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Qualitative understanding of the sign of t' asymmetry in the extended t-J model and relevance for pairing properties

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Numerical calculations illustrate the effect of the sign of the next-nearest-neighbor hopping term t' on the two-hole properties of the t-t'-J model. Working mainly on two-leg ladders, in the $-1.0 \leq t'/t \leq 1.0$ regime, it is shown that introducing t' in the t-J model is equivalent to effectively renormalizing J, namely t' negative (positive) is equivalent to an effective t-J model with smaller (bigger) J. This effect is present even at the level of a 2×2 plaquette toy model, and was observed also in calculations on small square clusters. Analyzing the transition probabilities of a hole pair in the plaquette toy model, it is argued that the coherent propagation of such hole pair is enhanced by a constructive interference between both t and t' for $t'>0$. This interference is destructive for $t'<0$.

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One of the most important unsolved problems in theoretical physics is the clarification of the nature of high-temperature superconductors. A popular approach in this context is the use of the t-J model, with holes moving in an antiferromagnetic (AF) spin background. In recent years, mainly due to an increase in the sensitivity and resolution of angle resolved photoemission spectroscopy (ARPES), it has been shown that extra hole hoppings beyond nearest neighbor (NN) are important in the t-J model, giving origin to the ‘‘extended’’ t-J model. For example, ARPES measurements in $Sr_2CuO_2Cl_2$,[1] and their subsequent interpretation,[2] have shown the importance of those extra hoppings to reproduce the experimental results. Subsequent efforts have concentrated on the effect of the extra hoppings on various properties of planar and ladder systems, such as stripe stability,[3] competition between pairing and stripes,[4] spin-charge separation in two dimensions,[5] stripe formation mechanism,[6] spin gap evolution,[7] and current-current correlations.[8] Most of these papers have compared and contrasted the dependence of different properties of the extended t-J model with the sign of the next-NN (NNN) hopping t'. Currently it is well established that a positive t' enhances hole pairing and AF correlations, while the opposite occurs for t' negative.[4,9] Nevertheless, to the best of our knowledge, these previous publications have not provided an intuitive mechanism that can explain why this happens, namely, for what reason there is an asymmetry between positive and negative t'. This is particularly puzzling considering the limit $t=0$, since in the t'-J model the sign of t' is irrelevant.[10]

It is the purpose of this paper to provide a qualitative explanation to this phenomenon, i.e., the sign of t' asymmetry. Our main result is that a quantum interference between NN and NNN hoppings identified in the hole-pair propagation was found to be constructive (destructive) for t' positive (negative); this accounts for the observed dependence of the hole-pair properties with the sign of t'. The t-t'-J model used here is defined as

$$H=J\sum_{\langle \mathbf{ij}\rangle}(\mathbf{S_i}\cdot\mathbf{S_j}-\tfrac{1}{4}n_{\mathbf{i}}n_{\mathbf{j}})-\sum_{\mathbf{im}}t_{\mathbf{im}}(c_{\mathbf{i}}^{\dagger}c_{\mathbf{m}}+\mathrm{H.c.}),\qquad(1)$$

where $t_{\mathbf{im}}$ is t for NN, t' for NNN, and zero otherwise. The rest of the notation is standard. Comparison with ARPES experiments[2,11] showed that $t'<0$ is physically relevant for the hole-doped cuprates. The density matrix renormalization group[12] (DMRG) and Lanczos[13] methods are used on ladders and small square clusters to study the Hamiltonian Eq. (1).

First, let us show that the dependence of hole-hole correlations with the sign of t' can be crudely described as a renormalization of the exchange interaction J. In Fig. 1 is shown, through calculations on ladders and square clusters, the dependence of the average distance $\langle d\rangle$ between two holes with the sign of t'. The result obtained is roughly consistent with a renormalization of J by t', in the sense that results for t' negative (positive) can be obtained by renormalizing J to a smaller (bigger) effective value, leading to an increase (decrease) in $\langle d\rangle$. To show that binding energy and phase separation (PS) tendencies are both affected in a way consistent with this interpretation the dependence of the PS line with t' is shown in Fig. 1(c) (squares). It can be observed that t' negative (positive) requires an increase (decrease) in the value of J needed for the holes to segregate (desegregate), if compared to the J value that leads to PS at $t'=0$. The circles display values of J/t and t'/t that result in the holes having a binding energy of $\approx 0.5t$ (as the boundary of the binding region that we can consider ‘‘robust’’). This binding energy line shows that at a fixed J, such as 0.4, increasing $t'>0$ leads to strong binding, with the opposite effect for $t'<0$. As expected, this line approximately follows the behavior of the PS line.[14] Thus, the essence of the results in previous studies,[4,9] showing pairing with $t'>0$, can be reproduced on a small cluster with two holes. Note that in Fig. 1, for $t'/t\approx1$, $\langle d\rangle$ reaches its minimum value and starts to increase. In the limit when $|t'|/t\gg1$ the hole-hole correlations (and other properties of the model) become *indepen-*

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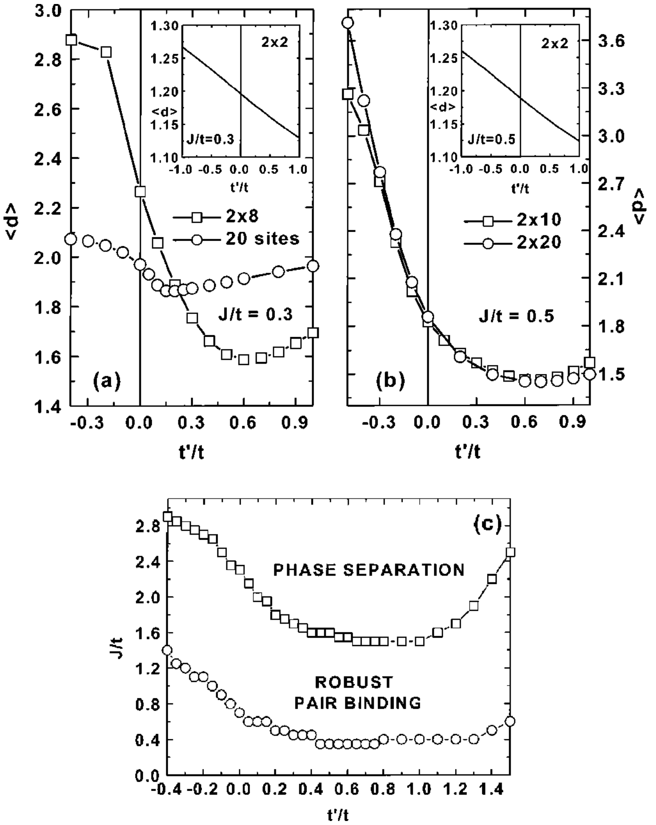

FIG. 1. (a) Exact diagonalization (ED) results showing the dependence with t' of the average distance $\langle d \rangle$ between two holes on a 2×8 ladder (squares) and on a 20 sites tilted two-dimensional cluster (circles). Periodic boundary conditions (PBC's) are used in both cases, $J/t=0.3$ and $-0.5\lesssim t'/t\lesssim1.0$. The tendency of the holes to separate when a negative t' is turned on can be observed. For $t'>0$, there is a tendency of the holes to form tighter pairs. However, in this last case, as t' keeps on increasing the holes will eventually tend to separate, showing a similar behavior to the t' negative case. The inset shows a calculation of $\langle d \rangle$ on a 2×2 plaquette with conclusions similar to those reached with the larger clusters. (b) Same as (a) except that now $J/t=0.5$ on a 2×10 ladder (ED) and the tilted cluster was substituted by a 2×20 ladder (DMRG) with open boundary conditions (OBC's). Again the inset shows results of $\langle d \rangle$ on 2×2, but now for $J/t=0.5$. (c) Phase diagram J/t vs t'/t showing regions of pair binding and phase separation (defined through the divergence of the compressibility). The pair binding line (circles) is defined by values of J/t and t'/t that give a robust binding energy of $\approx0.5t$ on a 2×8 ladder. Notice that close to $t'/t=0$ both lines behave in accordance with our qualitative picture, i.e., t' negative (positive) renormalizes J to smaller (bigger) values.

dent of the sign of t'.[10] Therefore, the renormalization of J described above mainly occurs in the region $-1.0\lesssim t'/t\lesssim1.0$.

It is important to note that it is not only $\langle d \rangle$ that behaves in accordance with this simple scenario. To a surprising accuracy, hole-hole correlations for, e.g., t' negative in the t-t'-J model, match those of the t-J model with an effective (smaller) J. To illustrate that, in Fig. 2 hole-hole correlations for a 2×8 ladder with two holes are calculated for

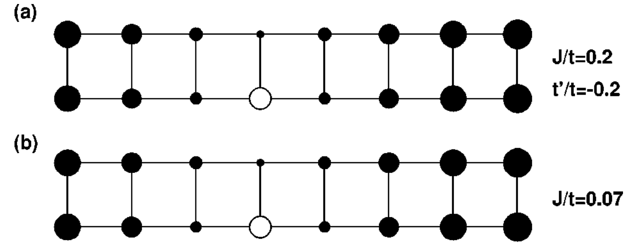

FIG. 2. Comparison of hole-hole correlations $\langle n_0 n_i \rangle$ between the t-t'-J model and an effective t-J model. (a) 2×8 ladder with two holes, $J/t=0.2$ and $t'/t=-0.2$, PBC's. The open circle stands for a projected hole at origin, while solid circles at site i have radius proportional to $\langle n_0 n_i \rangle$. (b) Same as (a) but for $J/t=0.07$ and $t'/t=0.0$.

the t-t'-J model with $J/t=0.2$ and $t'/t=-0.2$, and then compared to results for the t-J model with $J/t=0.07$. The open circle stands for a projected hole (at the origin of the coordinate system) and the radius of the solid circle on site i is proportional to $\langle n_0 n_i \rangle$. Most of the values match to high accuracy, as deduced from the similarity of the pictures. This is also the case for t' positive and for square clusters. Then, this seems an indication that the renormalization concept is robust. Preliminary results indicate that the main features of the dependence of the spin correlations with the sign of t' can be qualitatively explained through J's renormalization, although it is not possible to achieve the same degree of high accuracy as shown above in the charge sector.

The fact that the renormalization of the exchange interaction by t' is consistently observed on ladders and square clusters [compare result for 2×8 ladder and 20 sites cluster in Fig. 1(a)], and is observed for OBC's and PBC's [compare result for 2×10 PBC ladder with 2×20 OBC ladder on Fig. 1(b)], is an indication that this effect is associated with some local process and therefore could even be observable on a 2×2 plaquette with two holes. If this is correct then it should be possible, through a careful analysis of such toy model, to gain a better insight on the qualitative aspects of the physics associated with the sign of t'. In the insets for Fig. 1 is shown the dependence of $\langle d \rangle$ with t' on a 2×2 plaquette and the same trend found on ladders and square clusters is again reproduced. Also, the exact energy of the ground state for the plaquette with two holes is given by $E_0=-\frac{1}{2}[(J+2t')+\sqrt{(J+2t')^2+32t}]$, where the renormalization of J by t' can be explicitly seen. It is important to remark that in a reduced basis formed with spin singlets on the sides and diagonals of the plaquette, the coefficients describing the ground state also depended on t' through the same expression $(J+2t')$.

Encouraged by these results on the 2×2 plaquette, one can now try to understand qualitatively how the change of sign in one hopping amplitude can change the binding properties of a hole pair, a result that up to now is being rephrased as a renormalization of J. To make progress it has to be analyzed how this change of sign affects the dynamics of a hole pair. A hint in this direction is that for $t=0$ this asymmetry in the properties of the model caused by the sign of t'

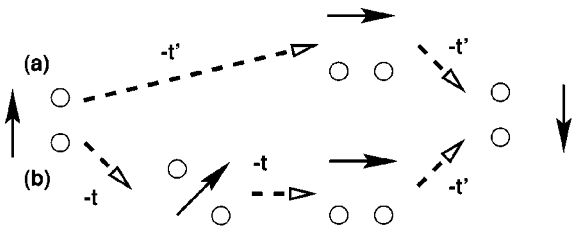

FIG. 3. (a) Second-order process that exchanges the positions of a hole pair (circles) and a spin singlet (solid arrow) localized on opposite sides of a 2×2 plaquette. (b) Third-order process for the same transition depicted in (a). Both processes will have the same amplitude if $t'=4t^2/J>0$ (see text). This leads to a constructive interference if t' is positive, which becomes destructive if t' is negative.

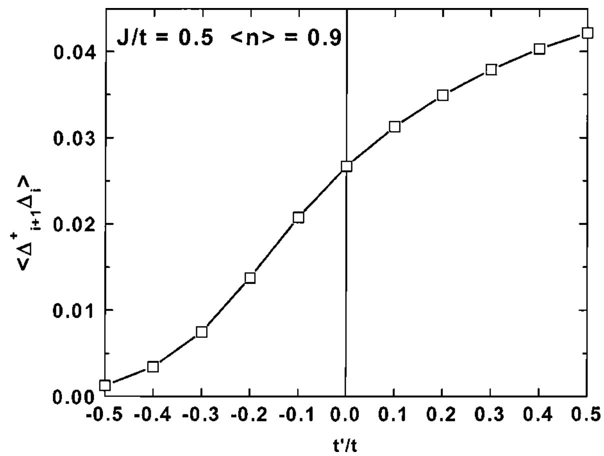

FIG. 4. Dependence with t'/t of the pair-pair correlations at distance 1 in a 2×10 ladder with two holes for $J/t=0.5$. The coherent propagation of a hole pair located in a rung is shown to have a dependence with t'/t consistent with the scenario described in Fig. 3.

vanishes, as implied above by the discussion of the $|t'|/t \gg 1$ regime. Then, for the hole-pair properties to be affected by the sign of t' it is important to have the possibility of NN t hoppings. Intuitively this resembles an interference of some sort: the movement of a hole pair, through a combination of both hoppings, may lead to a coherent propagation of the pair, for t' positive, or to its melting into independent quasiparticles,[7,15] for t' negative.[16] To check this idea, in the plaquette toy model, one can calculate the probability of a transition from an initial state composed of a hole pair and a spin singlet in opposite sides of the plaquette, to a final state where the hole pair and the spin singlet have exchanged places.[17] Such a transition is depicted in Fig. 3, where in (a) is shown the most probable second-order process (a process with two t hoppings would be less probable because the intermediate state would be an excited state[17]) and in (b) is shown a third order process (the other three are equivalent to the one discussed). The difference between processes (a) and (b) resides in the fact that the latter needs one more virtual state than the former. As such state is excited ($\Delta E=J$), and taking into account that there are three other third-order processes with two NN hoppings and one NNN hopping, it can be shown that second- and third-order processes will have amplitudes proportional to t'^2 and $4t^2t'/J$, respectively. This means that if t' is positive (negative) they will have the same (π-shifted) phase and their interference will be constructive (destructive). A similar reasoning can be applied to higher order processes, but it can be shown that they are less probable than the processes discussed above, given that they would pass by the same virtual state more than once.[18]

Through the mechanism described in Fig. 3, it is suggested that achieving coherency in the propagation of the hole pair depends on having the correct balance of short-range processes (1 and $\sqrt{2}$ hoppings). Then, it should not be a surprise that the plaquette can display this effect, as shown above. Nevertheless, it should be checked that such process also occurs on $2\times L$ ladders. That this is the case is shown in Fig. 4, where pair-field correlations at a distance of one lattice spacing are calculated through ED on 2×10 ladders with $J/t=0.5$ and $\langle n\rangle=0.9$. The pair operator is defined as $\Delta_i=c_{i1\uparrow}c_{i2\downarrow}-c_{i1\downarrow}c_{i2\uparrow}$, where i labels a rung and the legs are numbered 1 and 2. The result shows that the coherent propagation of a hole pair located in a rung is enhanced for t' positive, while a rapid decay is observed for t' negative, in agreement with the picture described in the toy model and with previous calculations.[4,9]

The physics of the $t'>0$ extended t-J model resembles results for the effective model discussed in Ref. 19, where holes were considered quasiparticles moving in a "perfect" antiferromagnetic background with hopping only within the same sublattice, and with an explicit NN attraction to mimic AF mediated pairing. In fact, in Ref. 20 it was shown that a *positive* t' is needed to generate a $d_{x^2-y^2}$ two-hole bound state in the quasiparticle model of Ref. 19. As a consequence, the regime of $t'>0$ of the extended t-J model, with its strong AF correlations and pair coherent movement, is likely mimicked by the simple toy model used in previous literature.[19,20]

Summarizing, here has been provided a qualitative picture to explain the dependence of hole pairing on the sign of the NNN hopping t' in the t-t'-J model. Through numerical calculations on square clusters, but mainly on ladders, using ED and DMRG, it was established that t' negative (positive) effectively reduces (increases) J. The variety of clusters and boundary conditions where this effect was consistently observed served as an indication of the locality of the process involved. This suggested the use of a 2×2 cluster with two holes as a guiding toy model. By solving analytically this cluster, the J renormalization was shown explicitly in the dependence of the ground-state energy with t', and the behavior of hole-pair size $\langle d\rangle$ was consistent with what was found on ladders and square clusters. The fact that for $t=0$ the properties of the t-t'-J model are not dependent on the sign of t' has indicated that some sort of interference process between t and t' should be responsible for the hole-pair dependence on t'. By analyzing transition probability amplitudes in the plaquette it was observed that indeed this is the case. A negative t' interferes destructively with t, causing a hole pair to have a tendency to split into two independent quasiparticles. A positive t', on the other hand, by interfering constructively with t, preserves the integrity of the hole pair while it propagates. This simple picture provides a better understanding of the t-t'-J model, adding more physical insight to the "effective J" picture.[5] By calculating pair-field correlations at a distance one on 2×10 ladders it was argued that this qualitative explanation holds also for larger systems.

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[10] It can be shown that changing the sign of t in the t-J model is equivalent to a shift in momentum by (π,π). Thus, by the expression of the dispersion relation of a hole in the t-J model $0.55J(\cos k_x+\cos k_y)^2$ it can be concluded that such a change of sign has no effect in the properties of the model. Changing the sign of t' in the t'-J model is also irrelevant; this can be concluded by noticing that the t'-J model is equivalent to a t-J model on a $\sqrt{2}a$ lattice. Therefore, in the t-t'-J model, in the limit where either $t=0$ or $t'=0$, a change of sign in the hopping amplitude is irrelevant.

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[16] In previous works by two of the authors (Ref. 5), indications of spin-charge separation were found in the negative t' regime. The connection of the ideas discussed here to these previous results is being presently analyzed.

[17] Since the objective is to analyze the hole-pair dynamics, a strong coupling regime ($J\gg t,\ t'$) is assumed. In this case the two states with spin singlets in the diagonal of the plaquette are excited configurations (with zero energy) and the four states with spin singlets in the sides of the plaquette form a degenerate ground state (with energy $-J$). Therefore, starting from a ground-state configuration (spin singlet on the side), a NN hopping takes it to an excited configuration (spin singlet on the diagonal), being therefore a less probable process, according to standard perturbation theory. Note that the fermionic commutation signs are included in the orientation of the singlets.

[18] A previous publication (Ref. 9), discussing differences between hole-doped and electron-doped cuprates, suggested as an explanation for the t' sign effect the stabilization of Néel-like configurations (containing NN hole pairs) in the ground state through a diagonal matrix element with value $-t'$. Such configurations would be energetically favored by a positive t', leading to an increase in pairing and AF spin correlations, with the opposite effect for t' negative, as compared to the $t'=0$ case. However, this argument does not address an important point: In the limit of $|t'|/t\gg1$ it would still give asymmetric results for positive and negative t'. It was checked by ED of a 2×8 ladder with two holes that the ground state for $J/t=0.2$ and $t'/t=\pm10.0$ has $\mathbf{k}=(0,0)$, that is a sufficient requirement for the matrix element argument to apply; nevertheless the probability of having the holes in the same rung is quite similar for positive and negative t'. The spin correlations are also similar, indicating the irrelevance of the sign of t' in the $t=0.0$ limit. Then, the interference mechanism, that takes into account the interplay of NN and NNN hoppings, supplements their argument, since in the limit $|t'|/t\gg1$ the interference becomes irrelevant. In Ref. 4, the 2×2 toy model was used to make an energetic consideration to explain the pair binding dependence on the sign of t'. The intuitive picture here discussed supplements their discussion and, regarding their assumption about the validity or not of generalizing results obtained in the 2×2 plaquette to larger systems, the results shown here (e.g., Fig. 2) give support to such a generalization.

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