Pairing of two holes by a single string

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The string mechanism of pairing in the t–J model is considered. It is shown that in the limit $J/t \ll 1$ and for low hole concentrations $x \lesssim (J/t)^{1/3}$ string pairing on a square lattice occurs for $J/t > 1.52\times 10^{-2}$; otherwise the holes condense into a ferromagnetic drop (spin bag). For $1.52\times 10^{-2} < J/t \ll 1$ a string pair has a binding energy $\Delta_s = 2.52(tJ^2)^{1/3}$ and an effective mass $m = (t\sqrt{3}/2)^{-1}$. Dispersion laws for a string pair and a single hole with a string are established.

1. INTRODUCTION

The discovery of high-T_c superconductivity initiated a series of papers devoted to the study of the Hubbard model with strong intrasite repulsion. When a band is nearly half-filled, the system is described by an effective Hamiltonian acting in the subspace of states that have no doubly occupied sites. The Hamiltonian is familiar as that of the t–J model and has the form $H = H_t + H_J$, with

$$H_t = -t \sum_{\langle ij\rangle\sigma} (\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^{+}_{j\sigma}\hat{c}_{i\sigma}), \tag{1}$$

$$H_J = J \sum_{\langle ij\rangle} (\mathbf{S}_i\mathbf{S}_j - \frac{1}{4} n_i n_j). \tag{2}$$

Here $\hat{c}^{+}_{i\sigma} = c^{+}_{i\sigma}(1 - n_{i,-\sigma})$, where $c^{+}_{i\sigma}$ is the electron creation operator; i and σ are, respectively, the site index ($i = 1,2,\ldots,N$) and the spin index ($\sigma = \uparrow,\downarrow$); $n_{i\sigma} = c^{+}_{i\sigma}c_{i\sigma}$; $n_i = \Sigma_\sigma n_{i\sigma}$; and S_i is the electron spin operator. The sum over $\langle ij\rangle$ indicates summation over all the edges of a square lattice.

By the very origin of the effective Hamiltonian specified by (1) and (2), there are two necessary conditions that must be met if we wish to apply it to a Hubbard system: (1) the relative weakness of the exchange interaction, or $J/t \ll 1$, and (2) the smallness of the hole concentration $x = N_h/N$, or $x \ll 1$. It is in this range of parameters that we must consider the t–J model if we wish to study pairing in a Hubbard system.

The string mechanism of pairing was suggested by Hirsch, Mohan, and Kumar.[1,2] The essence of this mechanism is as follows: two holes are coupled by an antiferromagnetic string, a line on which the initial Néel order is replaced by an alternative order. The string's energy is proportional to the string's length, as a result of which the attractive force between the two holes coupled by the string is distance-independent (confinement).

When a single hole moves against the Néel background, it leaves a string behind it that couples the hole with the initial site.[3] Hence, for a single hole to become delocalized, we must allow for processes more subtle than ordinary translation, namely, spin fluctuations and what is known as Trugman cycles.[4] Because of this, the effective mass of a single hole increases considerably as the hole moves against the Néel background. On the other hand, a pair is translated in an obvious manner without disrupting the magnetic order. Thanks to the presence of a "direct" mechanism of pair delocalization, the pair's effective mass must be considerably smaller than that of a single hole. This must lead to a certain gain in kinetic energy that stabilizes the hole-string-hole system as a whole.

The first attempts to apply these heuristic ideas to the building of a bound state of two holes were unsuccessful, however. Schraiman and Siggia[5] studied string pairing in the t–J_z model and found no pairing for $J_z/t \ll 1$. Somewhat later Eder[6] arrived at a similar result for the t–J model. Examining the possibility of string pairing, Eder, Schraiman, and Siggia[5,6] studied the region $J/t \sim 1$ and found bound states in it. Nevertheless, this left the question of the possibility of pairing in a Hubbard system unresolved because for $J/t \sim 1$ the t–J model does not describe such a system.

In another well-known paper[4] Trugman considered pair states on a truncated Hilbert space that allowed for the existence of a string no longer than three lattice constants. Numerical diagonalization of the Hamiltonian yielded a pair state with an infinite effective mass, which, naturally, was unfavorable energywise. Trugman argued that in the complete Hilbert space the paired hole-string-hole state has an infinite effective mass.

The general flaw in Refs. 4–6 is the unfortunate choice of the ansatz for the string pair, which ignores the possibility of the pair being translated as a whole without disrupting the magnetic order. A clear indication of this is the overestimated value of the pair's effective mass,[4] which contradicts the simple heuristic reasoning of Kumar and Mohan.[2]

In recent papers,[7,8] I suggested an ansatz free of the above drawback and resolved the contradiction between the qualitative picture of a string pair and a t–J model calculation. The ansatz allows explicitly for translational freedom of a string pair and provides for a fairly broad stability region in the Hubbard case $J/t \ll 1$. In this paper I consider this ansatz in the continuum approximation, whose meaningfulness is illustrated *a posteriori*. The main result is that in the interval $1.52\times 10^{-2} < J \ll 1$ there is string pairing when $x \lesssim (J/t)^{1/3}$ holds. The effective mass of the pair is $(t\sqrt{3}/2)^{-1}$, which is not very large, in contrast to Trugman's prediction[4] but in full agreement with Kumar and Mohan's heuristic reasoning.[2]

The plan of the paper is as follows. Section 2 is devoted

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to string states in the t–J_z model consisting of a single hole and a pair. Section 3 examines string states in the t–J model and clarifies the role of spin fluctuations. Section 4 analyzes ferromagnetic states in the t–J model and their competition with string states, which determines the lower limit on the existence of string states in parameter J/t. Section 5 compares the results with recent cluster calculations[9–12] and discusses the string interaction, which determines the upper limit on the existence of string states in the hole concentration x.

2. STRING STATES IN THE t–J_z MODEL

The most convenient way to analyze string states is to begin with the t–J_z model. The model Hamiltonian has the form $H_0 = H_t + H_{\rm Ising}$, with

$$H_{Ising} = J\sum_{\langle ij\rangle}\left(S_i^z S_j^z - \frac{1}{4}n_i n_j\right). \tag{3}$$

It differs from the Hamiltonian (1), (2) of the t–J model only in the absence of the term

$$H_\perp = H_J - H_{Ising} = \frac{J}{2}\sum_{\langle ij\rangle}\left(S_i^+ S_j^- + S_j^+ S_i^-\right), \tag{4}$$

which describes spin fluctuations. Below we account for this term perturbatively.

In the absence of holes the ground state of the t–J_z model is the Néel state $|N\rangle$. The corresponding energy value is $E_0 = -NJ$. Introducing one or two holes changes the structure and energy of the ground state. These changes are considered here using the concept of string states.

2.1. A single hole (string polaron)

As a hole moves against the Néel background, it leaves a string behind it that couples the hole with the initial site. Let l be an arbitrary configuration of the string with the fixed initial site i, $|l|$ being the length of the string, and $|1,l,i\rangle$ the corresponding state (Fig. 1). To build the ground state of the string polaron we select the following basis:

$$|1_\rho\rangle = [N(1,\rho)]^{-1/2}\sum_{|l|=\rho}|1, l, i\rangle, \quad \rho = 0, 1, 2, \ldots \tag{5}$$

These are symmetric normalized linear combinations of all possible states with a string of length ρ, with $N(1,\rho)$ the number of such states.

In describing string states we use what is known as the Cayley tree approximation, or simply the tree approximation. It is based on two assumptions:

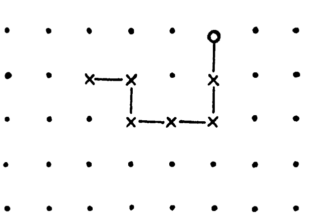

FIG. 1. The state of a string polaron (the ● denote spins whose orientation corresponds to the initial Néel state, the $\times$ denote spins with the opposite orientation, and ○ denotes the position of the hole).

(a) three new string states can be obtained from each string state by translating the hole by the lattice constant, and

(b) when the length of the string increases by unity, two bonds are frustrated, that is, the exchange energy $\langle H_{\rm Ising}\rangle$ increases by $(J/2)2 = J$. An exception is the initial state of the hole, from which four new string states can be obtained, with three bonds frustrated.

The tree approximation ignores the shape of the trajectory; for one thing, it does not allow for self-osculations and self-intersections. Substantiating it is a fairly complex topological problem. At the same time, intuitively it is clear that the relative number of trajectories with a large fraction of self-osculations and self-intersections is small.

In the tree approximation, the number of trajectories of length ρ is $N(1,\rho) = 4\times 3^{\rho-1}$ and the H_t, translational part of the Hamiltonian, acts on the base vectors $|1_\rho\rangle$ as follows:

$$H_t|1_0\rangle = -(4t/\sqrt{3})|1_1\rangle,$$

$$H_t|1_\rho\rangle = -t\sqrt{3}(|1_{\rho-1}\rangle + |1_{\rho+1}\rangle), \quad \rho \ge 1. \tag{6}$$

Moreover, the states $|1_\rho\rangle$ are eigenstates for the Ising part of the Hamiltonian:

$$H_{Ising}|1_0\rangle = -(N-2)J|1_0\rangle,$$

$$H_{Ising}|1_\rho\rangle = -\left(N - \rho - \frac{3}{2}\right)J|1_\rho\rangle, \quad \rho \ge 1. \tag{7}$$

The string polaron ground state is sought in the form of the linear combination

$$|1s\rangle = \sum_{\rho=0}^{\infty}\alpha(\rho)|1_\rho\rangle. \tag{8}$$

If we apply the Hamiltonian H_0 to this state and allow for the properties (6) and (7), we arrive at the discrete representation of the Schrödinger equation $H_0|1s\rangle = E|1s\rangle$ (see Ref. 5):

$$-(4t/\sqrt{3})\alpha(1) = E_{1s}\alpha(0),$$

$$-t\sqrt{3}[\alpha(\rho-1) + \alpha(\rho+1)]$$

$$+J\left(\rho + \frac{1}{2}\right)\alpha(\rho) = E_{1s}\alpha(\rho), \quad \rho \ge 1, \tag{9}$$

where $E_{1s} = E + (N-2)J$ is the string polaron energy measured from the Ising energy of the initial state $|1_0\rangle$.

In the continuum limit

$$\alpha(\rho \pm 1) \to \left[1 \pm \frac{d}{d\rho} + \frac{1}{2}\left(\frac{d}{d\rho}\right)^2\right]\alpha(\rho)$$

the recurrence relations (9) yield the Schrödinger equation $\mathscr{H}_{1s}\alpha = E_{1s}\alpha$ with the effective Hamiltonian

$$\mathscr{H}_{1s} = t\sqrt{3}[-2 + (d/d\rho)^2] + J\rho. \tag{10}$$

From the first recurrence relation in (9) follows the boundary condition on the "continuum" wave function $\alpha(\rho)$, that is, $\alpha(0) = 0$. The boundary condition at infinity corresponds to a variational problem with a free end: $\alpha'(\infty)=0$. The ground state of the Hamiltonian (10) satisfying these boundary conditions has the form

$$\alpha(\rho)=\mathrm{Ai}(s-s_0),\quad s=\rho/R_s,\quad R_s=(t\sqrt{3}/J)^{1/3},\qquad(11)$$

where $\mathrm{Ai}(s)$ is the Airy function, $-s_0=-2.338$ is the first zero of this function $[\mathrm{Ai}(-s_0)=0]$, and R_s is the characteristic length of the string in the string bipolaron. This state has the energy

$$E_{1s}=-2t\sqrt{3}+s_0(tJ^2\sqrt{3})^{1/3},\qquad(12)$$

which can be interpreted as the ground-state energy of the spin polaron. For further estimates it proves expedient to calculate the average length of the string in the string polaron:

$$\rho_1=\langle\rho\rangle=\int_0^\infty\rho\alpha^2(\rho)d\rho\Big/\int_0^\infty\alpha^2(\rho)d\rho=\frac{2s_0}{3}\left(\frac{t\sqrt{3}}{J}\right)^{1/3}.\qquad(13)$$

Since we are interested in the case $J/t\ll1$, we get $\rho_1\gg1$. This proves the self-consistency of the continuum approximation.

2.2. A pair of holes (string bipolaron)

A string pair, in contrast to a single hole, is translated in a natural way over the Néel background without disrupting the magnetic order. Hence, it is convenient to take for the basis states the following symmetric linear combinations of all possible states $|2,l\rangle$ (a hole plus a string plus a hole with a string of length $|l|=\rho$; Fig. 2):

$$|2_\rho\rangle=[N(2,\rho)]^{-1/2}\sum_{|l|=\rho}|2,l\rangle,\quad\rho=1,2,\ldots\qquad(14)$$

In contrast to the basis ansatz (5), the initial position of both holes is not fixed now, and because of this the state (14) is initially delocalized. We denote the total number of states $|2,l\rangle$ (a hole plus a string plus a hole with a string of length $|l|=\rho$) by $N(2,\rho)$. In the tree approximation this number is equal to $4\times3^{\rho-1}\times\frac{1}{2}N$. The additional factor N appears because of the N possible positions of the second hole, and the $\frac{1}{2}$ reflects the fact that the holes are identical. In the tree approximation, the translational part of the Hamiltonian, H_t, acts on the base vectors $|2_\rho\rangle$ in the following simple manner:

$$H_t|2_1\rangle=-2t\sqrt{3}|2_2\rangle,$$
$$H_t|2_\rho\rangle=-2t\sqrt{3}(|2_{\rho-1}\rangle+|2_{\rho+1}\rangle),\quad\rho\geq2.\qquad(15)$$

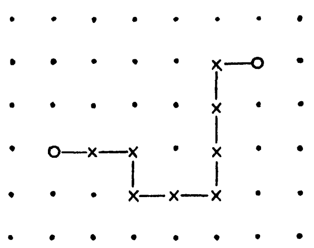

FIG. 2. The state of a string bipolaron.

Moreover, these vectors are the eigenvectors of the Ising part of the Hamiltonian:

$$H_{Ising}|2_1\rangle=-\left(N-\frac{7}{2}\right)J|2_1\rangle,$$
$$H_{Ising}|2_\rho\rangle=-(N-\rho-3)J|2_\rho\rangle,\quad\rho\geq2.\qquad(16)$$

The string bipolaron ground state is sought in the form of the linear combination

$$|2s\rangle=\sum_{\rho=1}^{\infty}\beta(\rho)|2_\rho\rangle.\qquad(17)$$

If we apply the Hamiltonian H_0 to this state, we arrive at the discrete representation of the Schrödinger equation $H_0|2s\rangle=E|2s\rangle$:

$$-2t\sqrt{3}\beta(2)-(J/2)\beta(1)=E_{2s}\beta(1),$$
$$-2t\sqrt{3}[\beta(\rho-1)+\beta(\rho+1)]$$
$$+J(\rho-1)\beta(\rho)=E_{2s}\beta(\rho),\quad\rho\geq2.\qquad(18)$$

Here $E_{2s}=E+(N-4)J$ is the string bipolaron energy measured from the background (Ising) energy of the Néel state containing two isolated holes.

In the continuum limit these recurrence relations yield the Schrödinger equation $\mathscr{H}_{2s}\beta=E_{2s}\beta$ with the effective Hamiltonian

$$\mathscr{H}_{2s}=2t\sqrt{3}[-2+(d/d\bar{\rho})^2]+J\bar{\rho},\quad\bar{\rho}=\rho-1\qquad(19)$$

and a wave function $\beta(\bar{\rho})$ specified on the semiaxis $0<\bar{\rho}<\infty$. The first recurrence relation in (18) yields the boundary condition $\beta(0)=0$. The boundary condition at infinity corresponds to a variational problem with a free end: $\beta'(\infty)=0$.

Thus, the effective Hamiltonian of a string bipolaron, $\mathscr{H}_{2s}$, differs from the effective Hamiltonian of a string polaron, $\mathscr{H}_{1s}$, only in that $2t$ has replaced t. This makes it possible to use Eqs. (12) and (13) directly to obtain the ground-state energy E_{2s} and the average string length ρ_2 for a string bipolaron:

$$E_{2s}=-4t\sqrt{3}+s_0(2tJ^2\sqrt{3})^{1/3},\qquad(20)$$

$$\rho_2=1+\langle\bar{\rho}\rangle=1+(2s_0/3)(2t\sqrt{3}/J)^{1/3}.\qquad(21)$$

The expression for the binding energy of the two holes in a string bipolaron follows directly from Eqs. (12) and (20) for E_{1s} and E_{2s}:

$$\Delta_s=2E_{1s}-E_{2s}=s_0(2-2^{1/3})(tJ^2\sqrt{3})^{1/3}\approx2{,}08(tJ^2)^{1/3}.\qquad(22)$$

It is quite obvious that the ansatz (14) and (17) describes a string bipolaron with zero total momentum. Building the states of a string bipolaron with an arbitrary momentum $\mathbf{k}\neq0$ requires generalizing the basis (14). We introduce the base vectors $|2_{\rho i}\rangle$ in which not only the string length ρ is fixed but so is the position $\mathbf{i}$ of the pair's center of mass:

$$|2_{\rho i}\rangle = [N(2,\rho,\mathbf{i})]^{-1/2}\sum_{|l|=\rho}|2,l,\mathbf{i}\rangle. \tag{23}$$

Here $\mathbf{i} = (i_x, i_y)$ is a vector index specifying the position of the center of mass (the components i_x and i_y are half-integers, generally speaking), l is the configuration of the string and $|2,l,\mathbf{i}\rangle$ is the respective state, and $N(2,\rho,\mathbf{i})$ is the number of such states with fixed values of $\mathbf{i}$ and $|l| = \rho$.

The momentum state of a string bipolaron is given by the linear combination

$$|2s,\mathbf{k}\rangle = N^{-1/2}\sum_{\rho,\mathbf{i}}\beta_{\mathbf{k}}(\rho)e^{i\mathbf{k}\mathbf{i}}|2_{\rho i}\rangle, \tag{24}$$

where the coefficients $\beta_{\mathbf{k}}(\rho)$ are found from a variational principle. These coefficients can be shown to satisfy the same recurrence relations (18) as the $\beta(\rho)$ do but with t replaced by $\frac{1}{2}t(\cos\frac{1}{2}k_x + \cos\frac{1}{2}k_y)$. Doing the same in the expression (20) for the ground-state energy E_{2s} and ignoring terms of the order of $J^{2/3}$ in the limit of $J/t \ll 1$, we obtain the dispersion law (see Appendix A)

$$E_{2s}(\mathbf{k}) = -2t\sqrt{3}[\cos(k_x/2) + \cos(k_y/2)] \tag{25}$$

and the effective string-bipolaron mass

$$m = (t\sqrt{3}/2)^{-1}. \tag{26}$$

3. STRING STATES IN THE t–J MODEL

Going from the t–J_z model to the t–J model requires allowing for spin fluctuations, whose source is the transverse part of the spin Hamiltonian,

$$H_\perp = \frac{J}{2}\sum_{\langle ij\rangle}(S_i^+S_j^- + S_j^+S_i^-).$$

First, we note that the recurrence relations (9) and (18) can be considered the result of minimizing the average energy $\langle H_0\rangle$ over the states (8) and (17). What happens if the Hamiltonian H_0 of the t–J_z model is replaced by the Hamiltonian $H = H_0 + H_\perp$ of the t–J model, or the total energy $\langle H\rangle = \langle H_0\rangle + \langle H_\perp\rangle$ is minimized? In this section we see that allowing for spin fluctuations has two effects, the renormalization of the string's tension (the same for the string polaron and the string bipolaron), and string-polaron delocalization. Let us briefly consider both.

3.1. Renormalization of the string's tension

We examine the action of the operator

$$H_\perp = \frac{J}{2}\sum_{\langle ij\rangle}(S_i^+S_j^- + S_j^+S_i^-)$$

on string states. The operator forces the spins at two neighboring sites to change places. It may, for instance, cause two neighboring spins on a straight segment of the string proper to change places. Such a process, depicted in Fig. 3b, "snaps" the string, and the "two-string" state is orthogonal to any "single-string" state, with the result that such processes contribute nothing to the variational energy. The same is true of processes of creation of a new string not linked to the initial one (Fig. 3c).

There is, however, a variant of such processes which does provide a contribution to the variational energy. In a process of this kind two spins in the immediate vicinity of the structure change places (Fig. 3d). The state remains "single-string" and the string's length increases by 2. In the reverse process the length diminishes by 2 (Fig. 3e). Allowing for such processes results in the appearance of nonzero matrix elements of operator $H_\perp$ between the base vectors (5) and also between the base vectors (14) (see Appendix B):

$$\langle 1_{\rho\pm2}|H_\perp|1_\rho\rangle = \langle 2_{\rho\pm2}|H_\perp|2_\rho\rangle = J\rho/3. \tag{27}$$

Going on to ansatz (8) and ansatz (17), we notice that in the limit of $J/t \ll 1$, where the coefficients $\alpha(\rho)$ and $\beta(\rho)$ are fairly smooth functions ($\alpha(\rho\pm2)\simeq\alpha(\rho)$ and $\beta(\rho\pm2)\simeq\beta(\rho)$), we can replace Eqs. (27) with the diagonal relations:

$$\langle 1_\rho|H_\perp|1_\rho\rangle \approx \langle 2_\rho|H_\perp|2_\rho\rangle \approx J\rho/3. \tag{28}$$

Thus, we arrive at a renormalization of the Ising energy of the string,

$$\langle 1_\rho|H_{Ising}|1_\rho\rangle \approx \langle 2_\rho|H_{Ising}|2_\rho\rangle \approx J\rho$$

by $J\rho/3$, that is, a renormalization of the exchange constant: $J\to J_{\text{eff}} = BJ$, with $B = 4/3$. Performing this substitution in Eqs. (12), (20), and (22) belonging to the t–J_z model, we find, respectively, the ground-state energies of a string polaron and a string bipolaron and the binding energy of a string bipolaron in the t–J model:

$$E_{1s} = -2t\sqrt{3} + s_0(tB^2J^2\sqrt{3})^{1/3}, \tag{29}$$

$$E_{2s} = -4t\sqrt{3} + s_0(2tB^2J^2\sqrt{3})^{1/3}, \tag{30}$$

$$\Delta_s = s_0(2 - 2^{1/3})(tB^2J^2\sqrt{3})^{1/3} \approx 2{,}52(tJ^2)^{1/3}. \tag{31}$$

Equation (21) yields the average string length for the string bipolaron in the t–J model:

$$\rho_2 = 1 + \frac{2s_0}{3}\left(\frac{2t\sqrt{3}}{BJ}\right)^{1/3} \approx 1 + 2{,}14\left(\frac{t}{J}\right)^{1/3}. \tag{32}$$

The results obtained in this manner exhaust the effect of spin fluctuations on a pair state within the "single-string" ansatz (17).

There is a reason for analyzing the possibility of allowing for "multistring" states similar to the one depicted in Fig. 3c. Apparently, this is equivalent to allowing for spin fluctuations over the Néel background. Since a new string can originate at any point of the lattice, the energy acquires an additional term proportional to N, the total number of sites. This renormalizes the energy of the antiferromagnetic background, the energy E_0 of the ground state in the t–J model in the absence of doping. For a Heisenberg antiferromagnet such a renormalization, as is known, reduces to replacing the exchange constant J in the energy of a Néel state with $\hat{J}_{\text{eff}} = \hat{B}J$, where $\hat{B}\simeq 1.332$ (see Ref. 13). In the t–J model this yields $E_0 = -NJ(1+\hat{B})/2$ for the electromagnetic-background energy.

An interesting fact is the extremely close values of the effective exchange constants in the string's tension ($B = 4/3$) and in the energy of the antiferromagnetic background ($\hat{B}\simeq 1.332$). In what follows we assume these constants equal: $\hat{B}\simeq B$.

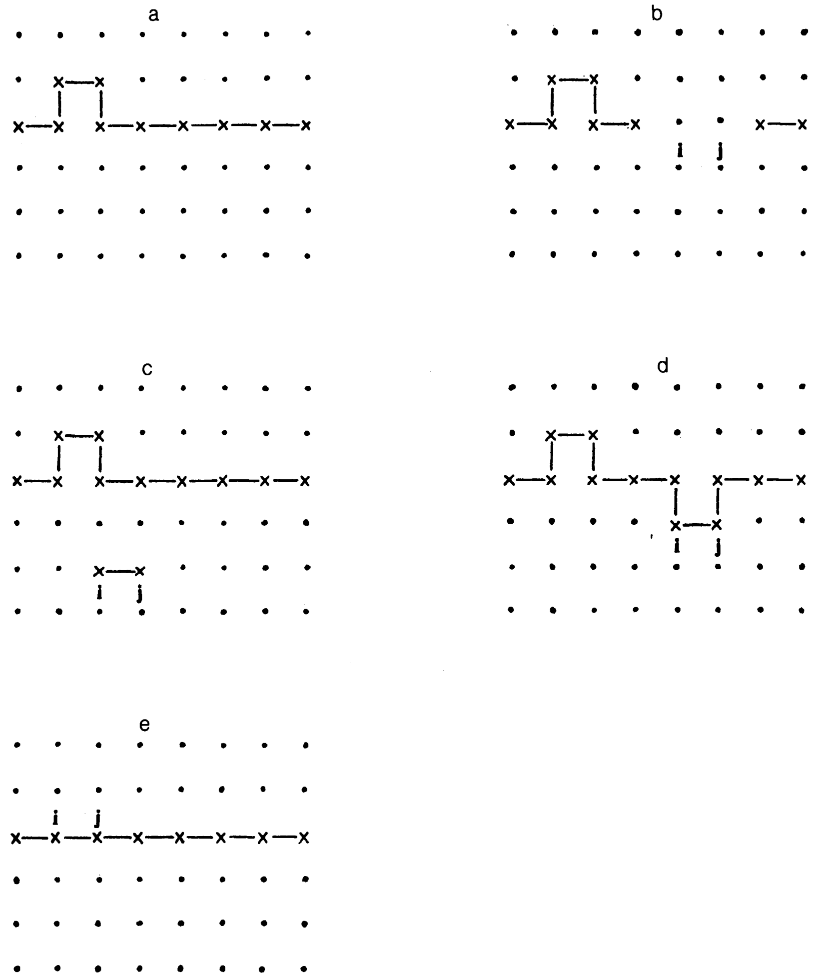

FIG. 3. The result of $H_\perp$ acting on a string: (a) the initial state of the string, (b) breaking of the string, (c) creation of a new string, (d) the length of the string decreases by a factor of 2, and (e) the length of the string increases by a factor of 2.

3.2. The momentum state of a string polaron

In the case of a string polaron one of the string's ends does not contain a hole (Fig. 4). Applying the operator $H_\perp$ to the first two spins of that end of the string, we obtain a new "single-string" state in which the string has become shortened by a factor of 2 (Figs. 4a and 4b). In a similar way the string can be made longer by a factor of 2 (Fig. 4c). To describe such processes we must provide the base vectors $|1_\rho\rangle$ corresponding to the states of a string polaron with a given string length ρ, with an additional vector index $\mathbf{i}=(i_x,i_y)$ that specifies the position of the string's end. Clearly, the respective matrix elements of $H_\perp$ are (see Appendix B)

$$\langle 1_{\rho'\mathbf{i}'}|H_\perp|1_{\rho\mathbf{i}}\rangle=\begin{cases} J/8 & \text{if} \quad |\rho'-\rho|=2, \ |\mathbf{i}'-\mathbf{i}|=2 \\ J/4 & \text{if} \quad |\rho'-\rho|=2, \ |\mathbf{i}'-\mathbf{i}|=\sqrt{2}. \\ 0 & \text{otherwise} \end{cases} \tag{33}$$

This enables finding the dispersion law for the delocalized state of a string polaron with a given momentum $\mathbf{k}$. Such a state has the standard form[14]

$$|1s,\mathbf{k}\rangle=\left(\frac{2}{N}\right)^{1/2}\sum_{\rho,\mathbf{i}} e^{i\mathbf{k}\mathbf{i}}\alpha_{\mathbf{k}}(\rho)|1_{\rho\mathbf{i}}\rangle, \tag{34}$$

in which the vector index $\mathbf{i}$ runs through $N/2$ values corresponding to one of the two sublattices. What is needed is the average value of operator $H_\perp$ on this state, where in the limit $J/t\ll 1$ we must put $\alpha_{\mathbf{k}}(\rho)\neq\text{const}$. This yields a $\mathbf{k}$-dependent term in the total energy:

$$\begin{aligned}\langle 1s,\mathbf{k}|H_\perp|1s,\mathbf{k}\rangle &=\frac{2}{N}\sum_{\mathbf{i}}\Big\{\sum_{\delta}\exp(2i\mathbf{k}\delta)(\langle 1_{\rho+2,\mathbf{i}+2\delta}|H_\perp|1_{\rho,\mathbf{i}}\rangle \\ &\quad+\langle 1_{\rho-2,\mathbf{i}+2\delta}|H_\perp|1_{\rho,\mathbf{i}}\rangle) \\ &\quad+\sum_{\delta\neq\delta'}\exp[i\mathbf{k}(\delta+\delta')](\langle 1_{\rho+2,\mathbf{i}+\delta+\delta'}|H_\perp|1_{\rho,\mathbf{i}}\rangle \\ &\quad+\langle 1_{\rho-2,\mathbf{i}+\delta+\delta'}|H_\perp|1_{\rho,\mathbf{i}}\rangle)\Big\} \\ &=2\frac{J}{8}\sum_{\delta}\exp(2i\mathbf{k}\delta)+2\frac{J}{4}\sum_{\delta\neq\delta'}\exp[i\mathbf{k}(\delta+\delta')] \\ &=J\{(\cos k_x+\cos k_y)^2-1\},\end{aligned} \tag{35}$$

where the δ are elementary translation vectors. Thus, the dispersion law for a string polaron in the t–J model is

$$E_{1s}(\mathbf{k})=J[\cos k_x+\cos k_y]^2+\text{const}. \tag{36}$$

A similar dispersion law for a single hole (with the coefficient J replaced by $J/2$) has been cited many times in Refs. 11 and 15 as a successful law for describing the results of

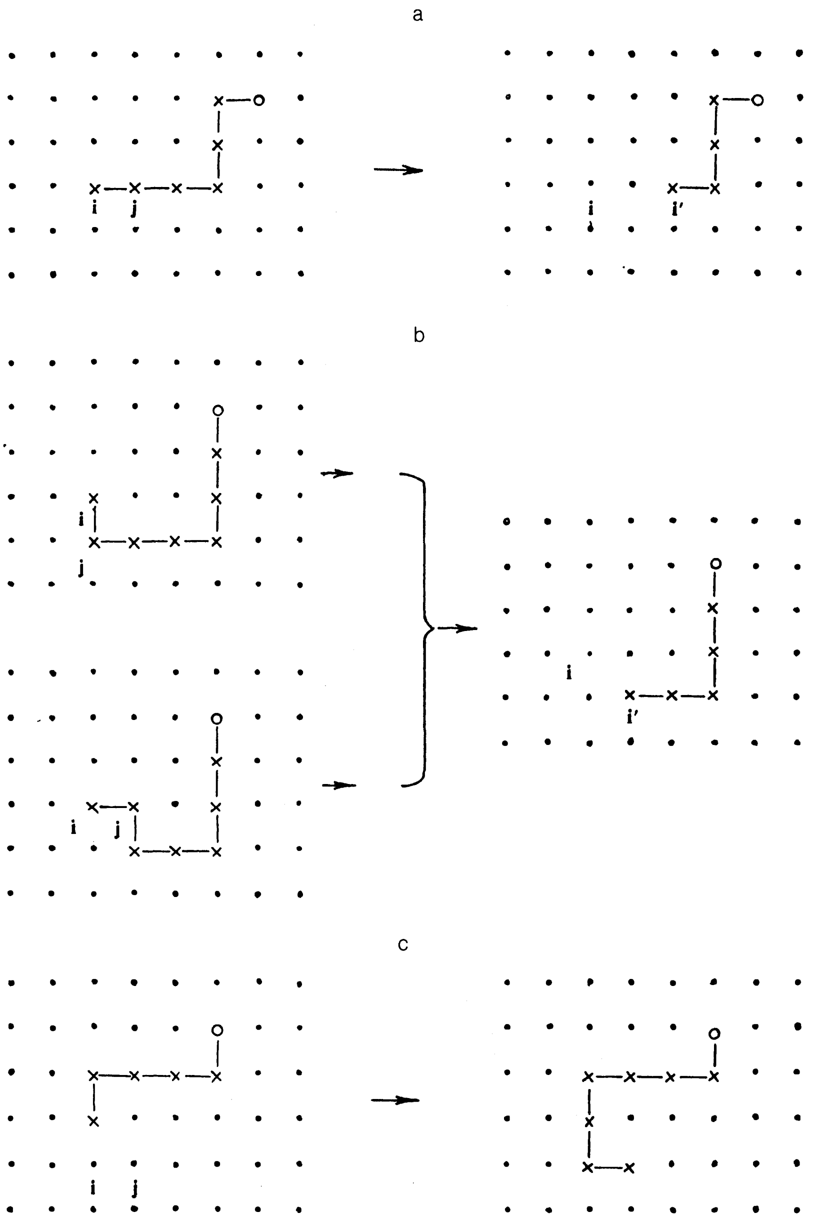

FIG. 4. The result of $H_\perp$ acting on the end of a string: (a) the length of the string decreases by a factor of 2 and the end shifts by a factor of 2, (b) the length of the string decreases by a factor of 2 and the end shifts by a factor of $\sqrt{2}$, and (c) the length of the string increases by a factor of 2.

numerical calculations on 4×4 and $\sqrt{18}\times\sqrt{18}$ clusters. Kane, Lee, and Read[16] arrived at a similar result for the anisotropic t–J model, which is close to the Ising model. In order to obtain such a law, Richter, Appel, and Hertel[17] went beyond the scope of the standard t–J model and allowed for the so-called triple term in the Hamiltonian. I believe the spectrum (36) has been obtained from the ordinary t–J model for the first time.

4. FERROMAGNETIC STATES IN THE t–J MODEL

In accordance with Nagaoka's theorem,[18] for $J/t\to0$ the ground state of a doped Hubbard system is ferromagnetic. As Nagaev, Emery, Kivelson, and Lin[19,20] demonstrated, at a fixed value of parameter J/t there is indeed a transition to a homogeneous ferromagnetic state as the average hole concentration $x=N_h/N$ grows. But before this happens, the system separates into two phases, the antiferromagnetic (without holes) and the ferromagnetic (with holes). What actually happens is that holes condense into a ferromagnetic drop.

Since for $J/t\to0$ a ferromagnetic state is the ground state, the competition of ferromagnetic states with string states must determine the point of crossover from one type of state to the other in the parameter J/t. In this section we consider ferromagnetic states in the t–J model and the competition of these states with string states.

4.1. A single hole (ferromagnetic polaron)

A ferromagnetic polaron constitutes a spherical ferromagnetically ordered region Ω of radius $R\gg1$. A hole moves freely only inside this region (the band mass of a hole is of order t^{-1}). Outside Ω, antiferromagnetic order blocks the free motion of the hole (the band mass is much larger than t^{-1}) and the wave function of the hole vanishes. Thus, calculating the energy of a ferromagnetic polaron reduces to solving the Schrödinger equation inside Ω with a zero boundary condition. The effective one-particle Hamiltonian has the form

$$\mathscr{H}_{1f}=t(-4+\nabla^2)+\pi R^2J(1+B)/2. \qquad (37)$$

The last term on the right-hand side allows for an increase in the energy of the exchange coupling of spins when the antiferromagnetic state ($-BJ/4$ per bond) transforms into the ferromagnetic state ($+J/4$ per bond). The ground state energy of this Hamiltonian is known:

$$E(R) = t(-4 + z_0^2/R^2) + \pi R^2 J(1 + B)/2, \tag{38}$$

where $z_0 \approx 2.405$ is the first zero of the zeroth Bessel function $J_0(z)$. Minimization of the function $E(R)$ yields the equilibrium radius $R = R_1$ and the ground-state energy $E_{1f} = E(R_1)$ of a ferromagnetic polaron:

$$R_1 = \left[\frac{2z_0^2}{\pi}\frac{1}{1+B}\frac{t}{J}\right]^{1/4}, \tag{39}$$

$$E_{1f} = -4t + 2z_0[\pi(1 + B)tJ]^{1/2}. \tag{40}$$

Comparison of this energy with the energy E_{1s} of the string-polaron ground state (29) shows that a ferromagnetic polaron is realized for $J/t < 4.70 \times 10^{-3}$ and a string polaron for $J/t > 4.70 \times 10^{-3}$.

4.2. A pair of holes (ferromagnetic bipolaron)

In the case of a ferromagnetic bipolaron the problem does not change drastically and remains one-particle in essence. It amounts to calculating the energy of two noninteracting fermions inside a sphere of radius R. After minimization in R, the energy of the ground state of a ferromagnetic bipolaron becomes

$$E_{2f} = -8t + (z_0^2 + z_1^2)^{1/2}[2\pi(1 + B)tJ]^{1/2}, \tag{41}$$

where $z_1 \approx 3.832$ is the first zero of the first Bessel function $J_1(z)$. This energy is lower than the energy of two noninteracting ferromagnetic polarons by the quantity

$$\Delta_f = [2z_0 - (z_0^2 + z_1^2)^{1/2}][2\pi(1 + B)tJ]^{1/2} \approx 1{,}09(tJ)^{1/2}, \tag{42}$$

which has the meaning of the binding energy of two holes in a ferromagnetic bipolaron.

Comparison of the energy of a ferromagnetic bipolaron with that of a string bipolaron shows that the ferromagnetic bipolaron is realized when $J/t < 4.74 \times 10^{-3}$ and a string bipolaron when $J/t > 4.74 \times 10^{-3}$. In both cases pairing is favorable energywise, although the pairing mechanisms differ considerably. The difference becomes apparent as the number of interacting holes grows.

4.3. A macroscopic number of holes (ferromagnetic drop)

If a system contains $N_h \gg 1$ holes, it may separate into two phases, the antiferromagnetic (without holes) and the ferromagnetic (with holes). Let N_f be the number of sites in the ferromagnetic phase. Then the energy of the system measured from the energy of the antiferromagnetic background, $E_0 = -NJ(1+B)/2$, is

$$E = N_h[-4t + 2\pi tx + J(1 + B)/2x] \equiv N_h\varepsilon(x), \tag{43}$$

where $x = N_h/n_f$ is the hole concentration in the ferromagnetic phase. The first and second terms (of order t) represent the kinetic energy of the holes, $\langle H_t \rangle$, and the third term (of the order of J) the exchange spin-coupling energy, $\langle H_J \rangle$.

Minimization in x yields the following expression for the equilibrium hole concentration in the ferromagnetic phase:

$$x_0 = \left(\frac{1+B}{4\pi}\right)^{1/2}\left(\frac{J}{t}\right)^{1/2}. \tag{44}$$

This is a constant quantity independent of N_h. The volume of the ferromagnetic phase increases linearly with the number of holes: $N_f = N_h/x_0$. Each new hole increases the volume of the ferromagnetic phase by the same quantity x_0^{-1}. This means that holes condense into a homogeneous ferromagnetic drop. When the number of holes $N_h = x_0 N$ becomes very great, the ferromagnetic drop fills the entire volume and hence degenerates into a homogeneous ferromagnetic phase.

The energy per hole in a ferromagnetic drop is

$$\varepsilon \equiv \varepsilon(x_0) = -4t + 2[\pi(1 + B)]^{1/2}(tJ)^{1/2}. \tag{45}$$

Any fission of the drop into smaller ones is disadvantageous because the surface energy would grow.[21] For instance, fission into ferromagnetic polarons or bipolarons is disadvantageous because of the inequality $\varepsilon < E_{2f}/2 < E_{1f}$. Among ferromagnetic states the ferromagnetic drop has the smallest energy.

At the same time, comparison of the energy of a ferromagnetic drop with that of $N_h/2$ noninteracting string pairs shows that for

$$J/t > 1{,}52 \cdot 10^{-2} \tag{46}$$

we have $E_{2s} < 2\varepsilon$. This means that for $1.52 \times 10^{-2} < J/t \ll 1$, string pairs are the leading candidate for the ground state of the doped t–J model. For $J/t < 1.52 \times 10^{-2}$, the variational "leader" is replaced by the ferromagnetic drop. As the J/t parameter further decreases ($J/t \to 0$), the ferromagnetic drop fills the entire volume and, in full agreement with Nagaoka's theorem, the ground state becomes homogeneous and ferromagnetic.

Here it is proper to compare the string and ferromagnetic mechanisms of hole interaction. The first clearly exhibits a saturation property and yields only pairing. The interaction energy of two string pairs is on the order of $J\rho_2 \sim (tJ^2)^{1/3}$, and for $t/J \ll 1$ is insufficient for pair coupling because of the small effective mass of a string pair ($\sim t^{-1}$). The ferromagnetic mechanism, on the other hand, does not exhibit saturation and leads to the condensation of all the holes into a single drop.

5. CONCLUSIONS

Below we list the main results that follow from a combined analysis of the string ansatz (17) and ferromagnetic states in the t–J model.

(1) Two separate holes form a bound state. This is a string pair with a binding energy $\Delta_s \approx 2.52(tJ^2)^{1/3}$ for $J/t > 4.74 \times 10^{-3}$ and a ferromagnetic bipolaron with a binding energy $\Delta_f \approx 1.09(tJ)^{1/2}$ for $J/t < 4.74 \times 10^{-3}$.

(2) A string pair has an effective mass $(t\sqrt{3}/2)^{-1}$.

(3) A system consisting of $N_h \gg 1$ holes separates into $N_h/2$ string pairs when $J/t > 1.52 \times 10^{-2}$, but for $J/t < 1.52 \times 10^{-2}$ the holes condense into a ferromagnetic drop.

TABLE I. The radius R_1 of a ferromagnetic polar and the average string length of a string polaron, ρ_1, and of a string bipolaron, ρ_2, as functions of parameter J/t.

J/t	R_1	ρ_1	ρ_2
0,01	3,5	7,9	10,9
0,02	3,0	6,3	8,9
0,05	2,4	4,6	6,8
0,1	2,0	3,7	5,6
0,2	1,7	2,9	4,7
0,5	1,3	2,1	3,8

Since all these results have been obtained by the variational approach, it is proper to compare them with those obtained by numerical analysis of the t–J model on finite clusters. Much work has been done in this area and several interesting results have been achieved (see Refs. 9–12). Practically all, however, belong to small clusters with dimensions ranging from 4×4 to $\sqrt{20}\times\sqrt{20}$. But are such sizes sufficient for a correct estimate of the effects of hole pairing and condensing? The answer is provided by Table I, which lists the radius R_1 of a ferromagnetic polaron and the average string length in the cases of a single hole (ρ_1) and a string pair (ρ_2) calculated for different values of parameter $J/t = 0.01$–0.5. We see that the finite size of a cluster (~ 4) begins to have an effect on ferromagnetic states for $J/t \lesssim 0.01$, on the string state of a single hole for $J/t \lesssim 0.1$, and on a string pair for $J/t \lesssim 0.5$.

Thus, numerical analysis of small clusters cannot serve as a meaningful description of pair states in the physical region $J/t \ll 1$. At the same time we note the presence of bound states of two holes in the region $J/t \geqslant 0.2$, a fact discovered by several researchers.[9,11,12] The binding energies of these states monotonically increase with J. The absence of a bound states for $J/t < 0.2$ on a 4×4 cluster is natural since when the volume is limited "ionization by pressure" occurs.

Barnes, Dagotto, Moreo, and Swanson[10] studied the state of a single hole in the t–J_z model using a 8×8 cluster. As Table I shows, their study may be considered meaningful for $J/t \geqslant 0.01$. The dependence of the ground-state energy on parameter J/t obtained by these researchers,

$$E_{1s}^{\exp}/t = -3,63 + 2,93(J/t)^{2/3} \tag{47}$$

agrees well with the theoretical formula that follows from the string ansatz (5),

$$E_{1s}^{theor}/t = -3,46 + 2,81(J/t)^{2/3}. \tag{48}$$

More than that, for $J/t \approx 0.01$ the beginning of a crossover from a string polaron to a ferromagnetic is observed. Thus, the string ansatz for a single hole has received unambiguous justification in a numerical experiment.

Table I implies that for a verification of the string-pair ansatz in the physical region $J/t \ll 1$ that is as reliable as the above, we must consider 6×6 clusters, and that obtaining the correct value of the crossover point, $J/t = 1.52\times10^{-2}$, requires considering 10×10 clusters. No data on the numerical analysis of pair states in the t–J model on clusters of such dimensions have been cited in the literature.

In conclusion we note that the string pairing of holes has been considered here in the low-concentration limit, $x \ll 1$. A simple mechanism that limits the effectiveness of string pairing precisely to low concentrations is worth mentioning. Namely for $(x/2)\rho_2 > 1/2$ strings involve more than half of the lattice sites. This leads to a reversal of the sign of the string tension: in this situation it is more advantageous for a string to stretch than to shrink. Since we have $\rho_2 \sim (t/J)^{1/3}$, this happens at $x \sim (J/t)^{1/3}$. Hence, string pairing takes place only for $x \lesssim (J/t)^{1/3}$.

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APPENDIX A. THE MOMENTUM STATE OF A STRING BIPOLARON

Let us study in greater detail the base vector of the state of a string bipolaron with a fixed position $\mathbf{i}$ of the center of mass and a string length ρ:

$$|2_{\rho,\mathbf{i}}\rangle = [N(2,\rho,\mathbf{i})]^{-1/2} \sum_{|l|=\rho} |2, l, \mathbf{i}\rangle. \tag{A1}$$

Here $\mathbf{i} = (i_x, i_y)$ is the radius vector of the center of mass, with components that can be both integers and half-integers. It is easy to see that for ρ even the norm $\mathbf{i} = |i_x + i_y|$ is an integer and for ρ odd it is a half-integer. In the continuum limit $\rho \gg 1$ and the tree approximation, the number of trajectories of a given length is $N(2,\rho,\mathbf{i}) \approx 3^{\rho-1}$.

The action of the translational part H_t of the Hamiltonian changes the string length by 1 and shifts the center of mass by 1/2. Hence, the matrix elements of H_t in this basis are

$$\langle 2_{\rho'\mathbf{i}'}|H_t|2_{\rho\mathbf{i}}\rangle = \begin{cases} -t\sqrt{3}/2 & \text{if} \quad |\rho'-\rho| = 1, \quad |\mathbf{i}'-\mathbf{i}| = 1/2 \\ 0 & \text{otherwise} \end{cases}. \tag{A2}$$

The origin of the factor $\sqrt{3}/2$ can be explained in the following way. When acting on the state with the center of mass at point $\mathbf{i}$, the Hamiltonian H_t must move the center of mass to point $\mathbf{i}' = \mathbf{i} + \delta/2$, with $\boldsymbol{\delta}$ a fixed elementary translation vector, and, in the process, change in a specified manner the string length ρ (for the sake of definiteness, to increase the length by 1). This can be achieved by shifting the first or second hole by vector $\boldsymbol{\delta}$. Here only 75% of all the $2\times3^{\rho-1}$ possibilities leads to an increase in string length (the remaining 25% decrease it). As a result we get $(3/2)3^{\rho-1}$ matrix elements ($-t$) whose sum should be multiplied by the normalization factors of the initial ($3^{-(\rho-1)/2}$) and final ($3^{-\rho/2}$) states. The result is $-t\sqrt{3}/2$.

If in the limit $J/t \ll 1$ we ignore the contribution to the energy of the momentum state (24) from the tension of the string [it is of the order of $(tJ^2)^{1/3}$] and the weak ρ-dependence of the coefficients $\beta_{\mathbf{k}}$ (i.e., by assuming that $\beta_{\mathbf{k}} \equiv \text{const}$), we arrive at the following dispersion law for a string bipolaron:

$$\begin{aligned} E_{2s}(\mathbf{k}) &\approx \langle 2s, \mathbf{k}|H_t|2s, k\rangle \\ &= N^{-1}\sum_{\mathbf{i},\boldsymbol{\delta}} \Big[\langle 2_{\mathbf{i}+\delta/2,\rho+1}|H_t|2_{\mathbf{i},\rho}\rangle \\ &\quad + \langle 2_{\mathbf{i}+\delta/2,\rho-1}|H_t|2_{\mathbf{i},\rho}\rangle\Big] e^{i\mathbf{k}\delta/2} \\ &= -2t\sqrt{3}[\cos(k_x/2) + \cos(k_y/2)]. \end{aligned} \tag{A3}$$

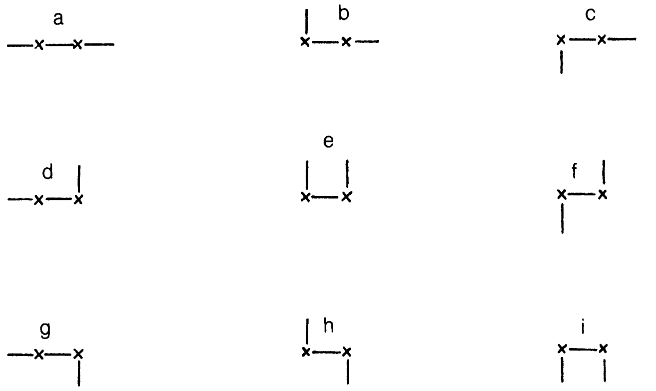

FIG. 5. Possible configurations of the neighborhood of a segment of the string.

Note that if in the energy we retain the contribution from the string tension (i.e., average $H_0 = H_t + H_{\rm Ising}$ rather than H_t) and keep the ρ-dependence in the $\beta_{\bf k}$ coefficients, after minimizing the total energy we arrive at recurrence relations for $\beta_{\bf k}(\rho)$ identical with the case ${\bf k} = 0$ except that t is replaced by $\frac{1}{2}t(\cos\frac{1}{2}k_x + \cos\frac{1}{2}k_y)$. Performing this manipulation with the energy (20) of a bipolaron at rest, we arrive at the same dispersion law (A3) with corrections on the order of $(tJ^2)^{1/3}$.

APPENDIX B. MATRIX ELEMENTS OF OPERATOR $H_\perp$

The matrix element of $H_\perp = \frac{1}{2}J\Sigma_{(ij)}(S_i^+S_j^- + S_i^-S_j^+)$ between "single-string" base vectors of string states is nonzero only if the initial and final lengths of the string differ by 2. Here either the shape of the string changes (see Figs. 3d and 3e) or, in the case of a string polaron, the end of the string is displaced (see Fig. 4).

First we consider the matrix element $\langle 2_{\rho-2}|H_\perp|2_\rho\rangle$ corresponding to shortening of the string in the string bipolaron (see Fig. 3e). Acting on the base vector $|2_\rho\rangle$, the operator $H_\perp$ may change the configuration of any of the ρ segments of the string. Altogether the neighborhood of a segment has nine possible configurations (Fig. 5). Only two of these, (e) and (i), allow for a decrease in string length.

In the tree approximation all nine configurations of the neighborhood of a segment are equally probable. Hence, the action of the operator $H_\perp$ on the state $|2_\rho\rangle$, a linear combination of $2N\times 3^{\rho-1}$ states of a string of length ρ, results in $(2/9)\rho\times 2N\times 3^{\rho-1}$ states with a string length $\rho - 2$. If we allow for the presence in $H_\perp$ of the factor $J/2$ and for the normalization factors $(2N\times 3^{\rho-1})^{-1/2}$ in state $|2_\rho\rangle$ and $(2N\times 3^{\rho-3})^{-1/2}$ in state $|2_{\rho-2}\rangle$, we obtain the desired matrix element $(J/2)(2/9)\rho\times 2N\times 3^{\rho-1}\times(2N\times 3^{\rho-1}2N\times 3^{\rho-3})^{-1/2} = J\rho/3$:

$$\langle 2_{\rho\pm 2}|H_\perp|2_\rho\rangle = J\rho/3. \tag{B1}$$

There is no need for a separate calculation of the matrix element $\langle 2_{\rho+2}|H_\perp|2_\rho\rangle$ corresponding to a decrease in the string length by 2, since operator $H_\perp$ is Hermitian.

Next we consider the matrix element $\langle 1_{\rho\pm 2,{\bf i}'}|H_\perp|1_{\rho,{\bf i}}\rangle$ corresponding to a variation in the string's length in a string polaron. If the end of the string does not change its position (${\bf i}' = {\bf i}$), the above reasoning remains valid and the value of the matrix element is the same:

$$\langle 1_{\rho\pm 2}|H_\perp|1_\rho\rangle = J\rho/3. \tag{B2}$$

But if the end of the string does change its position (${\bf i}'\neq{\bf i}$; Fig. 4), two situations are possible: either $|{\bf i}'-{\bf i}| = 2$ (Fig. 4a) or $|{\bf i}'-{\bf i}| = \sqrt{2}$ (Fig. 4b).

The first corresponds to initial configurations of the string in which two initial segments have the same fixed direction ${\bf i}'-{\bf i} = 2\delta$. The fraction of such configurations is $(4\times 3)^{-1}$ of all the $4\times 3^{\rho-1}$ states of the string, that is, $3^{\rho-2}$ configurations in all. Allowing for the presence of the normalization factor $(4\times 3^{\rho-1})^{-1/2}$ in the initial state and the normalization factor $(4\times 3^{\rho-3})^{-1/2}$ in the final state, we get the value of the desired matrix element, $(J/2)3^{\rho-2}(4\times 3^{\rho-1}\times 4\times 3^{\rho-3})^{-1/2} = J/8$.

The second case corresponds to initial configurations of the string in which the first two segments are at right angles. Here the position of the end of the second segment in relation to the beginning of the first is fixed by the vector ${\bf i}'-{\bf i} = \delta+\delta'$ $(\delta\neq\delta')$. The fraction of such configurations is $(4\times 3)^{-1}\times 2$. The additional factor 2 appears because of the two ways of passing from point ${\bf i}$ to point ${\bf i}'$ (see Fig. 4b). Repeating the previous reasoning, we arrive at $J/4$ for the value of the matrix element.

Thus, the matrix element of operator $H_\perp$ between the base states of a string polaron is (${\bf i}\neq{\bf i}'$)

$$\langle 1_{\rho'{\bf i}'}|H_\perp|1_{\rho{\bf i}}\rangle = \begin{cases} J/8 & \text{if} \quad |\rho'-\rho| = 2, \ |{\bf i}'-{\bf i}| = 2 \\ J/4 & \text{if} \quad |\rho'-\rho| = 2, \ |{\bf i}'-{\bf i}| = 2^{1/2}. \\ 0 & \text{otherwise} \end{cases} \tag{B3}$$

There is no need for a separate calculation of the matrix element $\langle 1_{\rho+2,{\bf i}'}|H_\perp|1_{\rho,{\bf i}}\rangle$ corresponding to an increase in string length (Fig. 4c), since operator $H_\perp$ is Hermitian.

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