Two-hole problem in the *t-J* model: A canonical transformation approach

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The *t-J* model in the spinless-fermion representation is studied. An effective Hamiltonian for the quasiparticles is derived using a canonical transformation approach. It is shown that the rather simple form of the transformation generator allows one to take into account the effect of hole interactions with the short-range spin waves and to describe the single-hole ground state. Obtained results are very close to ones of the self-consistent Born approximation. Further accounting of the long-range spin-wave interaction is possible on a perturbative basis. Spin-wave exchange and an effective interaction due to minimization of the number of broken antiferromagnetic bonds are included in the effective quasiparticle Hamiltonian. The two-hole bound state problem is solved using a Bethe-Salpeter equation. The only bound state found to exist in the region of $1<(t/J)<5$ is the d wave. Both types of the hole-hole interaction are important for its formation. A discussion of the possible relation of the obtained results to the problem of superconductivity in real systems is presented. [S0163-1829(97)04429-9]

I. INTRODUCTION

The problem of the hole motion in an antiferromagnetic (AF) background of local spins originally arose in connection with the study of the localized magnetic insulators,[1,2] and has received considerable attention since the discovery of the CuO_2 based high-temperature superconductors. It is well established that at zero doping these materials are insulators with the long-range AF order, and one is well described by the two-dimensional Heisenberg model.[3] The instability of long-range AF order under the small finite doping of carriers is due to the strong interaction of spins with mobile holes.[4,5] The simplest model, which contains in itself this strong interaction, is the t-J model.[6] Extensive studies of this model's validity for the description of the real CuO_2 plane result in a number of quantitative predictions for the range of parameters and in the set of possible t-J model generalizations.[7–11] It is widely believed that the essential low-energy physics of the high-T_c systems can be studied using the pure t-J model

$$H_{t-J}=t\sum_{\langle ij\rangle,\alpha}\tilde{c}^{\dagger}_{i,\alpha}\tilde{c}_{j,\alpha}+J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\mathbf{S}_j-\frac{1}{4}N_iN_j\right) \tag{1}$$

in the standard notation of the constrained fermion creation (annihilation) operators $\tilde{c}^{\dagger}_{i,\alpha}(\tilde{c}_{i,\alpha})$, $\langle ij\rangle$ denotes the nearest neighbor sites, $\mathbf{S}_i$ is a local spin operator, and N_i is the operator of the number of spins. Physically, the t term describes an additional hole (singlet) hopping on the background of hole spins, or, otherwise, the hopping of hole (vacancy) in the electron spin background. An important feature of this term is the absence of the double-particle occupancy at any site. Exclusion of doubly occupied states does not allow for the implementation of mean-field-type approximations.

The single-hole problem in the t-J model (1) has been extensively studied by the various analytical[12–22] and numerical[23–26] techniques, which have provided the deep understanding of the character of the hole motion. For a review see, e.g., Refs. 27 and 28. Analytical results obtained within the self-consistent Born approximation (SCBA) (Refs. 12, 13, 20, and 29) agree very well with the exact diagonalization studies on clusters,[28] variational,[16–18] and other approaches.[19] The main feature of hole motion revealed in these studies is the strong renormalization of the naive tight-binding result for the band energies due to the hole ''dressing'' by the cloud of spin excitations. This leads to a narrow band ($\sim 2J$ for $t/J>1$ and $\sim t^2/J$ for $t\ll J$) with minima at the $\pm(\pi/2,\pm\pi/2)$ points on the boundary of the magnetic Brillouin zone (MBZ).

The two-hole problem has received much attention due to the searching of possible pairing mechanisms. In spite of the large amount of work a full consensus on the existence of bound states in the t-J model is absent. There was much work devoted to the study of the spin-fluctuation pairing and corresponding type of superconductivity.[30–34] There is strong evidence that the long-range spin-wave exchange, which is the source of the dipolar interaction between holes,[32,35] can lead to the d-wave pairing in the t-J model. As was established in Ref. 36 the corresponding bound states are shallow and have a large size. Many efforts aimed at the study of the t-J model bound states originated from the fact that the two holes can minimize their energy by sharing the common link, that can lead to the picture of superconductivity by ''preformed'' pairs.[37] More specifically, numerical works in exact diagonalization on small clusters and Monte Carlo studies, which account for the latter interaction, provide negative energy of the bound state of the $d_{x^2-y^2}$ symmetry up to the values $t/J\sim 3-5$,[38–41] which are relevant to the real compounds. Variational[42] and a kind of quasiparticle calculation[43] yield the critical value of $t\simeq 2J$ for this interaction, which is somewhat lower than the realistic one. Generally, there is no agreement on the energy of the ground state of two holes and on their spatial correlation function[44] even between the similar approaches.

In this paper we propose a canonical transformation approach to the t-J model problems that allowed us to turn from the t-J model to an effective quasiparticle Hamiltonian,

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describing the ‘‘dressed’’ holes and their interaction of the (i) ‘‘contact’’ type and (ii) via spin waves, and then to find the ground state of two such quasiparticles. Both types of interactions are accurately accounted for by our approach. In some sense, we use the ideas of the earlier works by Sushkov *et al.*,[17,5,45,36] where the same scheme was realized using quite different approach.

To begin, let us describe the form of the Hamiltonian (1) we start with. The most popular analytical approach to the t-J model is the SCBA,[12,13,20,29] which is based on the spinless-fermion representation for the fermion operators and Holstein-Primakoff[12,20] or Dyson-Maleev[46] representation for the spin operators for the t-J model. Namely, this approach is applied to the spin-polaron Hamiltonian, which is followed from the t-J one (1) in the presence of the long-range AF order and in the linear spin-wave approximation:

$$H \simeq 2J\sum_{\mathbf{q}} \omega_{\mathbf{q}} a^\dagger_{\mathbf{q}} a_{\mathbf{q}} + t\sum_{\mathbf{k},\mathbf{q}} (M_{\mathbf{k},\mathbf{q}} h^\dagger_{\mathbf{k}-\mathbf{q}} h_{\mathbf{k}} a^\dagger_{\mathbf{q}} + \text{H.c.}) + \Delta H, \tag{2}$$

where $h^\dagger(h)$, $a^\dagger(a)$, are the spinless hole and magnon operators, respectively, $2J\omega_{\mathbf{q}} = 2J(1-\gamma_{\mathbf{q}})^{1/2}$ is the spin-wave energy, $M_{\mathbf{k},\mathbf{q}} = 4(\gamma_{\mathbf{k}-\mathbf{q}} u_{\mathbf{q}} + \gamma_{\mathbf{k}} v_{\mathbf{q}})$, $u_{\mathbf{q}}, v_{\mathbf{q}}$ are the Bogolubov canonical transformation parameters, $\gamma_{\mathbf{k}} = (\cos k_x + \cos k_y)/2$. The spinless-fermion representation fulfills the above-mentioned constraint on double occupation exactly[20] and, therefore, the only approximation made is the spin-wave one. As it was recently shown in Ref. 29, the two-loop corrections due to the higher-order terms in the t term of Eq. (2) are analogous to the higher-order nonlinear spin-wave corrections to the linear spin-wave theory, and have the same order of smallness.

To do mapping of the Hilbert space of the constrained fermion and spin operators onto one of the spinless fermions and bosons one has to care about projecting out the unphysical states with the boson and fermion at the same site. The procedure of including projection operators into the J term (1) is described in Sec. V B. This adds some interaction terms to the spin-polaron Hamiltonian (ΔH) (2). They are important for the consideration of the two-hole problem. Namely, the main part of them is an explicitly written term of the effective hole-hole attraction due to minimization of the number of the broken AF bonds.

We will study this version of the t-J model with the additional interaction terms arising from the projection operators in the J term. In such a formulation Eq. (2) is explicitly a problem with very strong interactions. The problem of the interaction of fermion excitations with a bosonic field and the resulting effective ‘‘dressing’’ of fermions by the virtual cloud of bosons is an old and well-investigated problem, and a powerful approach to it is the canonical transformation one.[47] Therefore, one can hope that a canonical transformation can be found for the t-J model too. Briefly, we will show that a rather simple transformation, which takes into account the main effect of the strong interaction $\sim t$ and allows one to consider the rest of the interaction perturbatively, exists.

To complete the consideration of the known facts about the Hamiltonian (2) let us note that in the recent work by Reiter[48] an exact wave function of the single hole in an AF background has been obtained within the SCBA:

$$\tilde{h}^\dagger_{\mathbf{k}}|0\rangle = \sqrt{Z_{\mathbf{k}}}\Bigg[h^\dagger_{\mathbf{k}} + \sum_{\mathbf{q}} M_{\mathbf{k},\mathbf{q}} G_{\mathbf{k}-\mathbf{q}}(E_{\mathbf{k}}-\omega_{\mathbf{q}}) h^\dagger_{\mathbf{k}-\mathbf{q}} a^\dagger_{\mathbf{q}} + \cdots + \sum_{\mathbf{q},\ldots,\mathbf{q}_n} M_{\mathbf{k},\mathbf{q}} G_{\mathbf{k}-\mathbf{q}}(E_{\mathbf{k}}-\omega_{\mathbf{q}}) \cdots M_{\mathbf{k}\cdots-\mathbf{q}_{n-1},\mathbf{q}_n} G_{\mathbf{k}\cdots-\mathbf{q}_n}$$
$$\times (E_{\mathbf{k}} \cdots - \omega_{\mathbf{q}_n}) h^\dagger_{\mathbf{k}\cdots-\mathbf{q}_n} a^\dagger_{\mathbf{q}} \cdots a^\dagger_{\mathbf{q}_n} + \cdots \Bigg]|0\rangle, \tag{3}$$

where Z_{k} is the quasiparticle residue, $G_{\mathbf{k}}(\omega)$ is an exact single-hole Green's function, and $E_{\mathbf{k}}$ is the hole energy. Since $\tilde{h}^\dagger_{\mathbf{k}}|0\rangle$ is an exact eigenfunction of the Hamiltonian (2), so the one-hole subspace of the Hamiltonian (2) is completely diagonalized, and the effective Hamiltonian for quasiparticles (3) has the form

$$H^{\text{SCBA}}_{\text{eff}} = 2J\sum_{\mathbf{q}} \omega_{\mathbf{q}} a^\dagger_{\mathbf{q}} a_{\mathbf{q}} + \sum_{\mathbf{k}} E_{\mathbf{k}} \tilde{h}^\dagger_{\mathbf{k}}|0\rangle\langle 0|\tilde{h}_{\mathbf{k}} + H^{h-h}_{\text{int}} + \cdots, \tag{4}$$

thus, the initially strong interaction is transformed exactly to the ‘‘dressing’’ of the bare hole, and to an effective interaction between such quasiparticles. Unfortunately, one cannot use Eq. (3) as the definition of the new Fermi operator $\tilde{h}^\dagger_{\mathbf{k}}$, and then obtain the hole-hole interaction $H^{h\text{-}h}_{\text{int}}$ by the averaging $H_{t\text{-}J}$ [Eq. (2)] over the two-hole wave function $\tilde{h}^\dagger_{\mathbf{k}} \tilde{h}^\dagger_{\mathbf{k}'}|0\rangle$, because $\tilde{h}_{\mathbf{k}}$, $\tilde{h}^\dagger_{\mathbf{k}}$ defined in this way, do not obey the usual anticommutation relations. In other words, to know $H^{h\text{-}h}_{\text{int}}$ one has to define the unitary operator, which corresponds to the transformation of the ‘‘bare’’ hole wave function $h^\dagger_{\mathbf{k}}|0\rangle$ to the ‘‘dressed’’ one $\tilde{h}^\dagger_{\mathbf{k}}|0\rangle$. This problem is very complicated.

Briefly, we present an approximate solution of the diagonalization problem of the initial Hamiltonian (2). An effective Hamiltonian is formulated for the ‘‘dressed’’ holes, which have the energy, bandwidth, and structure very close to SCBA ones. Our advantage is that we have an explicit expression for the hole-hole interaction. Then, the solving of the two-hole problem is straightforward.

Our described procedure is valid for the region $0<(t/J)<5$, and we consider this region as the actual one, since considering the t/J model as a result of the simple

Hubbard or many-band Hubbard model mapping, the t/J parameter has the lower boundary $t/J \sim 1$, below that the mapping procedure is not valid. Moreover, $t/J = 5$ corresponds to $U/t = 20$, which is well above that realized in the real compounds.

The paper is organized as follows. In Sec. II, we give a comparison of the lattice polaron problem with the spin-polaron one and write the general form of the transformed *t-J* Hamiltonian. In Secs. III and IV, we apply the proposed procedure to the Ising case as well as to the general case. Section V is devoted to the two-hole problem. Finally, Section VI states our conclusions. Technical details are available from the authors.[51]

II. CANONICAL TRANSFORMATION

From the formal point of view, the spin-polaron Hamiltonian (2) has a form that is very similar to one of the usual lattice polaron problem. We consider here the lattice polaron problem to compare these two models in detail, and to establish similarities and differences.

The Fröhlich Hamiltonian is

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \sum_{\mathbf{q}} \Omega_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \sum_{\mathbf{k},\mathbf{q}} \gamma_{\mathbf{q}} \Omega_{\mathbf{q}} c_{\mathbf{k}-\mathbf{q}}^{\dagger} c_{\mathbf{k}} (b_{\mathbf{q}}^{\dagger} + b_{-\mathbf{q}}), \tag{5}$$

where $c^{\dagger}(c)$ and $b^{\dagger}(b)$ are the electron and phonon operators, $E_{\mathbf{k}}$ and $\Omega_{\mathbf{q}}$ are their energies, respectively. $\gamma_{\mathbf{q}} \Omega_{\mathbf{q}}$ is the electron-phonon coupling. Diagonalization of the Hamiltonian (5) can be done using the Lang-Firsov (LF) transformation:[47]

$$H_{\mathrm{eff}} = e^{-S} H e^{S} = H + [H,S] + \frac{1}{2!}[[H,S]S] + \cdots,$$

with

$$S = -\sum_{\mathbf{k},\mathbf{q}} \gamma_{\mathbf{q}} c_{\mathbf{k}-\mathbf{q}}^{\dagger} c_{\mathbf{k}} (b_{\mathbf{q}}^{\dagger} - b_{-\mathbf{q}}). \tag{6}$$

In the limit of the ''static'' electron ($E_{\mathbf{k}} = E_0$) only the first two commutators in Eq. (6) are not equal to zero. One can easily obtain the effective Hamiltonian for the ''dressed'' electrons

$$H_{\mathrm{eff}} = \left(E_0 - \sum_{\mathbf{q}} \Omega_{\mathbf{q}} |\gamma_{\mathbf{q}}|^2 \right) \sum_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \sum_{\mathbf{q}} \Omega_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} - \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \Omega_{\mathbf{q}} |\gamma_{\mathbf{q}}|^2 c_{\mathbf{k}-\mathbf{q}}^{\dagger} c_{\mathbf{k}'+q}^{\dagger} c_{\mathbf{k}'} c_{\mathbf{k}}. \tag{7}$$

Thus, the electron-phonon interaction term in Eq. (5) results in the lowering of the electron energy (polaronic shift) and the direct $n_i^e n_j^e$ interaction. For the mobile electron an infinite series of terms in Eq. (6) may be summed and yields an effective hopping term describing the collective hopping process of a bare electron with a cloud of phonons. It was shown that the strong ''dressing'' leads to the exponentially narrow effective band.[47] The remaining part of the interaction with the phonons (multiple phonon processes) can be considered as the perturbation. The underlying physical idea of the LF approach is that the presence of an electron at the lattice site leads to change of the equilibrium position of the surrounding ions and that the new eigenfunction of phonons is a coherent state.

There are two main differences between phonon and magnetic polaron problems. The first one is the absence of the ''bare'' dispersion in the Hamiltonian (2), i.e., its hopping term is the hole-magnon vertex.[27] The second one is the nonlocal character of the hole-spin interaction, i.e., emission (absorption) of a magnon can be done only by hopping. Because of this there is no ''static'' limit of the problem even if $t \ll J$, and the evident *a priori* ideas about the structure of spin cloud around the hole are absent.

Nevertheless, the existing knowledge about the hole motion in an AF background can help one to succeed in transforming the *t-J* model to an effective one, which is much more appropriate to study. First, in the Ising background the ground state of the hole is a localized magnetic polaron, which is formed by a self-retraceable motion of the hole. For a Néel background there is the similar situation, i.e., spin waves in the virtual spin cloud around the hole are absorbed exactly in the reversed order that they were emitted. The contribution of the processes beyond these retraceable paths (or SCBA) approximation was found to be very small. Second, it was argued in a number of works that the hole ''dressing'' by the single spin wave provides results for the hole dispersion law, which are close to the exact ones.[17,18] Namely, the bottom of the band, band minima locations, and width of the band were determined with a sufficient accuracy in the framework of this approximation.[17] Therefore, this shows that the main contribution to the polaron well formation for the actual range of $(t/J) < 5$ is made by the ''one-string'' component of the hole wave function (3). The authors of some SCBA works also successfully used this approximation for the different *t-J* model studies.[48,49] These are the reasons to hope that the relatively simple transformation, in the spirit of Lang-Firsov, can be used to obtain an effective model which accounts for the main polaron effect (of the order of t) in the hole energy and hole-hole interaction, whereas the other included terms allow one to apply perturbation theory.

We propose the general form of the generator of such a transformation:

$$S = \sum_{\mathbf{k},\mathbf{q}} \mu_{\mathbf{k},\mathbf{q}} (h_{\mathbf{k}-\mathbf{q}}^{\dagger} h_{\mathbf{k}} a_{\mathbf{q}}^{\dagger} - \mathrm{H.c.}), \tag{8}$$

where $\mu_{\mathbf{k},\mathbf{q}}$ is the parameter of the transformation. It is natural to require that $\mu_{\mathbf{k},\mathbf{q}}$ should obey the same symmetry properties as the kinematic factor $M_{\mathbf{k},\mathbf{q}}$ of the t term in the Hamiltonian (2). Note that $M_{\mathbf{k},\mathbf{q}}$ is odd with respect to the transformations $M_{\mathbf{k},\mathbf{q}} = -M_{\mathbf{k}+\mathbf{Q},\mathbf{q}} = -M_{\mathbf{k},\mathbf{q}+\mathbf{Q}}$, here $\mathbf{Q} = (\pi,\pi)$. So, without loss of generality one can rewrite $\mu_{\mathbf{k},\mathbf{q}} = f_{\mathbf{k},\mathbf{q}} M_{\mathbf{k},\mathbf{q}}$, where $f_{\mathbf{k},\mathbf{q}}$ is even under mentioned symmetry transformations.

The transformed Hamiltonian (2) can be developed in the usual commutator expansion[50]

$$H_{\mathrm{eff}} = e^{-S} H e^{S} = H + [H,S] + \frac{1}{2!}[[H,S]S] + \cdots. \tag{9}$$

Using the generator given by Eq. (8) one can get

$$H_{\rm eff}\simeq\sum_{\mathbf{k}} E_{\mathbf{k}}h^{\dagger}_{\mathbf{k}}h_{\mathbf{k}}+2J\sum_{\mathbf{q}} \omega_{\mathbf{q}}a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}}+t\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V^{hh}_{\mathbf{k},\mathbf{k}',\mathbf{q}}h^{\dagger}_{\mathbf{k}-\mathbf{q}}h^{\dagger}_{\mathbf{k}'+q}h_{\mathbf{k}'}h_{\mathbf{k}}+t\sum_{\mathbf{k},\mathbf{q}} F_{\mathbf{k},\mathbf{q}}M_{\mathbf{k},\mathbf{q}}(h^{\dagger}_{\mathbf{k}-\mathbf{q}}h_{\mathbf{k}}a^{\dagger}_{\mathbf{q}}+\text{H.c.})$$
$$+t\sum_{\mathbf{k},\mathbf{q},\mathbf{q}'} V^{haa}_{1}(\mathbf{k},\mathbf{q},\mathbf{q}')(h^{\dagger}_{\mathbf{k}-\mathbf{q}-\mathbf{q}'}h_{\mathbf{k}}a^{\dagger}_{\mathbf{q}}a^{\dagger}_{\mathbf{q}'}+\text{H.c.})+t\sum_{\mathbf{k},\mathbf{q},\mathbf{q}'} V^{haa}_{2}(\mathbf{k},\mathbf{q},\mathbf{q}')h^{\dagger}_{\mathbf{k}-\mathbf{q}+\mathbf{q}'}h_{\mathbf{k}}a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}'}, \tag{10}$$

where we omit the terms, which are irrelevant for the one- and two-hole problems. General expressions for the hole energy $E_{\mathbf{k}}$, hole-magnon form factor $F_{\mathbf{k},\mathbf{q}}$ (up to the sixth order of the transformation), hole-hole vertex $V^{hh}_{\mathbf{k},\mathbf{k}',\mathbf{q}}$ (up to the fourth order), and the other vertices are presented in the full version of the paper.[51] The order of the transformation is equal to the number of the commutators in the expansion series (9).

There is the freedom in choosing of the transformation parameter (TP) $f_{\mathbf{k},\mathbf{q}}$. The systematic way of treating the problem is to do all calculations with the TP as a free parameter and then fix it using some physical reasons. In this paper we use the following procedure, which allows us to avoid the self-consistency in equations. We neglect the **q** dependence in the TP ($f_{\mathbf{k},\mathbf{q}}\Rightarrow f_{\mathbf{k}}$), and then determine $f_{\mathbf{k}}$ by minimizing the hole energy. The other thinkable condition for fixing the TP can be the equation for the hole-magnon form factor $F_{\mathbf{k},\mathbf{q}}=0$. Indeed, we investigated the different forms of the TP and found no significant changes in results. We will discuss the details of our approach in the next two sections. Here we claim that for the rather general form of the TP one can restrict oneself by the first four terms in the transformed Hamiltonian (10), namely

$$H_{\rm eff}\simeq\sum_{\mathbf{k}} E_{\mathbf{k}}h^{\dagger}_{\mathbf{k}}h_{\mathbf{k}}+2J\sum_{\mathbf{q}} \omega_{\mathbf{q}}a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}}+t\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V^{hh}_{\mathbf{k},\mathbf{k}',\mathbf{q}}h^{\dagger}_{\mathbf{k}-\mathbf{q}}h^{\dagger}_{\mathbf{k}'+q}h_{\mathbf{k}'}h_{\mathbf{k}}+t\sum_{\mathbf{k},\mathbf{q}} F_{\mathbf{k},\mathbf{q}}M_{\mathbf{k},\mathbf{q}}(h^{\dagger}_{\mathbf{k}-\mathbf{q}}h_{\mathbf{k}}a^{\dagger}_{\mathbf{q}}+\text{H.c.}) \tag{11}$$

keeping in mind that the transformed ''internal'' interactions [ΔH term in Eq. (2)] are included in $V^{hh}_{\mathbf{k},\mathbf{k}',\mathbf{q}}$. Moreover, the resulting effective hole-magnon vertex is perturbative, i.e., the second-order correction to the energy from the self-energy diagram is small. The importance of the effective hole-magnon vertex for the two-hole problem will be discussed in Sec. V.

III. ISING LIMIT

Let us start the general consideration of our approach from the Ising case. As was noted in Ref. 52, treating the t-J model in the Ising limit within the linear spin-wave approximation leaves the physics of the problem essentially unchanged. Moreover, it was shown[52] that the spin-wave formalism provides exactly the same result as one of the SCBA.

The t and J terms of the general spin-hole Hamiltonian (2) using the momentum independence of $\omega_{\mathbf{q}}$ in the Ising limit are ($\omega_{\mathbf{q}}=u_{\mathbf{q}}=1$ and $v_{\mathbf{q}}=0$):

$$H=t\sum_{\mathbf{k},\mathbf{q}} M^{I}_{\mathbf{k},\mathbf{q}}(h^{\dagger}_{\mathbf{k}-\mathbf{q}}h_{\mathbf{k}}a^{\dagger}_{\mathbf{q}}+\text{H.c.})+2J\sum_{\mathbf{q}} a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}} \tag{12}$$

with

$$M^{I}_{\mathbf{k},\mathbf{q}}=4\gamma_{\mathbf{k}-\mathbf{q}}.$$

The additional terms of the interaction Hamiltonian (ΔH) can be considered independently.

Following the analogy with the LF transformation we turn to the effective Hamiltonian with the help of the transformation (9) using

$$S=f\sum_{\mathbf{k},\mathbf{q}} M^{I}_{\mathbf{k},\mathbf{q}}(h^{\dagger}_{\mathbf{k}-\mathbf{q}}h_{\mathbf{k}}a^{\dagger}_{\mathbf{q}}-\text{H.c.}), \tag{13}$$

where generator of the transformation reproduces the kinematic structure of the hopping Hamiltonian and involves the single free parameter f. It is natural for the TP f to be **k** independent in this case, since the energy of the hole in the Ising background does not depend on **k**. Using the evident relation $[H_J,S]=f(2J/t)H_t$ one can get the effective Hamiltonian

$$H_{\rm eff}\simeq E_h\sum_{\mathbf{k}} h^{\dagger}_{\mathbf{k}}h_{\mathbf{k}}+2J\sum_{\mathbf{q}} a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}}+t\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V^{hh}_{\mathbf{k},\mathbf{k}',\mathbf{q}}h^{\dagger}_{\mathbf{k}-\mathbf{q}}h^{\dagger}_{\mathbf{k}'+q}h_{\mathbf{k}'}h_{\mathbf{k}}+tF\sum_{\mathbf{k},\mathbf{q}} M^{I}_{\mathbf{k},\mathbf{q}}(h^{\dagger}_{\mathbf{k}-\mathbf{q}}h_{\mathbf{k}}a^{\dagger}_{\mathbf{q}}+\text{H.c.})+t\sum_{\mathbf{k},\mathbf{q},\mathbf{q}'} V^{haa}_{\mathbf{k},\mathbf{q},\mathbf{q}'}h^{\dagger}_{\mathbf{k}-\mathbf{q}+\mathbf{q}'}h_{\mathbf{k}}a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}'} \tag{14}$$

with one-hole energy, hole-magnon form factor, hole-hole vertex, and hole-two magnon vertex given by

$$E_h=8t\left[f-\frac{4}{3}f^3+\frac{2J}{t}\left(\frac{1}{2}f^2-\frac{1}{3}f^4\right)\right],$$

$$F=1-4f^2+\frac{2J}{t}\left(f-\frac{4}{3}f^3\right), \tag{15}$$

$$V^{hh}_{\mathbf{k},\mathbf{k}',\mathbf{q}} = (M^I_{\mathbf{k},\mathbf{q}} M^I_{\mathbf{k}'+\mathbf{q},\mathbf{q}} + M^I_{\mathbf{k}-\mathbf{q},-\mathbf{q}} M^I_{\mathbf{k}',-\mathbf{q}}) \cdot f \left[1 + \frac{J}{t} f - \frac{4}{3} f^2 \left(1 + \frac{J}{2t} f \right) (4 + \gamma_{\mathbf{k}+\mathbf{k}'}) \right] - (M^I_{\mathbf{k},\mathbf{q}} M^I_{\mathbf{k}-\mathbf{q},-\mathbf{q}} + M^I_{\mathbf{k}'+\mathbf{q},\mathbf{q}} M^I_{\mathbf{k}',-\mathbf{q}}) \cdot \frac{8}{3} f^3 \left(1 + \frac{J}{2t} f \right), \quad (16)$$

up to the fourth order of transformation. The first peculiar feature of the Ising case is that the minimization of the energy provides an equation in f:

$$\frac{\delta E_h}{\delta f} \sim 1 - 4f^2 + (2J/t)\left(f - \frac{4}{3} f^3 \right) = 0, \quad (17)$$

which coincides exactly with the equation for the hole-magnon form factor $F=0$. This is closely connected to the facts that the each act of emission or absorption of the magnon is due to the hole hopping, and that the polaron is created by the self-retraceable motion of the hole. The role of the so-called Trugman processes[15] among the other fifth-order contributions was found negligibly small. The next simplifying fact is the absence of the two-magnon vertices with the $h^\dagger h a^\dagger a^\dagger$ (aa) terms in $H_{\rm eff}$ (14). This means that there are no contributions of the hole-two-magnon interaction (14) into the self-energy and to the hole-hole vertex. Hence, the $h^\dagger h a^\dagger a$ term can be omitted. Thus, after the energy minimization the effective quasiparticle Hamiltonian has the form, which is very similar to the lattice polaron one,

$$H_{\rm eff} = E_h \sum_{\mathbf{k}} h^\dagger_{\mathbf{k}} h_{\mathbf{k}} + 2J \sum_{\mathbf{q}} a^\dagger_{\mathbf{q}} a_{\mathbf{q}} + t \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V^{hh}_{\mathbf{k},\mathbf{k}',\mathbf{q}} h^\dagger_{\mathbf{k}-\mathbf{q}} h^\dagger_{\mathbf{k}'+q} h_{\mathbf{k}'} h_{\mathbf{k}}, \quad (18)$$

here the energy and hole-hole vertex are given by Eq. (15) with f obtained from Eq. (17).

Equation (17) shows that

$$f = -\frac{t}{2J}, \quad t/J \ll 1,$$

$$f^2 \simeq -\frac{1}{z}\left(1 - \frac{2J}{\sqrt{z}t} \right), \quad t/J \gg 1 \quad (19)$$

demonstrating the perturbative nature of our approach. The perturbative parameter is t/J for small t/J and $1/z$ for large t/J.

An exact result for the energy of the hole in the Ising background was obtained in Ref. 52 in the form of the difference equation. Also, there is an analytical solution of this equation in the $t/J \gg 1$ limit first proposed by Bulaevskii, Nagaev, and Khomskii:[2]

$$E = -2\sqrt{z}t - 2J + 2.34(2J)^{2/3}(\sqrt{z}t)^{1/3}. \quad (20)$$

Figure 1 presents the numerical solution of the exact equation[52] (bold solid curve) and approximate solution (20) (dashed curve) together with our results Eq. (15). Upper and lower curves correspond to the calculations performed up to the fourth and sixth orders of the transformation, respectively. This figure demonstrates that our single-hole energy is very close to an exact one.

We also have found a close agreement between the weights of the components of an exact wave function[52] and ones of our ‘‘dressed’’ hole $\tilde{h}^\dagger|0\rangle = e^{-S} h^\dagger |0\rangle$.

IV. NÉEL CASE

According to the above discussion (Sec. II) we transform the initial Hamiltonian $H = H_{t-J}$ (2) to an effective one $H_{\rm eff}$ (10) using

$$S = \sum_{\mathbf{k},\mathbf{q}} f_{\mathbf{k}} M_{\mathbf{k},\mathbf{q}} (h^\dagger_{\mathbf{k}-\mathbf{q}} h_{\mathbf{k}} a^\dagger_{\mathbf{q}} - \text{H.c.}). \quad (21)$$

The general form of H_{eff} is given by Eq. (10).

At the next step we use the same kind of variational principle to fix the TP $f_{\mathbf{k}}$. The technical advantage of the chosen form of the TP is that the **k**- and **q**-dependent parts in the integrals are separable and the integrals can be reduced to several functions.

Minimization of the energy by variation over the TP $f_{\mathbf{k}}$,

$$\frac{\delta}{\delta f_{\mathbf{k}}} \left(\sum_{\mathbf{k}'} E_{\mathbf{k}'} \right) = 0, \quad (22)$$

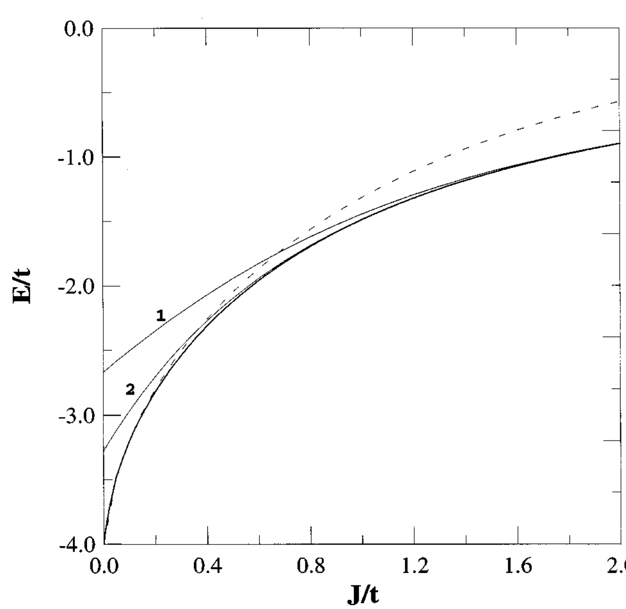

FIG. 1. Single-hole energy for the Ising limit. The bold solid curve is an exact result in the spin-wave approximation. The dashed curve is an exact result for the large $t \gg J$ limit. The solid curves (1) and (2) are the canonical transformation results up to the fourth and sixth orders of transformation, respectively.

gives an integral equation in $f_{\mathbf{k}}$. We use the following method to solve such an integral equation (22). Using the symmetry properties of the TP $f_{\mathbf{k}}$ one can see that $f_{\mathbf{k}}=f_{-\mathbf{k}}=f_{\mathbf{k}+(\pi,\pi)}=f(k_x\leftrightarrow k_y)$, and hence, $f_{\mathbf{k}}$ can be expressed as a power series in $\cos(k_x)^2$, $\cos(k_y)^2$, and $\cos(k_x)\cos(k_y)$, or more conveniently

$$f_{\mathbf{k}}=\sum_{n\geqslant m}^{\infty} C_{n,m}\gamma_{\mathbf{k}}^{2(n-m)}(\gamma_{\mathbf{k}}^{-})^{2m}=C_{0,0}+C_{1,0}\gamma_{\mathbf{k}}^{2} +C_{1,1}(\gamma_{\mathbf{k}}^{-})^{2}+\cdots, \tag{23}$$

where the shorthand notations are $\gamma_{\mathbf{k}}=[\cos(k_x)+\cos(k_y)]/2$, $\gamma_{\mathbf{k}}^{-}=[\cos(k_x)-\cos(k_y)]/2$. Then, substituting this form of $f_{\mathbf{k}}$ in expressions for the auxiliary functions one yields an infinite number of integrals of the type $\Sigma_{\mathbf{q}}[M_{\mathbf{k,q}}^{2}\gamma_{\mathbf{k-q}}^{2(n-m)}(\gamma_{\mathbf{k-q}}^{-})^{2m}]$, each of them is a finite series in $\gamma_{\mathbf{k}}^{2}$, $(\gamma_{\mathbf{k}}^{-})^{2}$ of the power $(n+2)$. Cutting $f_{\mathbf{k}}$ and all other series at the finite power n one obtains from Eq. (22) a set of $(n+1)(n+2)/2$ nonlinear algebraic equations in coefficients $C_{i,j}$ $(i\leqslant n)$. As a result, the integral equation (22) is transformed to the set of algebraic equations, which is much easier to solve. Keeping in mind the $1/z$ character of the expansion series for the hole energy $(t>J)$, one can hope that only a few terms are important, and the role of the higher orders is insignificant.

We solved these systems of equations numerically for the particular values of $0<t/J<5$, and found that extension of the series in Eqs. (22) and (23) from $n=3$ ($\cos^6$, 10 equations) to $n=5$ ($\cos^{10}$, 21 equations) changes results for the parameter $f_{\mathbf{k}}$, energy, and form factor for the relative value less than 0.5%. Note that including of the fifth- and sixth-order terms into the expression of the energy changes the results for approximately 10%. In all further calculations we used the largest $(n=5)$ set of equations.

With the solution for $f_{\mathbf{k}}$ of such a high accuracy in hand one can get explicit expressions for the energy, form factor, hole-hole, and hole-two-magnon vertices in the effective Hamiltonian, Eq. (10). Evidently, the hole energy has the shape with the minima at $\pm(\pi/2,\pm\pi/2)$ points and a large effective mass along the MBZ boundary, and also obeys the symmetry property $E_{\mathbf{k}}=E_{\mathbf{k}+(\pi,\pi)}$.

The next step of our consideration is to prove the negligible role of the hole-two-magnon vertices and the perturbative character of the renormalized hole-magnon one. We have calculated the second-order corrections to the single-hole energy from the one-magnon and two-magnon self-energy diagrams for the various t/J. Briefly, a correction to the depth of the band from the rest of the hole-magnon vertex is less than 10%, while a correction from the hole-two-magnon vertex (10) is of the next order of smallness. Namely, for $t/J=3$, $E_{(\pi/2,\pi/2)}=-2.22t$, $\delta E^{(1)}=-0.15t$, and $\delta E^{(2)}=-0.02t$. The relative correction to the effective hole-hole vertex $V_{\mathbf{k,k',q}}^{hh}$ from the hole-two-magnon exchange is even smaller. Single-magnon exchange is also negligible for the large transfer momentum ($|\mathbf{q}|\sim\pi$), but it is very important for the small one. Indeed, it has a ''quasisingular'' form at the small transfer momentum $\sim t(q_x+q_y)^2/q^2$, whereas $V_{\mathbf{k,k',q}}^{hh}$ is small at $|\mathbf{q}|\to 0$. Note also that the two-magnon exchange cannot provide the singular interaction anywhere.

Therefore, based on this argument we claim that the role of the higher-order magnon vertices is negligible, and the rather general type of transformation leads to a transfer of the initially strong hole-magnon interaction (2) mainly to the hole ''dressing'' and to the hole-hole interaction. Thus, for a wide region of t/J with the high level of accuracy, one can restrict oneself by consideration of the effective Hamiltonian (11)

$$H_{\mathrm{eff}}=\sum_{\mathbf{k}} E_{\mathbf{k}}h_{\mathbf{k}}^{\dagger}h_{\mathbf{k}}+2J\sum_{\mathbf{q}} \omega_{\mathbf{q}}a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}} +t\sum_{\mathbf{k,q}} F_{\mathbf{k,q}}M_{\mathbf{k,q}}(h_{\mathbf{k-q}}^{\dagger}h_{\mathbf{k}}a_{\mathbf{q}}^{\dagger}+\mathrm{H.c.}) +t\sum_{\mathbf{k,k',q}} V_{\mathbf{k,k',q}}^{hh}h_{\mathbf{k-q}}^{\dagger}h_{\mathbf{k'}+q}^{\dagger}h_{\mathbf{k'}}h_{\mathbf{k}}, \tag{24}$$

with all quantities defined as expressed through $\mu_{\mathbf{k,q}}=f_{\mathbf{k}}M_{\mathbf{k,q}}$, where $f_{\mathbf{k}}$ is defined from the integral equation (22).

The physical implication of the transformations (9) and (21) becomes clear if one considers the wave function of the ''dressed'' hole. One can see from Eq. (21) that since the hole-magnon vertex $M_{\mathbf{k,q}}\to 0$ at $\mathbf{q}\to 0$, the admixture of the long-range magnons in the polaron wave function should be small. Thus, the transformation (21) corresponds to taking into account the short-range spin-wave ''dressing'' of the hole. Following this statement one can conclude that it should be a strong $\mathbf{q}$ dependence of the form factor $F_{\mathbf{k,q}}$ (24). In agreement with this expectation we found that $F_{\mathbf{k,q}}$ tends to zero at large $|\mathbf{q}|\sim\pi$ and varies from 0.2 to 0.4 at $|\mathbf{q}|\ll\pi$ for $t/J>1$. The next thing, which is connected with the type of transformation, is the separation of the scales in the momentum space for the effective hole-hole interaction. The ''contact'' interaction $V_{\mathbf{k,k',q}}^{hh}$ tends to zero at $\mathbf{q}\to 0$, whereas the one-magnon-exchange interaction has the peak structure near $\mathbf{q}=0$. We focus on the long-range part of the interaction because, as was found earlier,[36] it is the key part of the pairing interaction for the $d_{x^2-y^2}$ two-hole bound state.

Figures 2 and 3 represent our results for the bottom and width of the single-hole band together with ones of the SCBA calculations from Refs. 20 and 49. The small gap between the bottoms in Fig. 2 is obviously due to the absence of the long-range magnon contribution in our quasiparticle.

After an exhaustive investigation we are certain that the wave function that results from the canonical transformation introduced in this paper is similar to those of other analytical studies, e.g., the SCBA, that numerical work,[53,26] has shown to be accurate. Thus, from now on we focus on the more interesting and complicated problem of two holes.

V. TWO-HOLE PROBLEM

A. Two-sublattice representation

Because of the AF long-range order there are two types of fermion and boson excitations in the system associated with two sublattices. For consideration of the one-particle subspace it is of no importance whether one has the model with

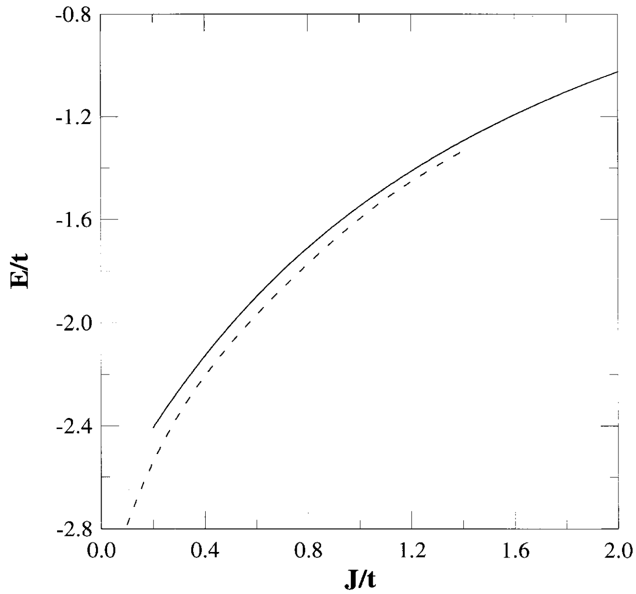

FIG. 2. Bottom of the hole band. The Solid curve is our result (sixth order of the transformation), the dashed curve is the SCBA result.

two degenerate branches of excitations, or the model with one type of them. Above we used the latter for the sake of simplifying the notations. One can easily prove the formal equivalence of these approaches. For the two-sublattice representation there are two types of holes and magnons both defined inside the first magnetic Brillouin zone, whereas for the one-sublattice representations holes and magnons are defined inside the full Brillouin zone.

For the calculation of the correlation function,[49] consideration of the hole-hole interaction,[54] or some other calculations in the two-hole subspace one should turn to the two-sublattice representation. It is convenient to do it using the following expressions for the operators $h_{\mathbf{k}}$ and $a_{\mathbf{q}}$:

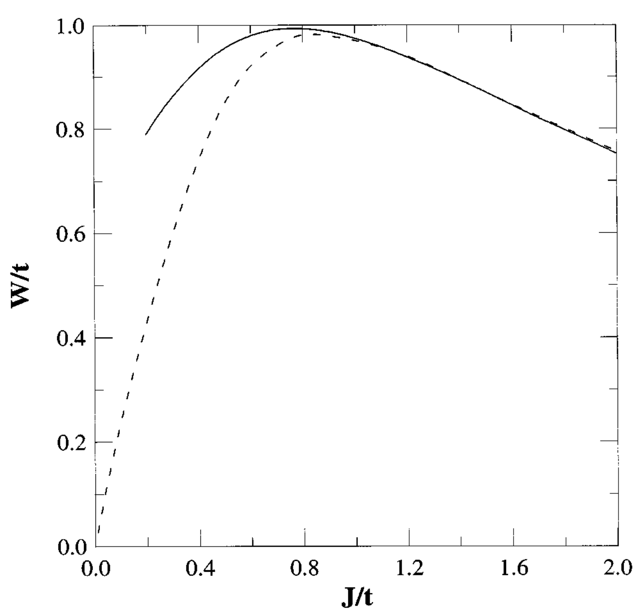

FIG. 3. Width of the hole band. The solid curve is our result (sixth order of the transformation), the dashed curve is the SCBA result.

$$h_{\mathbf{k}}=(f_{\mathbf{k}}+g_{\mathbf{k}})/\sqrt{2}, \quad h_{\mathbf{k}+(\pi,\pi)}=(f_{\mathbf{k}}-g_{\mathbf{k}})/\sqrt{2}, \tag{25}$$

$$a_{\mathbf{q}}=(\alpha_{\mathbf{q}}+\beta_{\mathbf{q}})/\sqrt{2}, \quad a_{\mathbf{q}+(\pi,\pi)}=(\alpha_{\mathbf{q}}-\beta_{\mathbf{q}})/\sqrt{2},$$

where $f_{\mathbf{k}}$ and $g_{\mathbf{k}}$ correspond to the fermionic excitations at the A and B sublattices, respectively. $\alpha_{\mathbf{q}}$ and $\beta_{\mathbf{q}}$ are the two types of Bogolubov spin-wave excitations. Transition to the new variables for the hole-magnon part of the effective Hamiltonian (24) is straightforward if one uses the odd parity of the vertex $M_{\mathbf{k},\mathbf{q}}$ with respect to the transformation $\mathbf{k}\rightarrow\mathbf{k}+(\pi,\pi)$:

$$H_{\rm eff}^{ha}\Rightarrow t\sum_{\mathbf{k},\mathbf{q}} F_{\mathbf{k},\mathbf{q}}M_{\mathbf{k},\mathbf{q}}(f_{\mathbf{k}-\mathbf{q}}^{\dagger}g_{\mathbf{k}}\beta_{\mathbf{q}}^{\dagger}+g_{\mathbf{k}-\mathbf{q}}^{\dagger}f_{\mathbf{k}}\alpha_{\mathbf{q}}^{\dagger}+\text{H.c.}), \tag{26}$$

where the summation is performed over the MBZ.

Expressing the hh-interaction (24) in the terms of new variables one has

$$H_{\rm eff}^{hh}\Rightarrow H^{fg}+H^{ff}+H^{gg}=t\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{k},\mathbf{k}',\mathbf{q}}^{fg}f_{\mathbf{k}-\mathbf{q}}^{\dagger}g_{\mathbf{k}'+\mathbf{q}}^{\dagger}g_{\mathbf{k}'}f_{\mathbf{k}} + t\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}[V_{\mathbf{k},\mathbf{k}',\mathbf{q}}^{ff}f_{\mathbf{k}-\mathbf{q}}^{\dagger}f_{\mathbf{k}'+\mathbf{q}}^{\dagger}f_{\mathbf{k}'}f_{\mathbf{k}} + (f\rightarrow g)]. \tag{27}$$

Thus, there are three different parts in the $H_{\rm eff}^{hh}$, which correspond to the interaction between the holes at the different sublattices (fg part) and at the same one (ff and gg parts). The first contribution to the latter arises in the third order of the transformation and physically corresponds to the process shown in Fig. 4(a). Generally, the ff (or gg) interaction does not have some important features of the fg one. Namely, there are no singularities in its long-range part, and the effective attraction due to reducing of the number of broken AF bonds is absent for the particles at the same sublattice as well. These physical reasons were checked earlier[43] and it was found that there are no bound states formed by the particles at the same sublattice in the region of $(t/J)>1$. So, we will concern ourselves with the interaction of the particles at the different sublattices.

To derive the fg interaction from the hh one, an accurate consideration of the parity of the hh vertex $V_{\mathbf{k},\mathbf{k}',\mathbf{q}}^{hh}$ with respect to the transformation $R=\mathbf{k}(\mathbf{k}')\rightarrow\mathbf{k}(\mathbf{k}')+(\pi,\pi)$ is required. There are two contributions of the different parity ($R=\mp$) in the effective fg interaction. Their diagrammatic analogues are presented in Figs. 4(b) and 4(c), respectively. Since the first contribution is due to the one-magnon exchange, by its origin it is of the ''exchange'' type ($V_{\rm ex}^{hh}$). The second one is due to the two-magnon exchange and the contact interactions (additions from the ΔH term), so it is of the ''direct'' type ($V_{\rm dir}^{hh}$). Obviously, these contributions enter in the fg vertex with the opposite signs

$$V_{\mathbf{k},\mathbf{k}',\mathbf{q}}^{fg}=[-V_{\rm ex}^{hh}(\mathbf{k},\mathbf{k}',\mathbf{q})-V_{\rm ex}^{hh}(\mathbf{k}',\mathbf{k},-\mathbf{q})+V_{\rm dir}^{hh}(\mathbf{k},\mathbf{k}',\mathbf{q}) + V_{\rm dir}^{hh}(\mathbf{k}',\mathbf{k},-\mathbf{q})]. \tag{28}$$

Note here that the first nonzero correction beyond the ladder approximation for the hole-hole (fg) scattering arises

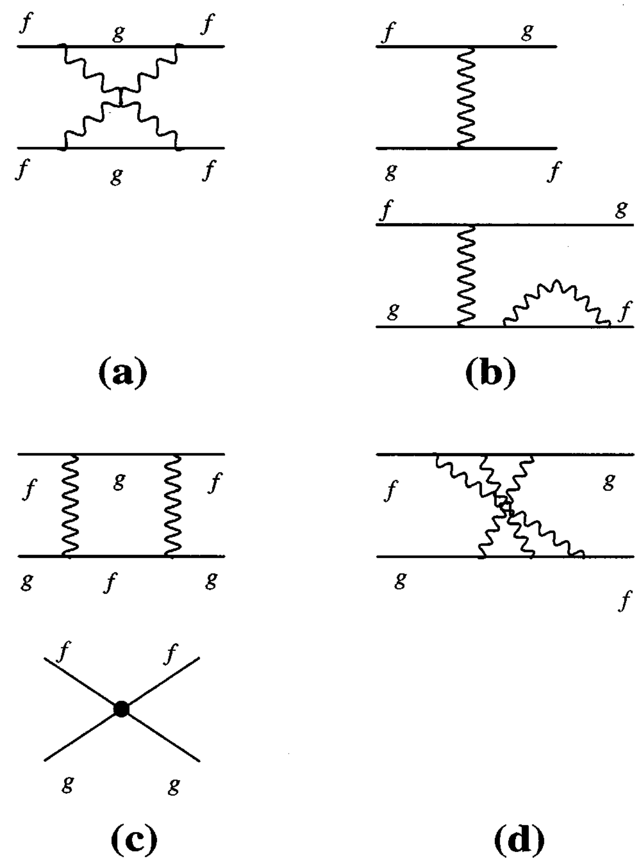

FIG. 4. Schematic view of the scattering diagrams: (a) $ff \rightarrow ff$, (b) $fg \rightarrow gf$, exchange type, (c) $fg \rightarrow fg$, direct type, (d) the first diagram of the $fg \rightarrow fg$ scattering beyond the ladder approximation. Here the wavy lines denote the interaction originated from the magnon exchange (t term). The point in the diagram (c) denotes the nearest neighbor attraction vertex (J term).

only in the sixth order over t [see Fig. 4(d)]. Moreover, structure of this correction resembles one of the Trugman-type diagrams for the single-hole self-energy. Therefore, keeping in mind the negligible role of the non-SCBA contributions to the hole energy, one can hope that the diagram in Fig. 4(d) can be omitted in all calculations. This leads to the conclusion that the ladder approximation should work well even for the initial (untransformed) t-J model (2). In our calculations we use the same approximation, but for already ''dressed'' quasiparticles and renormalized interactions.

B. Types of pairing interaction

Generally, there are two different types of hole-hole interactions in the t-J model. The first one is the spin-wave exchange and the second one is due to minimization of the number of broken AF bonds by the holes located at the nearest neighbor sites. We consider them separately.

The second type of interaction is usually introduced in the pure t-J model by adding projectors $P_i=(1-n_i^h)$ in the J term (1):

$$H_J=J\sum_{\langle i,j\rangle}\left[(1-n_i^h)\mathbf{S}_i\mathbf{S}_j(1-n_j^h)-\frac{1}{4}n_i^h n_j^h\right], \qquad (29)$$

which project out the subspace of the local spins at the sites with the holes, $n_i^h=h_i^\dagger h_i$ is the operator of the hole number. This procedure is necessary because the spinless fermion operators, unlike the constrained fermion ones, commute with the spin operators and hence, unphysical states of the spin and spinless fermion at the same site should be projected out. It is evident that due to the $h_i^\dagger(h_i)$ and $\mathbf{S}_i$ operators the commutativity projection procedure is exact, i.e., there is no spin-spin interaction between the sites with the holes. Thus, the additional part of the t-J Hamiltonian (2) can be written as

$$\Delta H=J\sum_{\langle i,j\rangle}\left[-(n_i^h+n_j^h)\mathbf{S}_i\mathbf{S}_j+n_i^h n_j^h\mathbf{S}_i\mathbf{S}_j-\frac{1}{4}n_i^h n_j^h\right], \qquad (30)$$

where summation runs over bonds. Treating this term in the spin-wave approximation yields

$$\Delta H=-2J(1-2\delta\lambda)\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\gamma_{\mathbf{q}}f^\dagger_{\mathbf{k}-\mathbf{q}}g^\dagger_{\mathbf{k}'+\mathbf{q}}g_{\mathbf{k}'}f_{\mathbf{k}}+\delta H_J, \qquad (31)$$

where the term δH_J consists of the two-magnon terms $n^h aa$ and $n^h n^h aa$.[51] The hole attraction (31) is enhanced by zero-point fluctuations $(-2\delta\lambda\simeq 0.16)$. Applying transformation (21) to the Hamiltonian (31) one can get the additional part of the effective Hamiltonian

$$\delta H^{fg}=J\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\delta V^{fg}_{\mathbf{k},\mathbf{k}',\mathbf{q}}f^\dagger_{\mathbf{k}-\mathbf{q}}g^\dagger_{\mathbf{k}'+\mathbf{q}}g_{\mathbf{k}'}f_{\mathbf{k}}. \qquad (32)$$

An explicit expression of the ''dressed'' vertex $\delta V^{fg}_{\mathbf{k},\mathbf{k}',\mathbf{q}}$ is cumbersome.

There is an evident result for the $n_i n_j$ interaction in the $t=0$ limit. Namely, the ground state of the two holes is the bound state with the energy $E_b=(1-2\delta\lambda)J/2\simeq -0.58J$. The states of s $[\cos k_x+\cos k_y]$, d $[\cos k_x-\cos k_y]$, and p $[\sin k_x, \sin k_y]$ symmetries are degenerate in this limit. The nn-type of interaction (31) has been intensively studied by a number of analytical,[42,43] and numerical techniques.[40] It was established that the increase of t leads to the gradual growth of E_b and disappearance of the bound states at some critical t_c. The largest critical value $t_c=(2-5)J$, which is close to the values of t proposed for the real CuO_2 planes, was found for the bound state of the d symmetry. There are two mechanisms of reducing the nn attraction. The first mechanism is due to the decrease of the ''bare'' hole part in the magnetic polaron. The second one is from the loss of the kinetic energy due to the close location of the holes.

Considered pairing interaction has nothing to do with the spin-fluctuation one, which has been investigated in Ref. 55 on the phenomenological basis and in Ref. 30 using the RPA for the Hubbard model. An essential contribution to the studying of the spin-wave exchange interaction in the t-J and Hubbard models has been done in Refs. 32 and 35, where authors found that the exchange by the long-range (small momentum transfer) spin wave leads to the dipolar interaction between holes which can be attractive or repulsive depending on the relative location of them. In the later work by

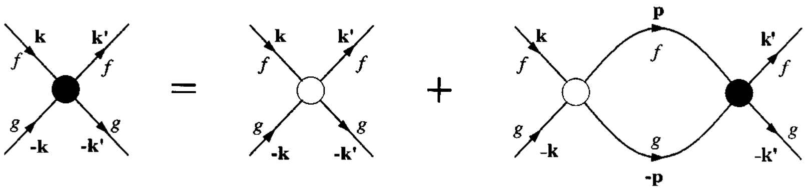

FIG. 5. Graphical identity for an exact vertex $\tilde{\Gamma}(k_f,-k_g,k'_f,-k'_g)$ for the fg scattering in the ladder approximation. The solid circle denotes $\tilde{\Gamma}(k_f,-k_g,k'_f,-k'_g)$, the empty circle denotes a ''compact'' vertex $\Gamma^0(k_f,-k_g,k'_f,-k'_g)$.

Kuchiev and Sushkov[36] this problem has been independently studied in great detail and several interesting features of the system have been found. First of all, neglecting the retardation effect and the finite size of the Brillouin zone one can obtain the Schrödinger equation for the two-hole problem with an effective potential $\sim(x^2-y^2)/r^4$, which can lead to the ''fall to the center'' effect and to the infinite number of bound states. It has been also found that the actual deepness of the bound states is very sensitive to the curvature of the hole band along the MBZ boundary.[36] This effect was explained by the strengthening of the pairing interaction due to the effective lowering of the dimensionality of the system. In Ref. 36 only d and g $[(\cos k_x-\cos k_y)\sin k_x \sin k_y]$ states were found to exist. This confirms the general statement[56] that in the AF state one-magnon exchange leads to repulsion of the carriers in the s-wave state and to attraction in the d-wave one.

C. Bethe-Salpeter equation

Thus, one has the Hamiltonian (24) with the hole-magnon (26) and ''contact'' hole-hole (28) and (32) interactions. As it was noted, the correct account of the retardation effect in the spin-wave exchange diagram is important, so let us consider this problem first. Since we turned to the effective Hamiltonian using a canonical transformation (21), the short-range spin-wave exchange [Fig. 4(b)] is included in the ''contact'' interaction, which does not contain the retardation.

The systematic procedure for searching the bound states is to look for the poles of the two-particle Green's function in the scattering channel considering it as a function of the total energy of the particles in the center of inertia system.[57] The corresponding integral equation for the two-hole Green's function for the holes with the total momentum $\mathbf{P}=0$ is presented in Fig. 5 in diagrammatic form. The standard way of solving this equation with the nonretarded ''compact'' vertex Γ^0 is given in the Appendix.

In our case the ''compact'' vertex Γ^0 consists of two parts (see Fig. 6) and one has to include the magnon propagator into the expression for the long-range spin-wave exchange part. A natural assumption that the two-particle Green's function has no singularities as the function of the difference of the energies of incoming particles provides a somewhat different way of solving the Bethe-Salpeter problem. Details are also given in the Appendix.

The resulting equation of the Bethe-Salpeter type for the problem with two vertices (Fig. 6) is given by

$$\psi(\mathbf{k},E)=\frac{1}{E-2E_{\mathbf{k}}}\sum_{\mathbf{p}}\left[\frac{-2V_{\mathbf{k},\mathbf{q}}V_{\mathbf{p},\mathbf{q}}}{E-E_{\mathbf{p}}-E_{\mathbf{k}}-\omega_{\mathbf{q}}}+tV^{fg}_{\mathbf{k},-\mathbf{k},\mathbf{q}} + J\delta V^{fg}_{\mathbf{k},-\mathbf{k},\mathbf{q}}\right]\psi(\mathbf{p},E), \qquad (33)$$

where $\mathbf{q}=\mathbf{k}+\mathbf{p}$ $(\mathbf{q}=\mathbf{k}-\mathbf{p})$ for the exchange (direct) parts of interactions (27) and (32), $V_{\mathbf{k},\mathbf{q}}=tF_{\mathbf{k},\mathbf{q}}M_{\mathbf{k},\mathbf{q}}$.

D. Results

Finally, having in hand vertices (26), (28), (32), and Eq. (33) one can hope to obtain reliable results for the bound states in the t-J model. Moreover, since we have considered the interactions of different natures independently one can demonstrate the role of each type of interaction in the formation of the bound states.

Briefly, our results are as follows. The bound state of the d symmetry $(d_{x^2-y^2})$ exists in the region $0<(t/J)<5$. The states of the other symmetries $(s,\ p)$ were not found at $(t/J)\geqslant 0.2$. The main thesis of this work is that the interplay of interactions which tend to d-wave pairing, namely the short-range J interaction (32) and the long-range spin-wave exchange (26), is important for the formation of the d-wave bound state.

Specifically, there are no bound states from the J term alone [the third term in Eq. (33)] for $(t/J)>2.1$. The spin-wave exchange [the first and second terms in Eq. (33)] provide a rather shallow bound state. Nevertheless, putting these interactions together one obtains a much deeper bound state than from the pure spin-wave exchange.

As was noted above in the limit $t=0$, the bound states of d, s, and p symmetry have the same energy. We have found that the s and p states disappear at $(t/J)\simeq 0.2$.

Considering terms in the equation for the bound state en-

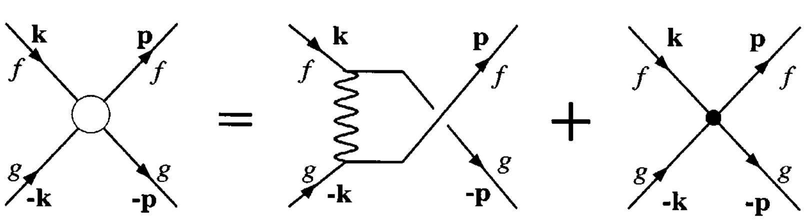

FIG. 6. Structure of the ''compact'' vertex $\Gamma^0(k_f,-k_g,k'_f,-k'_g)$ (empty circle). Here, the wavy line denotes the long-range spin-wave exchange (26), and the point denotes all vertices, which do not contain the retardation (28) and (32).

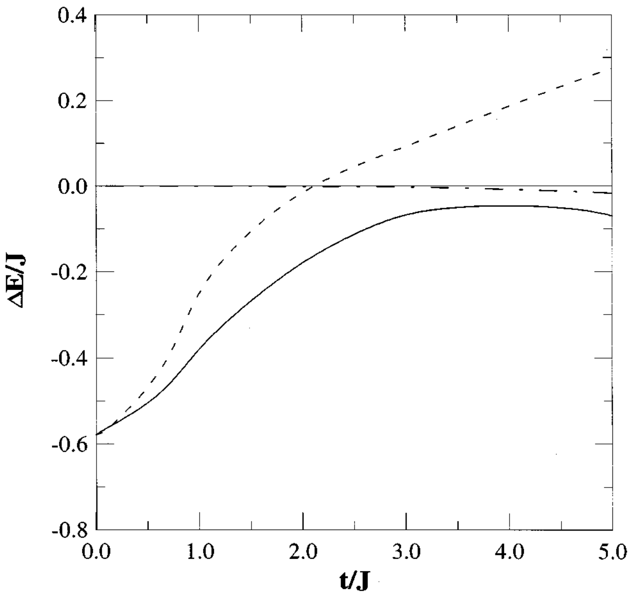

FIG. 7. Results for the energy of the d-wave pairing state. The dashed curve corresponds to the short-range bound state, the dash-dotted curve corresponds to the long-range one, and the solid curve corresponds to the resulting bound state.

ergy (33) separately and together, we have obtained results for the d-wave pairing state shown in Fig. 7. The dashed curve corresponds to taking into account the J term of interaction $\delta V^{fg}_{\mathbf{k},-\mathbf{k},\mathbf{q}}$ (32) alone. The obtained critical value of $t_c = 2.1J$ for disappearing this short-range-in-nature state is in excellent agreement with the variational approach,[42] finite-cluster calculations,[28,40] and other approaches.[43] The dash-dotted curve corresponds to the long-range bound state due to the first two terms in Eq. (33). According to Ref. 36 this state should have a small negative energy.

The actual value of the binding energy was found very sensitive to the curvature of the hole band along the MBZ boundary. As was noted in Ref. 36, the higher anisotropy leads to the more one-dimensional character of the spin polarons. The latter leads to the effective enhancement of the interaction. This feature of the problem is very close to the earlier idea by Schrieffer *et al.*[30] about the effective attraction of the ''cigarlike'' (one-dimensional) spin polarons. More generally, an attractive interaction itself does not immediately result in the bound state. One has to prove that the energy gain due to the pairing is larger than the energy loss due to the localization, or, in other words, to solve the Bethe-Salpeter equation. Hence, the less kinetic energy associated with the hole movement, the deeper bound state one can get.

We have found that the actual value of the mass (SCBA) along the MBZ boundary leads to very small binding energy $\sim 10^{-3} - 10^{-4} t$ for the long-range state. Actually, the bound state is almost pushed in the continuous spectra. The solid curve is our final result for the energy of the d-wave bound state in the t-J model. The bound state energy for $(t/J) = 3$ is equal to $\Delta E = E - 2E_{\mathbf{k}_0} = -0.022t$, which is two orders of magnitude deeper than was obtained earlier.[36] Thus we have obtained a strong enhancement of the coupling effect by the interplay of the two types of pairing interactions.

Note that the ''contact'' part of the spin-wave exchange interaction $V^{fg}_{\mathbf{k},\mathbf{k}',\mathbf{q}}$ (28) plays the minor role in such a strong effect. Namely, ignoring it in Eq. (33) one yields the energy $-0.01t$ $(t/J = 3)$, which is only two times smaller than the result of the integral effect.

It is useful to consider the structure of the wave functions of the two-hole bound states in $\mathbf{k}$ space. Figure 8(a) shows the wave function for $(t/J) = 1$. It is simply a short-range wave function from the ''bare'' J term $\psi_{\mathbf{k}} \sim (\cos k_x - \cos k_y)$ with the small addition of the higher harmonics. Figures 8(b)–8(d) show the wave functions for the (b) long-range state, (c) short-range one, and (d) resulting wave function, all for $(t/J) = 2$. The long-range bound state [Fig. 8(b)] is well localized near the band minima that is consistent with its large-$\mathbf{r}$ character. The short-range state [Fig. 8(c)] is more complex than one in Fig. 8(a) because its energy is smaller and the corresponding momentum space distribution involves more harmonics. The resulting wave function [Fig. 8(d)] reveals the features of the previous states.

The next problem is the influence of the next-nearest hopping terms (t' terms) on the bound states. Evidently, the small t' leads to the perturbative addition to the hole dispersion $\delta E_{\mathbf{k}} = 4t' \cos(k_x)\cos(k_y)$ which can change the physics of the system.[58,59] A positive value of t' makes the band more flat in the $(\pi/2,\pi/2) \rightarrow (\pi,0)$ direction. According to the above discussion it strongly enhances the interactions and makes the d-wave bound state much deeper. For instance, for the flat band $(m_{\parallel} = \infty)$ energy of the bound state is $E = -0.165t$ $[(t/J) = 3]$. Note that the neglecting of the short-range interaction provides the result $E = -0.043t$. For some region of $t' > 0$ existence of the long-range bound state of the g symmetry becomes possible. The g-state wave function obeys the symmetry of the product $[(\cos k_x - \cos k_y)\sin k_x \sin k_y]$, i.e., changes the sign in MBZ eight times. Because of the absence of the short-range attraction for such a state the energy associated with it is very small.

It is well established by now that, for the real CuO_2 compounds, t' has the negative sign and the t' terms result in the fully isotropic dispersion near the band minima.[60,61] Note that the change of the quasiparticle spectrum is the main effect from t' terms, so one can neglect their contribution to the effective interactions. Adding this statement to the sensitivity of the bound state to the anisotropy of the hole band one can suggest that there are no bound states in the t-t'-J models of the CuO_2 plane for the realistic parameters. We have studied the problem of the critical value of t' and found $t'_c \simeq 0.3J$ for $(t/J) = 3$, which is much lower than the realistic value $t'_{\text{eff}} \sim 1.5J$.

Turning back to the simple t-J model, one can say that the direct relation of the studied bound states to the t-J superconductivity is questionable, since we used the existence of the long-range AF order as the basis of the model (2), whereas the long-range order is unstable under very small hole doping. Therefore, to clear this subject one has to solve the problems of the pairing and stable spin state self-consistently.

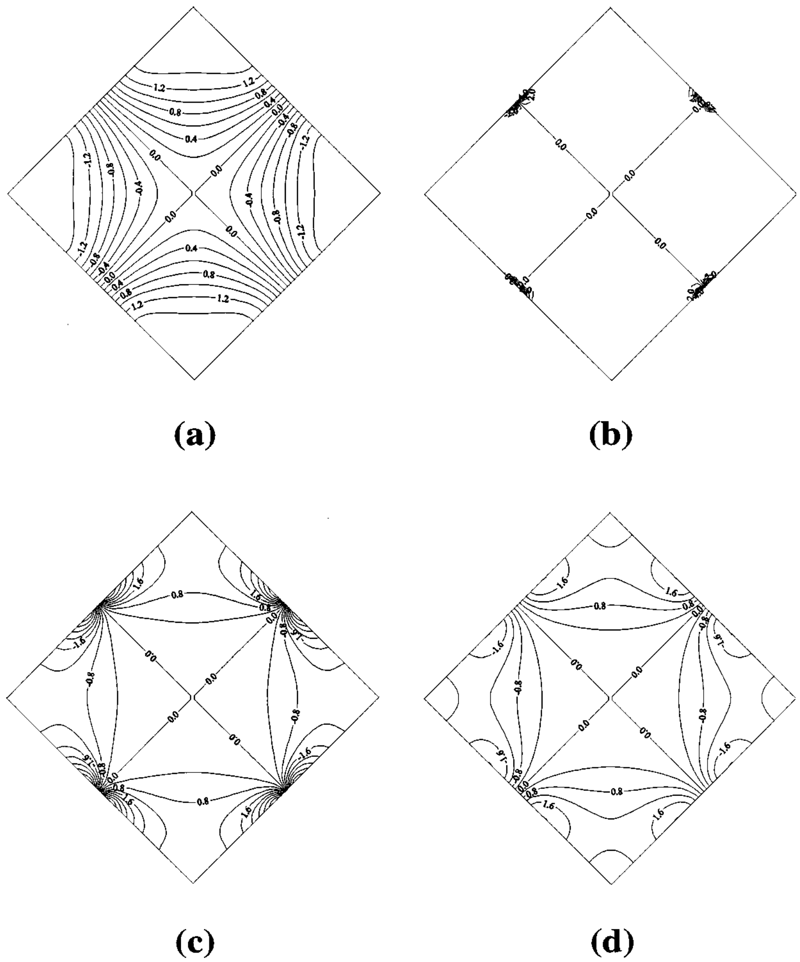

FIG. 8. Wave functions of the two-hole bound states: (a) $(t/J)=1$, (b) $(t/J)=2$, long-range state (c) $(t/J)=2$, short-range one, (d) $(t/J)=2$, wave function of the resulting bound state.

VI. CONCLUSION

We conclude by summarizing our results. We have put forward a canonical transformation of the t-J Hamiltonian using an analogy with the lattice polaron problem and some ideas based on the known properties of the hole in the AF background. We have shown that the rather simple transformation, which has some kind of $1/z$ expansion in the basis, allows one to extend the region of the analytical treatment of the problem up to $t/J \sim 5$ with appropriate accuracy. Generally, the powerful method applied provided us the straight way to the formulation of the quasiparticle Hamiltonian, which includes the free energy terms for the holes and magnons and all essential interactions.

Results for the single-hole bottom of the band, bandwidth, and other properties have been compared with ones of the SCBA calculations and remarkable agreement has been found. The idea that the ''canonically transformed'' quasiparticles have the properties which are close to ones of exact t-J model quasiparticles is supported.

Using the obtained Hamiltonian we have performed a study of the two-hole problem. The hole-hole interactions of different natures have been considered separately, and then together. Rather deep bound states of d-wave symmetry originating from the interplay of the two types of the pairing interactions have been found. The retardation effect for the long-range spin-wave exchange has been carefully taken into account. Other possible symmetries of the bound state wave function have been studied as well. The main effect of the so-called t' terms has been investigated and the critical value of t'_c, at which the bound state disappears, has been found.

Since we have used the presence of the AF long-range order as a foundation of setting up the problem, the direct relation of the considered two-hole problem to the case of finite hole doping of the real CuO_2 plane is unclear. We have briefly discussed the possible way of this relation and touched on questions which remain to be resolved.

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APPENDIX

For two holes with the total momentum $\mathbf{P}=0$ one can write the following integral equation:

$$\tilde{\Gamma}(k_f,-k_g,k_f',-k_g')=\Gamma^0(k_f,-k_g,k_f',-k_g')+\sum_{p_f}\Gamma^0(k_f,-k_g,p_f,-p_g)G(p_f)G(-p_g)\tilde{\Gamma}(p_f,-p_g,k_f',-k_g'),\quad \text{(A1)}$$

where we introduced four-momentum notations $k_f=(\mathbf{k},\epsilon_f)$, $-k_g=(-\mathbf{k},\epsilon_g)$, $p_f=(\mathbf{p},\epsilon_f'')$, $-p_g=(-\mathbf{k},\epsilon_g'')$ with momenta $\mathbf{k,p}$ and frequencies $\epsilon_{f(g)}$, $\epsilon''_{f(g)}$. $G(p)=1/(\epsilon-E_{\mathbf{k}}+i\delta)$ is the single-hole Green's function. This equation is equivalent to the graphic equality shown in Fig. 5. Near the pole $\Gamma^0\ll\tilde{\Gamma}$ and hence the first term in Eq. (A1) can be neglected. Then, one can see that $\tilde{\Gamma}$ dependence on outgoing four-momenta k, k' is the parametric one, i.e., it is not defined by equation itself. Omitting these parameters and introducing $E=\epsilon_f+\epsilon_g$, $\Delta\epsilon=(\epsilon_f-\epsilon_g)/2$, $\Delta\epsilon''=(\epsilon_f''-\epsilon_g'')/2$ we have

$$\tilde{\Gamma}(\mathbf{k},E,\Delta\epsilon)=\sum_{\mathbf{p},\Delta\epsilon''}\Gamma^0(\mathbf{k},\mathbf{p},E,\Delta\epsilon,\Delta\epsilon'')G(\mathbf{p},E/2+\Delta\epsilon'')G(-\mathbf{p},E/2-\Delta\epsilon'')\tilde{\Gamma}(\mathbf{p},E,\Delta\epsilon''). \quad \text{(A2)}$$

When Γ^0 has no frequency dependence (''static'' interaction),

$$\Gamma^0(\mathbf{k},\mathbf{p},E,\Delta\epsilon,\Delta\epsilon'')=U(\mathbf{k},\mathbf{p}), \quad \text{(A3)}$$

it is natural to change the variable $GG\tilde{\Gamma}=\chi$ and get

$$\chi(\mathbf{k},E,\Delta\epsilon)=G(\mathbf{k},E/2+\Delta\epsilon)G(-\mathbf{k},E/2-\Delta\epsilon)\sum_{\mathbf{p}}U(\mathbf{k},\mathbf{p})\int d(\Delta\epsilon'')\chi(\mathbf{p},E,\Delta\epsilon''). \quad \text{(A4)}$$

Integrating both sides over $\Delta\epsilon$ we get the Schrödinger equation

$$\psi(\mathbf{k},E)=\frac{1}{E-2E_{\mathbf{k}}}\sum_{\mathbf{p}}U(\mathbf{k},\mathbf{p})\psi(\mathbf{p},E), \quad \text{(A5)}$$

with $\psi(\mathbf{k},E)=\int d(\Delta\epsilon)\chi(\mathbf{k},E,\Delta\epsilon)$, which has the sense of the bound state wave function.

In our case the ''compact'' vertex Γ^0 consists of two parts (see Fig. 6) and one has to include the magnon propagator into the expression for the spin-wave exchange vertex

$$\Gamma_1^0(\mathbf{k},\mathbf{p},\Delta\epsilon,\Delta\epsilon'')=-\left[\frac{V_{\mathbf{k},\mathbf{p}}V^*_{-\mathbf{k},-\mathbf{p}}}{\epsilon-\epsilon''-\omega_{\mathbf{k}+\mathbf{p}}+i\delta}+\frac{V_{-\mathbf{k},-\mathbf{p}}V^*_{\mathbf{k},\mathbf{p}}}{\epsilon''-\epsilon-\omega_{-\mathbf{k}-\mathbf{p}}+i\delta}\right], \quad \text{(A6)}$$

where $V_{\mathbf{k,p}}=tF_{\mathbf{k,q}}M_{\mathbf{k,q}}$, $\epsilon-\epsilon''=\Delta\epsilon-\Delta\epsilon''$, $\mathbf{k}+\mathbf{p}=\mathbf{q}$. The negative sign on the right side and relation $\mathbf{q}=\mathbf{k}+\mathbf{p}$ are due to the exchange character of the diagram (Fig. 6). Thus, there are three $\Delta\epsilon''$-dependent denominators in the integral Eq. (A2) and the simple change of the variables is impossible.

It is natural to assume at this step that since one is looking for the poles of the two-particle Green's function as the function of E, $\tilde{\Gamma}$ has no singularities as the function of the difference of the energies of incoming particles $\Delta\epsilon$. Therefore, the integral over $\Delta\epsilon''$ in Eq. (A2) is determined by the poles of $G(\mathbf{p},E/2+\Delta\epsilon'')$, $G(\mathbf{p},E/2-\Delta\epsilon'')$, and $\Gamma_1^0(\mathbf{k},\mathbf{p},\Delta\epsilon,\Delta\epsilon'')$ (A6). These poles are $\Delta\epsilon''=(E_{\mathbf{p}}-E/2)-i\delta$, $\Delta\epsilon''=-(E_{\mathbf{p}}-E/2)+i\delta$, and $\Delta\epsilon''=\pm(\Delta\epsilon-\omega_{\mathbf{q}})\pm i\delta$, respectively. $+$ $(-)$ in the last pole corresponds to the first (second) term in Eq. (A6). The integration gives

$$\tilde{\Gamma}(\mathbf{k},E,\Delta\epsilon)=\sum_{\mathbf{p}}\left(-\frac{V_{\mathbf{k},\mathbf{p}}V^*_{-\mathbf{k},-\mathbf{p}}}{E-2E_{\mathbf{p}}}\right)\left[\frac{\tilde{\Gamma}[\mathbf{p},E,(E_{\mathbf{p}}-E/2)]}{\Delta\epsilon-(E_{\mathbf{p}}-E/2)-\omega_{\mathbf{q}}+i\delta}+\frac{\tilde{\Gamma}[\mathbf{p},E,-(E_{\mathbf{p}}-E/2)]}{-\Delta\epsilon-(E_{\mathbf{p}}-E/2)-\omega_{\mathbf{q}}+i\delta}\right]. \quad \text{(A7)}$$

The further way is close to the usual one. Multiplying both sides of Eq. (A7) by the external incoming Green functions one can integrate over $\Delta\epsilon$, using the evident parity of $\tilde{\Gamma}$ in $\Delta\epsilon$

$$\frac{\tilde{\Gamma}(\mathbf{k},E)}{E-2E_{\mathbf{k}}}=\frac{1}{E-2E_{\mathbf{k}}}\sum_{\mathbf{p}}\frac{-2V_{\mathbf{k},\mathbf{p}}V^*_{-\mathbf{k},-\mathbf{p}}}{E-E_{\mathbf{p}}-E_{\mathbf{k}}-\omega_{\mathbf{q}}}\times\frac{\tilde{\Gamma}(\mathbf{p},E)}{E-2E_{\mathbf{p}}}. \quad \text{(A8)}$$

Changing $\tilde{\Gamma}(\mathbf{k},E)/(E-2E_{\mathbf{k}})=\psi(\mathbf{k},E)$ one obtains

$$\psi(\mathbf{k},E)=\frac{1}{E-2E_{\mathbf{k}}}\sum_{\mathbf{p}}\frac{-2V_{\mathbf{k},\mathbf{p}}V^*_{-\mathbf{k},-\mathbf{p}}}{E-E_{\mathbf{p}}-E_{\mathbf{k}}-\omega_{\mathbf{q}}}\psi(\mathbf{p},E). \quad \text{(A9)}$$

Evidently, the ''usual'' Bethe-Salpeter equation (A5) can be obtained in the same way. Surprisingly, this result (A9) coincides exactly with one obtained in Ref. 36 using the Rayleigh-Schrödinger perturbation theory.

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