Large size two-hole bound states in $t$-$J$ model

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Abstract

Several series of shallow large-size ($l \gg$ lattice spacing) two-hole bound states are found in the two-dimensional $t-J$ model. Their binding energies depend exponentially on the inverse value of the hole-spin-wave coupling constant. Their parity is connected with the angular wave function in a nonstandard way. The possible role of these states in the formation of superconducting pairing is considered.

Keywords: Antiferromagnetic order, t-J model, spin fluctuations, energy gap.
I. INTRODUCTION

The problem of mobile holes in the $t$-$J$ model is closely related to high-$T_c$ superconductivity. The $t$-$J$ model with less than half-filling is defined by the Hamiltonian

$$H = H_t + H_J = -t \sum_{\langle nm \rangle \sigma} (d^\dagger_{n\sigma} d_{m\sigma} + \text{H.c.}) + J \sum_{\langle nm \rangle} S_n S_m,$$

where $d^\dagger_{n\sigma}$ is the creation operator of a hole with spin $\sigma$ ($\sigma = \uparrow, \downarrow$) at site $n$ on a two-dimensional square lattice. The $d^\dagger_{n\sigma}$ operator acts in the Hilbert space where there is no double electron occupancy. The spin operator is $S_n = \frac{1}{2} d^\dagger_{n\alpha} \sigma_{\alpha\beta} d_{n\beta}$. $\langle nm \rangle$ are neighbour sites on the lattice. Below we set $J = 1$.

At half-filling (one hole per site) the $t$-$J$ model is equivalent to the Heisenberg antiferromagnet model [1,2] which has the long-range antiferromagnetic order in the ground state [3–5]. The problem is the behavior of the system under doping by additional holes.

Single particle properties in the $t$-$J$ model are by now well established. A single hole is an object with complex structure due to virtual admixture of spin excitations. It has been shown that a single hole has the ground state with a momentum of $k = (\pm \pi/2, \pm \pi/2)$. The energy is almost degenerate along the line $\cos k_x + \cos k_y = 0$ which is the edge of the magnetic Brillouin zone (see e.g. Refs. [6–15]).

The two-hole problem is much more complicated. There is no doubt that for $t \ll 1$ there are short-range $d$- and $p$-wave two-hole bound states with a binding energy $\Delta E \approx -0.25$. These bound states could be relevant to the superconductivity. However the value of $t$ corresponding to the realistic high-$T_c$ superconductors is $t \approx 3$ (see, e.g. Refs. [16–18]). The early works on exact diagonalizations for finite-size clusters [10,19–23] indicated the existence of a short-range two-hole bound state for large $t$. However recent investigations [24–27] have demonstrated that the short-range two-hole bound state vanishes at $t \approx 2 – 3$. Moreover, in our opinion even for smaller values of $t$ the short-range Coulomb repulsion in realistic systems should destroy this
bound state (see the discussion in Ref. [27]). These arguments lead us to the conclusion that
theory predicts no short-range bound states at physical values of $t$. This conclusion makes the
investigation of the long-range dynamics in the $t - J$ model very important.

The long-range dynamics is determined by the interaction of a hole with spin-wave excita-
tions. Calculation of the hole-spin-wave coupling constant $f$ is straightforward if one treats
$H_t$ as perturbation and uses the condition $zS \gg 1$ ($z$ is the number of neighbour sites). The
value of the coupling constant obtained in this way is $f = \frac{1}{2}zt = 2t$ (see e.g. Ref. [9,12,13]). The
calculation of $f$ for realistic $zS$ and arbitrary $t$ has been done in recent works [28,29].

In the present work we prove the existence of shallow large-size two-hole bound states which
appear due to the exchange of a spin-wave. It is demonstrated that there are several infinite
series of such states. Their binding energies depend exponentially on the radial quantum
number: $E_n \propto e^{-\gamma n}$, where $\gamma$ is a numerical constant, $n = 0, 1, \ldots$. Very interesting is the
relation between the parity and the angular wave function of these states. A state with an
angular wave function without nodes (in this sense it is $s$-wave) has negative parity. A state
with two nodes in the angular wave function (in this sense it is $p$-wave) has positive parity.
This property may be considered as an additional negative “internal” parity of the pair. The
nonstandard parity relation is caused by two physical reasons. First, the ground state of the
system is the antiferromagnetic one. Second, the bottom of single-hole dispersion is at the face
of the Brillouin zone.

Our paper has the following structure. In Sec.II we derive an effective Hamiltonian describ-
ing the dynamics of the system in the long-range region. It is presented in terms of dressed
holes and spin-waves. The nontrivial properties of the system are caused by the strong interac-
tion between holes and spin-waves and the contact interaction between the holes. This section
is based on the results of Refs. [27,29]. In Sec.III we show that the exchange of a spin-wave
between two holes creates the long-range attracting potential which decreases as $1/r^2$ with the
separation \( r \) between the holes. This potential generates several infinitive series of bound states of the two holes. In Sec.IV we discuss the parity and the symmetry properties of these states. In Sec.V we compare the analytical solution with the results of exact numerical diagonalization of the equation for the bound states. In concluding Sec.VI we discuss scenario of possible superconducting pairing based upon the results of the present work.

II. INTERACTION BETWEEN THE HOLES WITH OPPOSITE SPINS.
EFFECTIVE HAMILTONIAN FOR THE DRESSED HOLES.

We treat the \( J \) term of the Hamiltonian (1) using the linear-spin-wave approximation (see Ref. [5] for a review). Define the following Fourier transformations

\[ a_q^\dagger = \sqrt{\frac{2}{N}} \sum_{n \in \uparrow} S_n^- e^{i q r_n}, \quad b_q^\dagger = \sqrt{\frac{2}{N}} \sum_{n \in \downarrow} S_n^+ e^{i q r_n}, \]  

where our notation \( n \in \uparrow (n \in \downarrow) \) means that site \( n \) is on the up sublattice (down sublattice). Introducing the Bogoliubov canonical transformation,

\[ \alpha_q^\dagger = u_q a_q^\dagger - v_q b_q^\dagger, \quad \beta_q^\dagger = u_q b_q^\dagger - v_q a_q^\dagger, \]  

we write the Heisenberg Hamiltonian \( H_J \) as

\[ H_J = E_0 + \sum_q \omega_q (\alpha_q^\dagger \alpha_q + \beta_q^\dagger \beta_q), \]  

where \( E_0 \) is the antiferromagnetic background energy. The summation over \( q \) is restricted inside the Brillouin zone of one sublattice where \( \gamma_q = \frac{1}{2} (\cos q_x + \cos q_y) \geq 0 \). The spin-wave dispersion and the transformation coefficients are given by

\[ \omega_q = 2\sqrt{1 - \gamma_q^2} \rightarrow \sqrt{2}|q|, \text{ at } q \ll 1 \]
\[ u_q = \sqrt{\frac{1}{\omega_q} + \frac{1}{2}}, \]
\[ v_q = -\text{sgn}(\gamma_q) \sqrt{\frac{1}{\omega_q} - \frac{1}{2}}. \]
The spin waves $\alpha_q$ and $\beta_q$ have definite values of the spin projections. Due to Eqs. (2), (3) $\alpha^\dagger_q |0\rangle$ has $S_z = -1$, and $\beta^\dagger_q |0\rangle$ has $S_z = +1$. Here $|0\rangle$ is the quantum Néel state wave function.

A single hole on the antiferromagnetic background is a composite object due to strong virtual admixture of the spin excitations. Therefore its dispersion is sufficiently complicated. Fortunately it may be well approximated by the simple analytical formula which was found in Refs. [15,29].

$$\epsilon_k = \sqrt{\Delta^2/4 + 4t^2(1+y)} - \sqrt{\Delta^2/4 + 4t^2(1+y) - 4t^2(x+y)k_x^2 + \frac{1}{4}\beta_2(\cos k_x - \cos k_y)^2}$$

(6)

$$\Delta \approx 1.33, \quad x \approx 0.56, \quad y \approx 0.14$$

The parameters $\Delta, x, y$ are some combinations of the ground state spin correlators [15]. The $\beta_2$ term gives the dispersion along the edge of the Brillouin zone. It is rather weak and may be estimated as $\beta_2 \sim 0.1 \times t$ at $t \geq \Delta/4$. Near the band bottom $k_0 = (\pm \pi/2, \pm \pi/2)$ the dispersion (6) can be presented in a usual quadratic form

$$\epsilon_k \approx \frac{1}{2}\beta_1 k_1^2 + \frac{1}{2}\beta_2 k_2^2, \quad \beta_2 \ll \beta_1,$$

(7)

where $k_2$ is projection of the momentum along the face of magnetic Brillouin zone, $k_1$ is orthogonal projection of the momentum, see Fig.1. Due to Eq.(3)

$$\beta_1 \approx \begin{cases} 
4\frac{x+y}{\Delta}t^2 \approx 2.1t^2 & \text{for } t \ll \Delta/4 = 0.33, \\
\frac{x+y}{\sqrt{1+y}}t \approx 0.65t & \text{for } t \gg \Delta/4.
\end{cases}$$

(8)

A comparison with numerical calculations (see e.g. Refs [11,13,15,25]) shows that simple formulas (6), (8) underestimate $\beta_1$ by 10-20%. This produces no serious effect on the results of the present work, but certainly this correction can to be included.

The wave function of a single hole may be written in the form $\psi_{k\sigma} = h^\dagger_{k\sigma} |0\rangle$. $h^\dagger_{k\sigma}$ is the creation operator of a dressed hole

$$h^\dagger_{k\uparrow} = \sqrt{\frac{2}{N}} \sum_{n \in \downarrow} h^\dagger_{n\uparrow} e^{ik\cdot r_n},$$

(9)
\[ h_{k \downarrow}^\dagger = \sqrt{\frac{2}{\mathcal{N}}} \sum_{n \in \uparrow} h_{n \uparrow}^\dagger e^{i\mathbf{k} \cdot \mathbf{r}_n}, \]

It was demonstrated in Refs. [15, 29] that \( h_{n \sigma}^\dagger \) may be well approximated by the following simple expressions:

\[
\begin{align*}
    h_{n \uparrow}^\dagger &\approx \nu d_{n \uparrow}^\dagger + \mu S_n^+ \sum_\delta d_{n+\delta \downarrow}^\dagger, \\
    \nu &= \frac{1}{2} \left( \frac{3/2 + 2S_t}{S_t} \right)^{1/2}, \\
    \mu &= \frac{t}{[S_t(3/2 + 2S_t)]^{1/2}},
\end{align*}
\]

(10)

where \( \delta \) is a unit vector corresponding to one step in the lattice. This form of trial wave function leads to the dispersion (9).

The effective interaction of a composite hole with a long wave-length spin-wave is of the form (see, e.g. Refs. [9, 12, 13, 28, 29]):

\[
H_{h,sw} = \sum_{\mathbf{k}, \mathbf{q}} g(\mathbf{k}, \mathbf{q}) \left( h_{\mathbf{k} + \mathbf{q}, \alpha}^\dagger h_{\mathbf{k}, \alpha} h_{\mathbf{k} + \mathbf{q}, \beta}^\dagger h_{\mathbf{k}, \beta} + H.c. \right),
\]

(11)

\[ g(\mathbf{k}, \mathbf{q}) = 2f \sqrt{\frac{2}{\mathcal{N}}} (\gamma_{\mathbf{k} \downarrow \mathbf{q} \uparrow} + \gamma_{\mathbf{k} \uparrow \mathbf{q} \downarrow}). \]

In the perturbation theory limit (\( t \ll \Delta/4 \)) and at \( zS \gg 1 \) (\( z \) is the number of neighbour sites) the coupling constant is \( f \approx f_0 = 2t \) (see e.g. Ref. [9, 12, 13]). Account of the first \( 1/zS \) correction gives \( f \approx f_1 = \frac{8}{3} t \), and summation of all \( 1/zS \) series gives \( f = 3.4t \) for \( t \ll \Delta/4 \) [28]. For an arbitrary \( t \) the coupling constant was calculated in Ref. [29]. The plot of \( f \) as a function of \( t \) is presented in Fig.2. For small \( t \): \( f \approx 3.4t \). For large \( t \) the coupling constant is \( t \)-independent: \( f \approx 2 \).

The interaction between the two holes can be caused by the exchange of single (or several) soft spin-wave. Alongside with that there is a contact hole-hole interaction. One can say that it is due to the exchange of several hard spin-wave excitations. Now we are going to derive the Hamiltonian of the contact hole-hole interaction. Interaction between two holes at large
momentum transfer \((q \sim 1)\) has been obtained in Ref. \cite{27} using a variational approach and 1/zS expansion.

\[
\Gamma(k_3 \uparrow, k_4 \downarrow; k_1 \uparrow, k_2 \downarrow) \approx \frac{8}{N} \left[ A \gamma_{k_1-k_3} + B (\gamma_1 \gamma_3 + \gamma_2 \gamma_4) + \frac{C}{2} (\gamma_{k_1+k_3} + \gamma_{k_2+k_4}) \right] \delta_{12,34},
\]

\(A = 16 \nu \mu^3 (1 - 7 \mu^2) - \frac{1}{4} - 2 \mu^2 - 18.5 \mu^4 + 84 \mu^6 + 10 \alpha \nu \mu^3,\)

\(B = 8 \nu \mu (1 - 9 \mu^2 + 32 \mu^4) - 4 \mu^2 (1 - 4 \mu^2) (1 - 12 \mu^2),\)

\(C = \frac{2}{3} \alpha \nu \mu^3.\)

Here \(\nu\) and \(\mu\) are the parameters of the wave function \(\text{(10)}\). We denote for simplicity \(\gamma_{k_i} = \gamma_i\).

The functions \(A\) and \(C\) in formula \(\text{(12)}\) have been derived in the first order in \(\alpha\), where \(\alpha\) is the coefficient in front of the transverse contribution to the Heisenberg energy: \(S_n S_m \rightarrow S_n^z S_m^z + \frac{\alpha}{2} (S_n^+ S_m^- + S_n^- S_m^+).\) The physical value is \(\alpha = 1\). The higher order contributions to \(A\) and \(C\) are essential. In order to fit them one has to set \(\alpha\) in Eq.(\text{12}) somewhere in between \(\alpha = 0.5\) and \(\alpha = 1\). The expression for \(B\) in formula \(\text{(12)}\) corresponds to the Ising background \((\alpha = 0)\). The difference is that \(A(\alpha = 0)\) and \(C(\alpha = 0)\) are small and therefore the corrections are crucial. The coefficient \(B\) is not small and the \(\alpha\) correction is not so important.

Expression \(\text{(12)}\) includes the contributions from the single spin-wave exchange as well as the many spin-wave exchange. It is important to separate them because, as it will be clear from further consideration, they play quite a different role in the physics of large-size bound states.

Let us demonstrate now that the \(B\)-term in \(\text{(12)}\) is due to the single spin-wave exchange, see Fig.3. For the Ising background there is no hole dispersion, the frequency of the spin-wave is equal \(\omega_q = 2\), and the Bogoliubov’s parameters in Eq.(\text{3}) are \(u_q = 1, v_q = 0\). Therefore due to Eq.(\text{11}) the single spin-wave exchange contribution (Fig.3) is equal

\[
- \frac{8 f^2}{N} \frac{1}{-\omega_q} (\gamma_1 \gamma_3 + \gamma_2 \gamma_4) = \frac{4 f^2}{N} (\gamma_1 \gamma_3 + \gamma_2 \gamma_4).
\]

We see that the single spin-wave exchange \(\text{(13)}\) possesses the same kinematic structure as the \(B\)-term in \(\text{(12)}\). Let us verify that their absolute values are also identical. The interaction \(\text{(12)}\)
has been derived in first order in $1/zS$ expansion. In this approximation for $t \ll \Delta/4$ the hole spin-wave coupling constant is $f = \frac{8}{3} t$ (see Ref. [28]). Substituting this value into expression (13) one can easily check that it perfectly agrees with $B = \frac{32}{9} t^2$ obtained from Eq.(12). At large $t$ the agreement between (13) and $B$-term in Eq.(12) cannot be perfect because the latter comes from an approximate variational solution. Nevertheless numerically the agreement is good enough. For example for $t = 3$ the coupling constant is $f \approx 1.8$ (see Fig.2) and the value of $B$ obtained from formula (13) is $B \approx 1.6$. From expression (12) one gets $B \approx 2.2$. This consideration demonstrates that the $B$-term in the short-range interaction (12) accounts for the single spin-wave exchange. Therefore $A$ and $C$ terms describe the contact hole-hole interaction.

Due to formula (12) the Hamiltonian of contact interaction is of the form

$$H_{hh} \approx \frac{8}{N} \sum_{1,2,3,4} \left[ A\gamma_{k_1-k_3} + \frac{C}{2} (\gamma_{k_1+k_3} + \gamma_{k_2+k_4}) \right] h_{3\uparrow} h_{4\uparrow} h_{2\downarrow} h_{1\downarrow} \delta_{12,34}. \quad (14)$$

We denote for simplicity $h_{k_i} = h_i$.

Let us formulate the result of the present section. Starting from the Hamiltonian of the t-J model (1) which is expressed in terms of operators $d_{n\sigma}$ we show that the dynamics of holes on the antiferromagnetic background is described by the effective Hamiltonian

$$H_{eff} = \sum_k \epsilon_k h_k^\dagger h_k + \sum_q \omega_q (\alpha_q^\dagger \alpha_q + \beta_q^\dagger \beta_q) + H_{h,sw} + H_{hh} \quad (15)$$

which is expressed in terms of composite operators $h_{k\sigma}$ and spin-waves $\alpha_q, \beta_q$. The interactions $H_{h,sw}$ and $H_{hh}$ are given by Eqs.(11) and (14).

### III. TWO-HOLE BOUND STATES

Consider a system of two holes with total momentum $P = 0$ and the projection of spin $S_z = 0$. Let $g_k$ be the wave function in the momentum representation describing the state of the system with the relative momentum $2k$:
\[ |P = 0\rangle = \frac{1}{\sqrt{N}} \sum_k g_k h_{k \uparrow}^\dagger h_{-k \downarrow}^\dagger |0\rangle. \quad (16) \]

The function \( g_k \) satisfies the equation of the type of Bethe-Salpeter one:

\[
(E - 2\epsilon_k) g_k = \sum_p \Gamma(E; k, -k; p, -p) g_p. \quad (17)
\]

Summation is carried out over the magnetic Brillouin zone \( (\gamma_p \geq 0) \). The kernel of this equation can be presented in the form

\[
\Gamma = \Gamma_{sw} + \Gamma_{contact}. \quad (18)
\]

The term \( \Gamma_{sw} \) in (18) is the contribution from the single spin-wave exchange (see Fig.3) for which we find with the help of Eq.(11)

\[
\Gamma_{sw} = -\frac{16f^2}{N} \frac{(\gamma_{-k} u_q + \gamma_p v_q)(\gamma_{-p} u_q + \gamma_k v_q)}{E - \epsilon_p - \epsilon_k - \omega_q}, \quad (19)
\]

where \( q = p + k \). The term \( \Gamma_{contact} \) in Eq.(18) describes the many spin-wave exchange. From Eq.(14) we derive

\[
\Gamma_{contact} = \frac{8}{N} \left[ A\gamma_{k-p} + C\gamma_{k+p} \right]. \quad (20)
\]

Let us apply Eq.(17) to the problem of the large-size bound state. In this case one can restrict the consideration to the two-hole dynamics near the band bottom in one pocket of the Brillouin zone, for example near the point \( k_0 = (\pi/2, \pi/2) \) (see Fig.1). We have to allow \( k_1 \) to be negative as well as positive. The hole state with negative \( k_1 \) is outside the Brillouin zone, but it is equivalent to one with \( k' = k - g \), which is inside the Brillouin zone. Here \( g = (\pi, \pi) \) is the vector of the inverse magnetic lattice. We will show that the single spin-wave exchange \( \Gamma_{sw} \) (19) plays the crucial role in the formation of these states. Therefore we consider it first. Later we will take into account the term \( \Gamma_{contact} \). Note also that the binding energy as well as the kinetic energy of the pair will be shown to be small compared to the spin-wave energy.
Therefore we can neglect $E - \epsilon_p - \epsilon_k$ compared to $\omega_q$ in the denominator in Eq.(19). As a result we obtain

$$\Gamma \approx \Gamma_{sw} \approx \frac{8f^2 q^2}{N q^2} = \frac{8f^2 (k_1 + p_1)^2}{N (k + p)^2}. \quad (21)$$

We have shifted the zero of momentum to the center of the pocket. Equation (17) is reduced with the help of (21) to the simple form

$$(E - \beta_1 k_1^2 - \beta_2 k_2^2)g_k = 8f^2 \int \frac{d^2 p}{(2\pi)^2} \frac{(k_1 + p_1)^2}{(k + p)^2} g_p. \quad (22)$$

The last equation is invariant in respect to the transformation $k \to -k, p \to -p$. That is why we can classify the wave function by its behaviour under the transformation:

$$g_k \to g_{-k} = R g_k, \quad (23)$$

where we introduce the quantum number $R = \pm 1$. Let us stress that $R$ is not the parity of the state because $k$ is the deviation from $k_0$ which is not the center of symmetry of the Brillouin zone. The relation between the quantum number $R$ and the parity will be discussed below.

From (22, 23) we get

$$(E - \beta_1 k_1^2 - \beta_2 k_2^2)g_k = 8f^2 R \int \frac{d^2 p}{(2\pi)^2} \frac{(k_1 - p_1)^2}{(k - p)^2} g_p. \quad (24)$$

Using the Fourier transformation

$$\psi(r) = \int g_k e^{i k r} \frac{d^2 k}{(2\pi)^2} \quad (25)$$

we can rewrite it in the coordinate representation as usual Schrödinger equation:

$$\left( -\beta_1 \frac{\partial^2}{\partial x_1^2} - \beta_2 \frac{\partial^2}{\partial x_2^2} + U(r) \right) \psi = E \psi, \quad (26)$$

where the potential energy is

$$U(r) = R \left( 2f^2 / \pi \right) \frac{x_2^2 - x_1^2}{r^4}. \quad (27)$$
It is convenient to perform the rescaling $x_1 = \sqrt{\beta_1} \eta$, $x_2 = \sqrt{\beta_2} \zeta$ and to introduce the polar coordinates $\eta = \rho \cos \varphi$, $\zeta = \rho \sin \varphi$. In new variables equation (26) has the form

$$
\left( -\frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} + \frac{V(\varphi)}{\rho^2} \right) \psi = E \psi,
$$

where

$$
V(\varphi) = RFa \frac{\sin^2 \varphi - a \cos^2 \varphi}{(\sin^2 \varphi + a \cos^2 \varphi)^2},
$$

$$
F = 2f^2 / (\pi \beta), \quad a = \beta_1 / \beta_2.
$$

The plot of the interaction constant $F$ as a function of $t$ is presented in Fig.2. Typical mass ratio in which we are interested is $a \sim 3 - 10$. The variables in equation (28) are separated, the solution is of the form

$$
\psi = R(\rho) \Phi(\varphi).
$$

From (28), (30) we find the following equations:

$$
\left( -\frac{d^2}{d\varphi^2} + V(\varphi) \right) \Phi(\varphi) = \lambda \Phi(\varphi),
$$

$$
\left( -\frac{1}{\rho} \frac{d}{d \rho} \rho \frac{d}{d \rho} + \frac{\lambda}{\rho^2} \right) R(\rho) = ER(\rho).
$$

The boundary condition for $\Phi(\varphi)$ follows from the symmetry relation (23):

$$
\Phi(\varphi + \pi) = R \Phi(\varphi).
$$

The boundary condition for $R(\rho)$ we will discuss later.

The crucial thing is the sign of the parameter $\lambda$, which is the eigenvalue of the angular equation (31). The latter has the form of the usual Schrodinger equation in which the function $V(\varphi)$ plays the role of a potential and the eigenvalue $\lambda$ plays the role of an energy. Note that $V(\varphi)$ depends on the symmetry of the wave function (33) through the symmetry parameter
If one neglects $V(\varphi)$ then the solution of Eq. (31) is trivial, $\lambda = m^2 \geq 0$, $m = 0, 1, \ldots$. The point is that $V(\varphi)$ provides the regions of attraction, where $V(\varphi) < 0$. For $\mathcal{R} = +1$ these regions are in the vicinity of points $\varphi = 0$ and $\varphi = \pi$, e.g. in the direction perpendicular to the edge of the Brillouin zone. For $\mathcal{R} = -1$ they are near points $\varphi = \pi/2$ and $\varphi = -\pi/2$, e.g. in the direction along the edge of the Brillouin zone, see Fig. 1. Hence one can expect that there are solutions of Eq. (31) with negative eigenvalues $\lambda$. They provide the attracting potential in the radial equation (32) and, as a result, the bound states for the two holes. Let us show these solutions do exist and examine their properties.

Consider first the case when the potential $V(\varphi)$ (29) is small, $F \ll 1$. Then the solutions of Eqs. (31), (31) in zero approximations are $\Phi_m^{(0)}(\varphi) = \exp(im\varphi)$, $\lambda_m^{(0)} = m^2$, $m = 0, \pm 1, \ldots$.

For the first level we have $m = 0$, $\Phi_0^{(0)}(\varphi) = 1$, $\lambda_0^{(0)} = 0$. Using Eq. (29) one can easily verify that first order correction to the eigenvalue vanishes: $\lambda_0^{(1)} = \frac{1}{2\pi} \int_0^{2\pi} V(\varphi) d\varphi = 0$. Therefore only the second order correction, which is definitely negative, is essential: $\lambda_0 \approx \lambda_0^{(2)} < 0$. This proves the existence of negative eigenvalue of Eq. (31) for small $F$. The considered solution belongs to $\mathcal{R} = 1$ symmetry.

Consider now the next level. It is degenerate: $m = \pm 1$, $\Phi_m^{(0)}(\varphi) = \exp(\pm i\varphi)$, $\lambda_m^{(0)} = 1$. The potential $V(\varphi)$ splits it. The splitting appears in the first order of perturbation theory because the level is degenerate. As a result one component of the doublet, $\lambda_1$, goes down with increasing $F$ as:

$$\lambda_1 \approx 1 - \frac{1}{\pi} \int_0^{2\pi} V(\varphi) \cos^2 \varphi d\varphi = 1 - \frac{2aF}{(1 + \sqrt{a})^2}. \quad (34)$$

Therefore for sufficiently large $F$ one has to expect that this eigenvalue is to become negative.

The corresponding eigenfunction possesses $\mathcal{R} = -1$ symmetry.

For large $F$ both eigenvalues $\lambda_0$ and $\lambda_1$ decrease, but $\lambda_1$ does it faster. Therefore for some $F$ there is an intersection of $\lambda_0$ with $\lambda_1$. The reason for this fact is the following. If $\mathcal{R} = -1$
then the potential \( V(\varphi) \) (29) has minima near the points \( \varphi = \pm \pi/2 \) which become deeper with increase of \( F \). As a result the ground-state function \( \Phi_{R=-1}(\varphi) \) is strongly localized in the vicinity of these points. Therefore we can approximate the potential \( V(\varphi) \) by the potential of a harmonic oscillator near the points \( \varphi = \pm \pi/2 \). This gives the following asymptotic expression for the eigenvalue \( \lambda_1 \) which is valid if \( Fa \gg 1 \):

\[
\lambda_1 \approx -Fa + \sqrt{Fa(3a - 1)} - \frac{15a^2 - 15a + 2}{4(3a - 1)}.
\] (35)

This proves that \( \lambda_1 \) becomes negative for sufficiently large \( F \).

The corresponding expression for \( \lambda_0 \) is more complicated, because the potential \( V(\varphi) \) for \( R = 1 \) can possess either two or four minima for different values of \( a \). Therefore we present only the lower estimation for \( \lambda_0 \):

\[
\lambda_0 > V_{\text{min}}(\varphi)|_{R=1} = \begin{cases} 
-F \frac{(a+1)^2}{8(a-1)} & \text{for } a \geq 3 \\
-F & \text{for } a \leq 3.
\end{cases}
\] (36)

Comparing inequality (36) with expression (35) we really see that \( \lambda_1 \) goes down with increase of \( F \) more rapidly than \( \lambda_0 \).

There is another parameter, the mass ratio \( a \), which governs the value of \( \lambda \). It is clear that the higher \( a \) the more our two-dimensional system looks like a one-dimensional one. The influence of the potential in one-dimension is stronger, the binding energies are deeper. Therefore both \( \lambda_0 \) and \( \lambda_1 \) decrease with the increase of \( a \). Due to formulas (35), (36) \( \lambda_1 \) decreases faster than \( \lambda_0 \).

Fig.4 presents the results of numerical solution of the eigenvalue problem (31),(33). In agreement with above consideration \( \lambda_0 \) (\( R = +1 \)) is negative for any positive \( F \). The negative \( \lambda_1 \) (\( R = -1 \)) appears when \( F \) is large enough.

For sufficiently large \( F \) there will appear other solutions with negative \( \lambda \). However we restrict our consideration to the lowest solutions because they are most important for the problem of
bound states. For illustration we present the eigenfunctions $\Phi(\varphi)$ for $F = 1.4$ and $a = 7$ in Fig.5. The solution with $R = -1$ has two nodes ($\varphi = 0, \pi$), and in this sense it is “p-wave”. There are no nodes in solution with $R = +1$, and in this sense it is “s-wave”.

Consider now the radial equation (32). For negative $\lambda$ there is the long-range attractive potential in Eq.(32). As a result for every such $\lambda$, $\lambda = \lambda_0, \lambda_1 < 0$, there appear the infinite series of bound states for the two holes. We can find their energies using the semiclassical approximation.

$$E_n \approx -\frac{4|\lambda|}{\rho_0^2} \exp\left(-2 - \frac{2\pi}{\sqrt{|\lambda|}}(n + 3/4)\right).$$

(37)

Here $\rho_0$ is a short-range cut off parameter. The point is that the interaction $-1/\rho^2$ is too singular at the origin and therefore it gives the “fall” of a particle to the center. To stabilize the solution we introduce infinite repulsion at $\rho \leq \rho_0$. It is obvious that the cut off parameter is due to the finite lattice spacing $\rho_0 \sim \beta_1/\beta_2$ as well as to the contact interaction. To find the exact value of $\rho_0$ one has to solve the equation (17) numerically with both short-range and long-range interactions taken into account. Below we will present examples of such calculations.

Formula (37) is one of the most important results in the paper. It states that there are two ($R = \pm 1$) infinite series of bound states for two holes with $S_z = 0$. However let us remember that there are two pockets in the Brillouin zone. Therefore we actually get four infinite sets of large-size bound states. The dependence of binding energies on the hole spin-wave coupling constant $f$ and on the mass ratio $a$ manyfests itself in Eq.(37) through the parameter $\lambda$. For realistic value of $t \sim 3 - 4$ the constant $F \approx 1$, see Fig.2. It makes both $\lambda_0$ and $\lambda_1$ not large: $|\lambda_0| \leq 0.7, |\lambda_1| \leq 1.5$, see Fig.4. Therefore the bound states (37) are shallow and long-range that.

Due to Eq.(37) typical momenta in these states are small:

$$q \sim \frac{1}{\rho} \sim \frac{1}{\rho_0} \exp\left(-\frac{\pi}{\sqrt{|\lambda|}}(n + 3/4)\right).$$

(38)
Therefore the neglect of \((E - \epsilon_p - \epsilon_k)\) in comparison with \(\omega_q\) in Eq.(21) is justified.

IV. SYMMETRY PROPERTIES

Let us discuss the relation connecting the parity \(P\) and the quantum number \(R\). The wave function of relative motion in coordinate representation is connected with that in momentum representation by relation (25). The inversed relation is

\[
g_k \propto \sum_n \psi(r_n) e^{-ikr_n}.
\] (39)

However let us remember that separation \(r_n\) between two holes of opposite spins is always equal to the odd number of lattice spacings. The reason for this is that the ground state of the system is an antiferromagnetic one, see Eq.(9). To avoid misunderstanding let us recall that we are considering dressed holes. Certainly due to the internal structure of the dressed hole (10) there are configurations with the separation between two bare holes equal to the even number of lattice spacings. However \(r_n\) is the separation between the centers of dressed holes, which is always odd. Thus only the terms with \(r_n\) corresponding to the odd number of lattice spacings should be taken into account in sum (39). Therefore

\[
g_{k-g} = -g_k,
\] (40)

where \(g = (\pm \pi, \pm \pi)\) is the inverse vector of the magnetic lattice. Remember that the vector \(k\) is the deviation from \(k_0\) which points to the band bottoms, \(k_0 = (\pm \pi/2, \pm \pi/2)\). The inversion is the transformation \(k \rightarrow -k, k_0 \rightarrow -k_0 = k_0 - g\). Therefore \(g_k\) is transformed under the inversion as

\[
P : g_k \rightarrow g_{-k-g}
\] (41)

Combining this with Eqs.(23),(40) we find
This is an important and surprising relation. Really, using the definition of $\mathcal{R}$ (23) it is easy to verify that it may be presented as $\mathcal{R} = (-1)^l$, where $l$ is the number of nodes of the angular wave function $\Phi(\varphi)$ in the region $0 \leq \varphi \leq \pi$. Eq.(12) states that the relation between $l$ and $\mathcal{P}$ is unusual: $\mathcal{P}$ is positive (negative) for odd (even) $l$.

It is useful to explain relation (12) using coordinate representation. The momentum with respect to the center of Brillouin zone is equal $p = k_0 + k$, where $k$ is deviation from the center of the pocket. Therefore

$$
\Psi(r_n) = \int g_k e^{i\mathbf{pr}_n} \frac{d^2p}{(2\pi)^2} = e^{i\mathbf{k_0}r_n} \int g_k e^{i\mathbf{k}r_n} \frac{d^2k}{(2\pi)^2}.
$$

(43)

Due to Eq.(25) the last integral here is $\psi(r_n)$, and we get

$$
\Psi(r_n) = \exp(i\mathbf{k_0}r_n) \times \psi(r_n) = \exp\left(i\frac{\pi}{2}(n_x + n_y)\right) \times \psi(r_n).
$$

(44)

Here $r_n = (n_x, n_y)$. Since $n_x + n_y$ is odd the exponent $\exp\left(i\frac{\pi}{2}(n_x + n_y)\right)$ is equal to $\pm i$. It changes the sign under reflection of coordinate $n_x \rightarrow -n_x$, $n_y \rightarrow -n_y$.

Relations (40), (42) permit one to find those representations of the symmetry of the system in which the bound states (37) should manifest themselves. The group of symmetry of the square lattice is $\mathcal{C}_{4v}$. It possesses four one-dimensional representations $A_1, A_2, B_1, B_2$ of positive parity and one two-dimensional representation $E$ of negative parity (see e.g. Ref. [30]).

Consider first the bound state with $\lambda = \lambda_1$. It has $\mathcal{R} = -1$ and hence the positive parity $\mathcal{P} = 1$. Therefore, we are to look for it among the one-dimensional representations. Further restriction comes from (11). In order to find it consider the nodes of the wave function $g_k$. We know that the angular function $\Phi_{\lambda_1}(\varphi)$ has two nodes, $\varphi = 0, \pi$, which are at the axis perpendicular to the face of the Brillouin zone, see Fig.5. The wave function in momentum representation $g_k$ has a similar angular behaviour. It vanishes when $k$ is orthogonal to the face
of the zone. This property does not contradict the symmetry in $A_2$ and $B_1$ representations, see Fig.6. For $A_1$ and $B_2$ there is a trouble: the function $g_k$ satisfying (40) in these representations must vanish at the edge, e.g. when $k$ is along the boundary. This means that the series of bound states (37) with $\lambda = \lambda_1$ have to appear in $A_2$ and $B_1$ representations only.

A similar consideration shows that the bound states with $\lambda = \lambda_0$ have to appear in two-dimensional $E$ representation.

We get the following full classification of the series of bound states (37): two of them with $\lambda = \lambda_1(R = -1, P = 1)$ are in $B_1$ and $A_2$ representations, the other two with $\lambda = \lambda_0(R = 1, P = -1)$ are degenerate, they belong to $E$ representation.

V. NUMERICAL CALCULATIONS

Now let us compare the analytical formula (37) with the exact numerical solutions of Eq.(17).

Consider first the states of positive parity with $R = -1$. One series of them belongs to the $B_1$ representation. The symmetry of the wave function for this case is shown schematically in Fig.6a. The short-range solution of this symmetry is usually called d-wave. The second solution belongs to the $A_2$ representation (Fig.6b).

The numerical solution of Eq.(17) is straightforward. We set the parameter $\alpha$ in the contact hole-hole interaction (20), (12): $\alpha = 0.6$; the mass ratio $a = \beta_1/\beta_2 = 7$. The value of hole-spin-wave coupling constant is taken from Fig.2. The kernel $\Gamma$ is calculated numerically with the help of Eqs.(18), (19), (20).

A few first energy levels of $B_1$ symmetry for different $t$ are presented in Table 1. For each energy level we present also the corresponding value of $\langle r^2 \rangle$

$$\langle r^2 \rangle = \int r^2 \psi^2(r) d^2r = \int \left| \frac{\partial g_k}{\partial k} \right|^2 \frac{d^2k}{(2\pi)^2}. \tag{45}$$

For $t = 0$ there is only one short-range bound state: $g_k = \sqrt{2}(\cos k_x - \cos k_y)$. It is due to
the contact hole-hole interaction. In agreement with Refs. [24–27] the short-range bound state disappears at $t \approx 2$.

The energies of large-size states are given in the second and the third sections of Table 1. The ratios $E_2/E_3$ are in agreement with formula $E_n/E_{n+1} = \exp(2\pi/\sqrt{|\lambda_1|})$ which follows from Eq.(37). Numerical values of $\exp(2\pi/\sqrt{|\lambda_1|})$ with $\lambda_1$ determined by Figs.4,2 are presented in the last line of the Table 1. The state at $t = 2$ with $E = -0.0417$ is actually intermediate between short range and long range one. Therefore the agreement in ratio $E_2/E_3$ is not so good as for the other states.

There are no short range bound states of $A_2$ symmetry. The situation with long-range states is quite similar to that of $B_1$ symmetry: they obey the Eq.(37).

The only difference for the states of negative parity ($\mathcal{R} = +1$) is that these states belong to the two-dimensional representation $E$, therefore each state is doubly degenerate. At $t = 0$ there is only short-range bound state $g_k = 2\sin k_x$ (or $g_k = 2\sin k_y$), which is due to the contact hole-hole interaction. The short-range state (usually it is called p-wave) disappears at $t \approx 2$ (see Refs. [24–27]). At $t \neq 0$ there is the series of long-range states whose binding energies are described by Eq.(37).

We conclude that there is a good agreement between the results of direct numerical calculations and the analytical approach developed in Sec.III.

VI. CONCLUSION

In the present work the long-range ($l \gg$ lattice spacing) positive and negative parity two-hole bound states have been found for the holes on the quantum Néel background. The parity of these states is related to the angular wave function in a nonstandard way. Their small binding energy depends exponentially on the hole-spin-wave coupling.
The natural question arises whether these states with the tiny binding energy could be relevant to high-$T_c$ superconductivity. There are the strong physical reasons which show that it is quite possible. We have demonstrated that there is the attraction between two holes caused by the spin-wave exchange. We have considered these two holes separately. If there is an ensemble of holes then one can expect that the attraction between a pair of two holes should be enhanced. The origin of this effect is the renormalization of spin-wave Green function caused by the particle-hole excitations. Therefore the binding energy of a pair is to be larger for the pair in the ensemble. The point is that a quite moderate enhancement of the interaction results in the very strong increase of the binding energy.

To illustrate the later statement let us consider $t = 3$, and let us enhance the hole-spin-wave coupling constant by a factor of $1.5$: $f = 1.79 \rightarrow f = 2.69$. Then solving Eq.(17) with this value of coupling constant numerically we find the bound state of the pair belonging to $B_1$ symmetry with the following characteristics:

$$E = -0.103, \quad \langle r_1^2 \rangle = 8.4.$$

This is the ground state with a reasonable energy of $E \sim 100K$ (we set $J = 1 \equiv 0.13eV$). The state is stretched along one direction, and its maximal size is about 6-7 lattice spacings.

The physical picture of the interaction enhancement is to be discussed in detail elsewhere.

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TABLES

TABLE I. The energies and the mean values of $r^2$ for a first few bound states of $B_1$ symmetry

| t  | 0   | 1   | 1.5 | 2   | 3   | 4   |
|----|-----|-----|-----|-----|-----|-----|
| $E_1$ | -0.250 | -0.262 | -0.146 | -   | -   | -   |
| $\langle r_1^2 \rangle$ | 1 | 1.22 | 1.95 | -  | -  | -  |
| $E_2$ | - | $-1.84 \cdot 10^{-3}$ | $-6.30 \cdot 10^{-4}$ | $-4.17 \cdot 10^{-2}$ | $-2.21 \cdot 10^{-4}$ | $-4.03 \cdot 10^{-6}$ |
| $\langle r_2^2 \rangle$ | - | $1.74 \cdot 10^2$ | $6.34 \cdot 10^2$ | 7.83 | $2.65 \cdot 10^3$ | $2 \cdot 10^5$ |
| $E_3$ | - | $-3.31 \cdot 10^{-5}$ | $-5.25 \cdot 10^{-6}$ | $-1.37 \cdot 10^{-4}$ | $\approx -2. \cdot 10^{-7}$ | ? |
| $\langle r_3^2 \rangle$ | - | $9.9 \cdot 10^3$ | $8.5 \cdot 10^4$ | $3.5 \cdot 10^3$ | $\approx 2.8 \cdot 10^6$ | ? |
| $(E_2/E_3)_{num}$ | - | 56  | 120 | 304 | 1105 | ? |
| $(E_n/E_{n+1})_{an}$ | - | 54  | 123 | 242 | 1071 | $2.15 \cdot 10^4$ |

\textsuperscript{a}The first section presents the small-size bound state which is due to the contact hole-hole interaction. It disappears at $t \approx 2$.

\textsuperscript{b}The large-size states are presented in the second and third sections.

\textsuperscript{c}In the last section the ratio $(E_2/E_3)_{\text{numerical}}$ is compared with $(E_n/E_{n+1})_{\text{analytical}}$ predicted by formula (37).

\textsuperscript{d}The accuracy of the code was insufficient to find extremely shallow levels denoted by “?”.
FIGURE CAPTIONS

FIG. 1. The Brillouin zone of a hole in the $t-J$ model.

FIG. 2. The coupling constants. Solid line represents the hole-spin-wave coupling constant $f$ calculated in Ref. [29]. Dashed line represents the effective constant $F = 2f^2/(\pi\beta_1)$ which governs the long-range interaction between two holes, see Eq.(29).

FIG. 3. Single spin-wave exchange between two holes. Its contribution to the kernel of Eq.(17) is given in (19).

FIG. 4. The eigenvalues $\lambda$ of the angular equations (31), (33) versus $F$. The number at every curve is the value of the mass ratio $a = \beta_1/\beta_2=3,5,7,9$. Fig.a - the solution $\lambda_0$ with $\mathcal{R} = +1$. Fig.b - the solution $\lambda_1$ with $\mathcal{R} = -1$. Note that the vertical scale in Fig.b is different from that in Fig.a.

FIG. 5. The angular wave functions $\Phi(\varphi)$ for $F = 2f^2/(\pi\beta_1) = 1.4$ and $a = \beta_1/\beta_2 = 7$. Solid line is the solution whose eigenvalue is $\lambda_1$ with $\mathcal{R} = -1$, and dashed line is the solution whose eigenvalue is $\lambda_0$ with $\mathcal{R} = 1$.

FIG. 6. The symmetry of the positive parity ($\mathcal{R} = -1$) bound state wave function. Fig.a - $B_1$ type, Fig. b - $A_2$ type.