

Unconventional pairing in a weakly doped antiferromagnet on the honeycomb lattice: Mechanism of symmetry selection

P. Wróbel^{1,2} and W. Suleja²¹Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany²Institute for the Low Temperature and Structure Research, P.O. Box 1410, 50-950 Wrocław 2, Poland

(Received 15 December 2006; revised manuscript received 8 February 2007; published 24 May 2007)

We discuss the mechanism of pairing-symmetry selection in the weakly electron-doped t - J model on the honeycomb lattice. Our analysis is motivated by some recent suggestions that due to charge ordering, which may take place in the unconventional superconductor $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ at doping levels near $x=1/3$, the physics of CoO_2 planes may be effectively described in terms of a model for a weakly electron-doped antiferromagnet on the honeycomb lattice. By applying the so-called string picture, we demonstrate that spin fluctuations may induce in the honeycomb lattice the formation of an unconventional two-particle bound state. This mechanism may give rise to unconventional pairing upon the condensation of bound particles. We do not evaluate the critical value of the ratio J/t , which is sufficient to induce binding. We assume instead that, in the case of cobaltates, some additional isotropic attractive interaction, for example, phonon mediated, is active. Nevertheless, the symmetry of the paired state is selected by the anisotropic interaction mediated by spin fluctuations. The relevant point group for the t - J model on the honeycomb lattice is C_{3v} . We argue that the bound state of two additional electrons doped to the half-filled antiferromagnetically ordered system has zero total momentum and p -wave symmetry of the irreducible representation E . Since the honeycomb lattice does not possess the inversion symmetry, the expected paired state is a mixture of a singlet and a triplet. This is an explicit prediction for the form of the superconducting order parameter in a weakly doped antiferromagnet on the honeycomb lattice.

DOI: [10.1103/PhysRevB.75.174522](https://doi.org/10.1103/PhysRevB.75.174522)

PACS number(s): 71.10.Fd, 74.20.Mn

I. INTRODUCTION

The discovery of superconductivity (SC) in a hydrated sodium cobaltate $\text{Na}_x\text{CoO}_2 \cdot y\text{H}_2\text{O}$ (Ref. 1) draws a lot of attention nowadays. Besides cuprates, cobaltates are the second class of layered $3d$ transition-metal oxides in which this phenomenon has been observed. A crucial difference between cuprates and cobaltates is that Cu ions form the square lattice in a single layer of the former system, while Co ions form the triangular lattice in a single layer of the latter system. Results of some experiments suggest triplet pairing²⁻⁵ in cobaltates. Other measurements have resulted in contradicting conclusions which indicate singlet pairing.^{6,7} In any case, there seems to be no controversy about the suggestion that pairing in layered cobalt oxides is unconventional.^{8,9} The mechanism of SC in those systems has been discussed in several theoretical papers,¹⁰⁻¹⁹ but no final conclusions regarding the symmetry and the total spin of the paired state have been drawn. On the other hand, even before the discovery of superconductivity in hydrated cobaltates, a theoretical analysis which may be relevant to that phenomenon has been performed.²⁰ That analysis concerned the t - J model (tJM) on the triangular lattice. Some arguments have been provided later that the electron-doped t - J model on the triangular lattice formed by cobalt ions is indeed suitable for analyzing them.¹⁰

Recently, the emergence of spin and charge ordering in Na_xCoO_2 at the doping level near $x=1/3$ has been suggested.²¹⁻²⁵ That ordering may be related to the appearance of SC, which occurs in the range $0.22 \leq x \leq 0.47$. Some experimental evidence that the scenario of charge modulations may be realized for $x=1/3$ has also been provided.

Namely, an angle-resolved photoelectron spectroscopy study²⁶ shows that, in this case, all parts of the Fermi surface have the nesting property for some fundamental reciprocal lattice vectors which are related with a well-defined superlattice structure. According to that observation, a natural assumption is that in the charge-ordered state exactly at $x=1/3$, cobalt atoms which are in the valence state Co^{3+} and in the spin-0 state form a new triangular lattice with a larger elementary cell. In the framework of the tJM , those sites are doubly occupied and therefore they do not influence magnetic and transport properties of the system at the doping level $x=1/3$ and slightly above that value. The rest of the cobalt atoms which are in the valence state Co^{3+} and in the spin- $\frac{1}{2}$ state forms the honeycomb lattice. Upon additional doping, some sites which belong to that newly effectively formed honeycomb lattice will become doubly occupied. Therefore, it seems that the analysis of the tJM on the honeycomb lattice in the limit of weak electron doping may give some insight into the physics of SC cobaltates for doping levels slightly higher than $x=1/3$. Since the honeycomb lattice is bipartite, the tJM on that lattice is invariant with respect to the particle-hole transformation for the filling of one electron per site, which may be proved by performing the particle-hole transformation and by changing additionally the sign of fermion operators for sites which belong to one of the sublattices. Therefore, it is, in principle, possible to analyze the equivalent hole-doped version of that model with the same number of holes created in the half-filled system as the number of additional electrons in the relevant electron-doped version of it. In fact, we will perform the calculation for the hole-doped system because, in that case, the graphical visualization of some relevant process involving doped holes is easier.

Recently, the properties of a single hole in the tJM on the honeycomb lattice have been analyzed by means of several methods²⁷ which have been before applied to the tJM on the square lattice, namely, an exact diagonalization based on the Lanczos method, the self-consistent Born approximation,^{28–33} and the series expansion.³⁴ The spin polaron approach^{35,37–40} based on the string scenario^{41,42} is another method which is applicable to the analysis of weakly hole-doped antiferromagnets described by the tJM . In particular, the mechanism of hole binding in the tJM on the square lattice,³⁷ the origin of the d -wave symmetry which appears in the two-hole ground state of that model,³⁸ and the full hierarchy of low-energy two-hole eigenstates transforming according to different irreducible representations of the C_{4v} point group for the square lattice⁴³ have been clarified by means of some analyses based on the spin polaron approach. That approach⁴⁴ also allows one to analyze the relation between hole binding and the formation by the current-current correlation function of a pattern,^{45,46} which corresponds to the so-called staggered flux phase.⁴⁷

The purpose of this paper is to understand the mechanism of pairing-symmetry selection in the cobaltates in the framework of the spin polaron approach applied to the hole-doped tJM on the honeycomb lattice. We will use the spin bipolaron (SBP) approach, which is the most basic version of this method. The SBP scenario is based on the assumption that antiferromagnetic (AF) spin fluctuations give rise to the formation of a tightly bound two-hole state and on the assumption that the problem of two holes in the honeycomb lattice may be reduced to the analysis of hopping performed by a single boson which represents a bound hole pair. A similar task has been successfully performed before for the tJM on the square lattice⁴³ where the bound state has been observed. We will not try to find out for what critical value of the ratio J/t hole binding starts to take place on the honeycomb lattice. In order to find this parameter, a calculation performed by means of a different method, as for example, an exact diagonalization, is necessary. On the other hand, an exact diagonalization usually does not give much insight into the underlying physics, the understanding of which is our aim; therefore, in this paper, we will concentrate on an analysis based on the SBP approach. In addition, it is not clear now if electron correlations alone can drive pairing in cobaltates or if a different source of attraction, as for example, phonon exchange, is involved in this process. Provided that the additional moderate effective attraction induced by phonons in the form of a density-density interaction is isotropic, it can be expected that the spin fluctuation mechanism will still decide the symmetry of the paired state. It is likely a similar situation we also encounter in the case of cuprates, where the phonons also seem to play an important role,⁴⁸ but the symmetry of the SC order parameter is most probably determined by the exchange of spin fluctuations.

The tJM which we will study is defined by the Hamiltonian,

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.}) + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \mathbf{S}_j - \frac{n_i n_j}{4} \right). \quad (1)$$

$\langle i,j \rangle$ denotes nearest-neighbor (NN) sites in the honeycomb lattice. The action of H is restricted to the subspace of states

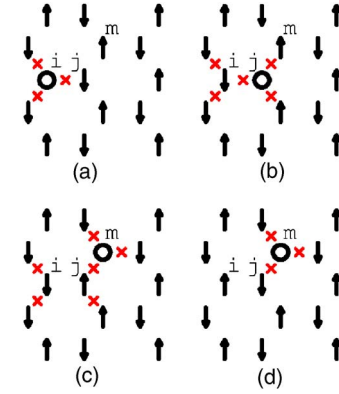


FIG. 1. (Color online) A process which gives rise to single-hole propagation in the tJM on the honeycomb lattice. Spin fluctuations induced in the antiferromagnet by a shift of a hole created at site i (a) to site j (b), and later to site m (c) have been removed by flips of spins at sites i and j (d).

in which there are no doubly occupied sites. Since our intention is to apply the tJM to cobaltates, in agreement with some recent estimations,¹⁰ we choose t to be negative, $t = -1$, and $J/t = -0.2$. On the other hand, it is worth mentioning that, since the honeycomb lattice is bipartite, the sign of the hopping integral is irrelevant in the tJM on that lattice with NN hopping only.

The outline of the paper is as follows. In Sec. II, we define SBPs and derive the lowest-order term in the SBP model. In Sec. III, we derive some higher-order terms which play a crucial role in determining the symmetry of the paired state. Next we find that symmetry. Finally, in Sec. IV, we present some conclusions.

II. SPIN BIPOLARONS IN THE WEAKLY DOPED ANTIFERROMAGNET ON THE HONEYCOMB LATTICE

The SBP model has been used before to analyze hole binding⁴³ and pairing⁴⁹ in the hole-doped antiferromagnet on the square lattice. Here, we will construct such a model for the honeycomb lattice. The scenario which underlies this construction is as follows. Since the honeycomb lattice is bipartite, we assume that at least short-range AF correlations exist in the weakly doped tJM on that lattice. This assumption is made while having in mind that, according to our scenario, the cobalt oxide plane may be modeled for doping levels slightly above the value $1/3$ by the weakly electron-doped tJM on the honeycomb lattice.

A hole which hops in the locally AF spin background shifts spins and creates defects in that background. This process, which has been depicted in Figs. 1(a)–1(c), gives rise to the increase of the exchange energy, due to the formation of “ferromagnetic” bonds at NN sites, and brings about temporal confinement of the hole by the defects. Defects which we discuss here can be also interpreted as fluctuations of the AF background. We will use those two notions interchangeably. Slanted crosses in Fig. 1 denote ferromagnetic or, in other words, “broken” bonds, the contribution of which to the diagonal Ising-like part H_I of the exchange term in the tJM ,

$$H_I = J \sum_{\langle i,j \rangle} \left(S_i^z S_j^z - \frac{n_i n_j}{4} \right), \quad (2)$$

is higher by $J/2$ in comparison to the contribution from a pair of sites occupied by antiparallel spins.

Defects form chains which lie on paths along which holes have traveled. Since the exchange energy grows linearly with their number, those chains act on holes as strings. Thus it is reasonable to assume, as we have actually done, that only short chains should be considered in detail, while details regarding longer strings can be neglected, for example, the possibility of path crossing. That assumption is true provided that the radius of regions in which holes are temporarily confined is shorter than the correlation length of the AF order. A stringlike chain of defects is shortened if the hole moves back along the same path towards the initial site where it has been created. An example of such a process is represented by the series of diagrams in Figs. 1(a)–1(c), analyzed in the inverse order. The retracable hopping of a hole forth and back along a chain plays an important role because charge dynamics is much faster than spin dynamics for $t \gg J$. The formation of strings determines the properties of the low-energy sector in the Hilbert space of a weakly doped antiferromagnet.^{28,29,35,41} In the string picture or, equivalently, within the spin polaron approach, that sector consists of spin polaron states representing holes quasiconfined by strings in regions around some sites. Spin polaron states are ground states of a trial “unperturbed Hamiltonian,” which by construction does not contain matrix elements that give rise to deconfinement of holes. In the case of a single hole, the trial Hamiltonian acts on string states obtained by the motion of it in all possible directions, with a starting point at an initial site. We will describe the construction of spin polarons with more details when we start to discuss the behavior of two holes.

Processes which give rise to hole deconfinement are considered at the next stage of the analysis, after spin polarons have been constructed. Those processes are often related to some path details neglected during the construction of spin polarons. They determine the coupling between spin polarons. For example, a single hole may escape from the potential well formed by strings because the transverse part of the Heisenberg model flips spins and removes defects formed in the AF spin arrangement by the hopping hole. This sequence of events has been presented in Figs. 1(a)–1(d). Such a mechanism gives rise to single-hole propagation. Within the common perturbation theory, the propagation of a single hole is governed by a third-order process which involves twice the action of the hopping term in the Hamiltonian with the prefactor t and once the action of the exchange term with the much smaller prefactor J . In reality, an object which propagates is not a bare hole but rather a spin polaron. The process of a hole escaping from the potential well formed by strings is complex because spin dynamics is much slower than charge dynamics and processes involving the exchange term are much less “frequent” than processes involving hole hopping.

The propagation of two holes together seems to be easier. We will analyze it now. The object which propagates is again

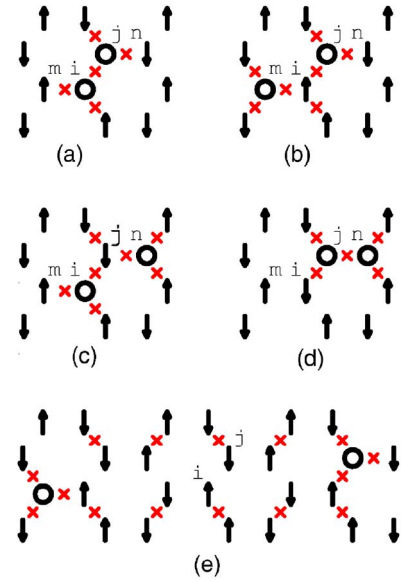


FIG. 2. (Color online) Some states which contribute to the superposition defining the wave function for the SBP created at sites i, j : (a)–(c) and (e). Also a process giving rise to the hopping of the SBP, which is represented in our effective model by a hard-core boson. One of two holes created in the Néel state at sites i, j (a) is being shifted from site j to site n (c). The move of the second hole from site i to site j gives rise to a state representing two holes created at sites j, n in the Néel state (d).

more complex than just a bare hole pair. It may be called an AF SBP because a deformation of the spin background accompanies it. We define a SBP wave function $|\Psi_{\langle i,j \rangle}\rangle$ as a combination of states which may be created by independent hopping of holes created at a pair of NN sites $\langle i, j \rangle$,

$$|\Psi_{\langle i,j \rangle}\rangle = \sum_{\mathcal{P}_i, \mathcal{P}_j} \alpha_{\mathcal{P}_i, \mathcal{P}_j} |\mathcal{P}_i, \mathcal{P}_j\rangle. \quad (3)$$

Examples of such states have been depicted in Figs. 2(a)–2(c). The zero-length string state representing two holes created in the Néel state at NN sites also contributes to the superposition defining the SBP wave function. It is a matter of convention to assume that this initial state has been obtained by the action of the fermion annihilation operator first on a site which belongs to the even sublattice and next on a site which belongs to the odd sublattice, and that hole hopping which creates different components of the SBP wave function is induced by operators in the form $c_{i,\sigma} c_{j,\sigma}^\dagger$, where i and j are NN sites. \mathcal{P}_i parametrizes the geometry of a path, along which the hole that starts from the site i has been moving and $|\mathcal{P}_i, \mathcal{P}_j\rangle$ is a state which has been created in this way. At this stage of considerations we prohibit, by definition, each hole from following the accompanying hole along the trace left by the latter. By means of that restriction, we achieve that SBP states are confined in the region around the pair of sites on which a bare hole pair has been initially created, which is a property useful for constructing an effective Hamiltonian for the weakly doped tJM on the honeycomb lattice.

Within the applied approximation, the coefficients $\alpha_{\mathcal{P}_i, \mathcal{P}_j}$ in Eq. (3) depend only on the lengths μ and ν of paths \mathcal{P}_i and \mathcal{P}_j , $\alpha_{\mathcal{P}_i, \mathcal{P}_j} \equiv \alpha_{\mu, \nu}$, $\alpha_{\mu, \nu}$ are solutions of the Schrödinger equation, which describes a hole pair in a potential well formed by stringlike lines of defects,

$$t[\alpha_{\mu-1, \nu} + (z-1)\alpha_{\mu+1, \nu} + \alpha_{\mu, \nu-1} + (z-1)\alpha_{\mu, \nu+1}] + \frac{J}{2}(6 + \mu + \nu - \delta_{\mu+\nu, 0})\alpha_{\mu, \nu} = E_2\alpha_{\mu, \nu}, \quad (4)$$

where $z=3$ is the coordination number. Since the lengths μ and ν cannot be negative, we also assume that $\alpha_{\mu, \nu}=0$ for $\mu < 0$ or $\nu < 0$. The form of this equation which defines the SBP is easy to understand. The first term originates from the fact that longer paths may be obtained from a given path by extending it during a hop in $z-1$ different directions. On the other hand, there exists only one possible hole move by means of which a string may be shortened by one step. The second term counts the number of pairs of NN sites which are not occupied by antiparallel spins. Every such broken bond raises the energy by $J/2$ in comparison to the energy of the Néel state. An additional normalization condition which should be obeyed by factors $\alpha_{\mu, \nu}$ is

$$\sum_{\mu=0, \nu=0} (z-1)^{\mu+\nu} \alpha_{\mu, \nu}^2 = 1. \quad (5)$$

The factor $(z-1)^{\mu+\nu}$ in the above formula represents the number of different paths obtained by means of μ and ν nonretraceable hops of the first and second holes, respectively.

The Schrödinger equation (4) represents a trial Hamiltonian, which does not describe all the processes contained in the tJM . We construct an effective Hamiltonian represented in terms of SBPs by analyzing matrix elements of the full tJM between SBP states defined as the ground state of Eq. (4). Therefore, processes responsible for SBP deconfinement are also considered now. They give rise to off-diagonal terms in the effective Hamiltonian.

The mechanism of hole-pair deconfinement in the AF spin background is actually rather simple. Let us consider two holes created at NN sites i, j in the honeycomb lattice [Fig. 2(a)]. A single hop of a hole from site j to site n gives rise to the creation of a defect in the AF spin background on site j [Fig. 2(c)] and to the increase of the exchange energy. That defect is removed when the hole initially created at site i moves to site j [Fig. 2(d)]. It turns out that during this process the hole pair has moved from the pair of sites i, j to the pair of sites j, n , while no defects in the AF environment have been left. Again, as in the case of a single hole, the hole-pair propagation is, in reality, more complex because it involves not only bare holes but also the cloud of spin fluctuations around them and longer strings, as one depicted in Fig. 2(e), which means that an object that moves is actually a SBP. Now, we will perform a quantitative analysis of the process depicted in Figs. 2(a), 2(c), and 2(d). Figures 2(a) and 2(c) depict string states which contribute to the SBP state $|\Psi_{\langle i, j \rangle}\rangle$ because they have been obtained by means of nonretraceable hopping of two holes, which started from sites i, j . The state depicted in Fig. 2(d) does not belong to this group.

Since the state presented in Fig. 2(d) represents two holes created at another pair of sites j, n , it is a string state which is a component of another SBP state $|\Psi_{\langle j, n \rangle}\rangle$. On the other hand, the state depicted in Fig. 2(d) can be obtained by the action of a term in the hopping operator in Eq. (1) on the state represented by Fig. 2(c). As we know, the latter state is a component of the SBP $|\Psi_{\langle i, j \rangle}\rangle$ created at sites i, j . Within the SBP formalism, this fact gives rise to the coupling of wave functions for SBPs created at different pairs of sites i, j and j, n by the hopping operator in the tJM and to a nonzero contribution to the matrix element $\langle \Psi_{\langle i, j \rangle} | H | \Psi_{\langle j, n \rangle} \rangle$. Longer strings which start at site i and lead through sites j and n but do not end at the latter site also contribute to the coupling between wave functions of SBPs formed on pairs of sites i, j and j, n . Those strings may be obtained by shifting in the nonretraceable way the hole which occupies the site n in Fig. 2(c). By applying a term in the hopping operator of the tJ model to one of such longer string states which are components of $|\Psi_{\langle i, j \rangle}\rangle$, we can create a string state which is a component of $|\Psi_{\langle j, n \rangle}\rangle$. Thus we see that the above-discussed process during which a bare hole pair has been shifted from the pair of sites i, j to the pair of sites j, n and which is represented by the sequence of diagrams in Figs. 2(a), 2(c), and 2(d) is an example of a whole class of analogous processes involving many different pairs of string states. In the same way as described above, a SBP may move between all bonds which share one end point. Thus, the appropriate contribution to an effective Hamiltonian H_{eff} defined in terms of operators $b_{i, j}^\dagger$ and $b_{i, j}$, which create and annihilate SBPs at links between NN sites i, j , is

$$H_{eff}^{(1)} = \tau_1 \sum_{\langle i, j, m \rangle} b_{i, j}^\dagger b_{j, m}. \quad (6)$$

To be more specific, the operators $b_{i, j}^\dagger$ and $b_{i, j}$ transform the ground state $|\Omega\rangle$ of the Heisenberg model on the honeycomb lattice into the wave function (3) of the SBP created at sites i, j and vice versa, respectively. It is clear that $|\Omega\rangle$ plays, in our description, the role of the vacuum state. The summation in Eq. (6) is carried over all sets containing three different sites $\langle i, j, m \rangle$, the first and third of which are NN of the second. The order of indices i and m in the sum is relevant. Since no more than one SBP which corresponds to a fermion pair can be created at a given pair of NN sites, operators b obey the hard-core constraint. In addition, it follows from the construction of SBPs that two of them cannot occupy two different links which end in the same site, which means that the effective Hamiltonian which we will derive actually belongs to the class of dimer models. The latter constraint that additionally restricts the Hilbert space in which H_{eff} is defined also originates from the Pauli principle and follows from the fact that a SBP created at the link between NN sites i, j has its origin in the state in which two holes have been created at this pair of sites. Since we concentrate here on single-particle properties of a SBP, the above remarks are not of great importance to our purposes.

The hopping integral τ_1 in $H_{eff}^{(1)}$ is

$$\tau_1 = -t \sum_{\mu=1} (z-1)^{\mu-1} \alpha_{0,\mu} \alpha_{0,\mu-1}. \quad (7)$$

We easily recognize the first term in the sum, which defines τ_1 as a product of the bare hole-hopping integral t and the prefactors $\alpha_{0,1}$ and $\alpha_{0,0}$. States depicted by Figs. 2(c) and 2(d) appear with those prefactors in the sums (3) representing bipolarons created at bonds $i-j$ and $j-n$. Thus the first term in the sum (7) originates from the above-discussed process represented by the sequence of diagrams in Figs. 2(a), 2(c), and 2(d). The rest of the terms stems from similar processes which involve longer strings. The overall sign which appears in the formula (7) has its origin from the convention which defines the form and the phase of components contributing to the wave function of the SBP (3). That sign has been determined by the form of quadratic fermionic operators creating in the AF background the bare hole pair on NN sites and by the form of operators applied to shift holes between NN sites during the construction of string states. It seems to be reasonable to state here that the change of the bare hopping integral induced by the gauge transformation supplementing the particle-hole transformation does not imply that the sign of hopping integrals for terms describing hopping of SBPs are differed in the case of holes and in the case of electrons. For example, the sign change induced in τ_1 by the sign change of t is compensated by the sign change of some prefactors α , which are given by a solution of Eq. (4) in which t also appears.

The SBP model which describes a weakly doped antiferromagnet on the honeycomb lattice is actually defined on the kagome lattice because midpoints of bonds between NN sites on which SBPs can be created form the latter type of lattice. After a little thought, it is easy to realize that the contribution (6) to the effective Hamiltonian represents the hopping between NN sites in the kagome lattice. The unit cell which reflects the periodicity of both the initial honeycomb lattice and the effective kagome lattice has been depicted in Fig. 3(a). Its basis vectors are \mathbf{a} and \mathbf{b} . The index “ i ” refers to the cell position. Disks shown in Fig. 3(a) are located in midpoints of bonds between NN sites. In each unit cell there are such three translationally nonequivalent midpoints. They are labeled by means of Greek letters. Instead of using the indices to refer to pairs of NN sites to label a bipolaron created at those sites, as we have done in Eq. (6), it is more convenient to use, for that purpose, those Greek indices which refer to midpoints between those sites. The advantage of the different convention will become obvious after we start to analyze more complicated contributions to the effective Hamiltonian than a term representing hopping of a SBP between pairs of NN sites. According to that convention, the first contribution to $H_{eff}^{(1)}$ can be written as

$$H_{eff}^{(1)} = \tau_1 \sum_i (b_{\mathbf{R}_i, \beta}^\dagger b_{\mathbf{R}_i, \alpha} + b_{\mathbf{R}_i + \mathbf{a}, \beta}^\dagger b_{\mathbf{R}_i, \alpha} + b_{\mathbf{R}_i, \gamma}^\dagger b_{\mathbf{R}_i, \alpha} + b_{\mathbf{R}_i - \mathbf{b}, \gamma}^\dagger b_{\mathbf{R}_i, \alpha} + b_{\mathbf{R}_i, \gamma}^\dagger b_{\mathbf{R}_i, \beta} + b_{\mathbf{R}_i - \mathbf{a}, \gamma}^\dagger b_{\mathbf{R}_i, \beta}) + \text{H.c.} \quad (8)$$

In the above formula, the first part of the index in operators b is a vector and labels elementary cells, while the second part of the index refers to the position of midpoints between

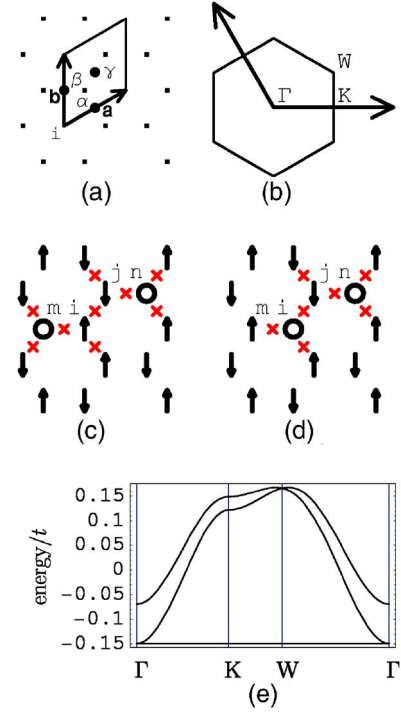


FIG. 3. (Color online) (a) The elementary cell in the honeycomb lattice and the first Brillouin zone, together with basis vectors in the reciprocal space (b). Greek letters and filled small circles in centers of links refer to three different positions of SBPs, which can be created at those links. Those SBPs are labeled by Greek letters and by the position vector of the presented elementary cell. Due to the fermionic character of particles, it is important to keep in mind that in order to form, for each SBP, the initial state representing two holes created at NN sites in the Néel state, the annihilation operator is, in all cases, first applied to the even site located in the center of the triangle formed by small filled circles. [(c) and (d)] A process which enables hopping of SBPs to second NN sites in the effective kagome lattice formed by midpoints between NN sites in the honeycomb lattice. (c) is a string state which is a component of the wave function for the SBP at link $m-i$. After the hole shift from site m to site i , a component of the wave function for the SBP at link $j-n$ is obtained. (e) The energy dispersion of a single SBP obtained by the diagonalization of a Hamiltonian, which consists only of terms representing hopping to first and second NN sites in the effective kagome lattice.

NN sites on which SBPs are created or annihilated in a given elementary cell. The form of the single-particle ground state of H_{eff} should give us some information about the form of the two-hole bound state, which, as we expect, will be generated on the honeycomb lattice in the t - J model supplemented by some isotropic short-range interaction term. The Hamiltonian (8) can be easily diagonalized by means of the Fourier transformation. The lowest band obtained in this way is dispersionless, which means that the analysis of the simplest process represented by the sequence of diagrams in Figs. 2(a), 2(c), and 2(d) is not sufficient to find out the form of the two-hole bound state in the t - J model on the honeycomb lattice. At $\mathbf{k}=(0,0)$, the ground state of Eq. (8) is doubly degenerate and transforms according to the irreducible representation E of the point group C_{3v} for the honeycomb

lattice, with a fixed point at a given site. We will see later, after analyzing higher-order processes, that the unique ground state of the full effective model is formed at $\mathbf{k}=(0,0)$ and also transforms according to the irreducible representation E .

III. GROUND-STATE ANALYSIS

Now, in an attempt to find a mechanism which lifts the degeneracy of the lowest band and in an attempt to find the unique form of the ground state, we start to discuss other processes which contribute to the effective Hamiltonian and involve only a small number of defects in the initial AF spin background. The state depicted in Fig. 3(c) can be obtained by the double action of some terms in the hopping operator of the t - J model on the state which represents two holes created at sites m and i in the AF background. Therefore, according to the definition (3), the state depicted in Fig. 3(c) contributes to the wave function of the SBP created at those sites. On the other hand, the state depicted in Fig. 3(d) is a component of the wave function of the SBP created at sites j , n because it has been obtained by shifting to a NN site one of two holes initially created in the AF background at sites j , n . Since string states depicted in Figs. 3(c) and 3(d) are coupled by the hopping term which moves the hole in Fig. 3(c) from site m to site i , the coupling between whole wave functions of two different SBPs created at pairs of sites m , i and j , n is generated. The amplitude of that coupling is $t\alpha_{0,2}\alpha_{1,0}$, which may be easily understood by realizing that states depicted in Figs. 3(c) and 3(d) contribute with prefactors $\alpha_{0,2}$ and $\alpha_{1,0}$ to wave functions (3) of SBPs created at pairs of sites m , i and j , n , respectively. Longer strings may also take part in the process of moving the SBP from the bond m - i to the bond j - n . Those longer strings may be obtained by shifting further the hole which occupies site n in Figs. 3(c) and 3(d). The new type of coupling, the origin of which we have just described, involves all pairs of sites which lie next to each other in the honeycomb lattice and thus it gives rise to a new term in H_{eff} .

$$\begin{aligned}
H_{eff}^{(2)} = \tau_2 \sum_i & (b_{\mathbf{R}_i+\mathbf{a}-\mathbf{b},\alpha}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i+\mathbf{b},\alpha}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i+\mathbf{a},\beta}^\dagger b_{\mathbf{R}_i,\alpha} \\
& + b_{\mathbf{R}_i-\mathbf{b},\beta}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i+\mathbf{a}-\mathbf{b},\gamma}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i-\mathbf{a},\gamma}^\dagger b_{\mathbf{R}_i,\alpha} \\
& + b_{\mathbf{R}_i+\mathbf{a},\beta}^\dagger b_{\mathbf{R}_i,\beta} + b_{\mathbf{R}_i+\mathbf{a}-\mathbf{b},\beta}^\dagger b_{\mathbf{R}_i,\beta} + b_{\mathbf{R}_i-\mathbf{a}+\mathbf{b},\gamma}^\dagger b_{\mathbf{R}_i,\beta} \\
& + b_{\mathbf{R}_i-\mathbf{b},\gamma}^\dagger b_{\mathbf{R}_i,\beta} + b_{\mathbf{R}_i+\mathbf{a},\gamma}^\dagger b_{\mathbf{R}_i,\gamma} + b_{\mathbf{R}_i+\mathbf{b},\gamma}^\dagger b_{\mathbf{R}_i,\gamma}) + \text{H.c.}
\end{aligned} \tag{9}$$

The hopping integral τ_2 is given by

$$\tau_2 = t \sum_{\mu=2} (z-1)^{\mu-2} \alpha_{0,\mu} \alpha_{1,\mu-2}. \tag{10}$$

$H_{eff}^{(2)}$ represents the hopping to second NN sites in the kagome lattice formed by centers of bonds which can be occupied by SBPs. Since the operator of hopping to second NN sites is a combination of the second power of the operator of hopping to first NN sites and the identity operator, the ground-state degeneracy of $H_{eff}^{(1)}$ which represents hopping to

first NN sites, is not lifted when $H_{eff}^{(2)}$ is added to the effective Hamiltonian. Figure 3(e) depicts the band structure obtained by the diagonalization of the operator $H_{eff}^{(1)}+H_{eff}^{(2)}$ originating from lowest-order processes which we have just described. The energy dispersion has been drawn along lines connecting some points. Their positions in the first Brillouin zone have been presented in Fig. 3(b). Those points are $\Gamma=(0,0)$, $K=(2\pi/3,0)$, and $W=(2\pi/3,2\pi/3\sqrt{3})$. Figure 3(b) also depicts basis vectors of the reciprocal lattice. Those basis vectors are $(4\pi/3,0)$ and $(-2\pi/3,2\pi/\sqrt{3})$. It is worth mentioning here that Fig. 3(e) also depicts the true energy dispersion of the SBP in the case of the antiferromagnet on the honeycomb lattice doped with two electrons. The particle-hole transformation, supplemented by the gauge transformation which changes the sign of fermions at sites belonging to one of the sublattices, does not influence the energy dispersion of the SBP because the initial state used in the construction of the SBP wave function represents two holes created at NN sites, one at a site belonging to an even sublattice and one at a site belonging to odd sublattices, and thus the influence of the sign change on the matrix elements of a Hamiltonian represented in the basis of SBP wave functions is compensated.

We can draw a conclusion from the previous considerations that, in order to find the form of the unique two-hole state in the t - J model on the honeycomb lattice, we need to analyze low-order process contributing to the Hamiltonian terms which are not polynomials of the NN-hopping operator. It turns out that some of those processes will involve quantum fluctuations in the ground state of the undoped antiferromagnet on the honeycomb lattice. In the framework of the second-order perturbation analysis which determines the correction to the ground state of $H=H_0+H_1$, $\delta|\phi_0\rangle$, as

$$\delta|\phi_0\rangle = - \sum_{i \neq 0} \frac{\langle \phi_i^{(0)} | H_1 | \phi_0^{(0)} \rangle}{E_i^{(0)} - E_0^{(0)}} |\phi_i^{(0)}\rangle, \tag{11}$$

where $|\phi_0^{(0)}\rangle$, $E_0^{(0)}$ and $|\phi_i^{(0)}\rangle$, $E_i^{(0)}$ are the wave function and the eigenenergy of the ground state and of an excited state i of H_0 , respectively; the excited states correspond to quantum fluctuations which take the form of spins flipped at pairs of NN sites, as has been depicted in Fig. 4(a) in the case of sites i and j . Here, we concentrate on the case of the undoped antiferromagnet and treat the transverse part of the exchange interaction as the perturbation. By calculating the fraction in Eq. (11) for Fig. 4(a) which represents an excited state of the operator (2) playing the role of H_0 , we deduce that the prefactor with which that state appears in the ground state of the Heisenberg model on the honeycomb lattice is $-1/4$. Similarly, as in the case of the square lattice,^{36,38} we expect that the presence of fluctuations in the ground state of the quantum antiferromagnet on the honeycomb lattice does not influence much the process of spin polaron formation. Therefore, in the lowest-order approximation, it is sufficient to assume that quantum spin fluctuations do not modify the form of the wave function (3) for the spin bipolaron, and, vice versa, that the presence of holes does not modify the weight with which quantum spin fluctuations appear in the ground state of the system, which means that prefactors re-

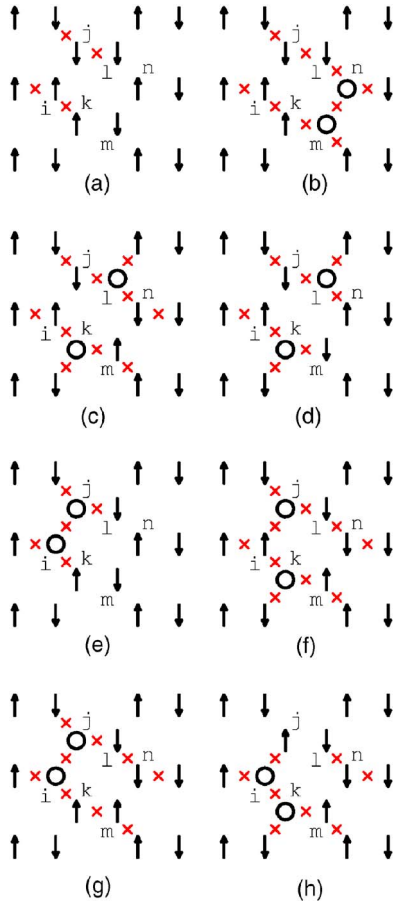


FIG. 4. (Color online) States which take part in low-order processes lifting the degeneracy of the lowest-energy band. These processes involve sites which belong to a single hexagonal plaquette in the honeycomb lattice and give rise to shifts of a SBP between every second and third sides of it. The presence of a spin fluctuation in the ground state of the antiferromagnet on the honeycomb lattice, as at sites i, j in (a), is a necessary prerequisite for the existence of those processes. The first of them can be described as follows. Two holes are created at sites m, n in the AF state with a spin fluctuation at sites i, j (b). Two additional fluctuations appear at sites m, n when holes are moved to sites k, l (c). Later, they are removed by flips (d). When holes jump on sites i, j , a state representing two holes created in the Néel state is created (e). Different sequences of events are also possible. For example, by applying some terms in the Hamiltonian, the intermediate state shown in (b) can be transformed via the state (f), either into the state (g) or (h) which represent holes created in the antiferromagnet at pairs of NN sites in the presence of a spin fluctuation at sites m, n .

lated to string states and prefactors related to AF spin fluctuations contribute as a product to the wave function representing a spin bipolaron formed in the AF background, which includes quantum fluctuations.

We proceed now to the consideration of a process which involves such a fluctuation. By applying twice some parts of the hopping operator to a state which represents a bare hole pair created at NN sites m, n and a spin fluctuation at NN sites i, j [Fig. 4(b)], we may transform it into the state depicted in Fig. 4(c) in which spins on sites m, n are turned upside down with respect to the direction which they have in

the Néel state. That additional fluctuation, on sites m, n , of the AF spin background may be removed by the action of the transverse part in the exchange term, which gives rise to the state depicted in Fig. 4(d). Again, by applying twice some parts of the hopping operator to the latter state, we may transform it into a state which represents two holes created in the Néel state [Fig. 4(e)], which means that the hole pair has been effectively shifted from the pair of NN sites m, n to the pair i, j . In the framework of the SBP formalism, that process can be interpreted in terms of coupling by the exchange term of the string state Fig. 4(c) with the string state Fig. 4(d). The former state is a component of the wave function (3) defining, in the presence of the quantum spin fluctuation on sites i, j , the SBP on sites m, n , while the latter state is a component of the wave function defining the SBP on sites i, j . The coupling between them gives rise to a matrix element τ'_3 of the effective Hamiltonian between wave functions of SBPs created at pairs of sites m, n and i, j ,

$$\tau'_3 = -\frac{J}{8} \sum_{\mu=1, \nu=1}^J (z-1)^{\mu+\nu+\delta_{\mu,1}+\delta_{\nu,1}-4} \alpha_{\mu,\nu}^2. \quad (12)$$

The prefactor in Eq. (12) is the product of the halved exchange integral, which originates from the action of the transverse part of the exchange term, and of the prefactor $-1/4$, with which the quantum spin fluctuation on sites i, j [Fig. 4(a)] appears in the ground state of the quantum antiferromagnet on the honeycomb lattice. The first term in the sum defining τ'_3 is a product of prefactors with which string states with “length” 2, Figs. 4(c) and 4(d), appear in the definition of the SBP (3). Further, terms in the sum refer to some “longer” string states which are involved in processes similar to the process depicted in Figs. 4(b)–4(e).

The hopping term in the tJM also couples the wave functions of a SBP created on sites i, j in Fig. 4 with the wave function of a SBP created on sites m, n . By applying a suitable term of the hopping operator to the state depicted by Fig. 4(c), we may shift a hole from site l to site j , which gives rise to the state depicted in Fig. 4(f). The different state [Fig. 4(f)] can also be obtained by shifting the hole in Fig. 4(g) from site i to site k . Since the state presented in Fig. 4(g) represents two bare holes created at sites i, j in the AF background with the quantum fluctuation on sites m, n , the state presented in Fig. 4(f) is, in fact, a component of the SBP created at sites i, j , and finally, since both states presented in Figs. 4(c) and 4(f) are components of SBPs created on some pairs of sites, m, n and i, j , respectively, the coupling between those SBPs is generated. The generated matrix element between wave functions of SBPs created on those pairs of sites is given by

$$\tau''_3 = \frac{t}{8} \sum_{\mu=1}^J (z-1)^{\mu+\delta_{\mu,1}-2} \alpha_{\mu,1} \alpha_{\mu,0}. \quad (13)$$

Formula (13) may be deduced by taking into account the prefactors for quantum spin fluctuations which are present in states depicted in Figs. 4(c) and 4(f) and by noticing that the prefactors related to strings which may be seen in those figures are given by $\alpha_{0,1}$ and $\alpha_{0,0}$, respectively. The fact that there exists a symmetric process analogous to the process

which we have just analyzed should be also kept in mind. States obtained by reflecting the states depicted in Figs. 4(c), 4(f), and 4(g) in the axis which leads through midpoints of bonds between sites m, n and i, j are involved in that additional process. Two processes of the kinds which we have just described, depicted in Figs. 4(b)–4(e) and 4(b)–4(d), 4(f), and 4(g), couple SBPs created at all pairs of bonds, which form opposite sides of hexagonal plaquettes in the honeycomb lattice. This coupling gives rise to the following contribution to the effective Hamiltonian:

$$H_{eff}^{(3)} = (\tau'_3 + \tau''_3) \sum_i (b_{\mathbf{R}_i+\mathbf{a},\alpha}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i+\mathbf{b},\beta}^\dagger b_{\mathbf{R}_i,\beta} + b_{\mathbf{R}_i+\mathbf{a}-\mathbf{b},\gamma}^\dagger b_{\mathbf{R}_i,\gamma}) + \text{H.c.} \quad (14)$$

Since the state presented in Fig. 4(f) is created when the hole on site i in Fig. 4(h), which represents two bare holes created at sites i, k in the Néel state with the quantum spin fluctuation on sites m, n , moves to site j , the former state is also a component of a SBP created at sites i, k . Furthermore, the state depicted in Fig. 4(f) can be obtained by the action of a suitable term in the hopping operator on the state depicted in Fig. 4(d), which is a component of the SBP created at sites m, n , which means that an additional contribution to the effective Hamiltonian is generated. That contribution represents the hopping of a SBP between second nearest sides of the plaquette in the honeycomb lattice,

$$H_{eff}^{(4)} = \tau_4 \sum_i (b_{\mathbf{R}_i+\mathbf{a},\beta}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i-\mathbf{b},\beta}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i+\mathbf{a}-\mathbf{b},\gamma}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i-\mathbf{a},\gamma}^\dagger b_{\mathbf{R}_i,\alpha} + b_{\mathbf{R}_i-\mathbf{a}+\mathbf{b},\gamma}^\dagger b_{\mathbf{R}_i,\beta} + b_{\mathbf{R}_i-\mathbf{b},\gamma}^\dagger b_{\mathbf{R}_i,\beta}) + \text{H.c.}, \quad (15)$$

where

$$\tau_4 = -\frac{t}{16} \sum_{\mu=0} (z-1)^{\mu+\delta_{\mu,0}-1} \alpha_{\mu,1} \alpha_{\mu+1,1}. \quad (16)$$

The prefactor in Eq. (16) contains the second power of the prefactor, with which a spin quantum fluctuation, as depicted in Fig. 4(a), appears in the ground state of the antiferromagnet on the honeycomb lattice. The sign of that prefactor originates from the convention determining the sign of the wave function (3) which defines the SBP, and from the fact that during the process which gives rise to the contribution (15), a hole which has initially occupied a site belonging to the even sublattice moves to a site belonging to the odd sublattice, and vice versa. The first term of the sum in Eq. (16) is the product of prefactors with which string states depicted in Figs. 4(d) and 4(f) contribute to the wave functions (3) of SBPs created at pairs of sites m, n and i, k , respectively. Further, terms in that sum refer to longer string states which are involved in processes similar to the process which we have just described.

Figure 5(a) depicts the band structure which has been obtained by the diagonalization of the full effective Hamiltonian H_{eff} . The degeneracy of states with different momenta present in the band structure obtained by the diagonalization of its first two terms, $H_{eff}^{(1)} + H_{eff}^{(2)}$, has been lifted. The single-particle ground state of the full model appears at the wave

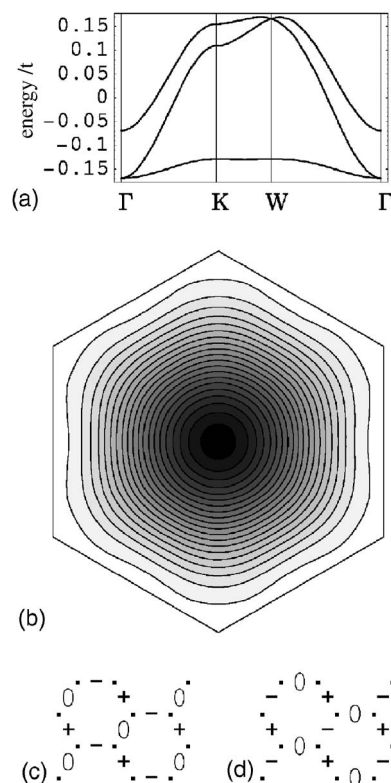


FIG. 5. (a) The energy dispersion of a single SBP obtained by the diagonalization of the full effective Hamiltonian. (b) Contour plot of the energy dispersion inside the first Brillouin zone for the lowest band. [(c) and (d)] The graphical representation of the degenerate ground state formed by two linearly independent superpositions of wave functions for SBPs created at pairs of NN sites (links). Symbols “+,” “-,” and the number “0” located between those sites represent absolute values and phases of prefactors which appear in those superposition at appropriate states.

vector $\Gamma=(0,0)$, which may be also seen in Fig. 5(b) depicting the contour plot for the energy dispersion of the lowest band. The ground state transforms according to the irreducible representation E of C_{3v} . Since that representation is two dimensional, the ground state is degenerate. E is realized by functions x and y , and thus, the name of p -wave symmetry can be applied to it. The properties of the representation E can be understood if one concentrates on one of the central sites in Figs. 5(c) and 5(d) represented in those figures by small squares. Signs “+,” “-,” and the number “0” nearest to that site should be also taken into account. For example, if we assume that the chosen site is a fixed point of the point group C_{3v} , it turns out that the first of two basis functions transforming according to the representation E is represented in Fig. 5(c) by that site and symbols around it, while the second basis function is represented by the same site and symbols in Fig. 5(d). The former function is odd with respect to the reflection in the axis forming the angle $\pi/3$ with the x axis. The function represented by the same site and characters around it in Fig. 5(d) is odd with respect to the reflection in the x axis. The same transformation properties have two appropriately chosen superpositions of x and y functions, which are $x-1/\sqrt{3}y$ and y , respectively. The terminology of

p -wave state may misleadingly suggest that the bound two-hole state represented by the single SBP state can have a triplet structure, which is impossible, because the honeycomb lattice lacks the inversion symmetry. Later, we will explicitly show that the obtained solution implies mixing of triplet and singlet pairing. Figures 5(c) and 5(d) also visualize two degenerate lowest-energy states at $\mathbf{p}=(0,0)$. For that purpose, the signs $+$, $-$, and the number 0 denote, now, prefactors with which states representing SBPs created at bonds between NN sites in the honeycomb lattice appear in coherent sums, which define two degenerate ground states. For example, the state symbolized by Fig. 5(c) is given by

$$|\phi_1\rangle = \sum_i (b_{\mathbf{R}_i, \alpha}^\dagger - b_{\mathbf{R}_i, \beta}^\dagger) |\Omega\rangle. \quad (17)$$

As has been stated before, the vacuum state $|\Omega\rangle$ is the ground state of the undoped antiferromagnet on the honeycomb lattice. In order to analyze in detail the nature of the degenerate bound state and the possible impact which it may have on the form of the SC state, we will represent it in terms of operators which create single spin polarons. We concentrate here on the case of two additional electrons added to the half-filled system. That case is relevant to cobaltates, but due to particle-hole symmetry at half-filling, it is equivalent to the system with two holes. We have just found the ground state of the latter system. Within the electron formulation, operators creating bipolarons which represent pairs of additional electrons created at NN sites and temporarily confined in the AF background are, by definition, equivalent to products of operators creating at those sites two single objects which may be called spin polarons,

$$b_{\mathbf{R}_i, \alpha}^\dagger = p_{\mathbf{R}_i, A, \downarrow}^\dagger p_{\mathbf{R}_i - \mathbf{b}, B, \uparrow}^\dagger, \quad (18)$$

$$b_{\mathbf{R}_i, \beta}^\dagger = p_{\mathbf{R}_i, A, \downarrow}^\dagger p_{\mathbf{R}_i - \mathbf{a}, B, \uparrow}^\dagger, \quad (19)$$

$$b_{\mathbf{R}_i, \gamma}^\dagger = p_{\mathbf{R}_i, A, \downarrow}^\dagger p_{\mathbf{R}_i, B, \uparrow}^\dagger. \quad (20)$$

As we have mentioned before, single spin polarons basically represent isolated quasicontained single electrons or, equivalently, holes, but it is clear that we can also represent a pair of electrons confined near a pair of NN sites and the related spin bipolaron in terms of two operators $p_{\mathbf{R}_i, A(B), \uparrow(\downarrow)}^\dagger$ which formally create spin polarons at those sites.^{38,43} The elementary cell in the honeycomb lattice [Fig. 3(a)] contains two sites, lower left and upper right, which belong to two different sublattices A (spin up at half-filling) and B (spin down at half-filling), respectively, which explains the origin of those letters in Eqs. (18)–(20). The spin polaron created at a site which belongs to the sublattice A has spin down because it is related to a state obtained by adding an additional electron to that site. Analogously, the spin polaron created at a site which belongs to the sublattice B has spin up. In the momentum representation, we formally have

$$p_{\mathbf{k}, \uparrow(\downarrow)}^\dagger = \sqrt{\frac{2}{N}} e^{i\mathbf{k}\mathbf{R}_i} \sum_i p_{\mathbf{R}_i, A(B), \uparrow(\downarrow)}^\dagger. \quad (21)$$

In terms of Fourier transformed operators, the degenerate ground state of the SBP model in the most general form is given by

$$|\phi\rangle = \sum_{\mathbf{k}} [C_1(e^{-i\mathbf{k}\mathbf{b}} - e^{-i\mathbf{k}\mathbf{a}}) + C_2(e^{-i\mathbf{k}\mathbf{b}} - 1)] p_{\mathbf{k}, \downarrow}^\dagger p_{-\mathbf{k}, \uparrow}^\dagger |\Omega\rangle, \quad (22)$$

where C_1 and C_2 are arbitrary numbers. The form of that state gives us information about the symmetry of the two-hole bound state, the formation of which is the prerequisite of pairing. Since the prefactor in the sum on the right side of Eq. (22) is neither even nor odd with respect to the parity transformation $\mathbf{k} \rightarrow -\mathbf{k}$, we expect that the paired state will be a mixture of singlet and triplet which transforms according to the irreducible representation $E(p)$ of the C_{3v} point group for the honeycomb lattice. The singlet-triplet mixing can be naturally attributed to the lack of the inversion symmetry in that lattice.

IV. DISCUSSION AND CONCLUSIONS

The aim of this paper is not to demonstrate that hole binding occurs in the t - J model on the honeycomb lattice when the J/t ratio is given by a value which may be relevant to the physics of layered cobalt oxides. The comparison of that value with the minimal ratio J/t for which a bound two-hole bound state is generated in a doped antiferromagnet on the square lattice^{50–53} suggests that a supporting attractive force should be involved in the generation of pairing in cobaltates. Also, a general theorem⁵⁹ which says that two electrons in the t - J model on any empty bipartite lattice do not form a bound state if $|J/t| < 1/2$, provides an additional argument that the ratio $|J/t|=0.2$ relevant to cobaltates may not be sufficiently high to induce binding of electrons. Provided that the attractive interaction is isotropic, it is most likely that the exchange of spin fluctuations determines the symmetry of a paired state. The scenario of SBP formation will also be true in this case. Thus the prediction which we make in this paper may be also valid if, for example, both spin fluctuations and phonons are involved in pairing in cobaltates. In order to test whether additional attractive interaction between charges changes the results reported in the previous section, we have calculated the shape of the SBP wave function (3) in the presence of it. To be precise, we have appropriately modified the Schrödinger equation (4) by adding to it a term representing short-range attractive density-density interaction. As can be seen in Figs. 2(b) and 2(c), for all strings formed by a single overturned spin between holes, the distance between holes at their ends is the same. Thus if we consider only short-range additional attraction between holes forming SBPs, we can assume that its strength depends only on string length, which simplifies the whole calculation. The outcome of the analysis performed along those lines suggests that the supplementary attractive force gives rise to the increase of the share which short string states have in the SBP wave

function, but the symmetry of the bound state is not changed.

The influence which the lack of the inversion symmetry may have on the symmetry and the spin of the paired state was discussed previously.^{54,55} In systems without space-inversion symmetry, the wave function cannot have well-defined parity with respect to an interchange of the spatial coordinates of two particles. Therefore, the other part of the wave function, the spin part, cannot have well-defined parity under particle interchange, which means that singlet-triplet mixing may be induced. Since the discovery of a superconductor without a center of symmetry,⁵⁶ there has been strong revival of interest in the theory of this phenomenon.^{57,58} In this paper, we present, for the layered cobalt oxide, a scenario according to which the inversion symmetry in that system is spontaneously broken owing to charge disproportionation. In the presence of charge ordering, the physics of a single CoO₂ layer can be described in terms of the t - J model on the honeycomb lattice, which is not centrosymmetric.

In summary, we have demonstrated that a bound state formed by two electrons or, equivalently, by two holes doped to the half-filled t - J model on the honeycomb lattice has

p -wave symmetry. The paired state which will be formed when that bound state condenses will be a mixture of a singlet and a triplet, which may be attributed to the fact that the honeycomb lattice is not centrosymmetric. Those conclusions are also valid if the exchange interaction in the t - J model is supplemented by some effective short-range isotropic attractive interaction, for example, induced by phonons. The presence of that interaction lowers the minimal value of the ratio J/t for which binding starts to take place. Provided that charge ordering, which effectively gives rise to freezing out of charge and spin fluctuations on every third cobalt atom, takes place in the superconducting layered cobalt oxide at the doping level $1/3$, the scenario presented here may be relevant to that system.

ACKNOWLEDGMENTS

P.W. acknowledges useful discussions with R. Eder, I. Ermin, P. Fulde, R. Micnas, J. A. Morkowski, A. M. Oleś, and J. Spałek.

-
- ¹K. Takada *et al.*, Nature (London) **422**, 53 (2003).
²T. Waki *et al.*, J. Phys.: Condens. Matter **18**, 669 (2006).
³W. Higemoto, K. Ohishi, A. Koda, S. R. Saha, R. Kadono, K. Ishida, K. Takada, H. Sakurai, E. Takayama-Muromachi, and T. Sasaki, Phys. Rev. B **70**, 134508 (2004).
⁴M. M. Maška, M. Mierzejewski, B. Andrzejewski, M. L. Foo, R. J. Cava, and T. Klimczuk, Phys. Rev. B **70**, 144516 (2004).
⁵M. Kato, C. Michioka, T. Waki, Y. Itoh, K. Yoshimura, K. Ishida, H. Sakurai, E. Takayama-Muromachi, K. Takada, and T. Sasaki, J. Phys.: Condens. Matter **18**, 669 (2006).
⁶Y. Kobayashi, M. Yokoi, and M. Sato, J. Phys. Soc. Jpn. **72**, 2453 (2003).
⁷G. Q. Zheng, K. Matano, D. P. Chen, and C. T. Lin, Phys. Rev. B **73**, 180503(R) (2006).
⁸T. Fujimoto, G. Q. Zheng, Y. Kitaoka, R. L. Meng, J. Cmaidalka, and C. W. Chu, Phys. Rev. Lett. **92**, 047004 (2004).
⁹G. Q. Zheng, K. Matano, R. L. Meng, J. Cmaidalka, and C. W. Chu, J. Phys.: Condens. Matter **18**, L63 (2006).
¹⁰G. Baskaran, Phys. Rev. Lett. **91**, 097003 (2003).
¹¹A. Tanaka and X. Hu, Phys. Rev. Lett. **91**, 257006 (2003).
¹²B. Kumar and B. S. Shastry, Phys. Rev. B **68**, 104508 (2003).
¹³C. Honerkamp, Phys. Rev. B **68**, 104510 (2003).
¹⁴Q. H. Wang, D. H. Lee, and P. A. Lee, Phys. Rev. B **69**, 092504 (2004).
¹⁵Y. Tanaka, Y. Yanase, and M. Ogata, J. Phys. Soc. Jpn. **73**, 319 (2004).
¹⁶H. Ikeda, Y. Nishikawa, and K. Yamada, J. Phys. Soc. Jpn. **73**, 17 (2004).
¹⁷K. Kuroki, Y. Tanaka, and R. Arita, Phys. Rev. Lett. **93**, 077001 (2004).
¹⁸M. D. Johannes, I. I. Mazin, D. J. Singh, and D. A. Papaconstantopoulos, Phys. Rev. Lett. **93**, 097005 (2004).
¹⁹K. Kuroki, Y. Tanaka, and R. Arita, Phys. Rev. B **71**, 024506 (2005).
²⁰M. Vojta and E. Dagotto, Phys. Rev. B **59**, R713 (1999).
²¹I. Terasaki, Physica B **328**, 63 (2003).
²²O. I. Motrunich and P. A. Lee, Phys. Rev. B **69**, 214516 (2004).
²³K. W. Lee, J. Kunes, and W. E. Pickett, Phys. Rev. B **70**, 045104 (2004).
²⁴W. Zheng, J. Oitmaa, C. J. Hamer, and R. R. P. Singh, Phys. Rev. B **70**, 020504(R) (2004).
²⁵H. Watanabe and M. Ogata, J. Phys. Soc. Jpn. **74**, 2901 (2005).
²⁶D. Qian *et al.*, Phys. Rev. Lett. **96**, 216405 (2006).
²⁷A. Lüscher, A. Läuchli, W. Zheng, and O. P. Sushkov, Phys. Rev. B **73**, 155118 (2006).
²⁸B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **60**, 740 (1988).
²⁹S. A. Trugman, Phys. Rev. B **37**, 1597 (1988); **41**, 892 (1990).
³⁰C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).
³¹S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988).
³²G. Martinez and P. Horsch, Phys. Rev. B **44**, 317 (1991).
³³A. L. Chernyshev and P. W. Leung, Phys. Rev. B **60**, 1592 (1999).
³⁴C. J. Hamer, Z. Weihong, and J. Oitmaa, Phys. Rev. B **58**, 15508 (1998).
³⁵R. Eder and K. W. Becker, Z. Phys. B: Condens. Matter **78**, 219 (1990).
³⁶R. Eder and K. W. Becker, Phys. Rev. B **44**, 6982 (1991).
³⁷R. Eder, Phys. Rev. B **45**, 319 (1992).
³⁸P. Wróbel and R. Eder, Phys. Rev. B **49**, 1233 (1994).
³⁹O. A. Starykh and G. F. Reiter, Phys. Rev. B **53**, 2517 (1996).
⁴⁰A. L. Chernyshev and R. F. Wood, in *Models and Methods of High-Tc Superconductivity: Some Frontal Aspects*, edited by J. K. Srivastava and S. M. Rao (Nova Science, Hauppauge, NY, 2003), Vol. 1, and references therein.
⁴¹L. N. Bulaeviskii *et al.*, Sov. Phys. JETP **27F**, 836 (1968).
⁴²W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).

- ⁴³P. Wróbel and R. Eder, Phys. Rev. B **58**, 15160 (1998).
- ⁴⁴P. Wróbel and R. Eder, Phys. Rev. B **64**, 184504 (2001).
- ⁴⁵D. A. Ivanov, P. A. Lee, and X. G. Wen, Phys. Rev. Lett. **84**, 3958 (2000).
- ⁴⁶P. W. Leung, Phys. Rev. B **62**, R6112 (2000).
- ⁴⁷F. C. Zhang *et al.*, Supercond. Sci. Technol. **1**, 36 (1988).
- ⁴⁸M. Zhao *et al.*, Nature (London) **385**, 236 (1997).
- ⁴⁹P. Wróbel *et al.*, J. Phys.: Condens. Matter **15**, 2755 (2003).
- ⁵⁰J. Bonča, P. Prelovšek, and I. Sega, Phys. Rev. B **39**, 7074 (1989).
- ⁵¹J. A. Riera and A. P. Young, Phys. Rev. B **39**, 9697 (1989).
- ⁵²Y. Hasegawa and D. Poilblanc, Phys. Rev. B **40**, 9035 (1989).
- ⁵³A. L. Chernyshev, P. W. Leung, and R. J. Gooding, Phys. Rev. B **58**, 13594 (1998).
- ⁵⁴P. W. Anderson, Phys. Rev. B **30**, 4000 (1984).
- ⁵⁵L. P. Gorkov and E. I. Rashba, Phys. Rev. Lett. **87**, 037004 (2001).
- ⁵⁶E. Bauer, G. Hilscher, H. Michor, Ch. Paul, E. W. Scheidt, A. Griбанov, Yu. Seropegin, H. Noël, M. Sigrist, and P. Rogl, Phys. Rev. Lett. **92**, 027003 (2004).
- ⁵⁷K. V. Samokhin, E. S. Zijlstra, and S. K. Bose, Phys. Rev. B **69**, 094514 (2004).
- ⁵⁸P. A. Frigeri, D. F. Agterberg, A. Koga, and M. Sigrist, Phys. Rev. Lett. **92**, 097001 (2004).
- ⁵⁹C. Y. Kadolkar and S. Basu, Phys. Rev. B **73**, 104501 (2006).