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Kinetic energy driven superconductivity and the pseudogap phase in weakly doped antiferromagnets

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Abstract

By analysing an effective Hamiltonian for spin polarons forming in weakly doped antiferromagnets represented by the t–J model we demonstrate that the driving mechanism which gives rise to superconductivity in such a system is the lowering of the kinetic energy, which is consistent with recent experimental observations. That source of attraction between holes is effective if the antiferromagnetic correlation length is longer than the radius of polarons. Notwithstanding that the attraction is strongest in the undoped system with long-range order, the superconducting order parameter vanishes when the doping parameter decreases, which can be attributed to emptying the spin polaron band and approaching the Mott insulator phase. Since the hypothetical normal phase of a low-density gas of fermions is unstable against formation of bound hole pairs the intensity of low-energy excitations is suppressed and a pseudogap forms in the underdoped region.

1. Introduction

The appearance of superconductivity (SC) with high T_c in doped antiferromagnetic (AF) insulators is one of the most intriguing problems in modern condensed matter physics. Some recent experimental observations shed new light on this problem. It has been observed [1] that the spectral weight of the optical conductivity is shifted toward lower energies below T_c and in the pseudogap region, which indicates that the lowering of the kinetic energy plays an important role in pairing. In addition, some recent measurements of optical conductivity in underdoped cuprates performed by Basov and collaborators [2] indicate that approaching the insulator regime in this system may be attributed to localization effects in a band which is emptied. A rigid band behaviour has also been recently observed by means of angle-resolved photoemission spectroscopy (ARPES) measurements in Na-doped $Ca_2CuO_2Cl_2$ by Shen, Takagi and collaborators [3, 4]. We shall argue that these findings are consistent with the spin polaron scenario for weakly doped AF.

The task of formulating a universal model capable of describing simultaneously all experimental aspects of different cuprates seems elusive. Nevertheless some general understanding of SC in doped AF may be gained from analysis of a minimal model for such systems; the t–J model (TJM). Recent numerical calculations based on a combination of various techniques, like quantum Monte Carlo (QMC) and Lanczos algorithms, performed for relatively large clusters have provided convincing evidence for pairing in the TJM [5, 6]. These calculations also indicate that short-range AF correlations are robust even for moderate doping. Some time ago an effective model was suggested to discuss SC in the TJM [7]. According to that suggestion the driving attractive force between holes may be attributed to the fact that by sharing a common link two holes minimize the the loss of the energy related to breaking AF links. This effect was represented in that effective model by a term corresponding to attraction between holes created at nearest neighbour (NN) sites. According to a different point of view, pairing in doped AF is mediated by an exchange of spin waves [8, 9]. In this paper we shall demonstrate that the main energetic gain in the paired state is due to formation of spin bipolarons which move in a way that conserves the kinetic energy.

Detailed knowledge about binding in weakly doped AF, about the role which symmetry plays in this process and about the internal structure of the bound pair [10] indicates that the static attraction between holes related to the minimization of the number of broken AF bonds if a hole pair occupies NN sites is ineffective because in the interesting parameter region $t \gg J$ the kinetic energy of each hole is raised due to the presence of the second hole at an NN site, which restricts the freedom of motion of holes. That insight gained by means of the spin polaron (string) approach and based on an assumption that short-range AF correlations prevail even for moderate doping has been verified by extensive comparisons with results of numerical analyses including QMC [11], exact diagonalization (ED) [12, 13] and density matrix renormalization group (DMRG) calculations [14]. A consistent picture which emerges from the collection of different pieces of data is that competition between different phases like the non-superconducting local pair phase, the SC state, phase separation or the stripe phase is governed by an obvious tendency to lower simultaneously the kinetic and the magnetic exchange energy.

In this paper, using knowledge gained about binding of holes in weakly doped AF [10], we analyse the formation of the SC state in such a system in terms of an effective model, which represents propagation and interaction of spin polarons. The basic assumption of this approach is that the AF correlation length is longer than the radius of spin polarons which seems to be valid at least in the region of weak doping. We will demonstrate that the shape of the curve representing the superconducting order parameter as a function of doping obtained in the numerical calculations [5] is reproduced within the Hartree–Fock (HF) approximation to an effective Hamiltonian represented in the basis of spin polaron states, and that the agreement for underdoped systems where the spin polaron approach should be valid is better than qualitative.

The standard version of the TJM [15] on the square lattice is used in this paper, which means that some possible effects related to the long-range Coulomb repulsion are not analysed here

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

The $\boldsymbol{S}_i$ are electronic spin operators, $\hat{c}^{\dagger}_{i,\sigma} = c^{\dagger}_{i,\sigma}(1 - n_{i,-\sigma})$ and the sum over $\langle i, j\rangle$ stands for a summation over all pairs of NNs.

2. Localized spin polarons and bipolarons

In order to make this paper self-sufficient we now outline the construction of spin polarons and the mechanisms of interaction between them. The spin polaron approach to binding of holes in doped AF [16–18] is based on the notion of a string. A moving hole inserted into the AF medium creates a line of defects (string) in the spin pattern, which raises the magnetic potential-like contribution to the energy. Since the rate of processes related to hopping is higher than the rate of magnetic exchange processes during which anti-parallel spins on NN sites are turned upside down, the latter category of processes may be temporarily neglected in the lowest-order approximation, when a trial 'unperturbed' Hamiltonian H_0 is solved. That Hamiltonian represents a hole attached to a site by a string, or in other words it describes a particle in a potential well. The eigenstates of the trial Hamiltonian, which we call in our terminology spin polarons span in principle the whole Hilbert space, but to discuss the low-energy properties of the system it is sufficient to concentrate on the ground state, which may be represented as

$$|\Psi_i\rangle = \sum_{\mathcal{P}_i} \alpha_{l(\mathcal{P}_i)} |\mathcal{P}_i\rangle. \tag{2}$$

$|\mathcal{P}_i\rangle$ denotes a state obtained by hopping along a path $\mathcal{P}_i$ without retreats of a hole created at the site i in the AF medium. For simplicity, we assume that the Néel state plays the role of that medium and that amplitudes $\alpha_{l(\mathcal{P}_i)}$ depend only on the length of paths $l(\mathcal{P}_i)$. If more holes are created at distant sites, the wavefunction of the multi-hole spin polaron representing many holes in separate potential wells is just a product of the wavefunctions for single independent polarons. If a hole pair is created at NN sites that approximation cannot be applied, because the holes share the same region in which the spin arrangement has been disturbed. Due to the size reduction of the disturbed area, the increase of the static potential contribution to the energy related to the part of the Hamiltonian which is equivalent to the Ising model is reduced. On the other hand, the proximity of holes may restrict their freedom of motion which raises the kinetic energy. In order to analyse these effects quantitatively we define a localized spin bipolaron as a combination of states which may be obtained by non-retraceable hopping of holes created at a pair of NN sites i, j,

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

The amplitudes $\alpha_{l(\mathcal{P}_i),l(\mathcal{P}_j)}$ represent the ground state solution of an approximate Schrödinger equation for an unperturbed Hamiltonian H_0 which describes two particles in the same potential well. The explicit form of the Schrödinger equations which determine α_μ and $\alpha_{\mu,\nu}$ will be presented in the appendix. It is sufficient to say here that H_0 couples string states of different length, counts the increase in the energy related to the destruction of the local AF environment and also takes into account the role of quantum spin fluctuations in the AF spin background, but neglects differences between paths of different geometry. A general lesson which we learn by comparing eigenenergies of localized single polarons and bipolarons is that the gain in the energy related to the reduction of the number of broken bonds when holes occupy NN sites is compensated by the loss of the kinetic energy which may be attributed to the fact that motion of each hole toward its partner is prohibited in such a case.

3. Effective Hamiltonian

During the process of constructing spin polarons we have solved a trial unperturbed Hamiltonian which is a part of the full TJM. We will take into account the remaining part

of the TJM by analysing all processes which have been neglected at the earlier stage of the calculation. These processes will be represented by a part of the Hamiltonian matrix which couples spin polaron states. This way of thinking about the TJM is very convenient, because eigenenergies of a spin polaron and a spin bipolaron already contain a substantial part of the energy related to the fast incoherent motion of holes inside potential wells. The formulation of the Hamiltonian in terms of the spin-polaron basis brings about some new features of the formalism. Since spin bipolaron states are not orthogonal, the particle-number operator contains two-body terms which consist of a pair of operators annihilating spin polarons and a pair of operators creating spin polarons at pairs of NN sites. The appearance of such terms may be understood by means of a simplest example depicted in figures 1(a)–(c). A wavy line represents a frustrated link for which the static contribution to the exchange energy, which is diagonal in the basis of spin up–down states, is raised in comparison with the Néel state. Diagrams (a) and (c) represent two holes created in the AF (Néel) background on different pairs of sites. These states are components of two different bipolarons $|\Psi_{i,j}\rangle$ created at these pairs of sites i, j. In both cases, by hopping outward from the accompanying hole, the hole at the central site creates a state depicted in figure 1(b) which is simultaneously the component of those two different bipolarons. Equivalence between components of bipolarons created at different sites gives rise to the overlap between them. By further hopping the holes create more equivalent states and the total overlap between bipolarons created on NN sites may be written as a sum, $-\sum_{\mu=0,\nu=1}(z-1)^{\mu+\nu-1}\alpha_{\mu,\nu}\alpha_{\mu+1,\nu-1}$, where $z=4$ is the coordination number and the minus sign is a matter of convention. Analogously, to each string state of arbitrary length, which consists of aligned magnons (flipped spins) and holes at both end-points, may be attributed overlap between bipolarons created at outer pairs of sites. In the language of the second quantization the overlap between bipolarons may be represented in terms of a pair of operators annihilating spin polarons and a pair creating them, as for example

$$\delta\hat{O} = -\sum_{\mu=0,\nu=1}(z-1)^{\mu+\nu-1}\alpha_{\mu,\nu}\alpha_{\mu+1,\nu-1}\sum_{i} h^{\dagger}_{i+\hat{\boldsymbol{x}}}h^{\dagger}_{i}h_{i}h_{i-\hat{\boldsymbol{x}}} \tag{4}$$

in the previously discussed case, where $\hat{O}$ is an operator representing the overlap. It turns out that each non-trivial contribution to the overlap operator brings about a new contribution to the effective Hamiltonian. By applying the kinetic energy term to the state depicted in figure 1(b), which is a component of the bipolaron created at a pair of sites represented by circles in figure 1(a), the left hole may be shifted to the central site and a state represented by figure 1(c) will be obtained, which means that spin polarons created at different pairs of sites marked by circles in figures 1(a) and (c) are coupled by the Hamiltonian. That coupling was neglected when we were solving the trial Hamiltonian because holes created at a pair of NN sites were not allowed to retrace each other. Longer strings obtained by further hopping of the right hole may also be involved in analogous processes. The contribution to the Hamiltonian is,

$$\delta\hat{H} = -t\sum_{\mu=1}(z-1)^{\mu-1}\alpha_{0,\mu}\alpha_{0,\mu-1}\sum_{i} h^{\dagger}_{i+\hat{\boldsymbol{x}}}h^{\dagger}_{i}h_{i}h_{i-\hat{\boldsymbol{x}}}. \tag{5}$$

Longer strings are crucial to the effectiveness, in lowering the energy, of processes driven by the kinetic term in the Hamiltonian. They have been neglected in previous analyses by different authors which lead them to an incorrect conclusion that the collective motion of a hole pair connected by a string cannot bring about pairing. We will discuss this issue later. At this stage of our considerations it is necessary to mention that the contributions to the energy which are brought about by the processes included in the trial Hamiltonian are incorporated into the eigenenergies of the polaron E_1 and the bipolaron E_2 and appear in the effective Hamiltonian

as diagonal terms

$$\delta\hat{H} = E_1 \sum_i h_i^\dagger h_i + (E_2 - 2E_1) \sum_{i,\delta} h_{i+\delta}^\dagger h_i^\dagger h_i h_{i+\delta}. \tag{6}$$

Since the absolute value of amplitudes α_μ, $\alpha_{\mu,\nu}$ declines, when the length of strings μ or $\mu+\nu$ grows only short string states may bring about considerable contributions to the effective Hamiltonian. This remark concerns only the shortest strings which are involved in a process of a given type, as in figures 1(a)–(c). As we have mentioned before, longer strings obtained by further hopping of holes in the state presented in figure 1 (b) may also take part in an analogous process. Since the number of such strings grows exponentially with the length, their contributions should also be taken into account as we did in (4) and (5). On the other hand, in this paper the analysis of processes is restricted to the shortest strings (of maximal length two lattice spacings) which are involved in a given process and 'initiate' the whole family of longer strings that may also take part in it. We apply an obvious defining convention that the string length is equal to the number of magnons created by hopping holes, which means that the maximal distance between holes connected by a string of length 2 is three lattice spacings. Restricting our calculation to processes which involve strings with the minimal length no longer than two lattice spacings needs some justification. By solving the Schrödinger equation determining the shape of spin polarons we deduce that the weight of a string state of length 3 for $J/t = 0.33$ is already smaller at least by one order of magnitude than the weight of states representing bare holes created in the Néel state and drops faster with increasing length. Thus, we immediately realize that the weight of the shortest strings involved in a given process basically determines the order of magnitude of its amplitude which may be also confirmed by an explicit evaluation of formulae like the sums (4) and (5). In addition, results of experiments with neutron scattering performed for $La_{2-x}Sr_xCuO_4$ [19] suggest that the AF correlation length in the cuprates follows the mean hole distance, which allows us to make an estimate that the spin polaron approach to pairing in weakly doped AF will provide reasonable results for the doping parameter $\delta \leqslant 1/9$ for which the AF correlation length is longer than the average distance between the holes that form the spin bipolaron, which we estimate to be about two to three distances between copper atoms. The applicability of the string approach to the whole underdoped region, for example for the doping parameter up to the value $1/4$ starts to be questionable because at that value the AF correlation length is surely no higher than two distances between copper atoms. Provided that the AF correlation length is bigger than the radius of spin polarons, the procedure of finding the effective Hamiltonian is well controlled. The string approach is an expansion with the controlling parameter $1/z$. Since the total weight of all string states is unity, the weight of a process which involves strings of length l is of order $1/z^l$ and decreases fast with l. No double counting is possible because contributions to the effective Hamiltonian are systematically found by analysing the matrix elements between spin polaron wavefunctions and their components which are string states. Since only spin polaron states with lowest eigenenergy are applied, the effective Hamiltonian is defined in the low-energy shell.

While constructing the effective Hamiltonian we not only take into account processes which were omitted when the trial Hamiltonian was solved, but also make some amendments to approximations we made previously. Since the wavefunction of a spin multipolaron representing holes created at a distance longer than one lattice spacing is approximated by the product of wavefunctions, some corrections are necessary. By considering that kind of product we tacitly assumed that such holes may jump on top of each other. Such artificial states should be removed, which gives rise to a necessary correction in the normalization condition for pairs of spin polarons located at a distance longer than one lattice spacing and an additional term in the operator representing the overlap between pairs of polarons. Also an appropriate correction

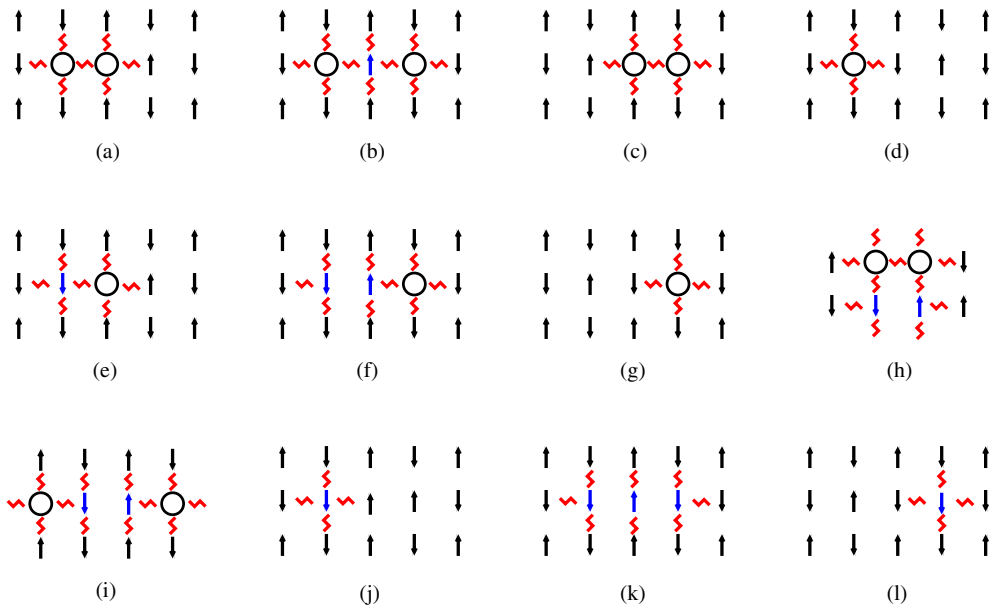

Figure 1. Graphical representation of some states and processes.
(This figure is in colour only in the electronic version)

to the eigenenergies of single polarons should be made for polarons created at such a small distance, because the obvious restriction on the possibility of hopping of holes on top of each other was neglected when we solved the Schrödinger equation defining single polaron states, which means that some spurious processes were taken into account during the evaluation of the kinetic energy.

Different spin polaron states may also be coupled by terms in the TJM related to the magnetic exchange. Their action, which occurs at a slower rate $\sim J$, turns anti-parallel spins at NN sites upside down. That coupling was neglected when the spin polaron basis was constructed. Figures 1(d)–(g) show a most obvious process, which gives rise to coherent propagation of a single hole in the AF medium. The diagram (d) represents a hole created in the AF spin background. This state is also a component of a spin polaron created at the same site. Other components of that polaron which are depicted in diagrams (e) and (f) will be obtained if the hole starts to hop. Two magnons created in this way may be annihilated if the transverse part of the Heisenberg model is applied to the state represented by figure 1(f). The new state, which is a component of the spin polaron localized at the site shifted by two lattice spacings, is represented by the diagram in figure 1(g). In a similar way a spin bipolaron may be shifted by one lattice spacing in the direction perpendicular to the bond occupied by the bipolaron. If two defects created by independent hops in that direction of each hole from the pair initially created at NN sites are removed by the transverse part of the exchange term, the hole pair is effectively moved, which brings about the shift of the whole spin bipolaron. The intermediate state has been depicted in figure 1(h). The initial and final position of the spin bipolaron is the middle pair of sites in the lower and upper row respectively. Such a process is of paramount importance for the selection of the symmetry of the bound state of two holes created in an AF [10], because it lowers the energy of the $d_{x^2-y^2}$-wave state and raises the energy of the p-wave state, while the remaining low-order processes which involve only

spin bipolarons are neutral. We expect that the preference for the $d_{x^2-y^2}$-wave symmetry will prevail in the hypothetical SC state, which may emerge after polaron pairs condense.

Some additional amendments to terms in the Hamiltonian which are diagonal in the spin-polaron representation are necessary. For example, our analysis should also take into account that holes initially created at sites which are not NN sites may gain some potential energy by lowering the number of broken bonds when they occupy such a pair after they have made a few hops. The discussion of quantum fluctuations in the AF state which lower the energy of the ground state of the Heisenberg model in comparison with the energy of the Néel state, that is the ground state of the Ising model, is also incorporated into our calculation. In the lowest order of the perturbation theory such fluctuations represent pairs of magnons created at NN sites in the Néel state and change the energy by the amount $-J/12$ for each link.

At the chosen level of accuracy there are altogether 14 different contributions to the overlap operator and 58 to the Hamiltonian, which may be classified according to processes that give rise to them and the positions of involved polarons. The physical picture which underlies the principle according to which the Hamiltonian is constructed is based on the assumption that the dynamics of holes should not destroy local AF correlations. For example in the process depicted in figures 1(a)–(c) the defects in the spin structure created by the motion of the right hole are annihilated by the subsequent hopping of the left hole. Thus, by the exchange of magnons forming a string which connects two holes, hole pairs initially created at NN sites avoid confinement. The process depicted in figures 1(d)–(g) which deconfines a single hole may be interpreted as cutting of the string formed by magnons attached to the initial site, by the transverse part of the exchange term in the Hamiltonian.

Due to space limitations we are not able to dwell upon further details and we now present the form of the effective Hamiltonian expressed in terms of operators h_i and $h_i^\dagger$ annihilating and creating spin polarons:

$$\begin{aligned}\hat{H}-\mu\hat{N} &= (E_1-\mu)\sum_i h_i^\dagger h_i + h\sum_{i,\delta,\delta';\delta'\neq-\delta} h^\dagger_{i+\delta+\delta'}h_i + (E_2/2-E_1+u_1)\sum_{i,\delta} h_i^\dagger h^\dagger_{i+\delta}h_{i+\delta}h_i \\ &+ u_2\sum_{i,\delta,\delta';\delta'\neq-\delta} h_i^\dagger h^\dagger_{i+\delta+\delta'}h_{i+\delta+\delta'}h_i + u_3\sum_{i,\delta,\delta';\delta'\perp\delta} h_i^\dagger h^\dagger_{i+\delta+\delta'}h_{i+\delta+\delta'}h_i \\ &+ u_4\sum_{i,\delta,\delta',\delta'';\delta'\neq-\delta,\delta''\neq-\delta'} h_i^\dagger h^\dagger_{i+\delta+\delta'+\delta''}h_{i+\delta+\delta'+\delta''}h_i + s_1\sum_{i,\delta,\delta';\delta'\neq-\delta} h^\dagger_{i+\delta+\delta'}h^\dagger_{i+\delta}h_{i+\delta}h_i \\ &+ s_2\sum_{i,\delta,\delta',\delta'';\delta'\neq-\delta,\delta''\neq-\delta'} h^\dagger_{i+\delta+\delta'}h^\dagger_{i+\delta+\delta'+\delta''}h_{i+\delta}h_i \\ &+ s_3\sum_{i,\delta,\delta';\delta'\perp\delta} [(h_i^\dagger h^\dagger_{i+\delta+\delta'}h_{i+2\delta}h_i + \text{H.c.}) + h_i^\dagger h^\dagger_{i+\delta+\delta'}h_{i+\delta-\delta'}h_i] \\ &+ s_4\sum_{i,\delta,\delta',\delta'';\delta'\neq-\delta,\delta''\neq-\delta'} (h_i^\dagger h^\dagger_{i+\delta+\delta'+\delta''}h_{i+\delta}h_i + \text{H.c.}) + s_5\sum_{i,\delta,\delta';\delta'\perp\delta} h_i^\dagger h^\dagger_{i+\delta'}h_{i+\delta}h_i \\ &+ s_6\sum_{i,\delta,\delta',\delta'';\delta'\neq\delta,\delta''\neq-\delta} (h^\dagger_{i+\delta+\delta''}h^\dagger_{i+\delta'}h_{i+\delta}h_i + \text{H.c.}) + s_7\sum_{i,\delta,\delta';\delta'\perp\delta} h^\dagger_{i+\delta+\delta'}h^\dagger_{i+\delta'}h_{i+\delta}h_i. \end{aligned} \tag{7}$$

Parameters which appear in this effective Hamiltonian are functions of E_1, E_2, μ, t, J and amplitudes α and include at once contributions from many different types of process. An important remark which we should also make is that the highest value for experimentally relevant ratios J/t has a parameter related to the motion as a whole of strings connecting a pair of holes, an example of which is depicted in figures 1(a)–(c). That type of caterpillar-like motion is so effective in lowering the total energy because by expanding at one end and shrinking at the other the whole string may move freely, while the number of magnetic defects

is kept low. Only the kinetic term in the Hamiltonian is involved in that movement, and the term related to the magnetic exchange does not have to intervene. Thus the gain in the energy is mainly due to lowering of the kinetic energy.

It is widely believed [20–22] that the motion of the hole pair is frustrated and cannot bring about lowering of the total energy and binding or pairing. Already the analysis of hole binding [10] has provided arguments that such an opinion is not correct. The notion of frustration was used in the literature to describe the fact that the effective hopping of the hole pair occupying NN sites, to nearest links that are parallel and perpendicular to the link at the ends of which the holes have been initially located, produces effective hopping integrals with the same positive sign, which is not very convenient in terms of lowering the kinetic energy but does not change a generally applicable rule that a mobile quantum object has lower energy than an immobile one. We have previously shown that the motion of a hole pair connected by a string formed by defects in the AF spin structure may give rise to formation of bound states with $d_{x^2-y^2}$- and p-wave symmetries, which agrees with results of numerical analyses including a recent work [13] performed for a relatively large cluster consisting of 32 sites. Also the energetic hierarchy of two-hole states representing symmetries and wavevectors allowed by the geometry of the 4×4 cluster observed by Hasegawa and Poilblanc [23] in the results of the ED has been reproduced by means of the spin polaron approach. Since the interaction between spin polarons mediated by the processes related to the motion of the string connecting two holes is dominating, the agreement between numerical and analytical analyses indicates that the spin polaron approach properly takes into account such effects. Arguments against the kinetic energy driven mechanism of binding in doped AF are based on the large d expansion [22]. A single hole created in the Néel background may lower the energy by virtual hopping to NN sites. If two holes occupy NN sites, the hopping of each hole in one direction is blocked and the energy is raised by the amount $2t^2/Jd$ in comparison with the energy of two separated holes. On the other hand if holes are created at NN sites one spoiled AF link is saved and a negative contribution $-J/2$ to the total energy is generated. In the first order of the $1/d$ expansion, the propagation of a hole pair occupying NN sites mediated by the process represented by figures 1(a)–(c) may only compensate the loss in the energy related to the blocking effect and no net gain in the energy related to the kinetics of the hole pair is observed. That picture changes qualitatively in lower dimensions for $t \gg J$. The energy scale $\sim t^2/J(d-1)$ related to kinetic processes dominates the scale $\sim J(d-1)$, which means that the energetic cost related to the creation of longer strings similar to the state represented by figure 1(i) is relatively lower. In addition, there is no blocking effect in the case of strings with at least one magnon. In simple terms, holes at the ends of longer strings can hop at least once in all directions without disturbing each other. All this makes the creep of strings more effective in lowering the energy. It seems that any calculation based on the $1/d$ expansion or an approach limited to a small basis of states related to short strings will not provide reliable results for a 2D system. During the construction of the spin polaron and the bipolaron the important contribution to the energy from incoherent motion in the potential wells and longer strings has also been taken into account. The energy of the spin bipolaron by construction contains contributions related to saving spoiled AF links and mutual restriction of the freedom of motion by two holes which oscillate chaotically around a pair of NN sites where they have been initially created. It turns out that for physically relevant range of parameters these two effects almost compensate each other and the eigenenergy of the localized spin bipolaron is roughly twice the energy of a localized polaron. Thus, truly kinetic effects related to motion of the centre of mass of a hole pair connected by a string bring about a net gain in the kinetic and total energy. These effects are represented in the effective Hamiltonian by terms related to the hopping of bipolarons. The difference between the behaviour in low and high dimensions may be associated with the

change in the relation between the energy scales $J(d-1)$ and $t^2/J(d-1)$ which means that the creation of longer strings is not so costly in lower dimensions and the system may lower its energy by kinetic processes which involve longer strings.

The wavefunctions of spin polarons are not orthonormal and the operator $\hat{O}$ representing overlap between them takes an unconventional form,

$$\hat{O} = 1 + d_1 \sum_{i,\delta,\delta';\delta'\neq-\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i + d_2 \sum_{i,\delta,\delta';\delta'\perp\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i + o_1 \sum_{i,\delta,\delta';\delta'\neq-\delta} h_{i+\delta+\delta'}^\dagger h_{i+\delta}^\dagger h_{i+\delta} h_i + o_2 \sum_{i,\delta,\delta',\delta'';\delta'\neq-\delta,\delta''\neq-\delta'} h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta} h_i + o_3 \sum_{i,\delta,\delta';\delta'\perp\delta} [(h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+2\delta} h_i + \text{H.c.}) + h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta-\delta'} h_i]. \quad (8)$$

Since the explicit formulae for the parameters of the Hamiltonian and the overlap operator are rather lengthy, they will be presented in the appendix.

4. Pairing versus the pseudogap phase in doped antiferromagnets

The distance between two holes which form a bound state in the AF background is a few lattice spacings [10] and it is natural to analyse their paring in real space. That approach is suitable for superconductors with a short coherence length. For the sake of simplicity we concentrate on anomalous Green functions $\mathcal{F}(i,\tau;i',\tau')$,

$$\mathcal{F}(i,\tau;i',\tau') = \langle T_\tau h_i(\tau) h_{i'}(\tau')\rangle, \quad (9)$$

which represent a pair of spin polarons annihilated at a pair of sites i, i' located at a distance no longer than three lattice spacings. The remaining anomalous Green functions which correspond to longer distances are neglected. That simplification will be justified by showing that $\mathcal{F}(i,\tau;i',\tau')$ decreases rapidly with distance between i and i'. Our intention is to understand the results of the recent numerical calculation performed by Sorella and collaborators [5] using numerical methods. Since they observe pairing correlations at some pairs of nearby sites we may also define the order parameter in real space for a few short distances. Possible symmetries of the order parameter are determined by irreducible representations of the point group C_{4v}. The order parameter, which is a singlet, may transform according to one-dimensional representations s, $d_{x^2-y^2}$, d_{xy} and g, while the triplet order parameter corresponds to the two-dimensional representation p. It turns out that in a full analysis of pairing in the real space at distances no longer than three lattice spacings, a 24-dimensional order parameter should be considered. Due to space limitations we omit a full analysis of the interplay between different symmetries. Since attraction between holes is strongest in the $d_{x^2-y^2}$-wave channel we shall discuss pairing only of that symmetry. If we restrict pairing in the real space to distances up to three lattice spacings, the $d_{x^2-y^2}$ symmetry will generate three different harmonics in the order parameter. The need to apply a non-monotonic order parameter was recently suggested after analysis of results of some experiments with Raman scattering performed for electron-doped cuprates [24].

We assume that the anomalous Green function is translationally invariant in space and time,

$$\mathcal{F}_e(\boldsymbol{x},\tau) = \langle T_\tau h_{i+\boldsymbol{x}}(\tau'+\tau) h_i(\tau')\rangle, \quad (10)$$

and that i in the previous definition belongs to the even sublattice. A relevant order parameter in the real space is defined as,

$$\Delta_{\boldsymbol{x}} = \mathcal{F}_e(\boldsymbol{x}, 0^+). \quad (11)$$

By proceeding in a standard way we derive HF equations for the SC order parameter in which vertex corrections have been neglected. Since retardation effects related to the exchange of magnons have already been taken into account during the derivation of the effective Hamiltonian, application of the weak coupling approach seems to be appropriate. The difference between the grand canonical potential at $T = 0$ in the superconducting and the normal state $\Omega_s - \Omega_n$ may be reconstructed from the equations for the order parameter. The inverse procedure is also possible:

$$\begin{aligned}\left.\frac{\Omega_s - \Omega_n}{N}\right|_{T=0} = \frac{1}{N}\sum_{\boldsymbol{k}} \frac{|\xi_{\boldsymbol{k}}| - \epsilon_{\boldsymbol{k}}}{2} - \{&(4u_1 + 8u_4 - 4s_1 + 4s_2 - 16s_4 - 8s_5 + 16s_6 + 8s_7) \\ &\times \Delta_{1,0}^2 + 24u_4\Delta_{2,1}^2 + 4u_4\Delta_{3,0}^2 + (16s_4 + 16s_6)\Delta_{1,0}\Delta_{2,1} \\ &+ (8s_4 + 8s_6)\Delta_{1,0}\Delta_{3,0}\},\end{aligned} \tag{12}$$

where $\xi_{\boldsymbol{k}}$ and $\epsilon_{\boldsymbol{k}}$ are quasiparticle energies in the normal and superconducting state

$$\xi_{\boldsymbol{k}} = E_1 + h(S_{\boldsymbol{k}}^{(2,0)} + 2S_{\boldsymbol{k}}^{(1,1)}) - \mu; \qquad E_{\boldsymbol{k}} = \sqrt{\xi_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2}. \tag{13}$$

The gap function is strongly anisotropic,

$$\begin{aligned}&\Delta_{\boldsymbol{k}} = d_{\boldsymbol{k}}^{(1,0)}\Delta_{e_x} + d_{\boldsymbol{k}}^{(2,1)}\Delta_{2e_x+e_y} + d_{\boldsymbol{k}}^{(3,0)}\Delta_{3e_x}; \\ &d_{\boldsymbol{k}}^{(1,0)} = (2u_1 + 4u_4 - 2s_1 + 2s_2 - 8s_4 - 4s_5 + 8s_6 + 4s_7)D_{\boldsymbol{k}}^{(1,0)} \\ &\qquad\qquad + (2s_4 + 2s_6)D_{\boldsymbol{k}}^{(2,1)} + (2s_4 + 2s_6)D_{\boldsymbol{k}}^{(3,0)}; \\ &d_{\boldsymbol{k}}^{(2,1)} = (4s_4 + 4s_6)D_{\boldsymbol{k}}^{(1,0)} + 6u_4 D_{\boldsymbol{k}}^{(2,1)}; \qquad d_{\boldsymbol{k}}^{(3,0)} = (2s_4 + 2s_6)D_{\boldsymbol{k}}^{(1,0)} + 2u_4 D_{\boldsymbol{k}}^{(3,0)},\end{aligned} \tag{14}$$

where

$$\begin{aligned}&D_{\boldsymbol{k}}^{(1,0)} = 2\cos(k_x) - 2\cos(k_y); \\ &D_{\boldsymbol{k}}^{(2,1)} = 2\cos(2k_x + k_y) + 2\cos(2k_x - k_y) - 2\cos(k_x + 2k_y) - 2\cos(k_x - 2k_y); \\ &D_{\boldsymbol{k}}^{(3,0)} = 2\cos(3k_x) - 2\cos(3k_y); \qquad S_{\boldsymbol{k}}^{(2,0)} = 2\cos(2k_x) + 2\cos(2k_y); \\ &S_{\boldsymbol{k}}^{(1,1)} = 2\cos(k_x + k_y) + 2\cos(k_x - k_y).\end{aligned} \tag{15}$$

The chemical potential applied in this formalism refers to the number of holes $\hat{N}$ which is given by the formula $\hat{N} = \sum_i h_i^\dagger h_i + 2(\hat{O} - 1)$, that within the HF approximation may be written at $T = 0$ as

$$\delta = \frac{1}{N}\sum_{\boldsymbol{k}}\left(1 - \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)\Big/ 2 - 8(o_1 - o_2)\Delta_{\hat{e}_x}^2, \tag{16}$$

where $\delta = \langle\hat{N}\rangle/N$. In the following we will restrict our analysis to the case of $T = 0$. $o_1 - o_2$ turns out to be negative. Thus it is clear that equation (16) will enforce disappearance of the SC order parameter when the number of holes decreases.

Figure 2 depicts anomalous Green functions that represent the SC order parameter related to pairs of spin polarons condensing on some nearest pairs of sites in the real space obtained within the weak coupling approximation applied to the effective Hamiltonian for $J/t = 0.33$. Numerical analyses of the TJM indicate that the AF correlations decrease with doping and that the correlation length becomes comparable to two or even one lattice spacing, when the doping exceeds 20%, which agrees with the phenomenology of the cuprates. Since the spin-polaron approach is based on the assumption that the polaron radius is smaller than the correlation length, this method will not work for the values of the doping parameter $\delta \geqslant 0.2$. In addition, according to our previous estimates we may expect that the spin polaron method should definitely provide reasonable results for doping levels δ below $1/9$. The agreement between our analytical approach and numerical results of Sorella and collaborators [5] turns

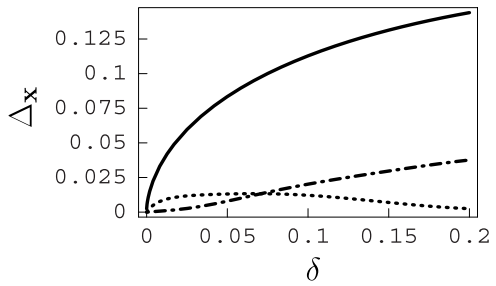

Figure 2. Anomalous Green functions Δ_x which represent pairs of spin polarons condensing at the distance of one lattice spacing (continuous curve), $\sqrt{5}$ lattice spacings (dotted curve) and three lattice spacings (dash–dotted curve).

out to be better than qualitative for the whole 'underdoped' region for which the results have been presented in figure 2. Our calculation also demonstrates that the energetic gain is not due to minimization of the number of broken bonds in the AF state if holes reside on a pair of NN sites, but pairing actually occurs because by formation of spin bipolarons, the magnetic and kinetic components of the energy may be simultaneously lowered. Since $t \gg J$, lowering of the kinetic energy plays a leading role in pairing, which confirms recent experimental observations [1] that the spectral weight in the plots of optical conductivity is shifted toward lower energies below T_c and in the pseudogap region. We also observe that the SC order parameter vanishes in the limit of low hole doping, which may be attributed to emptying the spin polaron band and approaching the Mott insulator (MI) phase in the nominally half-filled system. A rigid band picture which may be associated with propagating spin polarons has recently been observed by means of ARPES measurements in Na-doped $Ca_2CuO_2Cl_2$ by Shen, Takagi and collaborators [3, 4]. The only effect which has doping up to a level above 10% is the shift of the chemical potential.

The vanishing of the SC energy gap related to the coherent SC state does not necessarily mean that the underdoped AF should reveal features of an ordinary Fermi liquid-like normal state, because the system of freely propagating spin polarons becomes unstable against formation of bipolarons which brings about opening of the a pseudogap in the spectral function of a single quasiparticle. An earlier analysis [17] together with results presented in this paper and some numerical calculations [12, 13] demonstrate that the binding energy of a hole pair in the AF medium, which according to our scenario should be the energy scale of the pseudogap near half-filling, is a bigger fraction of J than the SC energy gap at optimal doping, which is in rough agreement with the phenomenology of the cuprates. Localization effects which should accompany a transition to MI in the limit of low doping and the intrinsic disorder [25] which is a characteristic feature of the cuprates may complicate the physical picture of the relation between the superconducting state and the pseudogap phase.

5. Conclusions

The analysis presented in this paper allows us to identify spin fluctuations which mediate pairing. It turns out that the coherent propagation of magnons which takes the form of spin waves is not relevant to pairing. A process which gives rise to magnon propagation has been depicted in figures 1(j)–(l). Figure 1(j) represents an isolated magnon. By swapping two spins the transverse part of the exchange interaction may create a state with three magnons which form a line as in figure 1(k). The magnon will be effectively shifted by two lattice spacings if

two left defects in the AF spin background are removed by the XY term in the Hamiltonian. The position change of the magnon between configurations depicted in figures 1(j) and (l) gives rise to the coherent propagation of the spin wave. It turns out that inclusion of such processes in our considerations does not influence the results, which proves that the standard propagation of spin waves does not play a crucial role in pairing. Emission of spin fluctuation by a hopping hole, which are later annihilated by the second hole that retraces the path of the first hole has a quite different nature and is a dominating factor in pairing.

The form of the effective Hamiltonian (7) indicates that the pairing mechanism is essentially non-retarded and effective interactions have a short range which agrees with conclusions drawn from the universal trends observed for the cuprates in the dependence of T_c on the hole and condensate density [26, 27].

The disappearance of SC in the underdoped region with decreasing number of holes should not be attributed to vanishing of the attractive force between quasiparticles but to emptying the spin polaron band. The later effect does not influence binding of hole pairs which gives rise to pseudogap phenomena. That rough scenario will in reality be modified by dimensionality effects, disorder, phase fluctuations, and some other phenomena like the tendency toward phase separation and stripe formation. A more detailed analysis of these effects is beyond the scope of this paper.

The Bardeen–Cooper–Schrieffer (BCS) mean-field type analysis employed in this paper needs some further improvements, due to short coherence length effects. This remark mainly concerns finite temperatures, where pairing correlation and fluctuation effects, processes related to formation of strongly coupled pairs and their condensation at lower temperatures are important. A full analysis of the transition and phenomena at finite temperatures requires a more involved method suitable for low density systems, which is the T matrix approach [28–33]. On the other hand, the detailed analysis is restricted in this paper to the case $T = 0$ where, as has been shown by many authors [29, 34–36], the BCS approach is expected to give rise to at least qualitatively correct results. This statement is true even in the case of strong coupling and for the scenario of condensing preformed pairs. Some more subtle effects, like the evolution of collective modes in the superconducting ground state, may be easily described in terms of the random phase approach which is a natural extension of the BCS method [37].

A phenomenological scenario in which SC is mediated by lowering of the kinetic energy has been suggested by Hirsch [38], who coined the notion of hole undressing, which may also be applied to the spin bag scenario. The kinetic mechanism of SC was also discussed by Imada and co-workers [39]. In both cases the standard Hubbard or TJMs were supplemented by additional terms which give rise to kinetic pairing. Our calculation demonstrates that such an effect may be observed in the original non-extended TJM.

In summary, by constructing an effective Hamiltonian we have identified spin fluctuations which mediate pairing in doped AF as local spin fluctuations which lie on a path connecting two holes. Creep-like motion of the whole object is an effective way of lowering the kinetic energy and the predominant factor which gives rise to pairing. This contradicts previous statements and widespread opinions, based on the $1/d$ expansion, that the collective motion of two holes in the locally AF background cannot effectively lower the energy. Experimental evidence that pairing may be associated with the change in the kinetic energy has recently been found by a second group [40]. These researchers were actually looking for the transfer of spectral weight from lower to higher energies in the pseudogap region, but observed an opposite behaviour, which supports the suggestion that the physics of the pseudogap may be also related to binding of holes.

A more detailed analysis, which is beyond the scope of this paper indicates that in the superconducting state both the hopping energy and the exchange energy defined at the level

of the TJM are lowered. Such behaviour has already been observed in the two-hole bound state [14], but this observation seems to contradict the virial theorem. The virial theorem which relates the mean values of the kinetic energy and the potential energy has a simple form if the energy of interaction of particles is a homogeneous function of a given degree n in their coordinates, which is not necessarily the case for low-energy effective models like the TJM. It may be shown that after a unitary transformation, the Coulomb potential energy defined at the level of the Hubbard model is represented at the level of the TJM by the exchange energy with a negative sign [41], and this quantity indeed increases in the SC state. The hopping term in the Hubbard model is represented in the TJM by the constrained hopping term plus twice the exchange energy. Thus, a relation which resembles the virial theorem for particles interacting by Coulomb law indeed holds for the Hubbard model in the large U limit, but not for the TJM. We also notice that the definition of the kinetic energy depends on the model which is applied. The total kinetic energy defined at the level of the full Hamiltonian derived from first principles does not have much experimental significance because it is not measurable. For effective models in which electrons may only hop to NN sites, the optical integral is proportional with the overall minus sign to the kinetic energy [42]. If the upper limit in the integral of the optical conductivity over the frequency is set below the charge excitation energy U, that integral measures the hopping energy in the lower Hubbard band, or in other words the kinetic energy defined at the level of TJM. Lowering of such a quantity is reported in some experimental papers [1, 40] and this meaning of the notion of kinetic energy, which has experimental significance, is applied in this paper.

The analysis of the effective Hamiltonian obtained by means of a method which has both a variational and perturbative character reproduces better than qualitatively the behaviour of the SC order parameter obtained by means of the numerical analysis [5] in the region where $\delta < 0.2$, which exceeds our expectations that the spin polaron method should be valid for $\delta \leqslant 0.11$. On the other hand the solution of the gap equation turns out to very sensitive to changes of the parameters defining the Hamiltonian. Since the effective Hamiltonian has been obtained by means of some approximations we can hardly expect quantitative accuracy of our results.

Some recent experimental results obtained by measuring optical conductivity [2] and ARPES [3] confirm the relevance of the band scenario at low doping, which is consistent with the spin polaron approach.

The strength of the attraction mediated by spin fluctuations decreases with increasing doping and diminishing AF correlation length. That effect may explain decreasing of the pseudogap with doping and the disappearance of SC in the overdoped region. On the other hand in the underdoped region SC disappears, because the quasiparticle band is emptied, while the density of low-energy excitations is still suppressed by formation of bound hole pairs.

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Appendix

We start the appendix with the presentation of parameters which define the Hamiltonian and the overlap operator in terms of operators creating and annihilating spin polarons:

$$
\begin{aligned}
&h = 2M_{\{(2,0)\}\{(0,0)\}}; \qquad u_1 = J^H_{\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} - J^H_{\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}};\\
&u_2 = (E_1-\mu)P_{\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}_{\}}} + P^H_{\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}}/2 + J^H_{\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}};\\
&u_3 = (E_1-\mu)R_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}} + R^H_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}}; \qquad u_4 = J^H_{\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}}/2;\\
&s_1 = (E_2-2\mu)C_{\left\{\begin{smallmatrix}(2,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} - 2M_{\{(2,0)\}\{(0,0)\}} + C^H_{\left\{\begin{smallmatrix}(2,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}};\\
&s_2 = (E_2-2\mu)C_{\left\{\begin{smallmatrix}(2,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} + C^H_{\left\{\begin{smallmatrix}(2,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}};\\
&s_3 = (2E_1-2\mu-J/2)S_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}} + S^H_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}}; \qquad \text{(A.1)}\\
&s_4 = M_{\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} + M_{\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}} - 2M_{\{(2,0)\}\{(0,0)\}};\\
&s_5 = 2M_{\left\{\begin{smallmatrix}(0,0)\\(0,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} - 2M_{\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} - 2M_{\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}} + 2M_{\{(2,0)\}\{(0,0)\}};\\
&s_6 = M_{\left\{\begin{smallmatrix}(2,0)\\(-1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}}/2; \qquad s_7 = 2M_{\left\{\begin{smallmatrix}(1,1)\\(0,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} - M_{\left\{\begin{smallmatrix}(2,0)\\(-1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} - (J/2)C_{\left\{\begin{smallmatrix}(2,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}};\\
&d_1 = P_{\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}}/2; \qquad d_2 = R_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}}/2;\\
&o_1 = C_{\left\{\begin{smallmatrix}(2,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}}; \qquad o_2 = C_{\left\{\begin{smallmatrix}(2,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}}; \qquad o_3 = S_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}}.
\end{aligned}
$$

Parameters which are presented below correspond to different categories of processes which involve string states.

$$
\begin{aligned}
&P_{\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}} = -\left[2\sum_{\mu=2,\nu=0}(z-1)^{\mu+\nu-2}\alpha_\mu^2\alpha_\nu^2 + \sum_{\mu=1,\nu=1}(z-1)^{\mu+\nu-2}\alpha_\mu^2\alpha_\nu^2\right];\\
&C_{\left\{\begin{smallmatrix}(2,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = -\sum_{\mu=0,\nu=1}(z-1)^{\mu+\nu-1}\alpha_{\mu,\nu}\alpha_{\mu+1,\nu-1};\\
&C_{\left\{\begin{smallmatrix}(2,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = \sum_{\mu=0,\nu=2}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu}\alpha_{\mu+2,\nu-2};\\
&S_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}} = -\sum_{\mu=2,\nu=0}(z-1)^{\mu+\nu-2}\alpha_\mu\alpha_\nu\alpha_{\mu-2}\alpha_{\nu+2};\\
&R_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}} = -\left[\alpha_1^2 + (z-2)\sum_{\mu=2}(z-1)^{\mu-2}\alpha_\mu^2\right]^2;\\
&M_{\{(2,0)\}\{(0,0)\}} = (J/2)\sum_{\mu=2}(z-1)^{\mu-2}\alpha_\mu\alpha_{\mu-2};\\
&M_{\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = (J/2)\sum_{\mu=0,\nu=2}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu}\alpha_\mu\alpha_{\nu-2};\\
&M_{\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}} = (J/2)\sum_{\mu=2,\nu=0}[\delta_{\mu,2}(z-1)^\nu + (1-\delta_{\mu,2})(z-2)(z-1)^{\mu+\nu-3}]\alpha_\mu\alpha_\nu\alpha_{\mu-2,\nu};\\
&M_{\left\{\begin{smallmatrix}(0,0)\\(0,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = (J/2)\sum_{\mu=2,\nu=0}[\delta_{\mu,2} + (1-\delta_{\mu,2})(z-2)(z-1)^{\mu-3}]\\
&\qquad\qquad \times[\delta_{\nu,0} + (1-\delta_{\nu,0})(z-2)(z-1)^{\nu-1}]\alpha_{\mu,\nu}\alpha_{\mu-2,\nu}; \qquad \text{(A.2)}\\
&M_{\left\{\begin{smallmatrix}(2,0)\\(-1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = (-J/2)\sum_{\mu=1,\nu=1}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu}\alpha_{\mu-1}\alpha_{\nu-1};\\
&M_{\left\{\begin{smallmatrix}(1,1)\\(0,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = (-J/2)\sum_{\mu=1,\nu=1}[\delta_{\mu,1} + (1-\delta_{\mu,1})(z-2)(z-1)^{\mu-2}]
\end{aligned}
$$

$$\times [\delta_{\nu,1} + (1-\delta_{\nu,1})(z-2)(z-1)^{\nu-2}]\alpha_{\mu,\nu}\alpha_{\mu-1,\nu-1};$$

$$C^{H}_{\left\{\begin{smallmatrix}(2,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = -t\sum_{\mu=1}(z-1)^{\mu-1}\alpha_{0,\mu}\alpha_{0,\mu-1};$$

$$C^{H}_{\left\{\begin{smallmatrix}(2,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = t\sum_{\mu=2}(z-1)^{\mu-2}\alpha_{0,\mu}\alpha_{1,\mu-2}; \qquad P^{H}_{\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}} = -2t(\alpha_0^2\alpha_1\alpha_2 + \alpha_0\alpha_1^3);$$

$$S^{H}_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}} = -t\sum_{\mu=2}\alpha_\mu\alpha_0\alpha_{\mu-2}\alpha_1; \qquad R^{H}_{\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,1)\end{smallmatrix}\right\}} = -t\sum_{\mu=1}\alpha_1\alpha_\mu^2\alpha_0;$$

$$J^{H}_{\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(1,0)\end{smallmatrix}\right\}} = (-J/2)\left[2\sum_{\mu=2,\nu=0}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu}^2 + \sum_{\mu=1,\nu=1}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu}^2\right];$$

$$J^{H}_{\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(3,0)\end{smallmatrix}\right\}} = (-J/2)\left[2\sum_{\mu=2,\nu=0}(z-1)^{\mu+\nu-2}(\alpha_\mu\alpha_\nu)^2 + \sum_{\mu=1,\nu=1}(z-1)^{\mu+\nu-2}(\alpha_\mu\alpha_\nu)^2\right];$$

$$J^{H}_{\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}\left\{\begin{smallmatrix}(0,0)\\(2,0)\end{smallmatrix}\right\}} = (-J/2)\sum_{\mu=1,\nu=0}[\delta_{\mu,1} + (1-\delta_{\mu,1})(z-2)(z-1)^{\mu-2}]$$
$$\times [\delta_{\nu,0} + (1-\delta_{\nu,0})(z-2)(z-1)^{\nu-1}](\alpha_\mu\alpha_\nu)^2.$$

Spin polarons are defined as a solution of the following eigenvalue problem

$$zt\alpha_1 + 2J\alpha_0 = E_1\alpha_0; \qquad t\alpha_{\mu-1} + (z-1)t\alpha_{\mu+1} + J(\tfrac{5}{2}+\mu)\alpha_\mu = E_1\alpha_\mu,$$

where $\mu \geqslant 1$. A solution of the following Schrödinger equation for two particles in the same potential well determines the wavefunction of the spin bipolaron,

$$t[\alpha_{\mu-1,\nu} + (z-1)\alpha_{\mu+1,\nu} + \alpha_{\mu,\nu-1} + (z-1)\alpha_{\mu,\nu+1}] + J(4+\mu+\nu-\tfrac{1}{2}\delta_{\mu+\nu,0})\alpha_{\mu,\nu} = E_2\alpha_{\mu,\nu}, \tag{A.3}$$

where $\alpha_{\mu,\nu} = 0$ for $\mu < 0$ or $\nu < 0$. The normalization conditions for spin-polaron wavefunctions are

$$\alpha_0^2 + z\sum_{\mu=1}(z-1)^{(\mu-1)}\alpha_\mu^2 = 1; \qquad \sum_{\mu=0,\nu=0}(z-1)^{(\mu+\nu)}\alpha_{\mu,\nu}^2 = 1. \tag{A.4}$$

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