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 canonical transformation approach. It is shown that the rather simple form of the transformation generator allows to take into account effect of hole interaction with the short-range spin waves and to describe the single-hole groundstate. Obtained results are very close to ones of the self-consistent Born approximation. Further accounting for the long-range spin-wave interaction is possible on the perturbative basis. Both spin-wave exchange and an effective interaction due to minimization of the number of broken antiferromagnetic bonds are included in the effective quasiparticle interaction. Two-hole bound state problem is solved using Bethe-Salpeter equation. The only d-wave bound state is found to exist in the region of \(1 < \frac{t}{J} < 5\). Combined effect of the pairing interactions of both types is important to its formation. Discussion of the possible relation of the obtained results to the problem of superconductivity in real systems is presented.

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I. INTRODUCTION

The problem of the hole motion in an antiferromagnetic (AF) background of the local spins, originally arisen in connection with the study of the localized magnetic insulators, 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, which is well described by the two-dimensional Heisenberg model. 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. The simplest model, which contains in itself this strong interaction is the t-J model. Extensive studies of this model validity for the description of the real CuO\(_2\) plane result in the number of quantitative predictions for the range of parameters and in the set of possible t-J model generalizations. It is widely believed that the essential low-energy physics of the high-T\(_c\) systems can be done using the pure t-J model

\[
H_{t-J} = t \sum_{\langle ij \rangle, \alpha} \tilde{c}_{i,\alpha}^\dagger \tilde{c}_{j,\alpha} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{2} N_i N_j)
\]

in the standard notation of the constrained fermion creation (annihilation) operators \(\tilde{c}_{i,\alpha}^\dagger, \tilde{c}_{i,\alpha}\), \(\langle ij \rangle\) denotes the nearest neighbor sites, \(\mathbf{S}_i\) is a local spin operator, \(N_i\) is the operator of the number of spins. For the consideration of the two- and many-hole problem one must include projection operators into \(J\)-term, which project out the unphysical states with both spin and hole at the same site. Such a procedure is described in Section V.B. Physically, \(t\)-term describes additional hole (singlet) hopping over the background of local spins, or, otherwise, the hopping of hole (vacancy) in the spin background. An important feature of this term is the absence of the double particle occupancy at site. Exclusion of doubly occupied states does not allow to apply mean field type approximations.

The single-hole problem in the t-J model has been extensively studied by the various analytical and numerical techniques, which have provided the deep understanding of the character of the hole motion. For a review see, e.g., Refs. 1, 2. Analytical results obtained within the self-consistent Born approximation (SCBA) agree very well with the exact diagonalization studies on clusters. Variational, and other approaches. The main feature of hole motion revealed in these studies is the strong renormalization of the naive tight-binding result for the band due to hole "dressing" by the cloud of spin excitations, which leads to a narrow band \((\sim 2J \text{ for } t/J > 1 \text{ and } \sim t^2/J \text{ for } t \ll J)\) 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 the full consensus on the problem of bound states in the t-J model is absent. There were a lot of works devoted to the study of the spin-fluctuation pairing and corresponding type of superconductivity. There is strong evidence that the long-range spin-wave exchange, which is the source of the dipolar interaction between holes, can lead to the d-wave pairing in the t-J model. As it was established in Ref. 3, the corresponding bound states are shallow and have the large size. Many efforts also have been aimed to 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 [17]. 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 $t/J \sim 3 - 5$ [33, 41], which are relevant to the real compounds. Variational [12], and some kind of quasiparticle calculations [13] yield the critical value of $t \sim 2J$ for this interaction, which is somewhat lower than the real one. Generally, there is no agreement on the energy of the groundstate of two holes and on their spatial correlation function [14] 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, describing the "dressed" holes and their interaction of the "contact" type and via spin waves, and then to find the groundstate of two such quasiparticles. Both types of interactions of the most interest are accurately accounted for by our approach. In some sense, we use the ideas of the earlier works by Sushkov et al [11,21], 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 [12,13,20,24], which is based on the spinless-fermion representation for the fermion operators and Holstein-Primakoff [12,20] or Dyson-Maleev [10] 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

$$H \simeq 2J \sum_{\mathbf{q}} \omega_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + t \sum_{\mathbf{k},\mathbf{q}} \left( M_{\mathbf{k},\mathbf{q}} h_{\mathbf{k}-\mathbf{q}}^{\dagger} h_{\mathbf{k}} + H.c. \right) ,$$

(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, $M_{\mathbf{k},\mathbf{q}} = 4(\gamma_{\mathbf{k}} - \omega_{\mathbf{q}}) \gamma_{\mathbf{k}}$, $\omega_{\mathbf{q}}, \gamma_{\mathbf{q}}$ 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 [21] and, therefore, the only approximation made is the spin-wave one. As it was recently shown in Ref. [27], the two-loop corrections due to the higher order terms in (1) is analogous to the higher-order nonlinear spin-wave correction to the linear spin-wave theory, and have the same order of smallness.

We will study this [12] version of the $t$-$J$ model with the additional interaction terms from the projection operators in $J$-term. In such a formulation (2) the $t$-$J$ problem is explicitly the problem with the extremely strong interaction. The problem of the interaction of fermion excitations with bosonic field and the resulting effective "dressing" of fermion by the virtual cloud of bosons is an old and well investigated problem, and the powerful approach to it is the canonical transformation one [17]. Therefore, one can hope that a canonical transformation will be found very helpful for the $t$-$J$ model too. Briefly, we will show that the rather simple transformation, which takes into account the main effect of the strong interaction $\sim t$ and allows 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 [25] an exact wave function of the single hole has been obtained within the SCBA

$$\tilde{h}_{\mathbf{k}}^\dagger |0\rangle = a_{\mathbf{k}} \left[ h_{\mathbf{k}}^\dagger + \sum_{\mathbf{q}} M_{\mathbf{k},\mathbf{q}} G_{\mathbf{k}-\mathbf{q}} (E_{\mathbf{k}} - \omega_{\mathbf{q}}) h_{\mathbf{k}-\mathbf{q}}^\dagger a_{\mathbf{q}} + \ldots + \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_{n-1}} M_{\mathbf{k},\mathbf{q}} G_{\mathbf{k}-\mathbf{q}_1} \ldots G_{\mathbf{k}-\mathbf{q}_{n-2}} (E_{\mathbf{k}} - \omega_{\mathbf{q}_1} - \ldots - \omega_{\mathbf{q}_{n-2}}) h_{\mathbf{k}-\mathbf{q}_1}^\dagger \ldots a_{\mathbf{q}_1}^\dagger \ldots a_{\mathbf{q}_{n-1}}^\dagger \right] |0\rangle ,$$

(3)

where $G_{\mathbf{k}}(\omega)$ is an exact hole Green function, $E_{\mathbf{k}}$ is the hole energy. Since it is an exact wave function of the Hamiltonian (2) (within the SCBA) there is no interaction of the corresponding quasiparticle with spin-waves, i.e. 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 simply obtain the hole-hole interaction extracting $\tilde{h}_{\mathbf{k}}^\dagger$ from the wave function (3) as a Fermi operator and averaging $H$ (Eq. (2)) over the two-hole wave function $h_{\mathbf{k}}^\dagger h_{\mathbf{k}}^\dagger |0\rangle$, since $\tilde{h}$, $\tilde{h}^\dagger$, defined by this way, do not obey the usual anticommutation relations.

Briefly, we present an approximate solution of the diagonalization problem of the initial Hamiltonian (2). An effective Hamiltonian is formulated for the quasiparticles, which have the energy, bandwidth, and structure very close to SCBA ones. Further solving of the two-hole problem is straightforward.

Described procedure is valid for the region $0 < (t/J) < 5$. We consider the region $1 < (t/J) < 5$ as an actual one, since considering $t/J$ model as a result of the simple Hubbard or many-band Hubbard model mapping, $t/J$ 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 hardly realized in the real compounds.

The paper is organized as follows. In Section II, we give the comparison of the lattice polaron problem with the spin-polaron one and write the general form of the transformed $t$-$J$ Hamiltonian. In Sections III, IV, we apply the
proposed procedure to the Ising case, small $t$ limit, and general case of the problem. Section V is devoted to the two-hole problem.

II. CANONICAL TRANSFORMATION

From the formal point of view the spin-polaron Hamiltonian \[^{[3]}\] has the 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, establish similarities and differences.

The Fröhlich Hamiltonian is

$$H = \sum_k E_k c_k^\dagger c_k + \sum_q \Omega_q b_q^\dagger b_q + \sum_{k,q} \gamma_k \Omega_q c_{k+q}^\dagger c_k (b_q^\dagger + b_{-q}),$$

where $c_k^\dagger (c)$ and $b^\dagger (b)$ are the electron and phonon operators, $E_k$ and $\Omega_q$ are their energies, respectively. $\gamma_k \Omega_q$ is the electron-phonon coupling. At the limit of the "static" electron ($E_k = E_0$) diagonalization of the Hamiltonian can be done exactly using the Lang-Firsov transformation \[^{[7]}\]:

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

$$S = - \sum_{k,q} \gamma_q c_{k-q}^\dagger c_k (b_q^\dagger - b_{-q}).$$

Only the first two commutators are not equal to zero in this limit. One easily obtains the effective Hamiltonian in the terms of the "dressed" electron

$$H_{\text{eff}} = \left( E_0 - \sum_q \Omega_q |\gamma_q|^2 \right) \sum_k c_k^\dagger c_k + \sum_q \Omega_q b_q^\dagger b_q - \sum_{k,k',q} \Omega_q |\gamma_q|^2 c_{k+q}^\dagger c_k c_{k'+q} c_{k'}.$$

Thus the electron-phonon interaction term in Eq. \[^{[3]}\] results in the lowering of the electron energy (polaronic shift) and the direct $n_i^n_j$ interaction. For the mobile electron an infinite series of terms in Eq. \[^{[3]}\] arises. It is summed up and yields the effective hopping term describing the collective hopping process of the bare electron with the cloud of phonons. It was shown that this "dressing" leads to the exponentially narrow effective band \[^{[7]}\]. The emitting of the phonons (multiple phonon processes) can be considered as the perturbation. In the basis of this approach there is a clear physical idea that the presence of the electron at the lattice site leads to the change of the equilibrium positions of the surrounding ions, and the new eigenfunction of phonons is a coherent state.

There are two main differences between the phonon and magnetic polaron problems. The first one is the principal absence of the "bare" dispersion in the Hamiltonian \[^{[3]}\], i.e. its hopping term is more likely the vertex than the usual tight-binding hopping integral \[^{[27]}\]. The second one is the nonlocal character of the hole-spin interaction, i.e. emission (absorption) of magnon can be done only by hopping. Because of that there is no "static" limit of the problem even if $t \ll J$, and the evident \textit{a priori} ideas about the structure of spin cloud around the hole are absent.

Nevertheless, the existing knowledge of the character of hole motion in AF background can help one to succeed in turning to an effective model, which is much more appropriate to study than the initial one. Firstly, at the Ising background the groundstate of the hole is the localized magnetic polaron, which is formed by self-retraceable motion of the hole. At the 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 than they were emitted. The contribution of the processes beyond these retraceable paths (or SCBA) approximation is found to be extraordinary small. Secondly, it was found in the number of works that taking into account the hole "dressing" even by the single spin wave already provides results, which are close to the exact ones \[^{[13], [15]}\]. Namely, the bottom of the band, hole minima locations, and width of the band are determined with a sufficient accuracy \[^{[17]}\]. Therefore, it 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 \[^{[3]}\]. Authors of some SCBA works also successfully used this approximation for some other $t$-$J$ model studies \[^{[13], [11]}\]. These are the reasons to hope that relatively simple transformation in the spirit of Lang-Firsov one can be used to get the 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 to apply the perturbation theory.

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

$$S = \sum_{k,q} \mu_k \left( h_{k-q} h_k a_q^\dagger - \text{H.c.} \right),$$

$$3.$$
where $\mu_{k,q}$ is the parameter of the transformation. It is natural to require for $\mu_{k,q}$ to obey the same symmetry properties as the kinematic factor $M_{k,q}$ of the $t$-term in the Hamiltonian (3). Note that $M_{k,q}$ is odd with respect to the transformations $M_{k,q} = -M_{k+Q,q} = -M_{k-q,Q}$, here $Q = (\pi, \pi)$. So, without loss of generality one can rewrite $\mu_{k,q} = f_{k,q} \mu_{k,q}$ where $f_{k,q}$ is even under mentioned symmetry transformations.

Main terms of the spin-hole Hamiltonian (3), which we wish to decouple are:

$$H = t \sum_{k,q} M_{k,q} \left( h_{k-q}^\dagger h_k a_q^\dagger + H.c. \right) + 2J \sum_{q} \omega_q a_q^\dagger a_q, \quad (8)$$

after the applying of the transformation (7) they provide transformed Hamiltonian

$$H_{tr} = \sum_{k} E_k h_k^\dagger h_k + 2J \sum_{q} \omega_q a_q^\dagger a_q + t \sum_{k,q} V_{k,q}^{hh} h_{k+q}^\dagger h_k^\dagger h_k^\dagger h_{k-q}^\dagger h_k + t \sum_{k,q} F_{k,q} M_{k,q} \left( h_{k-q}^\dagger h_k a_q^\dagger + H.c. \right)$$

$$+ t \sum_{k,q,q'} V_{k,q}^{hha}(k,q,q') \left( h_{k-q+q}^\dagger h_k a_q^\dagger a_q + H.c. \right) + t \sum_{k,q,q'} V_{k,q}^{hha}(k,q,q') h_{k-q+q}^\dagger h_k a_q^\dagger a_q + \ldots, \quad (9)$$

where we omit terms with six and more fermion operators. General expressions for the hole energy $E_k$, hole-magnon formfactor $F_{k,q}$ (up to the sixth order of the transformation), hole-hole vertex $V_{k,k',q}^{hh}$ (up to the fourth order) and other vertices are given in Appendix A. There is the freedom in the choosing of the parameter of the transformation $f_{k,q}$. By analogy with an exact single-hole wave function (3) one can propose the following form of the parameter $f_{k,q}$: $f_{k,q} = g_k G(k - q, E_k - 2J\omega_q)$, where $G(k, \omega)$ is the Green function of the dressed hole. As a result one obtains the very complex self-consistent integral equation on $E_k$ and self-energy $\Sigma_k(\omega)$, which is hardly soluble. There are some other ways of choosing the transformation parameter (TP), which allow to avoid self-consistency in equations and technically are more advantageous. The simplest one is to neglect $q$-dependence in $f_{k,q} = f_k$, and then to determine it as a solution of an equation obtained from the requirement of the minimum of the hole energy, or, for example, equality to zero of the hole-magnon formfactor. We will discuss this approach in the next two Sections. Here we claim that for the rather general form of TP one can restrict oneself by the first four terms in the transformed Hamiltonian (3), namely

$$H_{eff} = \sum_{k} E_k h_k^\dagger h_k + 2J \sum_{q} \omega_q a_q^\dagger a_q + t \sum_{k,q} V_{k,q}^{hh} h_{k+q}^\dagger h_k^\dagger h_k^\dagger h_{k-q}^\dagger h_k + t \sum_{k,q} F_{k,q} M_{k,q} \left( h_{k-q}^\dagger h_k a_q^\dagger + H.c. \right)$$

keeping in mind that the transformed ”additional” interactions ($J$-term) is included in $V_{k,k',q}^{hh}$. Moreover, resulting effective hole-magnon vertex is perturbative, i.e. its second-order addition to the energy $\delta E_k$ is small. Importance of this vertex for the two-hole problem we will discuss in the Section V.

### III. ISING LIMIT

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

One can get the Ising limit of the $t$ and $J$ terms from the general spin-hole Hamiltonian Eq. (2) using the momentum-independence of $\omega_q$ at the Ising background and the absence of the spin fluctuations $(u_q = 1$ and $v_q = 0)$:

$$H = t \sum_{k,q} M_{k,q}^I \left( h_{k-q}^\dagger h_k a_q^\dagger + H.c. \right) + 2J \sum_{q} a_q^\dagger a_q, \quad (11)$$

$$\text{with} \quad M_{k,q}^I = 4\gamma_{k-q},$$

the additional terms of the interaction Hamiltonian (from $J$-term) can be considered independently and we will include them later.

Following the analogy with the Lang-Firsov transformation we turn to the effective Hamiltonian with the help of the transformation:

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

$$S = f \sum_{k,q} M_{k,q}^I \left( h_{k-q}^\dagger h_k a_q^\dagger - H.c. \right), \quad (12)$$

$$\text{with} \quad M_{k,q}^I = 4\gamma_{k-q},$$

$$\text{the additional terms of the interaction Hamiltonian (from } J \text{-term) can be considered independently and we will include them later.}$$

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$$S = f \sum_{k,q} M_{k,q}^I \left( h_{k-q}^\dagger h_k a_q^\dagger - H.c. \right), \quad (12)$$

$$\text{with} \quad M_{k,q}^I = 4\gamma_{k-q},$$

$$\text{the additional terms of the interaction Hamiltonian (from } J \text{-term) can be considered independently and we will include them later.}$$
where the generator of the transformation simply reproduces the kinematic structure of the hopping Hamiltonian and involves the single free parameter \( f \). It is natural for parameter of the transformation \( f \) to be \( k \)-independent, since the energy of the hole for the Ising problem does not depend on \( k \). Using the evident relation \( [H_J, S] = f(2J/t)H_t \) one can make the effective Hamiltonian calculation and get:

\[
H_{eff} = H_h + 2J \sum_{\mathbf{q}} \mathbf{a}_\mathbf{q}^\dagger \mathbf{a}_\mathbf{q} + t \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{\mathbf{k}, \mathbf{k}', \mathbf{q}}^{hh} \mathbf{h}_\mathbf{k}^\dagger \mathbf{h}_{\mathbf{k}'} \mathbf{h}_\mathbf{q}^\dagger \mathbf{h}_\mathbf{q} + F \sum_{\mathbf{k}, \mathbf{q}} (\mathbf{h}_\mathbf{k}^\dagger \mathbf{h}_{\mathbf{k}-\mathbf{q}} \mathbf{h}_{\mathbf{q}}^\dagger + \text{H.c.}) + t \sum_{\mathbf{k}, \mathbf{q}, \mathbf{q}'} V_{\mathbf{k}, \mathbf{q}, \mathbf{q}'}^{haa} \mathbf{h}_\mathbf{k}^\dagger \mathbf{h}_{\mathbf{k}+\mathbf{q}} \mathbf{h}_\mathbf{q}^\dagger \mathbf{h}_\mathbf{q} + \ldots
\]

(13)

with the one-hole energy, hole-magnon formfactor, hole-hole vertex, and hole-two magnon vertex:

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

\[
F \approx 1 - 4f^2 + \frac{2J}{t} \left( f - \frac{4}{3} f^3 \right)
\]

(14)

\[
V_{\mathbf{k}, \mathbf{k}', \mathbf{q}}^{hh} = (M_{\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}+\mathbf{q}} + M_{\mathbf{k}-\mathbf{q}, \mathbf{q}, \mathbf{k}', \mathbf{q}+\mathbf{q}} - \mathbf{M}_{\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}-\mathbf{q}}) \cdot f \left[ 1 + \frac{J}{t} f - \frac{4}{3} f^2 \left( 1 + \frac{J}{2t} f \right) \left( 4 + \mathbf{g}_{\mathbf{k}+\mathbf{k}'} \right) \right] -
\]

\[
- (M_{\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}-\mathbf{q}} + M_{\mathbf{k}', \mathbf{q}, \mathbf{k}, \mathbf{q}+\mathbf{q}}) \cdot \frac{8}{3} f^3 \left( 1 + \frac{J}{2t} f \right)
\]

\[
V_{\mathbf{k}, \mathbf{q}, \mathbf{q}'}^{haa} = (M_{\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}-\mathbf{q}, \mathbf{q}'} - M_{\mathbf{k}-\mathbf{q}, \mathbf{q}, \mathbf{k}', \mathbf{q}+\mathbf{q}}) \cdot 2f^2 \left( 1 + \frac{J}{t} f \right)
\]

up to the fourth order of transformation for the hole energy and formfactor of the spin-hole vertex and for the hole-hole interaction and higher vertices. The first peculiar feature of the Ising case appears here. Minimization of the energy provides an equation on \( f \):

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

(15)

that coincides with equality to zero of the hole-magnon formfactor \( F \). This is closely connected to the fact that the each act of emission or absorption of magnon is due to the hole hopping, and the polaron is created by moving on the self-retraceable paths. The role of the so called Trugman processes \[15\] among the other fifth and sixth order contributions was found small (~ 1/8 of relative magnitude) and they remain all results essentially unchanged. The next simplifying fact is the absence of the two-magnon vertices with the \( h^\dagger ha^\dagger (aa) \) terms. It means that at zero temperature there are no contributions of the hole-two-magnon part into the self-energy and to the hole-hole vertex, and hence, the \( h^\dagger ha^\dagger \) can be omitted in the effective model. Thus, after energy minimizing the effective Hamiltonian has the form, which is very similar to the lattice polaron one:

\[
H_{eff} = H_h + 2J \sum_{\mathbf{q}} \mathbf{a}_\mathbf{q}^\dagger \mathbf{a}_\mathbf{q} + t \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{\mathbf{k}, \mathbf{k}', \mathbf{q}}^{hh} \mathbf{h}_\mathbf{k}^\dagger \mathbf{h}_{\mathbf{k}'} \mathbf{h}_\mathbf{q}^\dagger \mathbf{h}_\mathbf{q} ,
\]

(16)

Eqs. (14), (15) for the hole energy are given by Eq. (14) with \( f \) obtained from Eq. (15). Eqs. (14), (15) for the hole energy show that:

\[
f = - \frac{t}{2J}, \quad t/J \to 0
\]

\[
f^2 \approx \frac{1}{z} \left( 1 - \frac{2J}{\sqrt{z}t} \right), \quad t/J \gg 1
\]

(17)

demonstrating the perturbative nature of our approach at small \( t/J \) and some kind of \( 1/z \) expansion at large \( t/J \).

An exact result for the single-hole energy on the Ising background was obtained in Ref. \[34\] 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 \[3\]:

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

(18)
Figure 1 presents numerical solution of the exact equation (solid bold curve) and approximate solution (dashed curve) together with our results Eq. (14). Upper and lower curves correspond to the hole energy calculated up to the fourth and sixth order of the transformation, respectively. Figure 3 shows the components of magnetic polaron wave function for the exact solution (bold curves) and ones of our canonically transformed polaron:

$$h^\dagger |0\rangle = e^{-S} h^\dagger |0\rangle$$

These figures demonstrate that our single-hole energy is very close to the exact one, the higher orders for the actual \( t/J \) region play the role of corrections, and the components of exact and our polaron wave functions are close to each other. Therefore, one can hope that the consideration of the interaction of our quasiparticles will reveal the properties of exact eigenstates of the \( t-J \) Hamiltonian.

IV. NÉEL CASE.

A. Small \( t \) limit.

Let us consider first the small \( t/J \) limit of the model. Perturbation theory over this parameter works very well and the most results can be obtained analytically. Our transformation procedure in this limit also has a perturbative sense and it is possible to compare our results with ones of the usual perturbation theory. It is also useful to consider this limit for the demonstration of some details of our approach.

As it was mentioned in Section II, there are some evident forms of the TP \( f_{k,q} \). The first one we wish to study is \( f_{k,q} \Rightarrow f_k \). The second one is \( f_{k,q} \Rightarrow f_k/\omega_q \), which can be considered as the simplification of one proposed in Section II \( f_{k,q} \Rightarrow f_k G(k-q,k_0) \) in the small \( t \) limit when \( E_k \ll 2J/\omega_q \). Technical advantage of both cases for any \( t \) is that \( k \) and \( q \) dependent parts are separable and all arisen integrals can be reduced to the several functions.

It is interesting to clarify the physical meaning of both transformations. Let us show the polaron wave functions:

\[
\begin{align*}
\text{1st case} & \quad h^\dagger |0\rangle = \left[ \left( 1 - \frac{1}{2} t f_k^2 \sum_{q} M_{k,q} \right) h^\dagger_k + f_k \sum_{q} M_{k,q} h^\dagger_{k-q} a^\dagger_{q} + O(t/J)^3 \right] |0\rangle \\
\text{2nd case} & \quad h^\dagger |0\rangle = \left[ \left( 1 - \frac{1}{2} t f_k^2 \sum_{q} \frac{M_{k,q}^2}{\omega_q} \right) h^\dagger_k + f_k \sum_{q} \frac{M_{k,q}^2}{\omega_q} h^\dagger_{k-q} a^\dagger_{q} + O(t/J)^3 \right] |0\rangle.
\end{align*}
\]

Since at \( q \to 0 M_{k,q} \to 0 \) the admixture of the long-range magnons in the wave function of the "first case" polaron is small, i.e. this transformation corresponds to taking into account short-range spin-wave "dressing" of the hole. Comparing the Reiter’s wave function (3) with the "second-case" one suggests their identity for this limit.

Transformed Hamiltonian (9) for the small \( t \) limit takes the form:

\[
H_{eff} = \sum_k \left[ \sum_q f_{k,q} M_{k,q}^2 \left( 1 + \frac{J}{t} f_{k,q}\omega_q \right) \right] h^\dagger_k h_k + 2J \sum_q \omega_q a^\dagger_q a_q - t \sum_k M_{k,q} \left( 1 + \frac{2J}{t} f_{k,q}\omega_q \right) \left( h^\dagger_{k-q} h_{q} + \text{H.c.)} \right) (21)
\]

Here we omit hole-two-magnon vertices \( O(t^2/J^2) \) since they contribute in the energy and scattering amplitude only in the second order \( O(t^4/J^4) \). The hole energy for both types of the transformation:

\[
E_k = \begin{cases} I_k f_k + \frac{J}{t} \bar{I}_k f_k^2 & \text{1st case} \\ \bar{I}_k f_k \left( 1 + \frac{J}{t} f_k \right) & \text{2nd case} \end{cases}
\]

with useful notations \( I_k = \sum_q M_{k,q}^2 \), \( \bar{I}_k = \sum_q M_{k,q}^2 \omega_q \), \( I^2_k = \sum_q M_{k,q}^2/\omega_q \). Minimization of the energy averaging over the band provides the following parameters of the transformations and formfactors:
\[
\frac{\delta}{\delta f_k} \left( \sum_{k'} E_{k'} \right) = 0 \Rightarrow \begin{cases} f_k = -\frac{t}{2J} \frac{I_k}{f_k} & \text{1st case} \\
1 - \omega_q \frac{f_k}{I_k} & \text{2nd case} \\
0 \end{cases}
\]

(23)

and the effective Hamiltonians

\[
H_{eff}^1 = -\frac{t^2}{2J} \sum_k I_k^2 h_k^+ h_k + 2J \sum_q \omega_q a_q^+ a_q + t \sum_{k,q} M_{k,q} \left( 1 - \omega_q \frac{I_k}{I_k} \right) \left( h_{k-q}^+ h_k a_q^+ + H.c. \right)
\]

\[
-\frac{t^2}{2J} \sum_{k,k',q} \frac{M_{k,q} M_{k'+q,a_k}}{I_{k'+q}} \left( 1 - \omega_q \frac{I_k}{2I_k} \right) \left( h_{k-q}^+ h_{k'+q}^+ h_k h_a + H.c. \right)
\]

(24)

\[
H_{eff}^2 = -\frac{t^2}{2J} \sum_k I_k^2 h_k^+ h_k + 2J \sum_q \omega_q a_q^+ a_q - \frac{t^2}{2J} \sum_{k,k',q} M_{k,q} M_{k'+q,a_k} \omega_q \left( h_{k-q}^+ h_{k'+q}^+ h_k h_a + H.c. \right)
\]

The hole energies have the well known shape with the minima at \( \pm(\pi/2, \pm\pi/2) \) points and large effective mass along MBZ boundary. Note, that the "second-case" transformation, which is the Lang-Firsov one by the construction, diagonalizes starting Hamiltonian exactly. Evidently, the "second-case" results for the hole energy and hole-hole vertex coincide with these values obtained by the usual perturbation theory. The first case correspond to the separation of the scales and implies the perturbative account for the interaction with the long-range spin waves. Clearly, that accounting for the second-order contribution of the remaining part of the hole-magnon vertex \( (H_{eff}^1 (24)) \) into the hole energy and hole-hole vertex reproduces results of the simple perturbation theory.

B. General case.

At the first glance the use of the second-case approach at arbitrary \( t \) is more appropriate, since one can hope for better account of the long-range spin waves into the direct hole-hole interaction and for small effective formfactor, which will allow to omit hole-magnon vertex at all and to get the simplest \( (24) \) effective model. At the large \( t/J (> 1) \) it is not correct, i.e. this transformation cannot reduce the initial hole-magnon vertex exactly to zero and about a half of the long-range spin-wave interaction remains untransformed. Therefore, the rest of the hole-magnon interaction cannot be neglected and the general form of the second-case effective Hamiltonian coincides with the first-case one. This is due to the difference of the Green function from the simple \((-1/\omega_q)\) form at \( t/J > 1 \).

At the same time, the "first-case" approach is better in a certain sense, since the resulting long-range part of the hole-hole interaction is separated from the short-range one, i.e. \( V_{k,k,q}^{hh} \) tending to zero and the whole long-range part of interaction is from the rest of the single-magnon exchange. We focus on the long-range part of interaction since, as it was found earlier \([64]\), it is the key pairing interaction for the \( d_{x^2-y^2} \) two-hole bound state. Thus, for the consideration of the two-hole problem correct account of the long-range magnon exchange is very important. In the situation when we technically can try the energy and formfactor up to the sixth order of the transformation, while the hole-hole vertex up to the fourth, the "first case" approach \( (f_{k,a} \Rightarrow f_k) \) becomes preferable.

Shortly, we have performed the transformation using both approaches without significant differences in results, except the long-range magnon exchange amplitude, which 1.5 times less for the second case. Further we will discuss only the "first-case" results.

Thus, we transform the initial Hamiltonian \( H = H_{t-J} \) to an effective one \( H_{eff} \)

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

with

\[
S = \sum_{k,q} f_k M_{k,q} \left( h_{k-q}^+ h_k a_q^+ - H.c. \right),
\]

(25)

which has the form of one in Eq. 8 with parameters presented in Appendix A.

For the sake of simplifying the consideration of the technical details of our approach let us omit for a moment the fifth and sixth order terms in the general formulae for the hole energy (see Appendix A). Minimization of the average energy by variation over the TP \( f_k \) leads to the following integral equation:
\[
\frac{\delta}{\delta f_k} \left( \sum_{k'} E_{k'} \right) \sim I_k + f_k F_k^I - 2 f_k^2 T_k^I - \frac{1}{2} f_k^2 + \frac{1}{2} f_k^2 I_k Y_k \\
+ \frac{2 J}{l} \left[ f_k \tilde{I}_k + \frac{1}{2} f_k F_k^3 - \frac{1}{4} f_k^2 \tilde{I}_k I_k - \frac{1}{12} f_k^2 F_k^4 + \frac{1}{4} f_k^3 \tilde{I}_k Y_k - \frac{1}{12} f_k^3 \tilde{I}_k Y_k \right] = 0 ,
\]

where we use auxiliary functions \( F_k^I \) and \( Y_k, \tilde{Y}_k \) given in Appendix A and notations introduced in the previous Section:

\[
I_k = \sum_q M_{k,q}^2 = A_0 + A_{1,0} \gamma_k^2 + A_{1,1} (\gamma_k^{-})^2 ,
\]

\[
\tilde{I}_k = \sum_q M_{k,q}^2 \omega_q = \tilde{A}_0 + \tilde{A}_{1,0} \gamma_k^2 + \tilde{A}_{1,1} (\gamma_k^{-})^2 ,
\]

with the short-hand notations \( \gamma_k = (\cos(k_x) + \cos(k_y))/2 \), \( \gamma_k^{-} = (\cos(k_x) - \cos(k_y))/2 \) and numbers:

\[
A_0 = 4.3273 , \quad A_{1,0} = -3.5907 , \quad A_{1,1} = -0.2453 ,
\]

\[
\tilde{A}_0 = 3.7828 , \quad \tilde{A}_{1,0} = -3.2808 , \quad \tilde{A}_{1,1} = -0.1496 .
\]

We use the following way of solving such a type of integral equation \([26]\). According to the discussion of the symmetry properties of the TP \( f_k \) given in Section II and using the form of Eq. \([26]\) it is evident that \( f_k = f_{-k} = f_{k+(\pi, \pi)} = f(k_x \leftrightarrow k_y) \), and hence, it 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 convenient

\[
f_k = \sum_{n \leq m} \infty C_{n,m,\gamma_k^2} (\gamma_k^{-})^2 \gamma_k^2 = C_{0,0,0} + C_{1,0,0} + C_{1,1,0} + \ldots
\]

then, substituting this form of \( f_k \) in expressions for the auxiliary functions \( F_k^I \) (Appendix A), one gets an infinite number of integrals of the type \( \sum_q \left( M_{k,q}^2 \gamma_k^{2(n-m)} (\gamma_k^{-})^{2m} \right) \), each of them is a finite series in \( \gamma_k^2 (\gamma_k^{-})^2 \) of the power \( (n+2) \). Cutting \( f_k \) and all other series at the finite power \( n \) one gets from Eq. \([26]\) a set of \( (n+1)(n+2)/2 \) nonlinear algebraic equations on \( C_{i,j} \) \((i \leq n)\). Thus, the integral equation \([26]\) is transformed to the set of algebraic equations, which is much easier to solve. Keeping in mind \( 1/z \) character of the energy expansion one can hope that only a few first 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. \([26], [29]\) from \( n = 3 \) \( \cos^6, 10 \) equations) to \( n = 5 \) \( \cos^10, 21 \) equations) changes results for the parameter \( f_k \), energy and formfactor (coefficients in their series) for the relative value less than 0.5%. Note, that including of the fifth and sixth order terms into expression of the energy (see Appendix A) change results for approximately 10%. In all further calculations we used the largest \((n = 5)\) set of equations.

With the solution for \( f_k \) of such a high accuracy in hand one can get explicit expressions for the energy, formfactor, hole-hole, and hole-two-magnon vertices for the effective Hamiltonian Eq. \([1]\). Evidently, as in the small \( t \) limit, the hole energy has the shape with the minima at \( \pm (\pi/2, \pm \pi/2) \) points and large effective mass along MBZ boundary, and obeys the symmetry property \( f_k = f_{k+(\pi, \pi)} \).

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, correction to the depth of the band from the rest of the hole-magnon vertex is no more than 10%, while correction from the hole-two-magnon vertex 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 \( \delta E^{(2)} = -0.02t \). For the correction to the effective hole-hole vertex the relative contribution of the effective hole-two-magnon exchange is even smaller. Single magnon exchange is really negligible for the large transfer momentum, but is very important for the small one, indeed it has a "quasi-singular" form \( \sim t (g_x + g_y)/q^2 \) for the holes near the bottom of the band. As it was discussed above, this separation of the contributions to the effective hole-hole interaction in the momentum space leads from the construction of the transformation. Note also, that the two-magnon exchange cannot provide the singular interaction anywhere.

Therefore, our analysis has shown the negligible role of the higher magnon vertices and proved that the using of the rather general type of the transformation leads to the transfer of the initially strong hole-magnon interaction mainly into the single-hole dispersion and hole-hole interaction. Thus, for a wide region of \( t/J \) and with the high level of accuracy one can restrict oneself by consideration of the effective Hamiltonian \([10]\)

\[
H_{eff} = \sum_k E_k h_k^\dagger h_k + 2J \sum_q \omega_q a_q^\dagger a_q + \sum_{k, q} F_{k, q} M_{k, q} \left( h_{k-q}^\dagger h_k a_q^\dagger + \text{H.c.} \right) + \sum_{k, k', q} V^{h, h}_{k, k', q} h_{k-q}^\dagger h_{k'-q}^\dagger h_k h_k ,
\]
with all quantities defined in the Appendix A, expressed through $\mu_{k,q} = f_k M_{k,q}$, where $f_k$ is defined from the integral equation of the type of Eq. (29).

Figures 3-5 represent our results for the bottom and width of the single-hole band, and for the weights of the components of the magnetic polaron wave function together with ones from the SCBA calculations from Refs. [20], [49]. From these figures we notice that the bottoms slightly differ for the all region of $t/J$, whereas the bandwidth difference is absent at small $t$ and tends to rise at larger ($t/J > 5$). The gap between the curve corresponding to our result and SCBA one in Fig. 3 is obviously due to the absence of the long-range magnon contribution in the former. Taking into account the second-order correction to the energy from the long-range magnon virtual emission-absorption provides the depth of the band $E_{\pi/2,\pi/2}$ and difference $E_{\pi,0} - E_{\pi/2,\pi/2}$, which almost coincide with the SCBA ones. Surprisingly, at small $t/J (< 1 > 0.5)$ results for bandwidth are very close to each other (Fig. 3).

Figure 6 shows $t/J$ dependence of the hole-magnon formfactor $F_{k,q}$ at different momenta $k$ and $q$. Following the general procedure of expansion in a series one can get the general form of the formfactor

$$F_{k,q} = \sum_{n,m,i,j} \left[ (W_{n,m,i,j} + \omega_q W_{n,m,i,j}) \gamma_k^{2(n-m)}(\gamma_k^{2m})(\gamma_{k-q}^{2i-j}) \gamma_{k-q}^{2j} \right] (31)$$

Thus, our formfactor has strong $k$ and $q$-dependence at any $t/J$ that differs from the result of Ref. [49] where the same kind of variational approach has been used. Namely, at $t/J = 3$ $F_{k,q}$ changes from 0.4 at small $q$ to 0.0 at large ($\sim \pi/2, \pi/2$) one.

V. TWO-HOLE PROBLEM.

A. Two-sublattice representation.

Because of the AF long-range order there are two types of fermion and boson excitations associated with two sublattices. For considering the one-particle subspace it is of no importance whether one has the model with two different sorts of quasiparticles having the same properties (energy, wave function etc.), or the model with one type of quasiparticles. In the above consideration we used the latter for the sake of simplifying the notations. One can easily prove the formal equivalence of these approaches. For two-sublattice representation there are two types of holes and magnons both defined in the first magnetic Brillouin zone, whereas for the one-sublattice representations holes and magnons are defined inside the full Brillouin zone, because of that $E_k = E_{k+\{\pi,\pi\}}$.

For the calculation of the correlation function [49], consideration of the hole-hole interaction [30], or some other calculations into two-hole subspace one should turn back to the two-sublattice representation. It is convenient to do it using the following expressions of the $h_k$ and $a_q$ operators through the linear combinations of the new operators

$$h_k = (f_k + g_k)/\sqrt{2}, \quad h_{k+\{\pi,\pi\}} = (f_k - g_k)/\sqrt{2},$$

$$a_q = (\alpha_q + \beta_q)/\sqrt{2}, \quad a_{q+\{\pi,\pi\}} = (\alpha_q - \beta_q)/\sqrt{2},$$

where $f_k$ and $g_k$ correspond to the fermionic excitations at the A and B sublattice, respectively. $\alpha_q$ and $\beta_q$ are the two type of Bogolubov spin-wave excitations. Transition to these new variables for the hole-magnon part of the effective Hamiltonian is straightforward

$$H_{eff}^{hh} \Rightarrow t \sum_{k,q} F_{k,q} M_{k,q} \left( f_{k-q}^\dagger g_k^\dagger \beta_q^\dagger + g_{k-q}^\dagger f_k^\dagger \alpha_q^\dagger + H.c. \right),$$

where summation is performed over the MBZ.

Now we should obtain $h, h \rightarrow f, g$ transformation of the hole-hole interaction part of the effective Hamiltonian (30). Rewriting the $hh$ interaction term (30) in the form where summation is produced over MBZ leads to

$$H_{eff}^{hh} \Rightarrow H_{eff}^f + H_{eff}^g + H_{eff}^{gg} = t \sum_{k,k'} V_{k,k'}^f f_{k}^\dagger f_{k'}^\dagger + \sum_{k,k',q} V_{k,k';q}^f f_{k}^\dagger g_{k-q}^\dagger + g_k f_{k-q}^\dagger + t \sum_{k,k',q} \left( V_{k,k';q}^f f_{k}^\dagger f_{k'}^\dagger g_{k-q}^\dagger + f_{k}^\dagger g_{k-q}^\dagger + \text{H.c.} \right).$$

Thus, there are three different parts in the $H_{eff}^{hh}$, which correspond to the interaction between holes at the different sublattices ($fg$-part) and at the same one ($ff$- and $gg$-parts). The first terms for the interaction of the particles at
the same sublattice arise in the third order of the transformation and physically correspond to the process shown in the diagram Fig. 3. At the Ising background it is equivalent to the four-hopping process of the two holes staying at the apart corners of the minimal lattice square, when they move in the clockwise or anticlockwise direction doing the half of a turn. Generally, \(ff\) or \(gg\) interaction has no some important features of the \(fg\) one. Namely, there are no singularities in their long-range interaction as well as the gain of the energy due to reducing of the number of broken AF bonds is absent. These physical reasons were checked earlier \cite{43} and it was found that the bound states are absent for the particles at the same sublattice in the region of \((t/J) > 1\). Thus, we will restrict ourselves by consideration of the interaction of the particles at the different sublattices.

For obtaining \(fg\) interaction from \(hh\) one accurate consideration of the parity of the vertex \(V^{hh}\) under the transformation \(R = k(k') \rightarrow k(k') + (\pi, \pi)\) is required. There are two contributions of different parity \((R = \pi)\) in the effective \(fg\) interaction. Their diagrammatic analogues are presented in Figs. 3b and 3f, respectively. The first one is due to the one-magnon exchange and by its origin it is of the "exchange" type \((V^{hh}_{ex})\). The second one is due to the two-magnon exchange and the contact interaction (additions to \(J\)-term) and it is of "direct" type \((V^{hh}_{dir})\). Obviously, these contributions enter in the \(fg\) vertex with different sign

\[
V_{k,k',q}^{fg} = (-V^{hh}_{ex}(k, k', q) - V^{hh}_{ex}(k', k, -q) + V^{hh}_{dir}(k, k', q) + V^{hh}_{dir}(k', k, -q)) .
\]

Note here, that the first non zero correction beyond the ladder approximation for the hole-hole \((fg)\) scattering arises only in the sixth order over \(t\) (see Fig. 3l), that is the same order as one of the Trugman processes for the single hole movement and, as it seems, it has the similar reasons in the basis. Therefore, keeping in mind the negligible role of these non SCBA contributions to the hole energy, one can hope that the role of the diagram in Fig. 3l in the hole-hole interaction can be omitted and the ladder approximation will work well even for the initial (untransformed) \(t\)-\(J\) model. In our calculations we use the same approximation, but previously obtain the effective vertices, which are perturbative.

**B. Types of pairing interaction.**

Generally, there are two different types of the hole-hole interaction in the \(t\)-\(J\) model. The first one is due to the spin-wave exchange, whereas the second is from minimization of the number of broken AF bonds by the placing of the holes at the nearest neighbor sites. We will consider them separately.

The second type of interaction is usually introduced in the pure \(t\)-\(J\) model by adding projectors \(P_i = (1 - n^h_i)\) in \(J\)-term

\[
H_J = J \sum_{i,j} \left[ (1 - n^h_i)S_iS_j(1 - n^h_j) - \frac{1}{4} n^h_i n^h_j \right] ,
\]

which project out the subspace of local states (spins), \(n^h = h^\dagger h\) is the operator of the hole number. It is evident that due to the \(h^\dagger(h)\) and \(S\) operator commutativity projection procedure is exact, i.e. there is no spin-spin interaction between the sites with the holes. Thus, the addition part to the \(t\)-\(J\) model can be written as

\[
\Delta H_{t-J} = J \sum_{i,j} \left[ -(n^h_i + n^h_j)S_iS_j + n^h_i n^h_jS_iS_j - \frac{1}{4} n^h_i n^h_j \right] ,
\]

where summation run over bonds. Further treating this interaction term in the spin-wave approximation is straightforward and yields

\[
\Delta H_{t-J} = -2J(1 - 2\delta\lambda) \sum_{k,k',q} \gamma_4 f^\dagger_{k+q} \theta_4^{k+q} \theta_4^{k'} f_k + \delta H_J ,
\]

where term \(\delta H_J\), consisting of the two-magnon terms \(n^h aa\) and \(n^h n^h aa\), is presented in Appendix B. Hole attraction is enhanced by the zero-point fluctuations by the constant \((-2\delta\lambda \simeq 0.16\)\). Applying the transformation \cite{23} to the Hamiltonian \cite{38} one can get the addition part of the effective Hamiltonian

\[
\delta H^{fg} = J \sum_{k,k',q} \delta V_{k,k',q}^{fg} f^\dagger_{k+q} \theta_4^{k+q} \theta_4^{k'} f_k .
\]

The expression of the second-order (in \(f_k\) addition to the bare vertex \cite{38} is cumbersome and we present the general expression of \(\delta V_{k,k',q}^{fg}\) in Appendix B.
Generally, there is an evident result for the $n_in_j$ interaction in the $t = 0$ limit, namely, the groundstate of two holes is the bound state with the energy $E_b \simeq -0.58J$. Moreover, there is the full degeneracy among 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. The $nn$ type of interaction (38) was intensively studied by the number of analytical [42, 43], and numerical techniques [40], which established that increase of $t$ (taking into account the spin-wave exchange interaction) leads to the rapid growth of $E_b$ and disappearance of bound states. It was found that the largest critical value of $t_c$ is for the $d$ symmetry of the bound state and that it is somewhere between $t = (2 - 5)J$, which is very close to the values of $t$ proposed for the real CuO$_2$ planes. This fact has stimulated the developing of the idea of the superconductivity by the "preformed" pairs (bosons).

Considered pairing interaction has nothing to do with the spin-fluctuation one, which was investigated in Refs. 52 on the phenomenological basis and in Refs. 30 using the RPA for the Hubbard model. An essential addition to the studying of the spin-wave exchange (Fig. 7b) in the $t$-$J$ and Hubbard models has been done in the work by Frenkel and Hanke [33], 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 the holes. In the later work by Kuchiev and Sushkov [36] this problem was independently studied in great details and several interesting features of the system were found. First of all, neglecting the retardation effect and finite size of the Brillouin zone for the two-hole problem one can obtain the Schrödinger equation with the potential $\delta V_{fg}$ states were found to exist, and the lowest one was the $d$-state. This confirms a general statement [53] that in AF state one-magnon exchange leads to the repulsion in $s$-wave and attraction in $d$-wave state.

Note, that due to the long-range nature of the interaction and the large size of the proposed bound states it is not obvious how cluster analysis can directly reveal them.

C. Bethe-Salpeter equation.

Thus, one obtains the Hamiltonian 30 with the hole-magnon 33 and "contact" hole-hole 15, 38 interactions. Since we turned to an effective Hamiltonian by canonical transformation 24 the short-range spin-wave exchange (Fig. 7b) is now included in the "contact" interaction, which does not contain the retardation. Both interactions, according to above discussion, can lead to the pairing. As it was noted, the correct account for the retardation effect in the spin-wave exchange diagram is important, so let us consider this problem in details.

The systematical method to search the bound states is to look for the two-particle Green function poles in the scattering channel as the function of the particles summary energy in the system of their center of inertia 53. Corresponding integral equation for two holes with the total momentum $P = 0$ is presented in Fig. 8 in a diagrammatic form. The standard way of solving of such a type of equation with the non-retarded "compact" bare vertex $\Gamma^0$ is given in Appendix C.

In our case the "compact" vertex $\Gamma^0$ consists of two parts (see Fig. 8) and one has to include the magnon propagator into expression for the spin-wave exchange vertex. A natural assuming that the two-particle Green function has no singularities as the function of the difference of the energies of incoming particles provides somewhat different way of solving the Bethe-Salpeter problem. Details are also given in Appendix C.

Resulting parametric equation on the bound state energy $E$ of the Bethe-Salpeter type for the problem with two vertices (Fig. 8), which we will solve looks like

$$\psi(k, E) = \frac{1}{E - 2E_k} \sum_p \left[ \frac{-2(F_{k,k+p}M_{k,k+p})^2}{E - E_p - E_k - \omega_q + V_{k-k,q}^{fg} + \delta V_{k-k,q}^{fg}} \right] \psi(p, E),$$

where $q = k \pm q$ for the exchange (direct) parts of $V_{fg}^{fg}$ 34 and $\delta V_{fg}^{fg}$ 39.

D. Results.

Thus, having in hands the vertices 33, 35, 39 and equation 10 one can hope to obtain reliable results for the bound states in the $t$-$J$ model. Moreover, since we have done the separation of the scales in the momentum space
and consider the “minimization of the number of broken bonds” interaction separately, one can demonstrate the role of each type of interaction in forming of the bound states.

Shortly, our results are as follows. The single bound state of \( d \) symmetry \((d_{x-y^2})\) is exist in all region of \( 0 < (t/J) < 5 \). The states of other symmetries \((s, p)\) at \((t/J) \geq 0.2\) were not found. The main thesis of this work is that the interplay of both interactions, which tend to \( d \)-wave pairing, namely the short-range \( J \)-term \((33)\) and the long-range spin-wave exchange \((33)\), is important for the formation of this state. Specifically, there are no bound states from the \( J \)-term alone for \((t/J) > 2.1\). The spin-wave exchange itself provide the shallow bound state, but the actual magnitude of the mass along the MBZ boundary almost pushes out this state in the continuous spectra. Nevertheless, putting these interactions together we get the bound state with the energy of the two orders of magnitude deeper than one found in Ref. [30]. It was claimed in Ref. [30] that due to the \( 1/r^2 \) nature of the attractive potential accurate account for the “cutoff” parameter (finite size of the MBZ) and the retardation effect is required. We have taken into account both effects and have done calculations for the lowest bound state. Deviation of the model from the pure \( t-J \) one, i.e. taking into account next hopping integrals, can lead to the different physics of the system.

Let us discuss the other symmetry states. As it was noted above the limit \( t = 0 \) the \( J \)-term bound states of \( d, s \), and \( p \) symmetry are not distinguished in energy, but already at \((t/J) = 0.1\) \( s \)- and \( p \)-states are two times higher than the \( d \)-state and they are disappeared at \((t/J) = 0.2\).

Considering terms in equation in the bound state energy \((40)\) separately and all together, we have obtained results for the \( d \)-wave pairing state shown in Fig. 11. The dashed curve corresponds to taking into account the transformed \( J \)-term of interaction \((33)\) alone \((\delta \nu_{k_k^q}^{V_{19}})\). Obtained critical value of \( t \) for disappearing this, short-range in nature, state \( t_c = 2.1J \) is in excellent agreement with the variational approach [42], and in the good one with the finite-cluster calculations [28], [40], and other approaches [33]. Dashed-dotted curve corresponds to the long-range bound state due to the first two terms in Eq. \((40)\). According to Ref. [30] this state should have small negative energy. We found that if one takes into account the second-order correction to the single-hole energy due to the rest of the hole-magnon term \((33)\) it will lead to the slightly smaller mass along MBZ boundary and then to the very small binding energy \( \sim (10^{-3} - 10^{-4})t \) for the long-range state. Actually, corrected value of the mass almost pushed up the bound state in the continuous spectra. As we noted in Sec. IV resulting masses coincide with the SCBA ones. The solid curve is our final result for the \( d \)-wave bound state energy in the \( t-J \) model. Bound state energy for \((t/J) = 3\) equals to \( \Delta E = E - 2E_{k_0} = -0.022t \), which is of the two orders of magnitude deeper than it was obtained earlier [30]. Thus we obtained the strong enhancement of the coupling effect because of the interplay of both types of pairing interaction.

Note, that the "contact" part of the spin-wave exchange interaction \((V_{19})\) plays the minor role in such a strong effect, namely ignoring it in Eq. \((40)\) yields the energy \(-0.01t\), 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 the \( k \)-space. Figure 11a shows the wave function for \((t/J) = 1\). It is simply “bare” short-range \( \psi_k \sim (\cos k_x - \cos k_y) \) with the small addition of the higher harmonics. Figures 11b,c,d show wave functions for the (b) long-range state, (c) short-range one, and (d) resulting wave function, all for \((t/J) = 2\). Whereas the long-range bound state \(11b\) is well localized near the band minima, the short-range one \(11c\) looks like something average between Figs. 11a and 11d. It is not easily understandable, but one can say that in canonically transformed vertex \( \delta \nu_{k_k^q}^{V_{19}} \) except the simple \( \gamma_0 \) term there are some second-order terms with the same kinematic structure as in the \( V_{19} \) vertex, and since at \((t/J) = 2\) this state is shallow the higher harmonics with this structure become important. Resulting wave function \(11d\) reveals the features of the previous states. We believe that our results are very close to exact ones in all region of primary interest \( 1 < (t/J) < 5 \). Lowering of the bound state energy for \((t/J) = 5\) manifests the worse accuracy of our approach for the very large \( t \).

The next problem, which can be touched, is the influence of the next-nearest hopping terms \((t' \text{-terms})\) on the bound states. Evidently, small \( t' \) leads to the perturbative addition to the hole dispersion \( \delta E_k = 4t' \cos(k_x) \cos(k_y) \) and for the positive value of \( t' \) it makes the band more flat in \((\pi/2, \pi/2) \rightarrow (\pi, 0)\) direction. According to the above discussion it also strongly enhances the long-range interaction and makes the \( d \)-wave bound state much deeper. For instance, for the absolutely flat band \((m_j = \infty)\) at \((t/J) = 3\) energy of the bound state is \( E = -0.165t \). Note, that the neglecting of the short-range interaction \((J \text{-term})\) provides result of the next order of smallness \( E = -0.023t \). Further increase of \( t' \) will lead to the shift of the minima to the \((0, \pm \pi)\), \((\pm \pi, 0)\) points and will make the bound state shallower. For some region of \( t' > 0 \) the long-range bound state of \( k \) symmetry becomes possible. Its wave function obeys the same symmetry as \([\cos k_x - \cos k_y] \sin k_x \sin k_y\], i.e changes the sign in MBZ eight times. Since there is no short-range interaction for this state, the energy associated with it is very small.

It is well established by now, that for the real \( \text{CuO}_2 \) compounds \( t' \) has the negative sign and the total effect from \( t' \)-terms is the fully isotropic dispersion near the band minima [34,56]. Note, that it is the main effect from such terms and one can neglect their contribution to the effective vertexes up to the rather large values of \( t' \). Joining this statement together with the claimed sensitivity of the bound state to the anisotropy of the band one can suggest that
there are no bound states in the realistic model of the CuO$_2$ plane. We have studied the problem of the critical value of $t'$ and found that the difference $\Delta = E_{(\pi,0)} - E_{(\pi/2,\pi/2)}$, which is directly connected with the inverse mass along MBZ boundary, at which the bound state energy tends to zero is equal to 0.22$t$ for $(t/J) = 3$. Comparing it with the bare $t$-$J$ model value of $\Delta = 0.13t$ one can get the critical $t'_c \simeq 0.3J$, which is much lower than the realistic value $t'_c \sim 1.5J$.

Turning back to the simple $t$-$J$ model, one can say that, at the first glance, obtained result strongly supports the idea of the $t$-$J$ superconductivity by the condensate of the "preformed" pairs. In our opinion such a picture is not so obvious, since the existence of the long-range spin wave excitations is essential for the bound state formation, whereas the long-range order is unstable under very small finite concentration of holes. Therefore, for the clearing this subject one has to solve the pairing and stable spin state problem selfconsistently.

\section*{VI. CONCLUSION}

We conclude by summarizing our results.

We have put forward the canonical transformation of the $t$-$J$ model Hamiltonian using an analogy with the lattice polaron problem as well as some evident ideas based on the known single-hole properties in the AF background. We have shown that the rather wide type of the transformations, which has the some type of the $1/z$ expansion in the basis, allow to extend the region of the analytical treatment of the problems up to $t/J \sim 5$ with an appropriate accuracy. Generally, powerful method applied provided us the straight way to the formulating of the quasiparticle Hamiltonian, which includes the free energy terms and all essential interactions.

The proof of the correctness of the simple form of the effective quasiparticle Hamiltonian has been done. Results for the single-hole bottom of the band, bandwidth, and other properties have been compared with ones of the SCBA calculations and a remarkable agreement has been found. It is supported the idea that the "canonically transformed" quasiparticles have the properties, which are close to ones of exact $t$-$J$ model quasiparticles. Although the bandwidth and components of magnetic polaron wave function have discrepancies with the exact ones, which are grown for the larger $(t/J) > 5$, the bottom of the hole band remains very close to an exact one, confirming the basic idea that the effect of the polaron well formation (of the order of $t$) is taken into account by our transformation.

Using the obtained Hamiltonian we have performed the study of the two-hole problem. The hole-hole interactions of the different nature have been considered separately and all together. Rather deep bound state of $d$-wave symmetry originated from the interplay of two types of the pairing interactions has been found. 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 $t'_c$ for the bound state existence has been found.

Since we have used the presence of the AF long-range order as a foundation of the setting up the problem and the long-range interaction was found to be essential for the bound state formation, so 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 questions, which remain to be resolved.

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\section*{APPENDIX A:}

The series of commutators of the type $[\hat{\mathbf{r}}, \hat{\mathbf{S}}]$ with generator of the transformation $\hat{\mathbf{r}}$ provide the general expression for the hole energy and hole-magnon formfactor $\hat{\mathbf{h}}$

\begin{equation}
E_k = 2t \sum_q \left( M_{k,q} \mu_{k,q} + \frac{1}{3!} W_{k,q} \mu_{k,q} + \frac{2J}{t} \left[ \frac{1}{\pi^2} \delta \mu_{k,q}^2 + \frac{1}{\pi^3} \delta W_{k,q} \mu_{k,q} + \frac{1}{\pi^4} \delta^2 W_{k,q} \mu_{k,q} \right] \right) \quad (A1)
\end{equation}
\[ F_{k,q} = 1 + \left( \frac{1}{\pi} W_{k,q} + \frac{1}{4\pi} \delta W_{k,q} + \frac{2J}{t} \left[ \mu_{k,q} \omega_q + \frac{1}{\pi} \tilde{W}_{k,q} + \frac{1}{3\pi} \delta \tilde{W}_{k,q} \right] \right) / M_{k,q} , \]

with

\[ W_{k,q} = 3 \mu_{k,q} \left( V_{k-q} - V_k \right) - M_{k,q} \left( U_{k-q} + U_k \right) , \quad \tilde{W}_{k,q} = \mu_{k,q} \left[ 3 \left( \tilde{V}_{k-q} - \tilde{V}_k \right) - \omega_q \left( U_{k-q} + U_k \right) \right] \]

\[ \delta W_{k,q} = \mu_{k,q} \left( 15 \left( \delta W_{k-q} - \delta W_k \right) \right) + (5 \delta U_{k-q} - \delta U_k) + \omega_q \left( U_{k-q} + U_k \right) , \]

\[ \delta \tilde{W}_{k,q} = \mu_{k,q} \left( \tilde{W}_{k-q} - \tilde{W}_k \right) + \omega_q \left( U_{k-q} + U_k \right) , \]

where

\[ V_k = \sum_{q'} M_{k,q'} \mu_{k,q'} , \quad U_k = \sum_{q'} \mu_{k,q'}^2 , \quad \tilde{V}_k = \sum_{q'} \mu_{k,q'} \omega_q , \]

and \( \delta W_{k,q} , \delta \tilde{W}_{k,q} \) are the terms from the Trugman processes. They were found to play the negligible role for the energy and vertex.

Explicit expression of the energy up to the fourth order over the TP for the generator in the form \( (25) \) is

\[ E_k \approx 2t \left[ f_k I_k + \frac{1}{\pi} \left( 3 f_k^2 F_1^2 - 4 f_k^3 F_2^2 \right) - f_k F_2^2 \right] + \frac{J}{t} \left[ f_k^2 I_k + \frac{1}{\pi} \left( 3 f_k^2 F_3^3 - 4 f_k^3 I_k - f_k F_4^2 \right) \right] \]

with

\[ F_1 = \sum_q \left( M_{k,q}^2 I_{k-q} \right) , \quad F_2 = \sum_q \left( M_{k,q}^2 I_{k-q} - I_{k-q} \right) , \]

\[ F_3 = \sum_q \left( M_{k,q}^2 I_{k-q} \right) , \quad F_4 = \sum_q \left( M_{k,q}^2 I_{k-q} \omega_q \right) , \]

\[ Y_k = \sum_q \left( M_{k+q,q}^2 \right) \],

where \( I_k \) and \( \tilde{I}_k \) are defined by Eq. \( (25) \).

Hole-hole vertex \( V_{k,k',q}^{hh} = V_{ex}^{hh} (k,k',q) + V_{dir}^{hh} (k,k',q) \) is

\[ V_{ex}^{hh} (k,k',q) = \left( M_{k,q} \mu_{k-q} + M_{k-q} \mu_{-q} \right) \left[ 1 + \frac{1}{\pi} F_{k,q} \right] + \frac{2J}{t} \omega_q \left( \mu_{k,q} \mu_{k-q} + \mu_{k-q} \mu_{-q} \right) \left[ 1 + \frac{1}{\pi} F_{k,q} \right] + \frac{4}{t} \left( \mu_{k,q} \mu_{-q} - \mu_{-q} \mu_{-q} \right) \left[ \frac{1}{\pi} (V_k - V_{k'}) + \frac{2J}{t} \left( U_k - U_{k'} \right) \right] , \]

and

\[ V_{dir}^{hh} (k,k',q) = T_{dir}^{h} (k,k',q) + T_{dir}^{h} (k,k',q) + T_{dir}^{h} (k,k',q) + T_{dir}^{h} (k,k',q) , \]

\[ T_{dir}^{h} (k,k',q) = \sum_{q'} \left( \mu_{k',q} + \mu_{-q} \right) \left( \mu_{k,q} \mu_{k,q} - M_{k,q} \mu_{k,q} \right) \]
Two-magnon vertices are

\[
V_{1}^{ha}(k, q, q') = M_{k-q-q'} u_{k, q} - M_{k-q} u_{k, q'} + \frac{J}{t} (\omega_{q} - \omega_{q'}) \mu_{k-q, q} + \text{higher order terms}
\]

\[
V_{2}^{h}(k, q, q') = M_{k-q} u_{k, q'} - M_{k-q-q'} u_{k, q} + \frac{J}{t} (\omega_{q} + \omega_{q'}) \mu_{k-q, q'} - \mu_{k-q', q} + \text{higher order terms}
\]

APPENDIX B:

Hole-two-magnon addition \( \delta H_{J} \) (38) originated from the projectors applied to \( J \)-term has the form

\[
\delta H_{J} = J \sum_{k, k', q, q'} \left\{ V_{Q, q, q'}^{1, J} \left( h_{k-q-q'}^{\dagger} h_{k-q}^{\dagger} + h_{k-q} h_{k-q'}^{\dagger} + \text{H.c.} \right) + 2V_{Q, q, q'}^{2, J} \right\}
\]

\[
- J \sum_{k, k', q, q'} \left\{ \tilde{V}_{Q, q, q'}^{1, J} \left( h_{k-q-q}^{\dagger} h_{k-q}^{\dagger} + \text{H.c.} \right) + 2\tilde{V}_{Q, q, q'}^{2, J} \right\},
\]

where vertices are given by

\[
V_{Q, q, q'}^{1, J} = \gamma_{Q} (u_{q} u_{q'} + v_{q} v_{q'}) + \frac{1}{2} \left[ \gamma_{Q+q} + \gamma_{Q-q} \right] (u_{q} u_{q'} + v_{q} v_{q'}),
\]

\[
V_{Q, q, q'}^{2, J} = \gamma_{Q} (u_{q} u_{q'} + v_{q} v_{q'}) + \frac{1}{2} \left[ \gamma_{Q+q} + \gamma_{Q-q} \right] (u_{q} u_{q'} + v_{q} v_{q'}),
\]

\[
\tilde{V}_{Q, q, q'}^{1, J} = \left[ 1 + \gamma_{Q+q} \right] (u_{q} u_{q'} + v_{q} v_{q'}) + \left[ \gamma_{Q+q} \right] (u_{q} u_{q'} + v_{q} v_{q'}),
\]

\[
\tilde{V}_{Q, q, q'}^{2, J} = \left[ 1 + \gamma_{Q+q} \right] (u_{q} u_{q'} + v_{q} v_{q'}) + \left[ \gamma_{Q+q} \right] (u_{q} u_{q'} + v_{q} v_{q'}),
\]

where \( u_{q}, v_{q} \) are the parameters of Bogolubov transformation, \( U_{k} \) defined in (33).

Applying the transformation (33) to the Hamiltonian (33) one can get the additional part to the effective interaction

\[
\delta V_{k, k', q}^{fg} = \delta V_{k, k', q}^{fg} + \delta V_{k, k', q}^{fg}
\]

with the direct part

\[
\delta V_{k, k', q}^{fg} = - \gamma_{Q} (1 - 2\delta \lambda) \left[ 1 - U_{k} - U_{k-q} \right]
\]

\[
+ 4 \sum_{q} \mu_{k, q} f_{k-q} \left\{ \delta \gamma_{k-q} \left( u_{q} u_{q'} + \frac{1}{2} \gamma_{q} (u_{q} u_{q'} + v_{q} v_{q'}) \right) + \left[ k, q \Rightarrow k - q, -q \right] \right\}
\]

\[
+ 4 \sum_{q} \mu_{k, q} f_{k-q} \left\{ \delta \gamma_{k-q} \left( u_{q} u_{q'} + \frac{1}{2} \gamma_{q} (u_{q} u_{q'} + v_{q} v_{q'}) \right) + \left[ k, q \Rightarrow k + q, -q \right] \right\}
\]

\[
- \sum_{q} \delta \gamma_{k+q, q'} \left\{ \mu_{k+q, q} \tilde{V}_{k-q, q}^{1, J} + \mu_{k+q, q} \tilde{V}_{k-q, q}^{2, J} \right\} + \left[ k, q \Rightarrow k + q, -q \right],
\]

\[
\delta V_{k, k', q}^{fg} = 32 f_{k} f_{k'} \left\{ \frac{1}{2} \delta \gamma_{k} \gamma_{k'} (u_{q} u_{q'} + \frac{1}{2} \gamma_{q} (u_{q} u_{q'} + v_{q} v_{q'})) + \frac{1}{2} D_{1} \gamma_{k} \tilde{F}_{k, q} + \frac{1}{2} D_{2} \tilde{F}_{k, k'} + \frac{1}{2} D_{3} \tilde{F}_{k, k'} \right\}
\]

\[
- 2 \left\{ \mu_{k+q, q} f_{k+q, q} + \frac{1}{2} \gamma_{q} \mu_{k+q, q} f_{k+q, q} \right\} + \left[ k, k', q \Rightarrow k - q, k' + q - q \right],
\]
where functions
\[ \tilde{F}_{k_1,k_2} = D_1 \gamma_{k_1} \gamma_{k_2} + \frac{1}{2} D_2 \gamma_{k_1-k_2} + \frac{1}{4} D_3 \gamma_{k_1+k_2}, \] (B5)
\[ \Phi_{k,q}^I + \Phi_{k,q}^D = 4f_k \left\{ \delta \lambda \gamma_k (\gamma_q v_q + u_q) + \left( \frac{1}{4} + \delta \lambda \right) u_q \gamma_k + v_q \tilde{F}_{k,q} \right\} + |k,q \Rightarrow k - q, -q|, \]
with the numbers
\[ \delta \lambda = \sum_q (u_q^2 + \gamma_q v_q u_q) = -0.0790 , \quad D_1 = \sum_q (\gamma_q v_q u_q + u_q^2 \cos q_x \cos q_y) = -0.1301 , \] (B6)
\[ D_2 = \sum_q u_q^2 (1 - \cos q_x \cos q_y) = 0.2628 , \quad D_2 = \sum_q u_q^2 (2 \cos^2 q_x - 1 - \cos q_x \cos q_y) = -0.0077 . \] (B7)

APPENDIX C:

For two holes with the total momentum \( P = 0 \) one can write the following integral equation
\[ \tilde{\Gamma}(k_f, -k_g, k'_f, -k'_g) = \Gamma^0(k_f, -k_g, k'_f, -k'_g) + \sum_{pf} \Gamma^0(k_f, -k_g, p_f, -p_g) G(p_f) G(-p_g) \tilde{\Gamma}(p_f, -p_g, k'_f, -k'_g) \] (C1)
where we introduced four-momentum notations \( k_f = (k, \epsilon_f), -k_g = (-k, \epsilon_g), \) \( p_f = (p, \epsilon'_f), -p_g = (-k, \epsilon'_g) \) with momenta \( k, p \) and frequencies \( \epsilon_{f(g)}, \epsilon'_{f(g)}, \) \( G(p) = 1/(\epsilon - E_k + i\delta) \) is the single-hole Green function. This equation is equivalent to the graphical equality shown in Fig. 3. Near the pole \( \Gamma^0 \ll \tilde{\Gamma} \) and hence the first term in Eq. (C1) 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 determined by equation, and they can be omitted. Let us also introduce \( E = \epsilon_f + \epsilon_g, \Delta \epsilon = (\epsilon_f - \epsilon_g)/2, \) and \( \Delta \epsilon'' = (\epsilon'_f - \epsilon'_g)/2. \) Thus,
\[ \tilde{\Gamma}(k, E, \Delta \epsilon) = \sum_{p, \Delta \epsilon''} \Gamma^0(k, p, E, \Delta \epsilon, \Delta \epsilon'') G(p, E/2 + \Delta \epsilon'') G(-p, E/2 - \Delta \epsilon'') \tilde{\Gamma}(p, E, \Delta \epsilon'') . \] (C2)

When \( \Gamma^0 \) has no frequency dependence ("static" interaction),
\[ \Gamma^0(k, p, E, \Delta \epsilon, \Delta \epsilon'') = U(k, p), \] (C3)

it is natural to change the variable \( G \tilde{\Gamma} = \chi \) and get
\[ \chi(k, E, \Delta \epsilon) = G(k, E/2 + \Delta \epsilon) G(-k, E/2 - \Delta \epsilon) \sum_p U(k, p) \int d(\Delta \epsilon'') \chi(p, E, \Delta \epsilon'') . \] (C4)

Additional integration of both sides over \( \Delta \epsilon \) gives the Schrödinger equation:
\[ \psi(k, E) = \frac{1}{E - 2E_k} \sum_p U(k, p) \psi(p, E) , \] (C5)
with \( \psi(k, E) = \int d(\Delta \epsilon) \chi(k, E, \Delta \epsilon), \) which has the sense of the bound-state wave function.

In our case the "compact" vertex \( \Gamma^0 \) consists of two parts (see Fig. 3) and one has to include the magnon propagator into expression for the spin-wave exchange vertex
\[ \Gamma^0_1(k, p, \Delta \epsilon, \Delta \epsilon'') = -\left[ \frac{V_{k,p} V_{-k,-p}}{\epsilon - \epsilon'' - \omega_{k+p} + i\delta} + \frac{V_{-k,-p} V_{k,p}}{\epsilon'' - \epsilon - \omega_{-k-p} + i\delta} \right] \] (C6)
where \( V_{k,p} \) is the vertex of the type Eq. (33), \( \epsilon - \epsilon'' = \Delta \epsilon - \Delta \epsilon'', k + p = q. \) Both negative sign and \( q = k + p \) are due to exchange character of the diagram (Fig. 3). Thus, there are three \( \Delta \epsilon'' \)-dependent denominators in the integral Eq. (C4) and the above change of variables is impossible.

It is natural to assume that since one is looking for the poles of the two-particle Green function as the function of \( E, \) \( \tilde{\Gamma} \) has no singularities as the function of the difference of the energies of incoming particles. Therefore, the integration
over $\Delta \epsilon''$ in Eq. (C2) can be done and it is determined by the poles of $G(p, E/2 + \Delta \epsilon'')$, $G(p, E/2 - \Delta \epsilon'')$, and $\tilde{\Gamma}_0^\alpha(k, p, \Delta \epsilon, \Delta \epsilon'')$. Their poles are: $\Delta \epsilon'' = (E_p - E/2) - i\delta$, $\Delta \epsilon'' = -(E_p - E/2) + i\delta$, and $\Delta \epsilon'' = \pm(\Delta \epsilon - \omega_q) \pm i\delta$, respectively. $+$($-$) in the last pole corresponds to the first (second) term in Eq. (C6). The integration gives

$$\tilde{\Gamma}(k, E, \Delta \epsilon) = \sum_p \left( - \frac{V_{k,p} V_{k,-p}}{E - 2E_k} \right) \left[ \frac{\tilde{\Gamma}(p, E, (E_p - E/2))}{\Delta \epsilon - (E_p - E/2) - \omega_q + i\delta} + \frac{\tilde{\Gamma}(p, E, -(E_p - E/2))}{-\Delta \epsilon - (E_p - E/2) - \omega_q + i\delta} \right],$$

(C7)

The further way is close to the usual one. Multiplying both sides of Eq. (C7) by the external incoming Green functions one can integrate over $\Delta \epsilon$, using the evident parity of $\tilde{\Gamma}$ on $\Delta \epsilon$

$$\frac{\tilde{\Gamma}(k, E)}{E - 2E_k} = \frac{1}{E - 2E_k} \sum_p \frac{-2V_{k,p} V_{k,-p}}{E - E_p - E_k - \omega_q} \times \tilde{\Gamma}(p, E).$$

(C8)

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

$$\psi(k, E) = \frac{1}{E - 2E_k} \sum_p \frac{-2V_{k,p} V_{k,-p}}{E - E_p - E_k - \omega_q} \psi(p, E).$$

(C9)

Evidently, the "usual" Bethe-Salpeter equation (C5) can be obtained by the same way. Surprisingly, this result (C9) coincides exactly with one obtained in Ref. [6] using Rayleigh-Schrödinger perturbation theory.

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Figure captions

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

FIG. 2. Weights of the components of the magnetic polaron wave function (Ising limit). Bold curves are for an exact solution, light curves are for the canonical transformation results (fifth order). Solid curves correspond to the weights of the bare hole, dashed-double-dotted curves – hole+1 magnon, dashed curve – hole+2 magnons, long-dashed curve – hole+3 magnons.

FIG. 3. Bottom of the hole band. Solid curve is our result (the sixth order of the transformation), dashed curve is the SCBA result.

FIG. 4. Width of the hole band. Solid curve is our result (the sixth order of the transformation), dashed curve is the SCBA result.
FIG. 5. Weights of the components of the magnetic polaron wave function (Néel case). Bold curves are for an exact solution (SCBA), light curves are for the canonical transformation results (the fourth order). Solid curves correspond to the weights of the bare hole, dashed curves – hole+1 magnon, dashed-dotted curve – hole+2 magnons.

FIG. 6. $t/J$ dependence of the formfactor $F_{k,q}$. Solid curve $- k = (\pi/2, \pi/2)$, $q = (0,0)$, dashed curve $- k = (\pi/2, \pi/2)$, $q = (\pi/2, \pi/2)$, dashed-double-dotted curve $- k = (0,0)$, $q = (0,0)$.

FIG. 7. Schematic view of the scattering diagrams: (a) $ff \rightarrow ff$, (b) $fg \rightarrow gf$ of exchange type, (c) $fg \rightarrow fg$ of direct type, (d) the first diagram of the $fg \rightarrow fg$ scattering beyond the ladder approximation. Here, the wavy lines denote the interaction, which originates from the magnon exchange ($t$-term), and the point in the diagram (c) denotes the vertex, which is from the nearest neighbor interaction ($J$-term).

FIG. 8. Graphical identity for an exact vertex $\tilde{\Gamma}(k_f, -k_g, k'_f, -k'_g)$ for the $fg$ scattering in the ladder approximation. Black circle denotes $\tilde{\Gamma}(k_f, -k_g, k'_f, -k'_g)$, empty circle denotes a ”compact” vertex $\Gamma^0(k_f, -k_g, k'_f, -k'_g)$.

FIG. 9. Structure of the ”compact” vertex $\Gamma^0(k_f, -k_g, k'_f, -k'_g)$ (empty circle). Here, the wavy line denotes the interaction due to the long-range spin-wave exchange (33), and the point denotes all diagrams, which do not contain the retardation (33), (35).

FIG. 10. Results for the energy of the $d$-wave pairing state. Dashed curve corresponds the short-range bound state, dashed-dotted curve corresponds to the long-range one, and solid curve corresponds to the combined effect of both types of the state.

FIG. 11. 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 mixed state.
Fig. 2
Fig. 3
Fig. 4
Fig. 6
Fig. 7
Fig. 8
Fig. 9
