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Pairing-induced kinetic energy lowering in doped antiferromagnets

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Abstract

We analyse lowering of the kinetic energy in doped antiferromagnets at the transition to the superconducting state. Measurements of optical conductivity indicate that such unconventional behaviour takes place in underdoped Bi-2212. We argue that the definition of the operator representing the kinetic energy is determined by experimental conditions. The thermodynamic average of that operator is related to the integrated spectral weight of the optical conductivity and thus depends on the cut-off frequency limiting that integral. If the upper limit of the integral lies below the charge transfer gap the spectral weight represents the average of the hopping term in the space restricted to the energy range below the gap. We show that the kinetic energy is indeed lowered at the superconducting transition in the t–J model (tJM), which is an effective model defined in the restricted space. That result is in agreement with experimental observations and may be attributed to the formation of spin polarons and the change of roles which are played by the kinetic and the potential energy in the tJM and in some effective model for spin polarons. The total spectral weight represents the kinetic energy in a model defined in a broader space if the upper limit in the integral of the optical conductivity is set above the gap. We demonstrate that the kinetic energy in the Hubbard model is also lowered in the superconducting state. That result does not agree with experimental observations, indicating that the spectral weight is conserved for all temperatures if the upper limit of the integral is set above the charge transfer gap. This discrepancy suggests that a single band model is not capable of describing in some respects the physics of excitations across the gap.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Recent experiments on underdoped Bi-2212 samples seem to indicate that the kinetic energy of the system is lowered when the material becomes superconducting [1–3]. This is in sharp contrast to BCS theory [4] which predicts an increase in the kinetic energy when superconductivity sets in. The reason for the lowering of the kinetic energy in the BCS model is very simple. When Cooper pairs are formed they condense in a state with zero pairing momentum. This causes a broadening of the momentum distribution $\langle n_{k,\sigma}\rangle$ by an amount of the order of the order parameter Δ. The broadening of the Fermi distribution implies an increase in kinetic energy which is, of course, overcompensated by the potential energy gain in the superconducting state. Experimental measurements concerning the kinetic energy are obtained via a measurement of the temperature and frequency-dependent real part of the optical conductivity $\sigma_1(\omega, T)$. There exists a relation between the optical conductivity and the kinetic energy of a model lattice Hamiltonian with a nearest-neighbour hopping term [5–8], i.e.

$$T_\delta = -\sum_i t_\delta [c^\dagger_{i,\sigma} c_{i+\delta,\sigma} + \text{H.c.}]. \tag{1}$$

Here $c^\dagger_{i,\sigma}$ ($c_{i,\sigma}$) creates (destroys) an electron with spin σ on the lattice site i and δ is a direction, e.g. in the square lattice. The relation between $\sigma_1(\omega, T)$ and T_δ is given by

$$\int_0^{\Omega_\mu} \sigma_{1\delta}(\omega, T)\,\mathrm{d}\omega = \frac{\pi^2 a_\delta^2 e^2}{2\hbar^2\Omega}\langle -T_\delta\rangle. \tag{2}$$

Here a_δ is a lattice constant in the direction of δ and Ω is the volume. The expectation value $\langle -T_\delta\rangle$ refers to a thermodynamic average with respect to the model system under consideration. The upper cut-off Ω_μ excludes transitions to higher energy states which are not described by the model Hamiltonian. We want to draw attention to the following: when Ω_μ is chosen in an experiment, e.g. by the experimentally available frequency range, then $\langle -T_\delta\rangle$ is determined for a model Hamiltonian which is suitable for describing properly the energy excitations within the same frequency range.

As pointed out above, experiments in the normal and superconducting states of Bi-2212 were performed by several groups. They determined the evolution with temperature of spectral weight

$$W(t, \Omega_\mu) = \int_0^{\Omega_\mu} \sigma_1(\omega, T)\,\mathrm{d}\omega. \tag{3}$$

In conventional superconductors one finds that for all $\Omega_\mu \geqslant 4\Delta$

$$W(T > T_\mathrm{c}, \Omega_\mu \geqslant 4\Delta) = W(T < T_\mathrm{c}, \Omega_\mu \geqslant 4\Delta), \tag{4}$$

indicating that $\sigma_1(\omega > 4\Delta, T)$ does not change when the system becomes superconducting. For smaller frequencies $\sigma_1(\omega, T)$ is depleted in the superconducting state. The depletion is compensated for by a contribution of the form $A\delta(\omega)$, which is caused by the condensate [9, 10]. In contrast to the above it was found that, in underdoped Bi-2212, one has to go up to 2 eV (instead of 4Δ) in order that an equivalent of equation (4) holds, i.e.

$$W(T > T_\mathrm{c}, \Omega_\mu \geqslant 2\ \mathrm{eV}) = W(T < T_\mathrm{c}, \Omega_\mu \geqslant 2\ \mathrm{eV}). \tag{5}$$

This shows that states up to the charge-transfer gap contribute to the formation of the superfluid. When, for example, in the experiment Ω_μ is chosen to be $\simeq$0.125 eV, which is of the order of 4Δ and also of the order of the exchange integral J in the cuprates, it is found that [3]

$$W(T > T_\mathrm{c}, \Omega_\mu \simeq 0.125\ \mathrm{eV}) < W(T < T_\mathrm{c}, \Omega_\mu \simeq 0.125\ \mathrm{eV}). \tag{6}$$

The inequality is still very pronounced for $\Omega_\mu \simeq 0.7$ eV. Therefore, according to equation (2) the kinetic energy decreases in a model when the system becomes superconducting. It is important to realize that this conclusion is correct only if the model Hamiltonian describes the excitations just in the range up to Ω_μ. If it also describes much higher energy excitations the kinetic energy $\langle T_\delta \rangle$ also contains contributions from the latter. In that case the left-hand side of equation (2) is no longer the measure of the kinetic energy of the model Hamiltonian. Rather, it describes the kinetic energy of an effective Hamiltonian obtained by a reduction to the energy range below Ω_μ.

The model Hamiltonian conventionally used for the cuprates is that of the t–J model (tJM). Its energy scale is given by the hopping matrix element t and is much smaller than the one of the Hubbard model, i.e. U. Here the on-site Coulomb integral U defines the scale of charge excitations. In the limit of low doping the energy scale of the tJM is reduced even further and is given by J. ARPES measurements for undoped and underdoped oxychlorides [12, 11] and several theoretical analyses [13] provide evidence for that reduction. Measured values are $J \simeq 0.125$ eV, $t \simeq 0.4$ eV and $U \simeq 2$ eV. Therefore the experiments with a cut-off Ω_μ in the energy range $0.125 \text{ eV} \simeq J \leqslant \Omega_\mu \leqslant t \simeq 0.4$ eV should be used to draw conclusions for changes with temperature of the kinetic energy within the tJM, rather than within the Hubbard, model.

The kinetic energy, which is defined by the hopping energy in a given model, is not the same as the kinetic energy defined in the same way in a model which has been obtained from that model by means of a unitary transformation and is valid for a narrower range of low energy excitations. In the next section we will discuss that relation for the example on the HM and the tJM for which the values of the hopping energy are different. We will also show that the cut-off frequency Ω_μ, which appears in the total spectral weight $W(T, \Omega_\mu)$, determines the microscopic model, the kinetic of which is directly related to $W(T, \Omega_\mu)$ by means of the formula (2). The central issue of this paper is the demonstration that the change of kinetic energy of the tJM at the transition to the SC state is in agreement with the experimentally measured change of $W(T, \Omega_\mu)$, while for the HM the change of the kinetic energy disagrees with the change of $W(T, \Omega_\mu)$. That statement suggests that, despite the relation between the HM and the tJM which may be obtained from the former model by means of the unitary transformation, the tJM provides the correct description of low energy excitations in cuprates in the energy range below the gap, while the behaviour of the HM, which also describes excitations across the gap, does not agree with the experimental observations made for cuprates.

Except for some numerical work [14–16] it is presently not possible to treat the differences between the normal and superconducting states within the tJM. But this can be done within a simplified version of it, which is the spin-polaron model (SPM). It describes the motion of a hole moving in a system with short-range AF correlations. One may also consider a spin polaron as a hole surrounded by a spin bag [17]. This assumed that the correlation length of this short-range order is longer than the radius of the polaron so that the background can be simply described by a Néel ordered state with some quantum fluctuations. In contrast to the tJM the spin polaron model neglects excitations of the spin bag. The propagation of the spin polaron determines the quasiparticle energy dispersion. This dispersion is of the order of J. The incoherent motion takes place at the scale of t. Processes related to incoherent hopping are incomplete in the SPM as compared with the tJM because of the neglect of the spin bag excitations. The energy of incoherent motion determines the eigenenergy of a hole trapped in a spin bag and sets a level from which the quasiparticle energy dispersion is measured. That level is of the order of t. We may consider the SPM as a representation of the tJM within the restricted basis of spin-polaron states. The kinetic energy of the tJM contributes predominantly to the interaction in the spin polaron model and, to a lesser extent,

to the quasiparticle motion. Two quasiparticles attract each other and can form a bound state, i.e. a Cooper pair. This allows for a description of the superconducting state. We will show that the transition to the superconducting state results in an increase of the kinetic energy within the spin-polaron model. This kinetic energy is of the order of J. But when we determine the kinetic energy of the tJM we find indeed that it decreases below T_c. This resolves an apparent puzzle pointed out at the beginning of the introduction. We shall also calculate the kinetic energy due to superconductivity within the Hubbard model. We find again that it decreases in the SC state.

The HM reduces to the tJM in the limit of strong correlations. The exchange energy in the tJM represents the double occupancies of sites caused by the kinetic term in the HM [18, 19]. Thus, the kinetic energy defined as a thermodynamic average of the hopping term is not identical in the tJM and in the HM. Nevertheless, the ambiguity in the definition of kinetic energy is, to some extent, spurious. As we have already mentioned, the cut-off frequency Ω_μ applied to the integral (3) of the measured optical conductivity determines which model we should choose in order to compare the kinetic energy with the spectral weight $W(t, \Omega_\mu)$. The lowering of the kinetic energy in the HM in the superconducting state contradicts the experimental observation that the integral of the optical conductivity $W(t, \Omega_\mu)$ is conserved at the superconducting transition if the upper limit in that integral Ω_μ is set above the gap energy. Thus, we shall conclude that a single band model, such as the HM, is not capable of describing correctly excitations across the gap. But an effective model, such as the tJM, captures the essential physics of low-energy excitations.

2. Kinetic energy in the tJM and in the HM

In this section we will find the answer to the following question: depending on the value of the cut-off frequency Ω_μ, which is the appropriate model in that the kinetic energy is related to the weight $W(t, \Omega_\mu)$? First we separate the states above the gap from the states below the gap by means of a unitary transformation [20]. We will perform that transformation for the example of the HM which seems to be the conceptually simplest model for describing processes in the wide energy range including the charge transfer energy U:

$$H_{\mathrm{HM}} = H_{\mathrm{hHM}} + H_U \tag{7}$$

$$H_{\mathrm{hHM}} = -t \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + \mathrm{h.c.}) \tag{8}$$

$$H_U = U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \tag{9}$$

Here H_{hHM} represents hopping in the HM between nearest neighbour sites i, j and defines the kinetic energy for that model. H_U refers to the on-site Coulomb repulsion. The tJM is derived from the HM by means of a unitary transformation $\hat{U}$ which separates the lower Hubbard band lying below the gap from the upper Hubbard band lying above the gap [21]. $\hat{U}$ transforms an operator $\hat{O}$ into $\hat{P}\hat{U}^\dagger \hat{O} \hat{U} \hat{P}$. We have additionally applied the projector $\hat{P}$ which restricts the action of the transformed operator to the low-energy space, which consists of states without doubly occupied sites. The expressions for the transformed kinetic and Coulomb energies in the HM have been thoughtfully analysed by Eskes *et al* [6]. The hopping term in the HM transforms into

$$H^{(tJ)}_{\mathrm{hHM}} = P\hat{U}^\dagger H_{\mathrm{hHM}} \hat{U} P = -t \sum_{i,\delta,\sigma} \tilde{c}^\dagger_{i+\delta,\sigma} \tilde{c}_{i,\sigma} + J \sum_{i,\delta,\delta',\sigma} \left(S_{i+\delta} S_i - \frac{\tilde{n}_{i+\delta} \tilde{n}_i}{4} \right) \tilde{c}^\dagger_{i+\delta,\sigma} \tilde{c}_{i+\delta',\sigma}. \tag{10}$$

where $\tilde{c}_{i,\sigma} = c_{i,\sigma}(1 - n_{i,\bar{\sigma}})$, $J = 4t^2/U$. If we neglect the correlated hopping between second and third NN in the second term, $H_{\mathrm{hHM}}^{(tJ)}$ is given by

$$H_{\mathrm{hHM}}^{(tJ)} = -t \sum_{\langle i,j\rangle,\sigma} (\tilde{c}_{i,\sigma}^{\dagger} \tilde{c}_{j,\sigma} + \mathrm{H.c.}) + 2J \sum_{\langle i,j\rangle} \left(S_i S_j - \frac{\tilde{n}_i \tilde{n}_j}{4} \right). \tag{11}$$

It consists of the hopping term in the tJM, $H_{\mathrm{h}tJ}$ plus twice the exchange term H_J, i.e. $H_{\mathrm{hHM}}^{(tJ)} = H_{\mathrm{h}tJ} + 2H_J$. For the transformed interaction term we may write

$$H_U^{(tJ)} = P\hat{U}^{\dagger} H_U \hat{U} P = -\frac{J}{2} \sum_{i,\delta,\delta',\sigma} \left(S_{i+\delta} S_i - \frac{\tilde{n}_{i+\delta} \tilde{n}_i}{4} \right) \tilde{c}_{i+\delta,\sigma}^{\dagger} \tilde{c}_{i+\delta',\sigma}, \tag{12}$$

and

$$H_U^{(tJ)} = -J \sum_{\langle i,j\rangle} \left(S_i S_j - \frac{\tilde{n}_i \tilde{n}_j}{4} \right). \tag{13}$$

The operator $H_U^{(tJ)}$ represents the interaction in the HM and equals the exchange term in the tJM with the negative sign, $H_U^{(tJ)} = -H_J$. As seen in (13), that operator favours ferromagnetic correlations. This effect is easy to understand: when spins at NN sites point in the same direction the hopping term cannot create a virtual state with a doubly occupied site. If spins at NN sites are antiparallel they can virtually hop on top of each other. This process gives rise to a lowering of the kinetic energy and an antiparallel configuration is favoured by the transformed hopping term in the HM as may be seen in (11). By comparing (11) with (13) one can see that the exchange term in the tJM favours AF correlations.

The Hamiltonian of the tJM in the space with no doubly occupied sites represents the full Hamiltonian of the HM in the low-energy regime, i.e. $H_{tJ} = P\hat{U}^{\dagger} H_{\mathrm{HM}} \hat{U} P$. The tJM may be expressed in terms of the sums $H_{tJ} = H_{\mathrm{hHM}}^{(tJ)} + H_U^{(tJ)}$ or $H_{tJ} = H_{\mathrm{h}tJ} + H_J$. Both the transformed Hamiltonian of the HM, H_{tJ}, and the transformed kinetic energy operator $H_{\mathrm{hHM}}^{(tJ)}$ contain terms related to the hopping ($H_{\mathrm{h}tJ}$) and the exchange energy (H_J) in the tJM. Therefore, if the system manages somehow to lower simultaneously the hopping energy and the exchange energy in the tJM, lowering of the total and kinetic energies defined for the HM is an obvious consequence.

We will decide now on the proper definition of the kinetic energy under given experimental conditions. We perform the analysis for the HM, but the results of this discussion are independent of which model is relevant to the energy range covering charge excitations. The real part of the optical conductivity for the light polarized in the direction η is [6, 7, 22]

$$\sigma_{1,\eta}(\omega) = \frac{\pi}{VZ} \sum_{n,m} \frac{\mathrm{e}^{-\beta E_n}}{E_m - E_n} \langle n|J_\eta|m\rangle \langle m|J_\eta|n\rangle (\delta(\omega - (E_m - E_n)) + \delta(\omega + (E_m - E_n))), \tag{14}$$

where J_η is the current operator in the direction η and E_n is the energy of the eigenstate $|n\rangle$. The relation (2) between the integral of the real part of the optical conductivity and the average of the kinetic energy in the HM model is based on some commutation relations between the polarization operator, $\vec{P} = \sum_i \vec{R}_i n_i$, the current operator $\vec{J}$ and the hopping term H_{hHM}, i.e.

$$\vec{J} \propto [H_{\mathrm{hHM}}, \vec{P}], \tag{15}$$

$$H_{\mathrm{hHM}} \propto [\vec{J}, \vec{P}]. \tag{16}$$

The second relation is true for models with hopping to NN sites only.

We divide the optical conductivity (14) into four terms with contributions to the sums over eigenstates $|n\rangle_{\mathrm{L}}$ with low energies $E_n^{(\mathrm{L})}$ below the charge excitation energy U and with contributions to the sums over eigenstates $|n\rangle_{\mathrm{H}}$ with energies $E_n^{(\mathrm{H})}$ above U:

$$(\delta\sigma_{1,\eta}(\omega))_1 \propto \sum_{n,m} \frac{\mathrm{e}^{-\beta E_n^{(\mathrm{L})}}}{E_m^{(\mathrm{L})} - E_n^{(\mathrm{L})}} {}_{\mathrm{L}}\langle n|J_\eta|m\rangle_{\mathrm{LL}}\langle m|J_\eta|n\rangle_{\mathrm{L}} \times(\delta(\omega - (E_m^{(\mathrm{L})} - E_n^{(\mathrm{L})})) + \delta(\omega + (E_m^{(\mathrm{L})} - E_n^{(\mathrm{L})}))),$$

$$(\delta\sigma_{1,\eta}(\omega))_2 \propto \sum_{n,m} \frac{\mathrm{e}^{-\beta E_n^{(\mathrm{L})}}}{E_m^{(\mathrm{H})} - E_n^{(\mathrm{L})}} {}_{\mathrm{L}}\langle n|J_\eta|m\rangle_{\mathrm{HH}}\langle m|J_\eta|n\rangle_{\mathrm{L}} \times(\delta(\omega - (E_m^{(\mathrm{H})} - E_n^{(\mathrm{L})})) + \delta(\omega + (E_m^{(\mathrm{H})} - E_n^{(\mathrm{L})}))),$$

$$(\delta\sigma_{1,\eta}(\omega))_3 \propto \sum_{n,m} \frac{\mathrm{e}^{-\beta E_n^{(\mathrm{H})}}}{E_m^{(\mathrm{L})} - E_n^{(\mathrm{H})}} {}_{\mathrm{H}}\langle n|J_\eta|m\rangle_{\mathrm{LL}}\langle m|J_\eta|n\rangle_{\mathrm{H}} \times(\delta(\omega - (E_m^{(\mathrm{L})} - E_n^{(\mathrm{H})})) + \delta(\omega + (E_m^{(\mathrm{L})} - E_n^{(\mathrm{H})}))),$$

$$(\delta\sigma_{1,\eta}(\omega))_4 \propto \sum_{n,m} \frac{\mathrm{e}^{-\beta E_n^{(\mathrm{H})}}}{E_m^{(\mathrm{H})} - E_n^{(\mathrm{H})}} {}_{\mathrm{H}}\langle n|J_\eta|m\rangle_{\mathrm{HH}}\langle m|J_\eta|n\rangle_{\mathrm{H}} \times(\delta(\omega - (E_m^{(\mathrm{H})} - E_n^{(\mathrm{H})})) + \delta(\omega + (E_m^{(\mathrm{H})} - E_n^{(\mathrm{H})}))).$$

The contributions from $(\delta\sigma_{1,\eta}(\omega))_3$ and $(\delta\sigma_{1,\eta}(\omega))_4$ are exponentially small at temperatures $T \ll U$. $(\delta\sigma_{1,\eta}(\omega))_1$ contributes to the spectrum below the energy $\simeq U$ while $(\delta\sigma_{1,\eta}(\omega))_2$ contributes above that energy. Thus, if the upper limit Ω_μ of the integral of the real part of the optical conductivity $W(t, \Omega_\mu)$ is set below U only the term $(\delta\sigma_{1,\eta}(\omega))_1$ contributes and the summations in formula (14) are restricted to states of the lower Hubbard band. If effects related to correlated hopping are neglected, the current operator, the polarization operator and the hopping term defined for the tJM may be obtained by substituting $\vec{P}$, $\vec{J}$ and H_{hHM}, defined at the level of the HM, by projected operators $P\vec{P}P$, $P\vec{J}P$ and $PH_{\mathrm{hHM}}P = H_{\mathrm{h}tJ}$, which have the same commutation relations (15) and (16) as $\vec{P}$, $\vec{J}$ and H_{hHM}. As we have already mentioned, the projector P restricts the Hilbert space to states without doubly occupied sites. We may conclude from the above discussion that the spectral weight $W(t, \Omega_\mu)$ with the cut-off frequency Ω_μ set below the charge transfer energy is proportional to the thermodynamic average of the hopping term $\langle H_{\mathrm{h}tJ}\rangle$ in the tJM and that $\langle H_{\mathrm{h}tJ}\rangle$ represents the kinetic energy. If the range of the integral in (3) covers also charge excitations with the energy $\simeq U$, $W(t, \Omega_\mu)$ is related to $\langle H_{\mathrm{hHM}}\rangle$. To order $\mathrm{O}(t^2/U)$ it is the same as the average $\langle H_{\mathrm{hHM}}^{(tJ)}\rangle$ and in that case the latter represents the kinetic energy. The difference between both definitions has its origin in $(\delta\sigma_{1,\eta}(\omega))_2$. This contribution originates in virtual transitions to states with doubly occupied sites and is related to the exchange energy $\langle H_J\rangle$. That statement follows from the relation $H_{\mathrm{hHM}}^{(tJ)} = H_{\mathrm{h}tJ} + 2H_J$. We have neglected the correlated hopping in the whole discussion. That term does not change qualitatively the behaviour of the tJM. Experimental results indicate that the weight $W(t, \Omega_\mu)$ is conserved for all T if Ω_μ exceeds the gap energy. Therefore, lowering of the kinetic energy in the superconducting state should be expected only in models defined in the energy range below the charge transfer gap U.

The discrepancy between the lowering of the kinetic energy in the HM in the superconducting state and conservation of $W(T, \Omega_\mu)$ at the transition to the superconducting state in Bi-2212 indicates that a simple one-band model is not capable of describing the physics of excitations across the gap. However, there exists strong experimental and theoretical evidence [23] that the tJM model or a modification of it is a proper low-energy model and we will analyse that model in the remaining part of this paper. Paradoxically, the relation between

the HM and the tJM is, in this context, irrelevant. Later, we will merely refer to the HM to demonstrate that it fails to represent correctly the physics in the energy range above the gap.

3. Kinetic energy in the spin-polaron model

As we have already mentioned, we analyse the behaviour of weakly doped AF at three levels: at the level of the HM, for which the energy scale is U, at the level of the tJM, for which the proper energy scale is t (or J in the limit of low doping), and at the level of the SPM, for which the energy scale is J. Now, we concentrate on the tJM. We assume that short-range AF correlations exist in the spin background. A moving hole frustrates the spin arrangement. The contribution from the exchange term in the tJM to the energy increases if the short-range AF order is locally frustrated. The kinetic energy in the tJM results in both repulsion and attraction in the regime $t > J$. On the one hand, a second hole acts like a hard-core object for the first one—this always results in a loss of kinetic energy, because the holes block each other's hopping. On the other hand, unlike a single hole which can propagate coherently in an AF only by the action of the exchange term, a pair of holes can propagate by the hopping term alone, which is more efficient. This kind of propagation will result in an attractive interaction between the holes. Which mechanism dominates is a subtle question. Some answers to that question have been given by means of the spin-polaron approach. For example, binding of holes has been confirmed by variational calculations for two holes [24]. Many detailed results obtained within the spin-polaron scenario have been verified by extensive comparisons with results of numerical analyses including QMC [25], exact diagonalization (ED) [26, 27] and density matrix renormalization group (DMRG) calculations [28].

As we have already mentioned, a line consisting of frustrated spins left by the moving hole tends to confine the hole. That line acts on it like a string. Since $t \gg J$ the probability of a next hop is higher than for any process mediated by the exchange term. We may assume in the lowest-order approximation that the trapped hole oscillates in the potential well formed by strings which consist of frustrated spins. The spin-polaron wavefunction

$$|\Psi_i\rangle = \sum_{\mathcal{P}_i} \alpha_{l(\mathcal{P}_i)} |\mathcal{P}_i\rangle \tag{17}$$

represents the hole trapped in the potential well. The string state $|\mathcal{P}_i\rangle$ is obtained by the hopping along a path $\mathcal{P}_i$, without retreats, of a hole created at site i in the locally AF medium. We find parameters $\alpha_{l(\mathcal{P}_i)}$ by solving a Schrödinger equation for a trial Hamiltonian which, by definition, neglects all processes that might give rise to the escape of the hole from the potential well. The Néel state with some quantum fluctuations plays the role of the AF medium for the moving hole. We also assume that amplitudes $\alpha_{l(\mathcal{P}_i)}$ depend only on the length $l(\mathcal{P}_i)$ of the paths. The spin fluctuations which are present in the ground state of the quantum AF in two dimensions are taken into account to lowest order [29].

At this stage of the calculation we analyse in the restricted Hilbert space the problem of a hole in the AF background. That restricted space consists of states $|\mathcal{P}_i\rangle$ which may be obtained by shifting a hole which has been initially created at the site i. That part of the calculation is analogous to the analysis by Bulaevskii–Nagaev–Khomskii and Brinkman–Rice of a model for non-retracing paths in a Néel background [30, 31]. Parameters $\alpha_{l(\mathcal{P}_i)}$ are solutions of the Schrödinger equation for a truncated version of the tJM. In the truncated Hamiltonian all matrix elements which give rise to the escape of the hole from the potential well formed by defects created by the moving hole have been omitted. Within that approximation we obtain parameters $\alpha_{l(\mathcal{P}_i)}$ practically by solving a problem of a single particle (hole) hopping in an external potential on half of a chain. $l(\mathcal{P}_i)$ which is the distance from the initial site i, labels

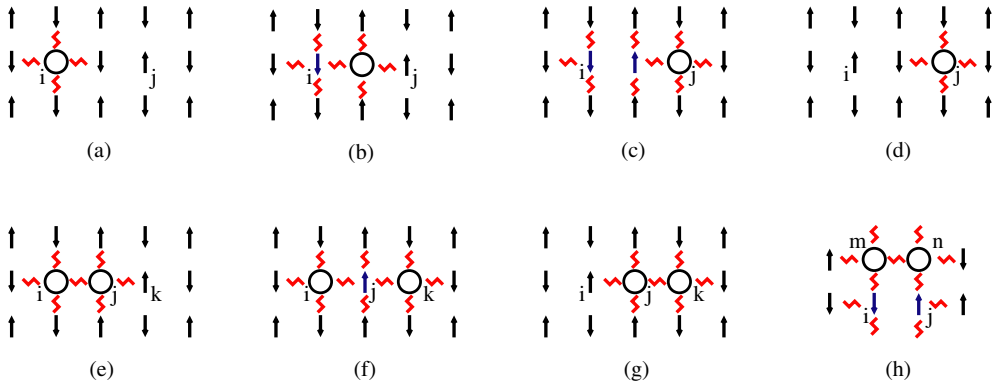

Figure 1. Graphical representation of the simplest processes which contribute to the effective Hamiltonian written in the language of spin polarons.

the sites in that chain. The external potential represents the increase of the exchange energy which is brought about by defects in the antiferromagnetic (AF) structure. These defects are created by the hopping hole, which means that the value of the potential increases linearly with the distance $l(\mathcal{P}_i)$. $|\Psi_i\rangle$, which is constructed in this way, resembles a confined orbital state with s-wave symmetry. Later we will derive a representation of the full tJM in the basis of these orbital-like states. That representation will have a standard form applied in the second quantization. In particular, an orbital-like state $|\Psi_i\rangle$ representing a trapped hole will be created by a single fermionic creation operator $h_i^\dagger$.

A product of wavefunctions (17) represents two holes trapped in distant potential wells. Such a product cannot be applied if potential wells trapping different holes overlap. Thus, for two holes created at a pair of nearest-neighbour sites i, j, we define a localized spin bipolaron as a combination of states which may be obtained by non-retraceable hopping of these holes:

$$|\Psi_{i,j}\rangle = \sum_{\mathcal{P}_i,\mathcal{P}_j} \alpha_{l(\mathcal{P}_i),l(\mathcal{P}_j)} |\mathcal{P}_i, \mathcal{P}_j\rangle. \tag{18}$$

By solving a Schrödinger equation for two particles in a potential well we derive amplitudes $\alpha_{l(\mathcal{P}_i),l(\mathcal{P}_j)}$. The basis consisting of (17) and (18) constitutes a low-energy shell of states. We will represent and solve the tJM in that basis. We may apply this construction because the eigenenergies of spin polarons (17) and (18) already contain the major portion of the total energy related to incoherent motion of holes on the scale of t. Some of the polaron states are not orthogonal. The nonorthogonality is weak and we will neglect it in this paper. The form of the effective low-energy Hamiltonian is determined by processes which restore AF correlations that are assumed to exist in the system, at least on a short-range scale. That Hamiltonian has already been presented in a previous article [32]. In order to make the present discussion self-sufficient we will now discuss three examples of processes which contribute to the effective Hamiltonian. The sequence of figures 1(a)–(d) represents a process during which the hole hops twice and creates two defects in the AF background. These defects are later annihilated by the transversal part of the exchange term in the tJM. A wavy line denotes a frustrated link for which the static, diagonal contribution to the exchange energy is higher than in the Néel state. Figure 1(c) represents a string state $|\mathcal{P}_i\rangle$ which is a component of the spin polaron state $|\Psi_i\rangle$ at site i. The exchange term in the tJM couples that string state to the state in figure 1(d). The latter state is a component of the polaron at site j. Such a sequence of events means, in the spin polaron language, that the polaron is shifted by two lattice spacings from site i to site

j and a term representing the hopping of that object will appear in the effective Hamiltonian. That term gives rise to the propagation of a single polaron. We may analogously find the remaining contributions to the SPM by analysing the coupling of spin-polaron wavefunctions by the tJM. Figures 1(e)–(g) represent the motion of a hole pair. The defect created by the right hole is later annihilated by the move of the left hole. The spin bipolaron is effectively shifted by one lattice spacing from the pair of sites i, j to the pair of sites j, k. Motion of spin bipolarons may also be mediated by the term in the Hamiltonian which flips antiparallel spins at NN sites. Two defects in figure 1(h) have been created by independent single upward hops of each hole. When they are annihilated, the hole pair and the bipolaron move upward by one lattice spacing from the pair of sites i, j to the pair of sites m, n.

The whole calculation is restricted to processes which involve strings with length not longer than 2 lattice spacings. That approximation 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 also be confirmed by an explicit evaluation. In addition, results of experiments with neutron scattering performed for $La_{2-x}Sr_xCuO_4$ [33] 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. We estimate that the latter parameter is equal to about 2–3 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 twice the distance between copper atoms.

The full low-energy Hamiltonian H_{SPM}:

$$\begin{aligned}
H_{\mathrm{SPM}} - \mu N_{\mathrm{SPM}} = {} & (E_1 - \mu)\sum_i h_i^\dagger h_i + h\sum_{i,\delta,\delta';\delta'\neq-\delta} h_{i+\delta+\delta'}^\dagger h_i \\
& + (E_2/2 - E_1 + u_1)\sum_{i,\delta} h_i^\dagger h_{i+\delta}^\dagger h_{i+\delta}h_i + u_2\sum_{i,\delta,\delta';\delta'\neq-\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'}h_i \\
& + u_3\sum_{i,\delta,\delta';\delta'\perp\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'}h_i + u_4\sum_{i,\delta,\delta',\delta'';\delta'\neq-\delta,\delta''\neq-\delta'} h_i^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta+\delta'+\delta''}h_i \\
& + s_1\sum_{i,\delta,\delta';\delta'\neq-\delta} h_{i+\delta+\delta'}^\dagger h_{i+\delta}^\dagger h_{i+\delta}h_i + s_2\sum_{i,\delta,\delta',\delta'';\delta'\neq-\delta,\delta''\neq-\delta'} h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta}h_i \\
& + s_3\sum_{i,\delta,\delta';\delta'\perp\delta} [(h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+2\delta}h_i + \mathrm{H.c.}) + h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta-\delta'}h_i] \\
& + s_4\sum_{i,\delta,\delta',\delta'';\delta'\neq-\delta,\delta''\neq-\delta'} (h_i^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta}h_i + \mathrm{H.c.}) + s_5\sum_{i,\delta,\delta';\delta'\perp\delta} h_i^\dagger h_{i+\delta'}^\dagger h_{i+\delta}h_i \\
& + s_6\sum_{i,\delta,\delta',\delta'';\delta'\neq\delta,\delta''\neq-\delta} (h_{i+\delta+\delta''}^\dagger h_{i+\delta'}^\dagger h_{i+\delta}h_i + \mathrm{H.c.}) \\
& + s_7\sum_{i,\delta,\delta';\delta'\perp\delta} h_{i+\delta+\delta'}^\dagger h_{i+\delta'}^\dagger h_{i+\delta}
\end{aligned} \tag{19}$$

is written in terms of operators creating (annihilating) a spin polaron at a site i, $h_i^\dagger$ (h_i). The operator $h_i^\dagger$ represents a combination of the products of raising and lowering spin operators and

an operator which annihilates the bare fermion defined for the $t\,J$M. These products create in the Néel state a string state which may also be obtained by letting a hole created at a given site hop in the AF background. Amplitudes $\alpha_{l(\mathcal{P}_i)}$ with which these products appear in the definition are obtained by solving a Schrödinger equation for the problem of a hole trapped in a potential well formed by spin fluctuations. More details are found in a previous publication [32]. Parameters of this Hamiltonian are functions of amplitudes α and eigenenergies of the spin polaron E_1 and the bipolaron E_2. N_{SPM} denotes an operator which represents the number of bare holes in the system. H_{SPM} represents the Hamiltonian of the $t\,J$M reduced to the space which spans polaron eigenstates with lowest energy:

$$H_{\mathrm{SPM}} = H_{\mathrm{h}tJ}^{(\mathrm{SPM})} + H_J^{(\mathrm{SPM})}. \tag{20}$$

The term $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$ corresponds to the hopping term $H_{\mathrm{h}tJ}$ in the $t\,J$M and $\langle H_{\mathrm{h}tJ}^{(\mathrm{SPM})}\rangle$ gives the kinetic energy for that model. The Hamiltonian H_{SPM} also represents the low-energy states of the Hamiltonian H_{HM}. It consists of two terms representing the kinetic and the potential energy of bare fermions in the HM:

$$H_{\mathrm{SPM}} = H_{\mathrm{hHM}}^{(\mathrm{SPM})} + H_U^{(\mathrm{SPM})}. \tag{21}$$

Here, $H_J^{(\mathrm{SPM})} = -H_U^{(\mathrm{SPM})}$ is equivalent to the exchange term in the $t\,J$M and to the Coulomb interaction in the HM multiplied by -1. This relation follows from an analogous formula $H_U^{(tJ)} = -H_J$ valid at the level of the $t\,J$M. In order to calculate the kinetic energy defined either by the hopping term in the $t\,J$M or by the hopping term in the HM, we should identify the operator $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$. Knowing that operator we can find the kinetic energy in the HM by means of the following relation:

$$H_{\mathrm{hHM}}^{(\mathrm{SPM})} = 2H_{\mathrm{SPM}} - H_{\mathrm{h}tJ}^{(\mathrm{SPM})}, \tag{22}$$

where $H_{\mathrm{hHM}}^{(\mathrm{SPM})}$ represents in the SPM the hopping term H_{hHM} in the HM.

In order to find $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$, we select terms in H_{SPM} which originate in the coupling of spin polarons by the hopping term $H_{\mathrm{h}tJ}$ in the $t\,J$M. Hopping in the $t\,J$M contributes to the eigenenergy of a spin polaron and a bipolaron. These contributions may be identified as portions of the eigenenergies $E_1^{(\mathrm{h})}$ and $E_2^{(\mathrm{h})}$, which are related to the motion of holes inside potential wells:

$$E_1^{(\mathrm{h})} = 2zt \sum_{\mu=0} P_{0,0}^{\mu} \alpha_{\mu}\alpha_{\mu+1} \tag{23}$$

$$E_2^{(\mathrm{h})} = 2(z-1)t \sum_{\mu=0,\nu=0} P_{0,0}^{\mu} P_{0,0}^{\nu} (\alpha_{\mu,\nu}\alpha_{\mu+1,\nu} + \alpha_{\mu,\nu}\alpha_{\mu,\nu+1}), \tag{24}$$

where z is the coordination number, $P_{\mu_1,\mu_2}^{\mu} = (z-2)^{(\mu-\mu_1)}$ for $\mu_2 \geqslant \mu \geqslant \mu_1$ and $P_{\mu_1,\mu_2}^{\mu} = (z-1)^{(\mu-\mu_2)}(z-2)^{(\mu_2-\mu_1)}$ for $\mu \geqslant \mu_2 \geqslant \mu_1$. P_{μ_1,μ_2}^{μ} is a number which represents the unfolding of new paths. Since $E_1^{(\mathrm{h})}$ and $E_2^{(\mathrm{h})}$ contribute to the eigenenergies of polarons they appear as the diagonal terms in the operator $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$ which, in the language of spin polarons, represents hopping in the $t\,J$M. We have already discussed (the sequence of figures 1(a)–(d)) an important process which gives rise to off-diagonal terms in $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$. This process is actually related to the motion of a string formed by defected spins. The string connects two holes which are attached to its ends. Hopping of these holes may give rise to an expansion of the string at an endpoint and a shrinking at the other and finally to a move of the whole string. In spin-polaron language this effect manifests itself as a coupling between wavefunctions of two different bipolarons (pairs of polarons on NN sites) by the hopping term in the $t\,J$M. A term which shifts the position of a bipolaron will appear in the effective operator $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$.

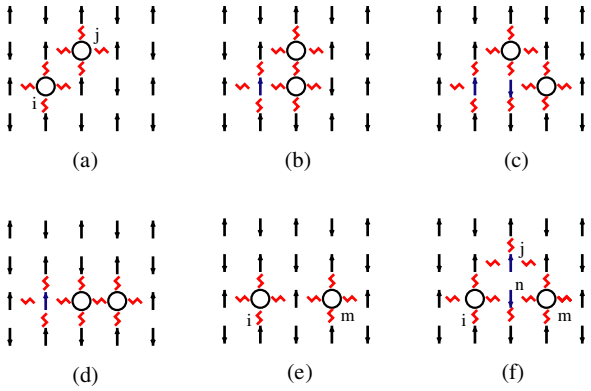

Figure 2. Graphical representation of two process which contribute to the operator representing the kinetic energy.

Next, we present in slightly more detail two other examples of processes related to hopping in the tJM. Let us consider figure 2(a) which depicts two holes that have been created in the AF background. Figure 2(a) also represents a string state which contributes to the wavefunction of two polarons occupying sites i and j. The lower hole starts to move, which gives rise to the states in figures 2(b) and (c). These states are also components of the wavefunction for the same polaron pair. If the hopping term is applied to the component represented by figure 2(c) a state depicted in figure 2(d) is created. This state is a component of the wavefunction for polarons representing two holes that have been initially created at two different sites i and m shown in figure 2(e). We find that $H_{\mathrm{h}tJ}$ couples wavefunctions of two different pairs of polarons. Thus, the process depicted in figures 2(a)–(e) shifts a polaron from site j to site m if site i is also occupied by a spin polaron and the term $-t\alpha_2\alpha_1\alpha_0^2 h_m^\dagger h_i^\dagger h_i h_j$ appears in the operator $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$. Indices of parameters α refer to the length of strings involved. The minus sign appears in front of t because an exchange of holes takes place. Further motion of the hole created at site j will not change the mechanism of the process that we have just discussed and contributions from longer strings will appear in $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$.

Figure 2(f) depicts a hole attached by a string to site j and a separate hole at site i. That state has been created from the state depicted in figure 2(a) by two hops of the hole from site j to site m. A process mediated by $H_{\mathrm{h}tJ}$ shifts the hole from site i to site n, removes a spin defect at the latter site and effectively moves a polaron from site i to site m. The new state may be interpreted as a string attached to site j and a hole at site m. That process also contributes to the operator $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$ which represents within the low-energy states the hopping term in the tJM. By collecting all contributions from different processes we can derive an approximate formula for $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$:

$$\begin{aligned} H_{\mathrm{h}tJ}^{(\mathrm{SPM})} = {} & E_1^{(\mathrm{h})} \sum_i h_i^\dagger h_i + (E_2^{(\mathrm{h})}/2 - E_1^{(\mathrm{h})}) \sum_{i,\delta} h_i^\dagger h_{i+\delta}^\dagger h_{i+\delta} h_i \\ & + u_2^{(\mathrm{h})} \sum_{i,\delta,\delta';\delta'\neq-\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i + u_3^{(\mathrm{h})} \sum_{i,\delta,\delta';\delta'\perp\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i \\ & + s_1^{(\mathrm{h})} \sum_{i,\delta,\delta';\delta'\neq-\delta} h_{i+\delta+\delta'}^\dagger h_{i+\delta}^\dagger h_{i+\delta} h_i + s_2^{(\mathrm{h})} \sum_{i,\delta,\delta',\delta'';\delta'\neq-\delta,\delta''\neq-\delta'} h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta} h_i \\ & + s_3^{(\mathrm{h})} \sum_{i,\delta,\delta';\delta'\perp\delta} (h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+2\delta} h_i + \mathrm{H.c.}) \end{aligned} \tag{25}$$

where the parameters representing hopping in the tJM, $u_2^{(\mathrm{h})}$, $u_3^{(\mathrm{h})}$, $s_1^{(\mathrm{h})}$, $s_2^{(\mathrm{h})}$ and $s_3^{(\mathrm{h})}$ are

$$u_2^{(\mathrm{h})} = E_1^{(\mathrm{h})} P_{\{\binom{0,0}{2,0}\}\{\binom{0,0}{2,0}\}} + P^{\mathrm{H}}_{\{\binom{0,0}{2,0}\}\{\binom{0,0}{2,0}\}}/2 \tag{26}$$

$$u_3^{(\mathrm{h})} = E_1^{(\mathrm{h})} R_{\{\binom{0,0}{1,1}\}\{\binom{0,0}{1,1}\}} + R^{\mathrm{H}}_{\{\binom{0,0}{1,1}\}\{\binom{0,0}{1,1}\}} \tag{27}$$

$$s_1^{(\mathrm{h})} = E_2^{(\mathrm{h})} C_{\{\binom{2,0}{1,0}\}\{\binom{0,0}{1,0}\}} + C^{\mathrm{H}}_{\{\binom{2,0}{1,0}\}\{\binom{0,0}{1,0}\}} \tag{28}$$

$$s_2^{(\mathrm{h})} = E_2^{(\mathrm{h})} C_{\{\binom{2,0}{3,0}\}\{\binom{0,0}{1,0}\}} + C^{\mathrm{H}}_{\{\binom{2,0}{3,0}\}\{\binom{0,0}{1,0}\}} \tag{29}$$

$$s_3^{(\mathrm{h})} = 2E_1^{(\mathrm{h})} S_{\{\binom{0,0}{1,1}\}\{\binom{0,0}{2,0}\}} + S^{\mathrm{H}}_{\{\binom{0,0}{1,1}\}\{\binom{0,0}{2,0}\}}. \tag{30}$$

Amplitudes P, P^{H}, R, R^{H}, C, C^{H}, S and S^{H} are related to different categories of processes have been defined in [32]. It is clear that we have derived the operator $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$ with the same accuracy which has been applied in [32] to the derivation of the full Hamiltonian (19).

4. Difference of the kinetic energy between the superconducting state and the normal state

By applying the standard mean-field procedure to the operator $H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$ we deduce the difference of the kinetic energy in the tJM between the SC and the normal state:

$$\left.\frac{\delta E_{\mathrm{h}tJ}}{N}\right|_{T=0} = \frac{1}{N}\sum_{\boldsymbol{k}}\left\{\frac{E_1^{(\mathrm{h})}}{2}\left(1-\frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right) - [(E_2^{(\mathrm{h})}/2 - E_1^{(\mathrm{h})}) - s_1^{(\mathrm{h})} + s_2^{(\mathrm{h})}]D_{\boldsymbol{k}}^{(1,0)}\Delta_{e_x}\Delta_{\boldsymbol{k}}E_{\boldsymbol{k}}\right\}$$
$$- 4[(E_2^{(\mathrm{h})}/2 - E_1^{(\mathrm{h})}) - s_1^{(\mathrm{h})} + s_2^{(\mathrm{h})}]\Delta_{e_x}^2, \tag{31}$$

where $\xi_{\boldsymbol{k}}$ and $E_{\boldsymbol{k}}$ are quasiparticle energies in the normal and the SC state:

$$\xi_{\boldsymbol{k}} = E_1 + h(S_{\boldsymbol{k}}^{(2,0)} + 2S_{\boldsymbol{k}}^{(1,1)}) - \mu, \tag{32}$$

$$E_{\boldsymbol{k}} = \sqrt{\xi_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2}. \tag{33}$$

Here $\Delta_{\boldsymbol{x}}$ represents an anomalous Green function:

$$\Delta_{\boldsymbol{x}} = \langle T_\tau h_{i+\boldsymbol{x}}(\tau + 0^+)h_i(\tau)\rangle, \tag{34}$$

and i belongs to the spin-up AF sublattice. The gap function is strongly anisotropic:

$$\Delta_{\boldsymbol{k}} = d_{\boldsymbol{k}}^{(1,0)}\Delta_{e_x} + d_{\boldsymbol{k}}^{(2,1)}\Delta_{2e_x+e_y} + d_{\boldsymbol{k}}^{(3,0)}\Delta_{3e_x}, \tag{35}$$

$$d_{\boldsymbol{k}}^{(1,0)} = (2u_1 + 4u_4 - 2s_1 + 2s_2 - 8s_4 - 4s_5 + 8s_6 + 4s_7)D_{\boldsymbol{k}}^{(1,0)}$$
$$+ (2s_4 + 2s_6)D_{\boldsymbol{k}}^{(2,1)} + (2s_4 + 2s_6)D_{\boldsymbol{k}}^{(3,0)}, \tag{36}$$

$$d_{\boldsymbol{k}}^{(2,1)} = (4s_4 + 4s_6)D_{\boldsymbol{k}}^{(1,0)} + 6u_4 D_{\boldsymbol{k}}^{(2,1)}, \tag{37}$$

$$d_{\boldsymbol{k}}^{(3,0)} = (2s_4 + 2s_6)D_{\boldsymbol{k}}^{(1,0)} + 2u_4 D_{\boldsymbol{k}}^{(3,0)}, \tag{38}$$

where

$$D_{\boldsymbol{k}}^{(1,0)} = 2\cos(k_x) - 2\cos(k_y), \tag{39}$$

$$D_{\boldsymbol{k}}^{(2,1)} = 2\cos(2k_x + k_y) + 2\cos(2k_x - k_y) - 2\cos(k_x + 2k_y) - 2\cos(k_x - 2k_y), \tag{40}$$

$$D_{\boldsymbol{k}}^{(3,0)} = 2\cos(3k_x) - 2\cos(3k_y), \tag{41}$$

$$S_{\boldsymbol{k}}^{(2,0)} = 2\cos(2k_x) + 2\cos(2k_y) \tag{42}$$

$$S_{\boldsymbol{k}}^{(1,1)} = 2\cos(k_x + k_y) + 2\cos(k_x - k_y). \tag{43}$$

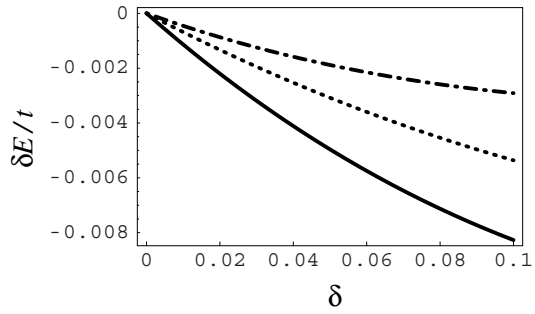

Figure 3. The differences between the total (full curve), kinetic (dotted curve) and potential (chain curve) energy in the superconducting and normal states defined at the level of the tJM at $T = 0$.

The differences between the total (full curve), kinetic (dotted curve) and potential (chain curve) energy in the SC state and in the normal state at $T = 0$ are shown in figure 3 for $J/t = 0.33$. The plot is restricted to the region of low doping. We believe that our approach may be applied there. It turns out that, in the tJM, both the kinetic energy and the potential energy decrease. We have used in the calculation the same numerical parameters defining the SPM (19) for the whole low doping range. We know from the analysis of the binding energy of holes that the strength of the pairing force is already overestimated in the system at half-filling, if effects related to quantum spin fluctuations in the ground state of the quantum AF in two dimensions are taken into account approximately [29]. We have applied the same simplified approximation in the calculation presented in this paper. If we ascribe the pairing in doped AF to the presence of AF correlations, we must also draw the conclusion that the strength of the pairing force between spin polarons weakens with doping because the correlation length becomes shorter. We have neglected this effect in the calculation of the energy change. The hopping parameter t for the cuprates is a fraction of an electronvolt. Having in mind the overestimation of the pairing force in our calculation we see that our assessment of the order of magnitude, by which the kinetic energy is lowered in the SC state, roughly agrees with the quantity $\sim$1 meV suggested by experiment [1, 3].

We proceed now to assess the difference of the kinetic energy in the HM between the SC state and the normal state. We evaluate the average of the operator $H_{\mathrm{hHM}}^{(\mathrm{SPM})} = 2H_{\mathrm{SPM}} - H_{\mathrm{h}tJ}^{(\mathrm{SPM})}$:

$$\begin{aligned}\left.\frac{\delta E_{\mathrm{hHM}}}{N}\right|_{T=0} = \frac{1}{N}\sum_{\boldsymbol{k}}\Bigg\{&|\xi_{\boldsymbol{k}}| - E_{\boldsymbol{k}} - \frac{E_1^{(\mathrm{h})}}{2}\left(1 - \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)\\ &+ [(E_2^{(\mathrm{h})}/2 - E_1^{(\mathrm{h})}) - s_1^{(\mathrm{h})} + s_2^{(\mathrm{h})}]D_{\boldsymbol{k}}^{(1,0)}\Delta_{e_x}\Delta_{\boldsymbol{k}}E_{\boldsymbol{k}}\Bigg\}\\ &- \{[8u_1 + 16u_4 - 8s_1 + 8s_2 - 32s_4 - 16s_5 + 32s_6 + 16s_7\\ &- 4((E_2^{(\mathrm{h})}/2 - E_1^{(\mathrm{h})}) - s_1^{(\mathrm{h})} + s_2^{(\mathrm{h})})]\Delta_{e_x}^2\\ &+ 48u_4\Delta_{2\boldsymbol{e}_x+\boldsymbol{e}_y}^2 + 8u_4\Delta_{3\boldsymbol{e}_x}^2 + (32s_4 + 32s_6)\Delta_{e_x}\Delta_{2\boldsymbol{e}_x+\boldsymbol{e}_y}\\ &+ (16s_4 + 16s_6)\Delta_{e_x}\Delta_{3\boldsymbol{e}_x}\}. \end{aligned} \tag{44}$$

Shown in figure 4 are the differences between the total (full curve), kinetic (dotted curve) and potential (chain curve) energies in the HM between the SC state and the normal state at $T = 0$ for $J/t = 0.33$. We notice that the kinetic energy in the HM decreases, while the potential energy increases. Our conclusions agree with results of a recent calculation performed for the HM in the low doping limit by means of the dynamical cluster approximation [34].

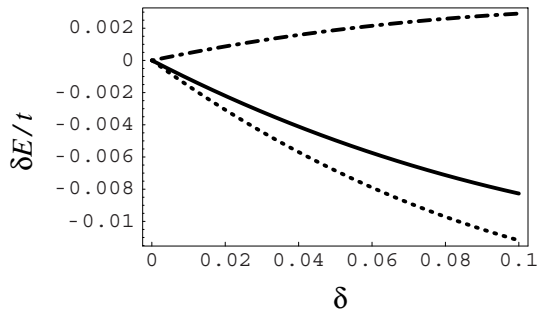

Figure 4. The differences between the total (full curve), kinetic (dotted curve) and potential (chain curve) energies in the superconducting and normal states defined at the level of the HM at $T = 0$.

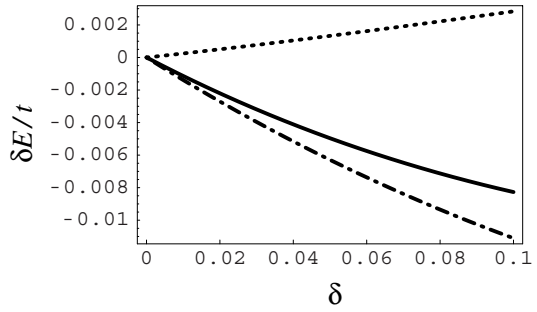

Figure 5. The differences between the total (full curve), kinetic (dotted curve) and potential (chain curve) energies in the superconducting and normal states defined for the dressed particles (spin polarons) at $T = 0$.

Experimental results do not indicate a strong change of $W(T <, \Omega_\mu)$ at $T = T_c$ if the cut-off frequency Ω_μ is set above the charge excitation energy [3]. This observation does not agree with our result, indicating that the kinetic energy is lowered in the HM. We conclude that experiments suggest that this model is not sufficient to describe the physics of cuprates in the energy range above the charge excitation energy U. The failure of the HM in this case is, to some extent, obvious because at such a high energy scale inter-band and multi-band effects may become important.

For comparison, we now calculate the change of the kinetic energy in the Hamiltonian (19). We define the kinetic energy by the term in the Hamiltonian

$$H_{\mathrm{hSPM}} = h \sum_{i,\delta,\delta';\delta'\neq-\delta} h^{\dagger}_{i+\delta+\delta'} h_i, \tag{45}$$

which represents the hopping of spin polarons. The change in the kinetic energy is then of the standard BCS form:

$$\delta E_{\mathrm{hSPM}} = \sum_{\boldsymbol{k}} (h/2)(S^{(2,0)}_{\boldsymbol{k}} + 2S^{(1,1)}_{\boldsymbol{k}})\left(1 - \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right). \tag{46}$$

The increase of this quantity in the SC state which we notice in figure 5 may be attributed to a smearing of the momentum distribution of spin polarons.

5. Summary and conclusions

The spectral weight $W(t, \Omega_\mu)$ defined by equation (3) determines the kinetic energy within the Hubbard model only when Ω_μ exceeds the energy $U \simeq 2$ eV, i.e. the charge transfer gap. As we have discussed above, in underdoped Bi-2212 equation (4) has to be replaced by equation (5). On the other hand, $W(t, \Omega_\mu)$ differs for $T > T_c$ and $T < T_c$ when Ω_μ is considerably less than U, i.e. when $\Omega_\mu < 0.6$ eV. In that case $W(T, \Omega_\mu)$ can be used to determine the kinetic energy of the tJM. For $J = 0.1$ eV and $J/t = 0.33$ we find a decrease of the kinetic energy within that model when the system is superconducting. At $T = 0$ this decrease is of the order of 1–2 meV per site, which is larger by approximately a factor of 1.5–2 than the experimental findings. This difference may result from the fact that the lowering of the AF correlations with increasing doping is not taken into account in the theory. In addition, the relation between the measured change in $W(T, \Omega_\mu)$ and the calculated change of the kinetic energy in the tJM which follows from (2) is already a crude approximation. We, like [34], see also for the HM a decrease of the kinetic energy due to superconductivity. But the relation (5) found from experiments would suggest that the kinetic energy remains unaffected in the superconducting state. This discrepancy suggests that modifications of the simple HM are required in order to explain the experimental findings as regards the spectral weight. In underdoped Bi-2212, as well as in the tJM, the difference in the sum of the kinetic and the exchange energy between the normal and superconducting states is of the order of 2 meV [1, 3, 35, 37, 36] per site. This is larger, by one order of magnitude, than the 0.1 meV per site which is obtained from the calorimetric measurements [38]. The tJM, as well as the HM, do not contain the long-range part of the Coulomb interactions. Based on an analysis of the dielectric function it has been suggested that the Coulomb energy increases when the system becomes superconducting [39]. This would imply that the decrease in the short-range or exchange part is compensated by an increase of the long-range part of the Coulomb interaction when superconductivity sets in.

It has been suggested that the violation of (4) may be attributed to the transition between an unconventional non-Fermi-liquid normal state with the frequency-dependent scattering rate and a more conventional SC state [40, 8, 39]. The authors of these suggestions deduce the frequency dependence of the scattering rate from fits to ARPES data at the $(\Pi, 0)$ point. The main argument is that, at the transition from the non-standard normal state to the SC state, a deformation of the electron momentum density profile takes place. The weight is shifted to states with lower momentum during that deformation. This scenario is actually realized in weakly doped AF as was discussed some time ago in the context of the Fermi surface evolution and binding in these systems [41, 42]. The rough picture may be described as follows. The electron momentum density in the unpaired state has an overall shape which resembles the electron momentum density of weakly interacting fermions on the square lattice. That form of the distribution has its origin in the fast incoherent hopping of holes trapped in a potential well. Dips in the distributions in the regions near points $(\pm\pi/2, \pm\pi/2)$ are related to a bigger concentration of holes. Points $(\pm\pi/2, \pm\pi/2)$ are minima of the energy dispersion of the spin polaron, which is a quasiparticle representing a propagating hole. These minima have been experimentally observed in an undoped system by means of angle-resolved photoemission spectroscopy (ARPES) [12]. A recent ARPES study of a metal to insulator transition in $Ca_{2-x}Na_xCuO_2Cl_2$ demonstrates that the rigid band picture, in which holes populate pockets about $(\pi/2, \pi/2)$, is true for some underdoped cuprates [11]. The rigid band is represented in our calculation by the quasiparticle dispersion in the normal state of the SPM. The spin-polaron propagation is not directly related to hopping of electrons between NN sites. That propagation is rather mediated by the exchange interaction which removes defects from the spin background. Pairing of holes is, to a much greater extent, mediated by hopping between

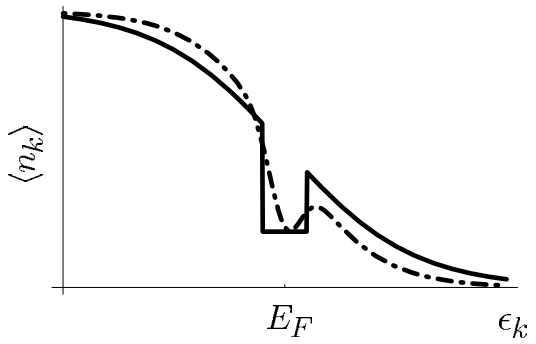

Figure 6. Electron momentum distribution along a line in the k space which crosses a region populated by spin polarons.

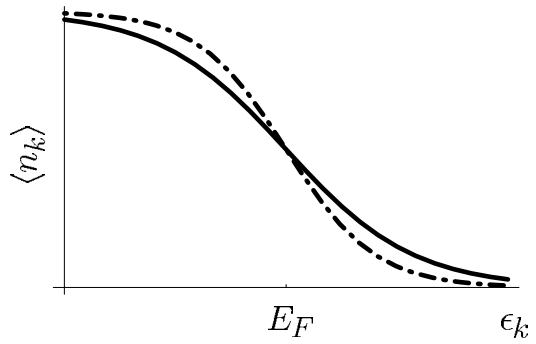

Figure 7. Electron momentum distribution along a line in the k space which does not cross a region populated by spin polarons.

NN sites. Dips in the electron momentum distribution become shallower, the weight is shifted toward lower momenta and the kinetic energy decreases in the paired state. The change of the momentum distribution plotted as a function of the band energy ϵ_k for a noninteracting system has been schematically presented in figures 6 and 7. Full curves represent the normal, while chain curves the SC state. Discontinuities in momentum distribution which form in the normal state are seen only along certain directions. They are much more pronounced near the zone centre. The weight is shifted in the SC state to the low-momentum region. This scenario takes into account the presence of quasiparticles in the normal state in some directions in the momentum and in this aspect is different from the suggestion that lowering of the kinetic energy may occur at the transition from a totally incoherent normal state to the SC state.

Binding of holes in the AF background in the state with d-wave symmetry has been found by means of the ED [43–47] of small clusters. These results also indicate that lowering of the kinetic energy is an important factor in that process. Binding of holes has also been found by means of the spin-polaron approach [48, 29, 24, 13].

Hopping of hole pairs between forming stripes will also bring about a lowering of the kinetic energy [49, 50] in a hypothetical superconducting state. The spin polaron scenario is also a suitable approach to discuss the dynamics of holes in the striped background [13].

In a model of hole superconductivity pairing and lowering of the kinetic energy take place simultaneously [51–53]. Electrons hop in this model in a correlated manner. Its mechanism

is effective only when the band is almost filled [54]. In contrast we deal in our scenario with a band which is nearly half-filled, i.e. close to the metal–insulator transition.

Lowering of the kinetic energy by the onset of SC has also been suggested within the RVB scenario [55, 56].

In a phenomenological model of a non-Fermi-liquid state with a frequency-dependent scattering rate a violation of the sum rule (4) has also been found [8].

The decrease of the kinetic energy at T_c has also been predicted in a scenario for a superconductor where there is a separation of the pairing amplitude formation from the phase coherence transition [57]. This scenario predicts the opening of a gap at low frequencies above T_c. Such an effect is not seen in the cuprates when the real part of the in-plane conductivity is measured [2].

The AF spin-polaron approach is based on the assumption of short-range AF correlations. An alternative would be to take them into account by a bond-ordered state [58].

Finally, we should point out that we have completely neglected the effects of phonons. According to Shen and collaborators, these effects are seen in the results of ARPES measurements [59].

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