Non-rigid hole band in the extended t-J model

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Abstract

The dispersion of one hole in an extended $t$-$J$ model with additional hopping terms to second and third nearest neighbours and a frustration term in the exchange part has been investigated. Two methods, a Green’s function projection technique describing a magnetic polaron of minimal size and the exact diagonalization of a 4 × 4 lattice, have been applied, showing reasonable agreement among each other. Using additional hopping integrals which are characteristic for the CuO$_2$ plane in cuprates we find in the nonfrustrated case an isotropic minimum of the dispersion at the point $(\pi/2, \pi/2)$ in $k$-space in good coincidence with recent angle-resolved photoemission results for the insulating compound Sr$_2$CuO$_2$Cl$_2$. Including frustration or finite temperature which shall simulate the effect of doping, the dispersion is drastically changed such that a flat region and an extended saddle point may be observed between $(\pi/2, 0)$ and $(\pi, 0)$ in agreement with experimental results for the optimally doped cuprates.

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1 Introduction

It is well known that many properties of the high-$T_c$ superconductors (HTSC’s) are determined by the spectrum of holes in the doped two-dimensional (2D) CuO$_2$ planes. Recent experiments by angle resolved photoemission (ARPES) reported a small band width providing evidence for the existence of strong correlations in cuprates [1-5]. Moreover they indicate the existence of a flat dispersion region close to the Fermi surface for the optimally doped cuprates Bi2212, Bi2201, Y123 and Y124 (for the notation see [5]). The flat region of the quasiparticle band is located close to the point $(\pi, 0)$ in the irreducible part of the Brillouin zone (where the lattice constant has to be set to unity $a = 1$) and it has the form of an extended saddle point between $(\pi, 0)$ and $(\pi/2, 0)$. The existence of the flat band region leads to the appearance of a strong Van-Hove (VH) singularity which is close to the Fermi level. This circumstance is often used by different theories for the explanation of the high superconducting transition temperature [3, 6-9]. Then, the existence of the optimal value of doping is naturally connected with the movement of the chemical potential over the position of the VH singularity when the hole density is increased. So, the investigation of the hole spectrum in the CuO$_2$ plane is of great importance for a microscopic theory of HTSC.

Important new results were obtained recently by ARPES experiments for the insulating, antiferromagnetic compound Sr$_2$CuO$_2$Cl$_2$ [10]. These results correspond to the situation of one hole in the quantum antiferromagnet and they serve as a test for different theoretical approaches. It was found [10] that the bottom of the hole band is close to the point $(\pi/2, \pi/2)$ and the band width is of order 0.3 eV. It is essential, that the effective mass was shown to be isotropic at the bottom of the band.

One generally believes that the $t$-$J$ model describes qualitatively the hole spectrum of the CuO$_2$ plane in HTSC. There are numerous studies of the hole spectrum in the framework of the $t$-$J$ model based on the exact diagonalization of small clusters [11, 12], the self-consistent Born approximation [13, 14] or a “string” ansatz for the hole wave function [15]. One can either start from the two-sublattice Néel-type state [13, 14, 15] or a spin rotational invariant spin liquid state [11] and obtains qualitatively the same result: the hole motion occurs mainly on one sublattice, i.e. the dispersion relation is dominated by an effective hopping to next nearest neighbours with the minimum of the dispersion at $(\pi/2, \pi/2)$. One finds a flat region of the dispersion near to the point $(\pi, 0)$. That was used for an attempt to interpret the experimental data of the optimally doped compounds [17], where a rigid-band picture was assumed (see also [15]). However, the anisotropic minimum of the pure $t$-$J$ model is in contrast to the experimental result in Sr$_2$CuO$_2$Cl$_2$ which shows an isotropic band bottom and a large energy difference between $(\pi/2, \pi/2)$ and $(\pi, 0)$.

Recently it was shown [19] that the qualitative agreement with the experimental results [10] may be improved in the framework of the $t_1$-$t_2$-$J$ model, which takes into account the next-nearest-neighbour hopping $t_2$ of the hole. The inclusion of a $t_2$-term substantially improves the correspondence of the calculated spectrum near the band bottom with the experimentally observed isotropic minimum of $\varepsilon(k)$ at the point $(\pi/2, \pi/2)$. On the other
hand, the hole spectrum of the $t_1$-$t_2$-$J$ model does not reproduce the flat band region near the point $(\pi,0)$. So, we have the following theoretical problem: the one-hole approach in the pure $t$-$J$ model can reproduce the flat band region of the optimally doped cuprates [1-5] but not the isotropic band bottom of the insulating compound [10]. And vice versa, one hole in the $t_1$-$t_2$-$J$ model leads to an isotropic band bottom but not to a flat band region near $(\pi,0)$. One possible solution could be that we have to choose different microscopic models for the different compounds. Here, we will investigate the other possibility, whether it is possible that the hole band is changed by doping so that a flat band region between $(\pi,0)$ and $(\pi/2,0)$ arises.

To simulate the effect of doping in a study of the one-hole motion there were recently compared two possibilities, namely the influence of frustration and temperature [20]. The inclusion of frustration leads to a $t$-$J_1$-$J_2$ model, where $J_1$ and $J_2$ denote the antiferromagnetic exchange interaction between nearest and next nearest neighbours. The influence of frustration was investigated by two different methods, namely by a variational ansatz where the spin-spin correlations in the frustrated Heisenberg model had been calculated by a spin rotational invariant procedure [21] and by the exact diagonalization of a $4 \times 4$ lattice. It was found that the frustration shifts the minimum of the hole dispersion from $(\pi/2,\pi/2)$ to the point $(\pi,0)$. Both methods had a quite reasonable agreement where the variational method showed the effect in a more pronounced way. Flat dispersion regions were found in the nonfrustrated and frustrated cases. Without frustration, the flat region occurs around $(\pi/2,\pi/2)$, whereas for frustration $J_2/J_1 \gtrsim 0.4$ it occurs between $(\pi,0)$ and $(\pi,\pi/2)$. Such a flat region is similar to the experiment [1-5], but there it appears between $(\pi,0)$ and $(\pi/2,0)$.

The mentioned above investigations demonstrate that the extension of the $t$-$J$ model by the inclusion of additional hopping terms, frustration or by taking into account a finite temperature may strongly modify the initial features of the hole spectrum. But at the same time, none of these extensions alone can lead to an adequate description of the experimental picture.

In the present paper we will investigate the hole spectrum in the framework of the $t_1$-$t_2$-$t_3$-$J_1$-$J_2$ model, e.g. we will take into account the hole hoppings between first ($t_1$), second ($t_2$) and third ($t_3$) nearest neighbours and the frustration in the spin subsysten simultaneously. The additional hoppings $t_2$ and $t_3$ naturally appear in the Hamiltonian if one reduces the well known three band Hubbard model of the CuO$_2$ plane to an extended $t$-$J$ model [22, 23, 24]. Throughout the present paper we will fix $t_2$ and $t_3$ to such values which can be derived from the characteristic parameters of the three band Hubbard model for the CuO$_2$ plane which were given by Hybertsen et al. [23]. The frustration will be understood to simulate the doping as proposed, for instance, in Ref. [26]. The effect of a finite temperature will also be discussed.

Two methods will be used to investigate the problem. The projection Mori-Zwanzig method [27] for two-time retarded Green’s functions will be employed to treat the hole excitation as a magnetic polaron of minimal size. Simultaneously we will use the exact diagonalization of a $4 \times 4$ lattice. Within the projection method the dispersion is determined by static spin-spin correlation functions. These are calculated here in a spin rotational
invariant method [21] (see also the zero temperature version [28]). We describe the state of the magnetic subsystem as a spin liquid state in contrast to the widely used two-sublattice Néel-type state due to several reasons. At first, our choice gives the possibility to avoid the degeneracy of the hole-spectrum between the points \((0,0)\) and \((\pi, \pi)\) which always occurs in the Néel-type state. Second, the spin liquid state does not contradict the Mermin-Wagner theorem [29] which forbids magnetic order in two dimensions for any finite temperature. So it gives the possibility to investigate the one-hole motion at non-zero temperatures. Of course, the Mori-Zwanzig projection method is an approximate one. Therefore, it is reasonable to investigate the problem by the exact diagonalization method and to compare the results of two independent procedures.

The paper will be organized as follows. At first, in Sec. 2 we will present the spin polaron approach in the framework of the projection method. Then we show the results of both methods for zero temperature and increasing frustration (Sec. 3) and discuss the influence of temperature. Finally we present our conclusions.

## 2 Small spin-polaron approach for the hole spectrum

We consider an extended \(t-J\) model on a square lattice with hoppings between first, second and third nearest neighbours and with a frustration term in the exchange interaction. The Hamiltonian of the model is given by

\[
H = H_t + H_J = -\sum_{i\alpha l} t_l X^0_{\alpha 0 i} X^0_{\alpha 0 i+l} + \frac{1}{2} \sum_{i\alpha m} J_{\alpha \beta} \vec{S}_i \cdot \vec{S}_{i+m},
\]

where

\[
t_l = \begin{cases} 
1 & \text{if } l \text{ is a nearest neighbour vector} \\
2 & \text{if } l \text{ is a second nearest neighbour vector} \\
3 & \text{if } l \text{ is a third nearest neighbour vector} \\
0 & \text{else}
\end{cases}
\]

and

\[
J_{\alpha \beta} = \begin{cases} 
1 & \text{if } m \text{ is a nearest neighbour vector} \\
2 & \text{if } m \text{ is a next nearest neighbour vector} \\
0 & \text{else}
\end{cases}
\]

The Hamiltonian is expressed in terms of the Hubbard projection operators which exclude the double occupancy at site \(i\): acting on the vacuum state \(X^0_{\alpha 0 i}\) creates the electron (annihilates the hole) at site \(i\) with spin \(S = 1/2\) and spin projection \(\sigma/2\) (\(\sigma = \pm 1\) is a spin index). The following operator equations are fulfilled

\[
X^0_{\alpha 0 i} = c_{i\alpha}^\dagger (1 - n_{i-\sigma}) , \quad X^{\sigma\sigma}_{i} = n_{i\sigma} (1 - n_{i-\sigma}) , \quad X^{\sigma - \sigma}_{i} = c_{i\sigma}^\dagger c_{i-\sigma} , \\
n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} , \quad S^\sigma_i = X^{\sigma\sigma}_{i} , \quad S_i^z = \frac{1}{2} \sum_{\sigma} \sigma X^\sigma_i , \\
X_{i}^{00} + \sum_{\sigma} X_{i}^{\sigma\sigma} = 1 , \quad \lambda_{\lambda_1\lambda_2} X_{i}^{\lambda_1\lambda_2} = X_{i}^{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_3} ,
\]

where \(\lambda_n = 0\) or \(\sigma\) in the last equation. The hopping parameters \(t_l\) in (1) are not free but have to be determined by a reduction procedure from the three band Hubbard model.
of the CuO$_2$ plane. We use here an analytical reduction procedure, the so-called “cell perturbation method” [22, 23, 24]. For the parameters of the three band Hubbard model we choose the values which were found by Hybertsen et al. [25] for La$_2$CuO$_4$ by a constrained density-functional calculation, namely: $t_{pd} = 1.3$ eV, $t_{pp} = 0.65$ eV, $\varepsilon_p - \varepsilon_d = 3.6$ eV, $U_d = 10.5$ eV, $U_p = 4$ eV and $U_{pd} = 1.2$ eV [24]. Band structure calculations for Sr$_2$CuO$_2$Cl$_2$ [30] show only few differences to the La-compound. Therefore, we expect that the parameter values of Hybertsen et al. are also responsible for the Sr-compound.

From the reduction procedure (details will be published in Ref. [24]) we found the following hopping parameters:

$t_1 = 498$ meV, $t_2 = -41$ meV and $t_3 = 77$ meV. They are within the limits which have been found in [23] and also near to the results of a numerical mapping in [25]. But in difference to Hybertsen et al. we found it necessary to include the $t_3$-term also. In the following we will choose $t_1$ as the unit of energy, i.e. $t_2 = -0.08$, $t_3 = 0.15$. So you see that the additional hopping terms are rather small, but nevertheless essential as will be shown below. The reduction procedure gives also the possibility to calculate the exchange energy $J_1$. That is however less important for our purpose, since we will show that the results for different values of $J_1$ can be roughly transformed into each other by scaling the bandwidth with $J_1$.

Let us discuss the one-hole excitations on the background of the half-filled rotationally invariant singlet states $|\Psi \rangle$ of the pure spin system $H_J$. We are interested in the energetically lowest branch of these excitations and it is known that the bottom of its band is represented by the states with total spin $S_{tot} = 1/2$. We will treat the problem within the framework of the spin polaron of small radius. That means that we restrict ourselves to spin excitations in the immediate neighbourhood of the hole. It may be seen that the full basis of such excitations is given by the following 5 basis operators $\phi^a_i \dagger$ with $a = 0, 1, \ldots, 4$:

$$\phi^0_i = X^0_i$$, \quad $\phi^a_i = \sum_s X^s_{i-a} X^{a0}_i$ \quad ($a = 1, \ldots, 4$), \quad (5)

where we will use the following notation hereafter: the small latin letters $a$ and $b$ denote either a number between 0 and 4 or the corresponding lattice vector

$$0 \leftrightarrow (0, 0) \quad 1 \leftrightarrow (1, 0) \quad 3 \leftrightarrow (-1, 0)$$

$$2 \leftrightarrow (0, 1) \quad 4 \leftrightarrow (0, -1)$$ \quad (6)

in a synonymous way. Any vector $\phi^a_i \dagger |\Psi \rangle$ corresponds to a one hole state with $S_{tot} = 1/2$ and $S_{tot}^z = -\sigma/2$, where $S_{tot}$ and $S_{tot}^z$ are the spin and its projection of the total system.

To obtain the one-hole spectrum $\varepsilon(k)$ we use the two-time retarded matrix Green’s function $G^{ab}(t, k)$ for the Fourier transformation of the operators $\phi^a_k$:

$$G^{ab}(t, k) = \langle \langle \phi^a_k(t); \phi^b_k \rangle \rangle = -i\Theta(t) \langle \lbrace \phi^a_k(t); \phi^b_k(0) \rbrace \rangle$$, \quad (7)

$$\phi^a_k = \frac{1}{\sqrt{N}} \sum_j e^{ikj} \phi^a_j$$, \quad (8)

where $\lbrace \ldots, \ldots \rbrace$ denotes the anticommutator and where we have used Zubarev’s notation [31].
The equation of motion for the Green’s function \( \langle \phi_k^a; \phi_k^b \rangle \) after going over from time \( t \) to frequency \( \omega \) by Fourier transformation \( \langle \langle \phi_k^a; \phi_k^b \rangle \rangle \) has the form

\[
\omega \langle \langle \phi_k^a; \phi_k^b \rangle \rangle \omega = S^{ab}(k) + \langle \langle \phi_k^a; \phi_k^b \rangle \rangle ,
\]

with the commutator \([\ldots,\ldots]\). To restrict ourselves to the above chosen set of 5 operators \( \{ \phi_k^a \} \) we use the standard Mori-Zwanzig projection method \[27\] for the operators \( \phi_k^a \):

\[
\phi_k^a \simeq \sum_b \Omega^{ab}(k) \phi_k^b , \quad \Omega(k) = H(k) S^{-1}(k) ;
\]

\[
H^{ab}(k) = \langle \{ \phi_k^a, H \phi_k^b \} \rangle = \langle \Psi | \phi_k^a H \phi_k^b | \Psi \rangle - E_0 S^{ab}(k) ,
\]

where \( E_0 \) denotes the ground state energy of the spin system \( H_J \) without any hole. Note that the expression with the anticommutator in (12) can be simplified considerably for the one-hole problem. Using (12) the eqn. (9) takes the following matrix form

\[
(\omega E - H(k) S^{-1}(k)) G = S(k) ,
\]

where \( E \) is a unit matrix. The quasiparticle spectrum \( \varepsilon(k) \) is determined by the poles of the Green’s function \( G \) from the condition

\[
\det [\varepsilon(k) S(k) - H(k)] = 0 .
\]

The matrix elements of \( H \) and \( S \) may be calculated in a straightforward way and the explicit expressions are given in the Appendix. These matrix elements are expressed through spin-correlation functions of the spin system for an undoped lattice which is described by the frustrated \( S = 1/2 \) Heisenberg model. As mentioned in the Introduction we treat this model in the framework of the spherical symmetric approach which gives values of pair spin-spin correlation functions at any value of frustration parameter \( J_2/J_1 \) and temperature. Let us note that the Ritz variational principle with the 5 basis vectors \( \phi_k^a \) leads exactly to the same condition \( [13] \) and the same matrices \( H \) and \( S \) \[16, 20\]. So, at least for the case of the one-hole motion, the Mori-Zwanzig projection technique is identical to the Ritz variational principle.

### 3 Numerical results and discussion

As mentioned above we calculate the spectrum \( \varepsilon(k) \) using the hopping parameters \( t_1, t_2, t_3 \) which were obtained for La-cuprates and take \( t_1 \) as the unit of energy. So we have the values \( t_2 = -0.08 \) and \( t_3 = 0.15 \). In the calculations of the magnetic polaron of minimal size we choose \( J_1 = 1 \) since our relevant set of operators is too limited to describe the small \( J_1 \) case. But we will see that one can reach the physically relevant region by a simple rescaling.

Simultaneously with the Green’s function method the Lanczos exact diagonalization scheme is used as a complementary method to calculate the low-lying eigenstates for a
square lattice of 4 * 4 sites (with periodic boundary conditions). These low-lying states are classified by its momentum $k$ and the total spin. Here we will concentrate on the band with total spin $1/2$. There are only few exceptions where the lowest states have spin $3/2$ and that happens only for higher lying levels with momentum $(\pi, \pi)$ or $(0, 0)$. The Mori-Zwanzig projection method gives the energy difference between the lowest state with one hole for total spin $1/2$ and fixed momentum and the ground state without any hole. The same energy difference is calculated for the 4 * 4 lattice.

To clarify the importance of the additional hopping terms and frustration, in Fig. 1 we represent the results for $J_1 = t_1 = 1$ without frustration (Fig. 1a) and with $J_2 = 0.4$ (Fig. 1b). For convenience we have chosen a finite temperature $T = 0.2$ to calculate the static spin-spin correlation functions [21, 28], but we have checked that the differences to the zero temperature case can be neglected. One observes a quite reasonable agreement between the Green’s function method and the exact diagonalization data for these parameter values. As it is seen in Fig. 1a, in the absence of frustration, the spectrum demonstrates an isotropic band bottom close to the point $(\pi/2, \pi/2)$ in accordance to the experimental dispersion of one hole [10]. The same result was obtained in Ref. [19] for the $t_1$-$t_2$-$J$ model where the following parameter values were taken: $t_2 = -0.35t_1$, $J = 0.3t_1$. Let us mention that the isotropization of the band bottom in comparison with the $t$-$J$ model may be obtained in a rather wide range of parameters $t_2$ and $t_3$. For example, also the values $t_2 = -0.15t_1$ and $t_3 = 0.1t_1$ give a dispersion which is similar to that one shown in Fig. 1a. It is important that the spectrum in Fig. 1a does not demonstrate a flat band region near the point $(\pi, 0)$.

Before considering the spectrum of Fig. 1b let us remind that we suppose that the frustration simulates doping [26]. Of course there is no full equivalence between doping and frustration. For example, the doped $t$-$J$ model and the frustrated $J_1$-$J_2$ model give different results for the dynamical spin-spin structure factor and for the spectrum of Raman scattering [32]. Nevertheless, it is well known that both doping and frustration lead to a decrease of the magnetic correlation length. Furthermore, numerical calculations on finite lattices indicate the equivalence of the mentioned models if we are interested in the static spin-spin correlation functions [33]. Note that this is especially relevant in our present Green’s function method where the spectrum $\varepsilon(k)$ is determined by the static spin-spin correlation functions of the spin subsytem.

Fig. 1b represents the spectrum for the same energetical parameters as Fig. 1a, except the inclusion of a frustration term $J_2 = 0.4J_1$. The comparison of Figs. 1a and b indicates that the frustration dramatically changes the spectrum in the vicinity of the point $(\pi, 0)$. It leads to the appearance of a flat band region close to that point. Moreover, this flat band region has the form of an extended saddle point which stretches in the direction $(\pi/2, 0)$-$(\pi, 0)$. Such a band structure corresponds to the ARPES results for optimally doped cuprates [1-5].

So, we can describe the experimental results for insulating (no frustration, Fig. 1a) and optimally doped compounds (Fig. 1b, the case with the frustration) by the same set of hopping parameters. It is important that at the same time our approach demonstrates the non-rigid band behavior in the framework of a simple and natural mechanism: the doping leads to the frustration in the spin subsystem and to the variation of spin-spin
correlation functions, and correspondingly the alteration of these functions results in the non-rigid behaviour of the spectrum. Or, in other words: the doping changes the state of the magnetic background which strongly determines the form of the spectrum. Let us mind that this mechanism doesn’t take into account the direct interaction between holes which will be of course important in the regime of heavy doping.

In Figs. 2a and b we compare the exact diagonalization and the Green’s function projection method for several momenta in dependence on the frustration \( J_2/J_1 \). The non-rigid band behaviour is clearly seen. Both figures demonstrate the following common features. First, without frustration, the order of the levels coincides. Then, the change of the energy due to frustration is quite similar for the lowest four levels. The energy difference between the levels \((\pi/2, \pi/2)\) and \((\pi,0)\) decreases as the frustration increases, i.e. the level \((\pi,0)\) goes down with the respect to the band bottom (in the case \(t_2=t_3=0\) there is even an inversion of the levels and the band bottom occurs close to \((\pi,0)\))\(^{20}\). One finds a crossing for the levels \((\pi/2,0)\) and \((\pi,\pi/2)\) at \(J_2/J_1 = 0.17\) and 0.27 for the projection and exact diagonalization methods, respectively. In addition, the energy difference \(\varepsilon(\pi,0) - \varepsilon(\pi/2,0)\) decreases in both methods, and both levels cross in the Green’s function projection technique. That corresponds to the appearance of the flat band region and the extended saddle point in the vicinity of the \((\pi,0)\)-point. Of course, there are also remarkable deviations of the Green’s function method, especially for the level \((\pi,\pi)\). But fortunately, that concerns only a high lying state.

As a general tendency, the effect of frustration is more pronounced in the projection method and it seems to be overestimated. This is already known for the static spin-spin correlation functions treated in the spherical symmetric approach \(^{21, 28}\) which is incorporated in the present calculation. This approach leads to a critical value \(J_2/J_1 = 0.11\) for the second order transition between long range order and the spin-liquid state of the frustrated Heisenberg model \(^{28}\) which is rather low in comparison with other theories \(^{34, 35}\).

The reasonable coincidence of the Green’s function method with the exact diagonalization data at \(J_1 = 1\) is understandable since for such large values of \(J_1\) the magnetic energy stabilizes the size of the magnetic polaron and our concept of a polaron of small radius is justified. Let us note that for \(J_1 \ll t_1\) the bandwidth tends to be proportional to \(J_1\) \(^{11-15}\). In principle this result may also be obtained within our projection procedure if we enlarge the polaron size by enlarging the space of operators. To clarify the problem, in Fig. 2c we represent the dependence of the levels on the frustration for the same parameters as in Fig. 2b, but for a more realistic value of the exchange interaction \(J_1 = 0.4\). Comparing Figs. 2b and 2c we observe that the bandwidth for \(J_1 = 0.4\) is scaled from its value for \(J_1 = 1\) by a factor of 0.4 with surprising accuracy. The scaling of the spectrum as a whole is not as good, especially the three levels \((\pi/2,0)\), \((\pi,0)\) and \((\pi,\pi/2)\) are shifted with respect to the bottom of the band. But the order of the levels coincides nearly and the effects which have been discussed above may also be observed in Fig. 2c. Especially, the appearance of a flat band region, i.e. the decrease of the energy difference \(\varepsilon(\pi,0) - \varepsilon(\pi/2,0)\) is visible. So, we can conclude that the results for \(J_1 = 1\) are already responsible for the realistic value \(J_1 = 0.4\) if we scale the energies by a factor of roughly 0.4. Such a scaling is already known for the case without additional hopping parameters.
(t_2 = t_3 = 0) [11-15, 20] where the scaling is fulfilled with a slightly higher accuracy than may be observed here. Furthermore, comparing Figs. 2b and 2c with former results [22, 23] we see that the additional hopping parameters do not increase the bandwidth. That is in contradiction to the work [23] where it was conjectured that the inclusion of the t_2- and t_3-terms leads to an increase of the bandwidth up to a factor of four.

Finally, in Fig. 3 we represent the results for finite temperature T = 1 and zero frustration. As can be expected, in some sense the inclusion of temperature simulates the effect of doping by decreasing the antiferromagnetic correlation length in a similar way as does the frustration. But now, the exact diagonalization method is not applicable. The dispersion in Fig. 3 is similar to that one of Fig. 1b. In particular, the extended saddle point between (π/2, 0) and (π, 0) can be observed. There is one important difference that the saddle point in Fig. 3 lies much higher with respect to the band bottom than in Fig. 1b. That may have consequences for the position of the Fermi level if we fill the band with holes. That question, however, is beyond the scope of the present investigation.

4 Conclusion

The ARPES experiments show different dispersions in the insulating and optimally doped cuprates. One observes an isotropic band minimum but no flat band in the insulating compound and a flat band region in the optimally doped ones. We have shown here that the isotropic band minimum of the undoped case may be explained due to additional hopping parameters in a t-J-like Hamiltonian which naturally appear in a proper reduction scheme from the three band Hubbard model. The doping changes the spin background and in the present study we have assumed that it may be simulated by a frustration term in the exchange energy. We have seen that frustration (doping) leads to a non-rigid change of the bands such that a flat band region appears.

Let us emphasize the importance of taking into account the t_2- and t_3-hopping-terms. As mentioned above, these hoppings lead to the isotropization of the band bottom in the non-frustrated case. But these terms are also important for an adequate description of the spectrum in the vicinity of the point (π, 0). As it was shown in [20] the frustration leads to a flat band region with an extended saddle point near the point (π, 0) also in the case of the t-J_1-J_2 model. But then, in contrast to Fig. 1b, this saddle point is extended in the direction (π, 0)-(π, π/2) and not in the direction (π/2, 0)-(π, 0) as in the experiment. So, only the simultaneous consideration of t_2-, t_3-hoppings and of frustration leads to the extended saddle point in the direction (π/2, 0)-(π, 0).

In the present study we proposed to explain the different dispersion in insulating and doped cuprates by one characteristic set of hopping-parameters and a non-rigid band behaviour. Since up to now the experiments in the insulating and doped cases have been done at different compounds, another theoretical approach is possible as well: different compounds lead to different hopping parameters and to different one-hole dispersions which behave more or less rigid with respect to doping. Such a point of view can be found in [13] and [30]. In the latter work it was proposed that the microscopic hopping
parameters are influenced especially by the position of the apex-oxygen. Which of the two approaches is the correct one can be decided in the end only by an experiment which shows explicitly the difference in the dispersion of the undoped and doped case of one substance.

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APPENDIX

The procedure to calculate the matrix elements $S_{ab}(k)$ (10) and $H_{ab}(k)$ (12) is close to that one given in [20], and we present only the final expression. Let us introduce the following notations for static correlation functions of Hubbard operators with noncoinciding indices:

\[
Z_a = \sum_s \langle X^\sigma s_i X^{\sigma} i \rangle ,
\]

\[
D_{a,b} = \sum_{s_1 s_2} \langle X^{\sigma s_1} i X^{s_2 \sigma} i \rangle ,
\]

\[
V_{a,b,c} = \sum_{s_1 s_2 s_3} \langle X^{\sigma s_1} i X^{s_2 s_3} i X^{s_3 \sigma} i \rangle .
\]

These expressions can be further reduced to static spin-spin correlation functions (for details see [20]). A straightforward calculation gives for the overlap matrix:

\[
S_{aa} = 1/2 \quad (a = 0, \ldots, 4)
\]

\[
S_{0a} = Z_a \quad (a = 1, \ldots, 4)
\]

\[
S_{ab} = D_{a,a} - D_{b,a} \quad (a, b = 1, \ldots, 4) \quad (a \neq b) ,
\]

and we see that it doesn’t depend explicitly on the momentum $k$. Analogously, the Hamilton matrix may be expressed as:

\[
H(k) = K(k) + \tilde{E}
\]

\[
K^{00}(k) = \sum_l t_l Z_l e^{ikl} ,
\]

\[
K^{0a}(k) = \frac{1}{2} t_a e^{ika} + \sum_l \tilde{\delta}_{al} t_l D_{l,l-a} e^{ikl} ,
\]

\[
K^{aa}(k) = t_a Z_a (e^{ika} + e^{-ika}) + \sum_l \tilde{\delta}_{al} \tilde{\delta}_{-l,a} t_l V_{a,a+l,l} e^{ikl} ,
\]

\[
K^{ab}(k) = \tilde{\delta}_{-a,b} t_b Z_a e^{ikb} + t_b Z_b e^{-ika} + t_{b-a} Z_{b-a} e^{ik(b-a)} + \sum_l \tilde{\delta}_{-a,l} \tilde{\delta}_{b,l} t_l V_{a,a+l,l-b} e^{ikl} ,
\]

\[
\tilde{E} = (J_1 + J_2) \mathbf{S} + \tilde{E} ,
\]

\[
\tilde{E}^{00} = -\frac{1}{2} \sum_m J_m Z_m ,
\]

\[
\tilde{E}^{0a} = -\sum_m J_m \left( \frac{\delta_{am}}{4} + \frac{\delta_{am}}{2} D_{m,m-a} \right) ,
\]

\[
\tilde{E}^{aa} = -\sum_m J_m \left( \frac{\delta_{am}}{2} Z_m + \tilde{\delta}_{am} (Z_m - \frac{Z_{m-a}}{2}) \right) ,
\]

\[
\tilde{E}^{ab} = \frac{1}{2} \sum_m J_m \left[ -\delta_{bm} Z_{a-b} - \delta_{am} Z_{b} + \delta_{m-a,-b} (Z_{a-b} - Z_{a})
\right.
\]

\[+ \delta_{am} \tilde{\delta}_{bm} V_{a-m,a-b} + \tilde{\delta}_{am} \tilde{\delta}_{m-a,-b} (V_{m,a-a-b} - V_{-m,a-m,a-b}) \right] .
\]
where $\delta_{am} = 1$ for $a = m$ and zero else, and $\bar{\delta}_{am} = 1 - \delta_{am}$. The indices $a$ and $b$ ($a \neq b$) run over 1 to 4 and the above summation on $l$ and $m$ are restricted to that neighbours which are defined in the kinetic (2) and exchange (3) parts of the Hamiltonian, respectively.
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FIGURE CAPTIONS

FIG. 1: Quasiparticle dispersion along the line $M$-$G$-$X$-$M$ and contour plot for $J_1 = t_1 = 1, t_2 = -0.08, t_3 = 0.15, T = 0.2$ without frustration (a) and for $J_2 = 0.4$ (b). The points in $k$-space mean: $M = (\pi, \pi), G = (0, 0)$ and $X = (\pi, 0)$. The circles are the result of the exact diagonalization of a $4 \times 4$ lattice at $T = 0$ with total spin $S_{tot} = 1/2$.

FIG. 2: Energy difference between the lowest state of one hole with total spin $S_{tot} = 1/2$ for several momenta and the groundstate without any hole in dependence on the frustration within the Green’s function method (GF) for $J_1 = 1$ (a), and for the $4 \times 4$ lattice for $J_1 = 1$ (b) and $J_1 = 0.4$ (c). The hopping parameters are the same as in Fig. 1.

FIG. 3: Dispersion and contour plot for $J_2/J_1 = 0$ and finite temperature $T = 1$. The other parameters are as in Fig. 1.