductivity in the strongly correlated Hubbard model.\textsuperscript{27,28} This model, as opposed to the $t$-$J$ model, is called the SC model below. Second, we include the next-neighbor hopping $\sim t'$ to simulate the situation in doped CuO$_2$ planes of the HTSO.\textsuperscript{13,14} It has been argued\textsuperscript{29} that the next-neighbor hopping term $\sim t'$ might be responsible for different physical properties as a hole can then propagate on the same sublattice without disturbing the underlying spin background (in contrast to the $t$ term). Recently, further justification to the $t'$ hopping was given, as it is necessary to reproduce the observed Fermi surfaces in the cuprates.\textsuperscript{30} The latter model which includes both contributions is called here the extended $t$-$t'$-$J$ model.

The paper is organized as follows. In Sec. II we present the SCBA for the $t$-$t'$-$J$ model. As shown, unlike in $t$-$J$ model, two-magnon processes arise due to the intrasublattice hopping terms. The numerical results obtained using the SCBA are presented and analyzed in Sec. III. The summary of the results and general conclusions are given in Sec. IV.

II. SPECTRAL FUNCTION IN $t$-$t'$-$J$ MODEL

A. $t$-$t'$-$J$ model

We start from the Hubbard model with the nearest-neighbor hopping $\sim t$, and next-neighbor hopping $\sim t'$, respectively,

\[
H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + H.c.) - t' \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + H.c.) + U \sum_{i} c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}.
\]

(2.1)

c_{i\sigma}^{\dagger}$ are electron creation operators at site $i$ with spin $\sigma$, and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, $\langle ij \rangle$ and $\langle \langle ij \rangle \rangle$ represent nearest and next-nearest neighbors, respectively, and each pair $\langle ij \rangle$ is included only once. The first two terms give one band of bandwidth determined by $t$ and $t'$. For large on-site repulsion $U \gg |t|, |t'|$ the Hubbard Hamiltonian Eq. (2.1) can be transformed to the following $t$-$t'$-$J$ Hamiltonian up to second order in hopping elements $\sim t^2/U$, etc., by a canonical transformation,\textsuperscript{9}

\[
H_{t-t'-J} = H_{t-J} + H_{t'-J} + H_{3\text{-site}},
\]

(2.2)

which consists of the usual $t$-$J$ and $t'$-$J$ Hamiltonians with restricted hoppings in the subspace without double occupancies $\tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i\downarrow - \sigma})$,

\[
H_{t-J} = -t \sum_{\langle \langle ij \rangle \rangle, \sigma} (\tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma} + H.c.) + \sum_{\langle \langle ij \rangle \rangle} (S_i S_j - \frac{1}{4} n_{i\downarrow} n_{j\downarrow}),
\]

(2.3)

\[
H_{t'-J} = -t' \sum_{\langle \langle ij \rangle \rangle, \sigma} (\tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma} + H.c.) + \sum_{\langle \langle ij \rangle \rangle} (S_i S_j - \frac{1}{4} n_{i\downarrow} n_{j\downarrow}),
\]

(2.4)

where $n_{i\sigma} = \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{i\sigma}$. The superexchange interactions are characterized by the exchange couplings, $J = 4t^2/U$ and $J' = 4t'^2/U$. The last part in our extended $t$-$t'$-$J$ model stands for the three-site terms which play an important role in the propagation of a hole,

\[
H_{3\text{-site}} = - \frac{1}{U} \sum_{\langle i \rangle, \sigma} \left[ t^2 \sum_{j', j''} n_{j'\sigma} n_{j''\sigma} + t'^2 \sum_{j', j''} n_{j'\sigma} n_{j''\sigma} + 2tt' \sum_{j', j''} n_{j'\sigma} n_{j''\sigma} \right] \times (c_{j'\sigma}^{\dagger} n_{i\downarrow - \sigma} c_{j''\sigma} - c_{j'\sigma}^{\dagger} n_{i\downarrow - \sigma} c_{j''\sigma} c_{j''\downarrow - \sigma}).
\]

(2.5)

Here the inner sums describe different three-site processes denoted by $tt'$, $tt'$, and $tt'$, respectively (e.g., $tt'$ means that a hole hops first between nearest neighbors and next between next-nearest ones). We note that the sites which may be reached in the hopping due to the $t^2/U$ term are not only the next-nearest neighbors, but also the third neighbors which are coupled by the forward hopping term.\textsuperscript{28} The other terms in $H_{3\text{-site}}$ have similar topology. Below we consider the hole propagation in the extended $t$-$t'$-$J$ model, Eq. (2.2), as well as in the SC model which results from the Hubbard model (2.1) at $t' = 0$,

\[
H_{SC} = H_{t-J} + H_{3\text{-site}}(t' = 0).
\]

(2.6)

B. Linear spin-wave order

Considering the motion of a single hole in the $t$-$t'$-$J$ model, Eq. (2.2), one has to implement the constraint of no double occupancy. A powerful method of doing this is to introduce the “slave fermion” representation for fermion operators,\textsuperscript{31}

\[
c_{i\sigma}^{\dagger} = f_i^{\dagger} b_{i\sigma},
\]

(2.7)

with $b_{i\sigma}$ standing for a Schwinger boson at site $i$, subject to the constraint that $f_i^{\dagger} f_i + \sum_{\sigma} b_{i\sigma}^{\dagger} b_{i\sigma} = 2S$ at each site. This automatically fulfills the condition of no double occupancy. Following the standard procedure,\textsuperscript{23} one considers mean-field theory in the Schwinger bosons and the Lagrange multipliers $\lambda_i$ to implement the constraints, which in an AF case is equivalent to the expansion around a saddle point of the following form:

\[
b_{i\uparrow} = b_{i\downarrow} = 0,
\]

\[
b_{i\uparrow} = b_{i\downarrow} = \sqrt{2S},
\]

\[
\lambda_i = \lambda_j = 0,
\]

(2.8)

where $i \in A, j \in B$, and $A$ and $B$ are the sublattices of $\uparrow$ and $\uparrow$ spins in the Néel state, respectively. Our general approach can be now simplified neglecting $\sim t^2/U$ terms in Eqs. (2.4) and (2.5) which are negligible in the realistic case, where $t'$ is small, i.e., $t' \ll t^2$. Thus we remove the frustration of AF interactions and obtain the spin waves as in $t$-$J$ model.\textsuperscript{24,21} Expanding up to quadratic order about the saddle point one finds from $H_{t-t'-J}$ (2.2) an effective spin-hole Hamiltonian,

\[
H_{\text{eff}} = H_{\text{eh}} + H_h + H_s,
\]

(2.9)
where
\[ H_{h-h} = -\sqrt{2St} \sum_{(ij) \in (AB)} \left[ f_i^f_j (b_{i \uparrow} + b_{j \downarrow}) + \text{H.c.} \right] \]
\[ + (1 - \delta) \left( 2S \right)^{\frac{3}{2}} \frac{t'U}{U} \sum_{(ij) \in (BAA) \cup (BBA)} \left( b_{ij \uparrow} - b_{ij \downarrow} \right) \left( f_i^f_j + \text{H.c.} \right), \]

\[ H_h = -2St' \sum_{(ij) \in (AB)} f_i^f_j \]
\[ + (1 - \delta) \left( 2S \right)^{\frac{3}{2}} \frac{t^2}{2U} \sum_{(ij) \in (ABA) \cup (BAB)} f_i^f_j, \]

\[ H_s = SJ \sum_{(ij) \in (AB)} \left( b_{i \uparrow}^\dagger b_{i \uparrow} + b_{j \downarrow}^\dagger b_{j \downarrow} + b_{i \uparrow}^\dagger b_{j \downarrow}^\dagger + b_{i \uparrow}^\dagger b_{j \downarrow} \right). \]

Here \( \delta = (f_i^f_i) \) is the average concentration of holes in the ground state, which can be neglected near to half-filling \( (\delta \approx 0) \). After Fourier,

\[ b_q = \sum_{i \in A} b_{i \uparrow} e^{iq \cdot r_i} + \sum_{j \in B} b_{j \downarrow} e^{iq \cdot r_j}, \]

and Bogoliubov transformations,

\[ \beta_q = u_q b_q - v_q^* b_q^\dagger, \]
\[ u_q = \left[ 1 + (1 - \gamma_q^2) \frac{1}{2} \right]^{\frac{1}{2}}, \]
\[ v_q = -\text{sgn}(\gamma_q) \left[ 1 - (1 - \gamma_q^2) \frac{1}{2} \right]^{\frac{1}{2}}, \]

with \( \gamma_q = 1/2 \sum_q \exp[iq(R_{i,z} - R_{i,x})], \) and with \( z = 4 \) in a 2D case. Neglecting an irrelevant constant one finds after somewhat lengthy calculations the following Hamiltonian in linear spin-wave (LSW) order:

\[ H_{LSW} = \sum_k \varepsilon(k) f_k^f f_k^\dagger + \sum_q \omega_q \beta_q^\dagger \beta_q \]
\[ + \frac{1}{\sqrt{N}} \sum_{kq} \left[ M(k, q) f_k^f f_{k-q}^\dagger - \text{H.c.} \right], \]

where \( \omega_q \) is the magnon dispersion in the unfolded Brillouin zone (BZ) for the Holstein-Primakoff spin waves which diagonalize \( H_s (2.12) \),

\[ \omega_q = 2J(1 - \gamma_q^2)^{1/2}. \]

\( M(k, q) \) is the hole magnon bare vertex depending on the geometrical factors which follow from the Bogoliubov transformation (2.14),

\[ M(k, q) = zt(u_q \gamma_{k-q}^\dagger + v_q \gamma_k^\dagger), \]
\[ + \frac{zt'}{U} (1 - \delta)(\eta_{k-q} - \eta_k)(u_q \gamma_{k-q}^\dagger - v_q \gamma_k^\dagger), \]

(2.17)

with \( \gamma_q = \frac{1}{2}(\cos q_x + \cos q_y) \), and \( \eta_q = \cos q_x \cos q_y \) for a 2D lattice with the lattice constant \( a = 1 \). Similarly as in the \( t-J \) model,\(^{21} \) here the vertex function Eq. (2.17) vanishes at \( q = (0, 0) \) and \( (\pi, \pi) \) being large at intermediate values of the momentum transfer \( q \). Moreover, unlike in the \( t-J \) model, we have here the free band \( \epsilon(k) \) for spinless \( f_k \) fermions, with the dispersion at low doping \( \delta \) given by

\[ \epsilon(k) = zt' \gamma_k^\dagger + \frac{zt^2}{U} (1 - \delta)(\gamma_k^\dagger - 1). \]

(2.18)

This propagation in the large \( U \) limit results from the intrasublattice processes \( A(B) \rightarrow A(B) \), occurring without disturbing the underlying AF spin background, realized by the \( t' \) (direct hopping) element, and by the three-site \( A \rightarrow B \) hopping terms \( \sim t^2/U \). The hole-spin couplings due to the \( t' \) and \( t^2/U \) terms involve even number of emission or absorption magnon processes around the saddle point, and are described by the last part in Eq. (2.10). Such processes are neglected in the lowest order used to write \( H_{LSW} \).

Using the SCBA\(^{23} \) we find the hole Green function of the form,

\[ G(k, \omega) = \frac{1}{\omega - \epsilon(k) - \Sigma(k, \omega)}, \]

(2.19)

with the self-energy \( \Sigma(k, \omega) \) determined self-consistently with the above Green functions,

\[ \Sigma(k, \omega) = \frac{1}{N} \sum_q M^2(k, q) G(k - q, \omega - \omega_q). \]

(2.20)

The system of the above equations, Eqs. (2.19) and (2.20), can be solved self-consistently to obtain the spectral functions,

\[ A(k, \omega) = \frac{1}{\pi} \text{Im} G(k, \omega + i\epsilon), \]

(2.21)

with \( \epsilon \rightarrow 0^+ \). In numerical calculation a finite value of \( \epsilon \) \( (\epsilon \approx 0.02 \text{ eV}) \) leads to a smoothing of spectral functions for the used finite number of \( k \) points in BZ. Omitting crossed diagrams, we ignore altogether such processes in which the spin excitations are absorbed in a different order than that in which they were created. Although a hole must absorb every emitted spin excitation, it is mobile as it moves together with the spin waves by which it dresses.

**C. Higher-order magnon processes**

In order to clarify the quality of the conventionally used LSW approximation for the hole propagation in the \( t-J \) model,\(^{21-24} \) we take into account also the higher-order magnon processes, existing in the performed expan-
sion about the saddle point. In Sec. II B we had for the hole propagation (i) zeroth order terms, \( f_i^\dagger f_j \), giving free hole dispersion, Eq. (2.18), and (ii) one-magnon terms, \( f_i f_j^\dagger b_{i\sigma} \) and \( f_j f_i^\dagger b_{i\sigma} \) (coupling to spin waves), while the free two-magnon processes, \( \sim \langle t_i \rangle \langle t_j \rangle \), give ordinary spin waves. Now we turn to two-magnon processes which couple to the moving hole, as, e.g., \( f_i^\dagger f_j^\dagger b_{i\sigma}^\dagger b_{j\sigma}^\dagger \), and the like. Such processes are described by more complicated Feynman diagrams in SCBA which come both from \( t' \) and \( t^2/U \) corrections. The \( t' \) and \( t^2/U \) terms modify the previously derived effective Hamiltonian in LSW order \( H_{\text{eff}} \), Eq. (2.9), in the following way:

\[
\tilde{H}_{\text{eff}} = H_{\text{eff}} - t' \sum_{\langle ij \rangle \in (AA)} b_i^\dagger b_{j+1} + \sum_{\langle ij \rangle \in (BB)} b_i^\dagger b_{j+1} \right] f_i f_j^\dagger \\
+ \frac{2t^2}{U} (1 - \delta) S \left[ \sum_{\langle (ji) \rangle \in (ABA)} (b_j^\dagger b_{i+1}^\dagger + b_i b_{j+1}) + \sum_{\langle (ij) \rangle \in (BAB)} (b_i^\dagger b_j^\dagger + b_j b_i) \right] f_i f_j^\dagger,
\]

(2.22)

where \( \sim \) in \( \tilde{H}_{\text{eff}} \) indicates the corrected Hamiltonian, and \( i \neq j, j' \) and \( j' \neq j \) in all sums. Making Fourier and Bogoliubov transformations one obtains in the reciprocal space the Hamiltonian which includes second order spin-wave (SOSW) processes,

\[
H_{\text{SOSW}} = H_{\text{LSW}} + \frac{1}{N} \sum_{k q_1, q_2} \left[ V_1(k, q_1, q_2) f_k^\dagger f_{k - q_1, q_1, -q_2, \beta_{q_1}, \beta_{q_2}, \text{h.c.}} \right] \\
+ \frac{1}{N} \sum_{k q_1, q_2} \left[ V_2(k, q_1, q_2) f_k^\dagger f_{k - q_1, q_1, -q_2, \beta_{q_1}^\dagger, \beta_{q_2}^\dagger, \text{h.c.}} \right],
\]

(2.23)

with \( V_1(k, q_1, q_2) \) and \( V_2(k, q_1, q_2) \) of a complicated form,

\[
V_1(k, q_1, q_2) = -\frac{z}{2} \left[ t'(\eta_{k - q_1, u_{q_1}, u_{q_2}, v_{q_1}} + \eta_{k - q_2, u_{q_2}, v_{q_1}}) \\
+ \frac{t^2}{U} (1 - \delta) 2S (\xi(k - q_1, q_2, -q_1, -q_2) u_{q_1, u_{q_2}, v_{q_1}} + \xi(k, q_1, q_2) v_{q_1}) \right],
\]

(2.24)

\[
V_2(k, q_1, q_2) = -\frac{z}{2} \left[ t'(\eta_{k - q_1, u_{q_1}, u_{q_2}, v_{q_1}} + \eta_{k - q_2, v_{q_1}, v_{q_2}}) \\
+ \frac{t^2}{U} (1 - \delta) 2S (\xi(k - q_1, q_2, -q_1, -q_2) u_{q_1, v_{q_2}, v_{q_1}} + \xi(k, q_1, q_2) u_{q_1} v_{q_1}) \right],
\]

(2.25)

where

\[
\xi(k, q_1, q_2) = z \gamma_k (\gamma_{k - q_1} + \gamma_{k - q_2}) - \gamma_{q_1} - \gamma_{q_2}.
\]

(2.26)

The SCBA can be straightforwardly generalized for our two-magnon couplings in \( H_{\text{SOSW}} \). Using the same rules as in Ref. 24 one can draw all one- and two-magnon non-crossing diagrams for the self-energy shown in Fig. 1, and next replace the free Green functions by full ones due to the self-consistent procedure. As a result we have the following rainbow approximation:

\[
\Sigma(k, \omega) = \Sigma_I(k, \omega) + \Sigma_{II}(k, \omega) \\
+ \Sigma_{III}(k, \omega) + 2\Sigma_{IV}(k, \omega),
\]

(2.27)

where the different contributions in Eq. (2.27) correspond to the diagrams I–IV shown in Fig. 1,
The factor “2” in the last contribution $\Sigma_{IV}(\mathbf{k}, \omega)$ follows from two topologically equivalent diagrams represented in diagram $IV$ of Fig. 1.

First we find it important to check whether the QP’s survive when the above more complex two-magnon processes are included, and whether they might give significant changes of the overall picture. In order to evaluate the role of these second order processes we used the self-energy given by Eqs. (2.27) and (2.28), instead of the lowest order expression (2.20), and solved self-consistently the hole Green function (2.19), as described in Sec. II B. In this way we have obtained the improved spectral functions $A(\mathbf{k}, \omega)$ (2.21) shown in Fig. 2. Because of numerical complications posed by four-dimensional sums present in Eqs. (2.28), we have carried out the self-consistent procedure for $N = 8 \times 8$ lattice and treated both contributions ($t'$ and $t^2/U$) independently.

As one can see in Fig. 2, the effect of $t^2/U$ hopping is really insignificant. It changes the energy of the ground state by $\sim 0.1|t|$, and leaves the shape of the incoherent part almost intact. The $t'$ corrections are even by about an order of magnitude smaller than the $t^2/U$ ones, if $|t'/t| < 0.4$, as it is the case for the realistic parameters. Therefore, they are not presented explicitly here. These higher-order findings justify $a$ posteriori the standard self-consistent procedure in LSW order and confirm that one-magnon couplings included within the SCBA23 are accurate enough to reproduce the realistic properties of the $t$-$J$-like models.

### III. NUMERICAL RESULTS

In this section we present some representative numerical results for different sets of parameters. After demonstrating the insignificance of higher-order magnon processes, the spectral functions $A(\mathbf{k}, \omega)$ are obtained by iterating the self-energy (2.20) and the Green function (2.19) with the lowest-order vertex (2.17). We adopted the nearest-neighbor hopping $t = 1.0$ (eV) as the energy unit, and the superexchange $J = 0.4t$ in almost all performed calculations. These values were obtained for the effective one-band model4-8 for realistic values of parameters in the three-band model.32,33 The realistic value of the next-nearest-neighbor hopping $t'$ has been estimated to be in the range $|t'/t| \sim 0.2-0.4$ using Cu$_2$O$_8$ cluster,5,30 but from local density approximation (LDA) calculations and comparisons with x-ray-absorption experiments for La$_{1-x}$Sr$_x$CuO$_4$ the lower ratio was extracted 0.16. Here we follow more recent literature13,14 and assume $|t'/t| = 0.3$ for numerical analysis. The energy scale $\omega$ consists of 100 points per energy unit and our lattice has 16 x 16 points in $\mathbf{q}$ space with periodic boundary conditions. We have verified that the results for the 16 x 16 lattice are hardly distinguishable from the ones for the 12 x 12 lattice. Hence we claim that $N = 16 \times 16$ is representative of the thermodynamic limit, in spite of other opinions on this subject in the literature.34

The two main new features of the extended $t$-$t'$-$J$ model with respect to the $t$-$J$ model are (i) the dispersion of free holes, Eq. (2.18), and (ii) $t'$-$U$ corrections to the hole-magnon vertex. First, we present the free hole bands in Fig. 3. As one can see, both propagating terms, $t^2/U$ [Fig. 3(a)], and $t'$ [Fig. 3(b)] give similar dispersions, with the maxima at $\Gamma = (0, 0)$ and $M = (\pi, \pi)$ points, and minima at $X = (\pi, 0)$ point, respectively, if $t' > 0$. Thus, if $t' > 0$, the effect of the three-site hopping $\sim t^2/U$ is amplified by the direct next-neighbor hopping $\sim t'$. On the contrary, if $t' < 0$, the overall dispersion due to $t^2/U$ terms is reduced by the direct hopping to second neighbors. As a result, the dispersion relation $\varepsilon_{k}$ (2.18) is relatively flat and may even be reversed for larger negative $t'$. The 2D character of the fermion bands given by Eq. (2.18) may be recognized from the density of states (DOS) with a van Hove singularity close to $\omega = 0$, displayed in Fig. 4. Remarkably, the van Hove singularity is found at negative $\omega$ both for $t' = 0.3t$ [Fig. 4(a)], and for $t' = -0.3t$ [Fig. 4(b)]. In agreement with the above
discussion, the band for $t' = 0.3t$ is much broader than the band obtained for $t' = -0.3t$.

First, we turn to the SC model, i.e., to the $t$-$J$ model extended by the $t'^2/U$-hopping terms. The free hole band is asymmetric and has a width of $W = 4J$. The hole energy $\varepsilon_k$ amounts to $3J$ at the $\Gamma$ and $M$ points which causes the disappearance ofQP states in the vicinity of $k = (0,0)$, as shown in Fig. 5(a), in contrast to the $t$-$J$ model, where the QP states form for each $k$ value. At $k = (\pi,0)$ the free hole energy $\varepsilon_k = 0$ is much smaller than at $k = (0,0)$, and the QP peak is visible already at small $J = 0.1t$. However, the QP is still considerably damped at this point and the incoherent processes absorb more weight than in the $t$-$J$ model [see Fig. 5(b)]. The reverse is true at the $X$ point [shown in Fig. 5(c)], where the QP state is more pronounced at small $J/t$ than in the $t$-$J$ model. The coherent state strengthens with increasing $J$, both for $k = (\pi/2,0)$ and $k = (\pi,0)$, as shown in Figs. 5(e) and 5(f). In contrast, the incoherent peak moves to the higher energies due to the increasing value of $\varepsilon_k$ at the $\Gamma$ point, and no QP is found [Fig. 5(d)]. Altogether, we found a striking difference in spectral functions between the generic $t$-$J$ model, as obtained by Martínez and Horsch, caused by the three-site hopping terms. The resulting hole dispersion $\varepsilon(k)$ is strongly $k$ dependent and renormalizes the self-energy obtained in SCBA particularly in some parts of the BZ.

In the extended $t$-$t'$-$J$ model we included both parts of the hole dispersion $\varepsilon(k)$, as given in Eq. (2.18), and the $t't'/U$ corrections to the hole-magnon vertex [see Eq. (2.17)]. For numerical evaluation we used realistic parameters for electron- and hole-doped CuO$_2$ planes of HTSO: $J/|t| = 0.4$, and $t' = \pm 0.3$, with $t = \mp 1.0$, respectively. For $t' = 0.3$ and $t = -1.0$ (electron doping) the spectral functions $A(k,\omega)$ (2.21) are qualitatively similar to those found in the SC model, but the QP’s become stronger due to increased dispersion at those $k$ points, where the free hole energy $\varepsilon_k$ is negative, or close to zero. Thus the sharp QP’s are found at the $M' = (\pi/2,\pi/2)$ (not shown) and $X = (\pi,0)$ points [Fig. 6(c)], while no QP is found at the $\Gamma$ point. In Fig. 6(b) we present the spectral function $A(k,\omega)$ for $k = (\pi/2,0)$, where the effect of hole dispersion is the most significant. As opposed to the generic $t$-$J$ model, our full $t$-$t'$-$J$ model gives here a completely incoherent spectrum with a broad irregular maximum at $\omega \sim -1.5$ eV. In contrast, at the $X$ point $A(k,\omega)$ has a strong QP peak and almost no incoherent part [Fig. 6(c)], contrasting sharply with that found at $k = (0,0)$ [Fig. 6(a)]. The changes in the spectrum are the smallest for $k = (\pi/2,\pi/2)$ (halfway between $\Gamma$ and $M$ point), where the $t'$ term in the free hole band disappears, and the $t'^2/U$ one is small (see Fig. 3). In spite of these well formed QP states at the $k$ values corresponding to the local minima of $\varepsilon_k$, the total weight of the QP states is somewhat reduced with respect to the $t$-$J$ model as no QP’s were found in part of the BZ, which results in the reduced weight in the QP DOS at low energy [see Fig. 6(d) and inset]. We note that the incoherent processes now give flat spectrum which spreads up to $\sim 6|t|$, i.e., the total width of the QP DOS has increased from $\sim 7|t|$ in the $t$-$J$ model to $\sim 9|t|$ due to the intrasublattice hopping. As seen in Fig. 6, the incoherent part is more flat not only in the integrated spectrum, but also for each $k$ point separately.

A comparison between $t = -1.0$, $t' = 0.3|t|$, and
$t = 1.0$, $t' = -0.3t$ (Figs. 6 and 7) shows that the existence of QP states at particular $k$ values depends on the actual value and sign of the next-nearest-neighbor hopping $t'$. We note that the sign of $t$ is irrelevant in LSW order, as the squared vertex (2.17) in Eq. (2.20) contains only $t^2$. In general, taking $t' < 0$ one finds coherent hole propagation (QP states) in the whole BZ (Fig. 7), with the strongest QP for $k = \left(\frac{\pi}{2}, \frac{\pi}{2}\right)$ at $\omega \approx -2.2t$ [Fig. 7(b)]. The QP has low weight, but is already well formed around $k = (0, 0)$ (Γ point), as shown in Fig. 7(a). At the X point we found significantly more coherent weight than in the $t$-$J$ model at the same value of $J/t$ (compare Fig. 7(c) and the inset of Fig. 6(c)). Furthermore, examining the DOS of QP states shown in Fig. 7(d), we notice that for $t' < 0$ one cannot identify some main QP peaks (or “group” of peaks as for $t' > 0$ in Fig. 6), but QP’s spread regularly in a broad band $\delta E_{\text{QP}} \approx 2.5t$. The reason is that the free dispersion $\epsilon(k)$ which results from the three-site hopping term is here overcompensated by $t' = -0.3t$. As a result, the QP peaks occur in the whole BZ, but turn out to be weaker than in the $t$-$J$ model. At the same time, the structures in the incoherent part of the spectrum are more pronounced than in the $t$-$J$ model.

The dispersion of the obtained QP band is drawn in Fig. 8 for the $t$-$J$ model, the SC model, and the extended $t$-$t'$-$J$ model with negative $t'$. For convenience, the curves were continued up to the Γ point, in spite of the absence of QP’s at this point in the SC and extended $t$-$t'$-$J$ models. One finds that the three-site hopping renormalizes...
the QP dispersion $E_{QP}(k)$, with the larger positive shifts at the $\Gamma$ and $M$ points. As a result, the overall dispersion is somewhat larger than in the $t$-$J$ model. The flat character of the QP near the $X$ point is preserved, with even a weaker dependence on the momentum $k$ in the neighborhood of the $X$ point. These main features are similar to those found from the exact diagonalization studies, and from the earlier analytic approach of Krier and Meissner. More substantial changes are found by adding the next-neighbor hopping $t' = -0.3t$. The QP energy $E_{QP}(k)$ moves to lower energies along the $\Gamma$-$X$ line, with larger shifts for the maxima at the $\Gamma$ and $X$ points. In contrast, the QP's move to higher energies near the $X$ point which gives a local maximum, being much stronger than in the $t$-$J$ model. The absolute minimum appears at the same $k = (\pi/2, \pi/2)$ point in the BZ, as in the $t$-$J$ (and SC) model, but its energy is lower by about 0.3t. The width of the QP band is somewhat smaller than for the generic $t$-$J$ model. Of course, the next-neighbor hopping with the opposite (positive) sign of $t'$ lowers the QP energy at the $X$ point and increases the QP bandwidth. The width is then larger than in the $t$-$J$ model.

Finally, we compare the QP wave functions for the generic $t$-$J$ model and for the extended $t$-$t'$-$J$ model with $t' = -0.3$ and $t = 1.0$. The wave function of a hole dressed by spin waves has the following form:

$$|\Psi_k^\pm\rangle = a_k \left[ f_k^1 + N^{-\frac{1}{2}} \sum_{q_1} M(k, q_1) G(k_1, \omega_1) f_{k_1}^1 \beta_{q_1}^1 \right. 
+ \left. \cdots + N^{-\frac{n}{2}} \sum_{q_1, \ldots, q_n} M(k, q_1) \cdots M(k_{n-1}, q_n) G(k_n, \omega_n) f_{k_n}^1 \beta_{q_n}^1 \cdots \beta_{q_1}^1 \right] |0\rangle,$$

(3.1)

with $k_i = k - q_i - \cdots - q_1$, $\omega_i = \varepsilon_k - \varepsilon_{q_i} - \cdots - \varepsilon_{q_1}$, and $|0\rangle$ standing for the vacuum of fermions and magnons. This wave function is a solution of the Schrödinger equation for the $t$-$J$ model in LSW approximation and gives the QP energy in SCB from $\varepsilon_k = \Sigma(k, \varepsilon_k)$, while the QP spectral weight $a_k$ is then given by

$$a_k = \frac{1}{1 - \frac{\beta}{\Sigma} \sum_{\mu}(k, \omega)|_{\omega = \varepsilon_k}}.$$

(3.2)

In a two-sublattice antiferromagnet we consider the linear combinations $|\Psi_k^\pm\rangle = 2^{-1/2}(|\Psi_k^\pm\rangle \pm |\Psi_k^\mp\rangle)$, which corresponds to the QP moving either on $\downarrow$ or on $\uparrow$ sublattice, respectively. In Fig. 9 we present the result of the numerical calculation of $N_k(n) = \langle \Psi_{k+1}^{(n)} | \Psi_{k+1}^{(n)} \rangle$ for various numbers of magnons $n = 0, 1, 2, 3$, for the $t$-$J$ and $t$-$t'$-$J$ models. As one can see the results are practically indis-
tistinguishable for $J/t < 0.2$, while the difference between
the wave function becomes more significant at larger values
of $J$. For example, the spectral weight of a QP peak
in the extended $t$-$t'$-$J$ model is by about 25% larger
than in the $t$-$J$ model for $J/t = 0.6$. For $J = 0.4t$ it is prac-
tically sufficient to use the expansion up to two magnons
in both cases. Of course, the higher-order magnon terms
are equally important for $J/t \to 0$, when $N_k \to 0$.

IV. SUMMARY AND CONCLUSIONS

We studied the dynamics of a single hole in a Heisen-
berg antiferromagnet using the SCBA scheme in which
one sums up an infinite class of “noncrossing” diagrams,
as shown by diagram I of Fig. 1. We focused here on sev-
eral physically relevant extensions of the $t$-$J$ model.
The SCBA turns out to be surprisingly accurate for this latter
model, as shown for the $S = 1/2$ $t$-$J$, and $S = 1$ and $3/2$
models. Our main conclusion is that coherent quasipar-
ticles similar to those found earlier in the $t$-$J$ model exist
as well when the hole has a possibility of free propaga-
tion on one of the sublattices. The coherent propagation
promoted by quantum-spin fluctuations dominates the
coherent motion of the hole and destroys the initial propa-
gation on the energy scale $\sim t^2/U$ (or $\sim t'$) completely.
We notice that the mean-field approximation (classical
limit) fails completely in the description of the spectral
function; there is nothing left of the broadband $\sim z t'$,
characteristic of the classical limit. As in the $t$-$J$ model,
the hole gets dressed up with spin waves because of the
near to singular coupling to the spin background. Rather
remarkably, although one needs self-consistency (rainbow
resummation), the vertex corrections are utterly harm-
less, as we showed once more in a somewhat different
context in our Sec. III C.

As expected, the QP pole strength $a_k$ increases with the
increasing ratio $J/t$. We note that this QP is physi-
cally different from a normal polaron, as the hopping of
the hole ($\sim t$) acts to increase locally the quantum spin
fluctuations, melting the “spin solid” in its immediate
neighborhood. The motion of the hole is accompanied
by a backflow of spin fluid, allowing it to move coher-
ently through the lattice (“spin liquid polaron”). In order
to make the comparison between the different cases more
explicit, we extracted the QP weight at $k = (\pi/2, \pi/2)$
and $(\pi, 0)$ for a few representative values of $J$ in Table I.
First of all, the QP’s are somewhat stronger in the SC
model than in the $t$-$J$ model due to the lowered reference
energy $\varepsilon_k$ by the free propagation via the effective $t^2/U$
hopping for these values of $k$, corresponding to the mini-
num in Fig. 3(a). If we turn the next-neighbor $t'$ hopping,
the QP at the $k = (\pi/2, \pi/2)$ point hardly changes and
has the weight in between those found for the $t$-$J$ and
SC models. The reason is that the $t'$ contribution in $\varepsilon_k$
vanishes at this $k$ value, and therefore only the incoher-
ent processes are averaged out in a different way. The
situation is quite different at $k = (\pi, 0)$, however, where
the two propagating terms $(t^2/U$ and $t'$) frustrate each
other (see Fig. 3), and the QP is damped, having almost
the same weight of $a_k \approx 0.18$ for $J/t = 0.1$ and 0.4, and

<table>
<thead>
<tr>
<th>$J/t$</th>
<th>$t$-$J$</th>
<th>SC</th>
<th>$t' = -0.3$</th>
<th>$t' = 0.3$</th>
<th>$t$-$t'$-$J$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.1648</td>
<td>0.1746</td>
<td>0.1540</td>
<td>0.1355</td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>0.2405</td>
<td>0.2700</td>
<td>0.2389</td>
<td>0.2224</td>
<td></td>
</tr>
<tr>
<td>0.4</td>
<td>0.3512</td>
<td>0.4228</td>
<td>0.3910</td>
<td>0.3899</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>0.5720</td>
<td>0.7202</td>
<td>0.7204</td>
<td>0.7178</td>
<td></td>
</tr>
</tbody>
</table>

$J = (\pi/2, \pi/2)$ and $k = (\pi, 0)$ as a function of $J$, found for the $t$-$J$, strong-coupling (SC), and the extended $t$-$t'$-$J$ model with $t' = -0.3$ and $t' = 0.3$ ($t = 1.0$).

TABLE I. Quasiparticle weight $a_k$ at $k = (\pi/2, \pi/2)$

We have demonstrated that the $t$-$t'$-$J$ model leads to qualitatively different and richer behavior
than that of the standard $t$-$J$ model. Depending on the
sign of the next-nearest neighbor hopping, the QP’s

and a minimum of about 0.14 in between. These weights are
less than one-half of the respective weights obtained in
the $t$-$J$ and SC models. Of course, the three-site hopping
terms $\sim t^2/U$ increases with $J$, so the coherent motion
takes over at larger $J$ (see Table I). In fact, the damp-
ing of the QP’s is found everywhere along the $\Gamma$-$X$ direc-
tion, and we reported earlier that the QP practically dis-
ppears for $k = (\pi/2, 0)$ at $t' \approx -0.2t$. The situation is
reversed for $t' > 0$, where the effective three-site hop-
ping and the direct $t'$ hoppings add to each other. There
is only little change at $k = (\pi/2, \pi/2)$ point, with the
weight very similar to the other cases. On the contrary,
the QP at $k = (\pi/2, 0)$ is much more pronounced than
in the $t$-$J$ and the SC model, with the weight $a_k = 0.42$,
0.52, and 0.63 at $J = 0.1, 0.2$, and 0.4, respectively (see
Table I). The difference is reduced at $J = 1.0$, as the QP
dominates at large values of $J$, practically indepen-
dently of the details of the effective Hamiltonian.

Recently, the $t$-$J$ model was used to interpret$^{39}$ the
angle-resolved photoemission experiments (ARPES) data of
Dessau et al.,$^{40, 41}$ who reported extended regions of flat
bands near the Fermi energy for Bi2212, Bi2201, Y123,
and Y124 superconductors. From the present study we have
to conclude that the agreement between the QP disper-
sion obtained from exact diagonalization of Dagotto,
Nazarenko, and Boninsegni$^{39}$ and the experimental data of
Dessau et al.$^{40}$ was somewhat accidental. It is well known from the cluster studies that the extended $t$-$t'$-$J$ model,
rather than the $t$-$J$ model, corresponds to the low-energy physics of HTSO.$^{42-45}$ We have shown, taking the realistic values of $t = 0.4$ eV,
$J = 0.13$ eV, and $t' = -0.12$ eV for a hole-doped system,
one finds a local maximum at the $X$ point, corresponding
to the minimum in the electronic bands measured in the
experiment.$^{40}$ The flat band was found by us instead for
positive $t' = 0.12$ eV, in agreement with the exact dia-
gonalization data of Ref. 39, obtained with $t' = 0.15$ eV. As
this value of $t'$ corresponds to the electronic doping, it
remains a puzzle to what extent the extended $t$-$t'$-$J$
model might be used to understand the ARPES data for
HTSO, except for just fitting its parameters.

In conclusion, we have demonstrated that the $t$-$t'$-$J$
model leads to qualitatively different and richer behavior
than that of the standard $t$-$J$ model.
are damped or enhanced, and their dispersion changes. In any case, they survive for those $k$ values which correspond to the QP energy minima, and thus might be observed in the strongly correlated systems which map on the extended $t-t'-J$ model, provided the interaction between the quasiparticles is weak. It is a bit surprising, however, that the free hole bands of considerable bandwidth $W = 2\pi|t'|$ ($W = 2.4|t|$ for realistic parameters used in this paper, $t = \pm 1.0$, $t' = 0.3$) disappear completely, not altering the QP energies in a significant way, and the low-energy QP states still appear in the energy range of $\sim 2J$, as in the $t-J$ model. Thus it turns out that the coherent motion of a hole is here possible only by its coupling to the quantum fluctuations in an antiferromagnet. In this respect these models are more restricted than the spin-fermion models which may be derived for strongly correlated transition metal oxides, as NiO (Ref. 42) and HTSO. In this latter case the moving hole interacts with the magnetically ordered lattice by the Kondo interaction, while the direct hopping connects only the oxygen orbitals and as such is only weakly dressed by the incoherent processes. As a result, the free propagation is there damped, but still visible, and shows up at higher energies (in hole notation). Such states are of importance for more realistic description of the photoemission data of doped charge-transfer insulators, including HTSO, away from the Fermi level. This confirms the notion that the effective models of the $t-t'-J$ type might be useful only for the low-energy phenomena.

**ACKNOWLEDGMENTS**

We thank Lou-Fé Feiner and Peter Horsch for valuable discussions on different parts of this work. J.B. and A.M.O. acknowledge support by the Committee of Scientific Research (KBN) of Poland, Project No. 2 P03B 144 08. J.Z. acknowledges support by the Royal Dutch Academy of Sciences (KNAW).

---

15. For a review, see E. Dagotto, Rev. Mod. Phys. 66, 763 (1994).