Pairing properties of the t-t'-t''-J model

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We study the pairing properties of the two-dimensional t-t'-t''-J model, where t' and t'' are second and third neighbor hoppings, at a doping level $x \approx 0.1$. Recent studies of the t-t'-J model find strong pairing for $t' > 0$, associated with electron doping, but an absence of pairing for $t' < 0$, associated with hole doping. This is in contrast to the cuprates, where the highest transition temperatures appear for hole doping. Model parametrizations for the cuprates estimate a t'' comparable to t', which, in principle, might fix this discrepancy. However, we find that it does not; we observe a suppression of pairing for the hole-doped system ($t' < 0, t'' > 0$), while for the electron-doped system ($t' > 0, t'' < 0$) d-wave pairing is robust. Extended hoppings appear to be insufficient to make the one-band t-t'-J model capable of describing the pairing in the hole-doped system.

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Can a single-band two dimensional t-t'-t''-J model capture the physics of both the hole- and electron-doped high-T_c cuprates? This model, with near-neighbor t, next nearest neighbor t', and third nearest neighbor t'' hopping parameters, a near neighbor spin exchange J, and the restriction of no double-site occupancy, has been found to describe a number of properties seen in these materials. For example, (1) the asymmetrical behavior of the commensurate antiferromagnetic (AFM) spin correlations which rapidly decrease with hole doping ($t' < 0, t'' > 0$) but remain strong for a much longer range of electron doping ($t' > 0, t'' < 0$) [1,2], the appearance of stripes in the hole-doped region and their absence in the low electron-doped region [3,4], and (3) a single particle spectral weight where doped holes lead to the appearance of Fermi arcs around the $(\pm\pi/2, \pm\pi/2)$ regions of the Brillouin zone while doped electrons are accommodated near the $(\pm\pi, 0)$ and $(0, \pm\pi)$ regions [1,2].

However, while the material itself has clear superconductivity with a high transition temperature, it has been unclear whether these models have a superconducting ground state. In many cases the t-J model and its "parental" Hubbard model have competing/intertwined orders [5–26], particularly stripes and uniform d-wave superconductivity, that are very close in energy. Recently, density-matrix renormalization group (DMRG) studies found that while $t' > 0$ (electron doping) can lead to strong and unambiguous d-wave superconductivity in the ground state [27–29], for $t' < 0$ (hole doping) the model exhibits charge stripes with the pairing suppressed [27]. While the coexistence of superconductivity and short range AFM correlations have been reported on the electron-doped side [30], the absence of a superconducting phase for the hole-doped case is clearly at odds with the long held belief that the t-t'-J model provides an appropriate model for understanding the cuprate superconductors.

The third neighbor hopping t'' is thought to be roughly the same size as t' in the cuprates [2,31–33]. For the case of the hole-doped cuprates, it reflects the extended nature of the orthogonalized Zhang-Rice singlet [34] of the three-band CuO_2 model [35]. Can the addition of t'' fix the discrepancy? In this paper, we use DMRG to investigate pairing properties of the t-t'-t''-J model at a doping level $x \approx 0.1$. Our main conclusion is that t'' does not resolve the discrepancy. We find that the parameters used for the electron-doped cuprates ($t' > 0, t'' < 0$) enhance superconductivity, both individually and in combination. However, the ones used for the hole-doped cuprates ($t' < 0, t'' > 0$) suppress it. In most of the region with pairing there is coexisting antiferromagnetic (AFM) order and uniform electron/hole density, i.e., an absence of charge stripes. These results imply that the extended t-t'-t''-J model fails to capture the superconducting phase of the hole-doped cuprates. The Hamiltonian of the t-t'-t''-J model that we will study is

$$H = \sum_{\langle ij\rangle\sigma} -t(c^\dagger_{i\sigma}c_{j\sigma} + \text{H.c.}) + \sum_{\langle\langle ij\rangle\rangle\sigma} -t'(c^\dagger_{i\sigma}c_{j\sigma} + \text{H.c.}) + \sum_{\langle\langle\langle ij\rangle\rangle\rangle\sigma} -t''(c^\dagger_{i\sigma}c_{j\sigma} + \text{H.c.}) + \sum_{\langle ij\rangle} J\left(\vec{S}_i\cdot\vec{S}_j - \frac{1}{4}n^{\text{tot}}_i n^{\text{tot}}_j\right) + \sum_i -\mu n^{\text{tot}}_i, \quad (1)$$

with the restriction of no double site occupancy. The single/double/triple brackets under the summations denote first/second/third nearest neighbor pairs of sites and $n^{\text{tot}}_i = n_{i\uparrow} + n_{i\downarrow}$ is the total particle density on site i. The nearest neighbor hopping t is set to 1 and the spin exchange J is set to 0.4 for all calculations. It has been proposed [31,32] that the parameters $t' = -0.3$, $t'' = 0.2$ correspond to hole-doped cuprates.

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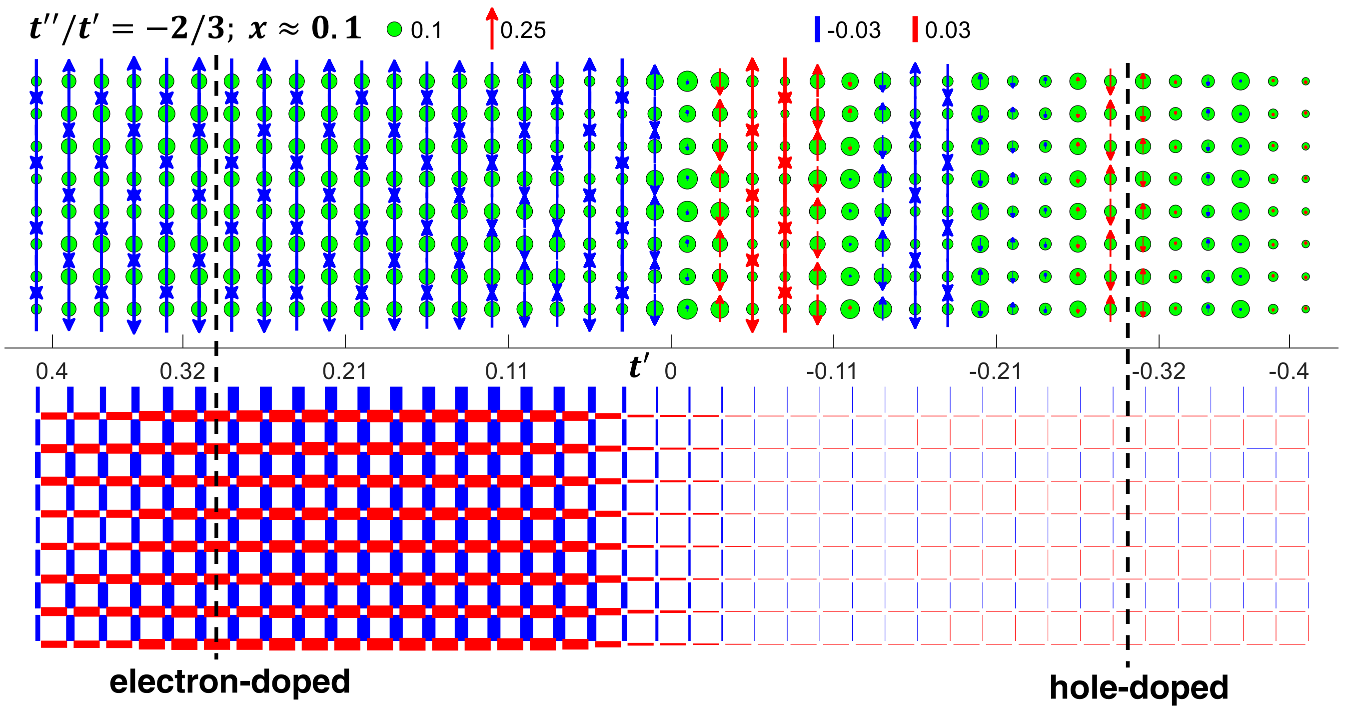

FIG. 1. Scan where both t'' and t' vary with a fixed ratio of $-2/3$. The system crosses from a parameter region corresponding to electron doping to one corresponding to hole doping [31,32]. In the upper plot, the area of the circles represents the local fermion density x_i at site i such that, for the electron-doped system, the electron density $n_i = 1 + x_i$ and for the hole-doped system $n_i = 1 - x_i$; the arrows represents the local $\langle S^z \rangle$ with the colors indicating different AFM regions. In the lower plot the width/color of the links represent the magnitude/sign of the singlet pairing between two adjacent sites. The electron-doped region has coexisting AFM, uniform hole density, and strong d-wave pairing, while the hole-doped region is striped with the pairing suppressed.

Under a particle-hole transformation which changes the signs of both hoppings, the set ($t' = 0.3, t'' = -0.2$) corresponds to electron doping with a filling $n = 1 + x$. Here we treat both t' and t'' as adjustable parameters to investigate their individual and combined effects on superconductivity. A chemical potential μ is used to control the doping level x. We keep $x \approx 0.1$, where with $t'' = 0$ it is known to have one phase for $t' > 0$ (electron doping) with clear superconductivity and another phase for $t' < 0$ (hole doping) where superconductivity is suppressed [27].

The DMRG calculations are carried out using the ITensor library [36]. We study cylinders, with open boundary conditions in the x direction and periodic boundary conditions in the y direction. We typically perform around 20 sweeps and keep a maximum bond dimension $m \sim 3000$, which provides good convergence for local observables of interest: the local doping on site i, $n_{\rm dope}(i) = 1 - n_i^{\rm tot}$, the local magnetization on site i, $S^z(i) = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$, and the local singlet pairing order parameter $\Delta(i, j)$ on nearest neighboring sites i and j, $\Delta^\dagger(i, j) = \frac{1}{\sqrt{2}}(c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} - c^\dagger_{i,\downarrow} c^\dagger_{j,\uparrow})$. Note that this bond dimension would not be sufficient for more difficult observables, such as long-range pairing correlations [21,28]. Our main interest is the overall phase diagram. We allow symmetry to break in these phases (encouraging the breaking with initial states or boundary fields) so that local observables describe them. Although our results are limited to width-8 cylinders, there are no indications that larger widths would give a qualitatively different phase diagram. A potential difficulty for DMRG simulations on large systems is the tendency to get stuck in metastable phases. This issue is most serious near phase boundaries where different competing phases are close in energy. To reduce this problem, we employ "scan" calculations where along the length of a 40×8 cylinder we vary one or two parameter(s) [27] linearly and slowly. A varying chemical potential is also used to keep the doping level constant—the variation of μ down the cylinder is manually adjusted with repeated runs to keep the doping constant. In this way the cylinder forms different phases in different regions along the length of the cylinder. The competition between phases occurs over a few columns of sites which automatically "regularizes" or controls the competition so that no large length scales or large entanglement can occur. The converged position of the phase boundary translates to the parameter values of the boundary. The phases are particularly stable near the center of each region. Near the centers of each region, we have also performed separate nonscan/fixed-parameter simulations to verify the phase.

In Fig. 1 we show a scan calculation which crosses a parameter region in which the system changes from electron-doped to hole-doped cuprates. The upper panel shows the local fermion density x_i and spin $\langle S^z \rangle$ observables which gives an immediate view of the phases and their spin/charge orders. Restricted by the t-J space, we simulate the electron-doped system by staying below half filling and performing a particle-hole transformation which changes the sign for both t' and t''. Therefore, one can treat the fermion density x_i (green circles)

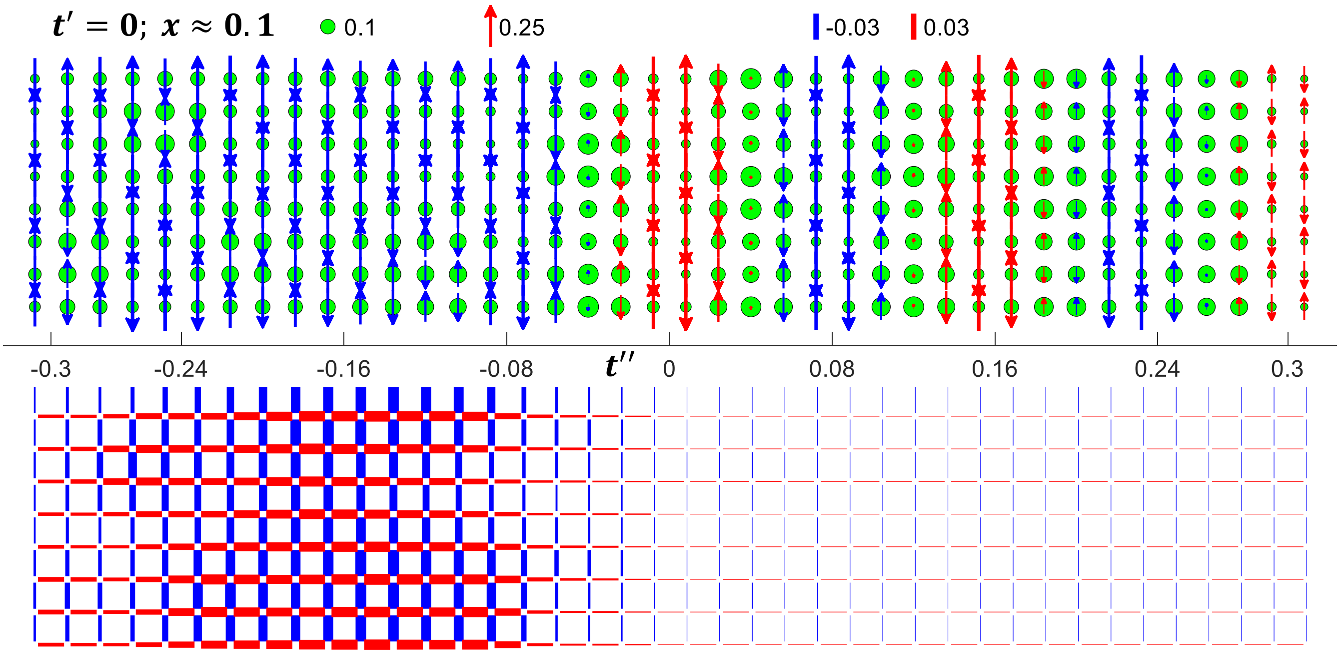

FIG. 2. t''-varying scan at $t' = 0$ and $x \approx 0.1$ plotted in the same way as in Fig. 1. For $t'' < 0$ the system shows AFM order with a slightly nonuniform hole density and d-wave pairing that peaks for $t'' = -0.16$. For $t'' > 0$ stripes appear and the pairing is suppressed.

in the left half of the system ($t' > 0$) as the density of doped electrons added to the half-filled band and in the right half of the system ($t' < 0$) as doped holes. For the parameter set ($t' = 0.3, t'' = -0.2$) corresponding to the electron-doped case, the system exhibits commensurate AFM with uniform density and a strong d-wave pairing shown in the lower plot. The pairing reaches its maximum around $t' \approx 0.2, t'' \approx -0.13$ instead of increasing monotonically with $|t'|$, $|t''|$. On the other hand, the parameter set ($t' = -0.3, t'' = 0.2$) associated with the hole-doped system shows a charge density wave with the pairing suppressed. One can see that its spin pattern which has much smaller spin moments differs from the conventional striped state near the $t' = 0$ region. As discussed in the Supplemental Material [37], the spin correlations in this unconventional striped phase are short ranged, mimicking the behavior of the two-leg Heisenberg ladders.

Next in Fig. 2 we present another scan calculation which varies t'' with t' fixed at zero to investigate the individual effect of t''. For $t'' < 0$ corresponding to the electron-doped cuprates we see commensurate AFM with a slight nonuniformity in density, while for $t'' > 0$ related to hole-doped cuprates it shows conventional stripes. The d-wave pairing only exists for $t'' < 0$ and its magnitude peaks around $t'' = -0.16$. Roughly speaking, the effect of having a t'' alone is very similar to having a t' alone [27] with opposite sign. The small differences are that the enhancement of pairing by $t'' > 0$ is overall weaker and happens over a narrower window. The rest of the scan calculations are presented in the Supplemental Material [38].

By collecting all the scans, we have constructed the approximate phase diagram in the t'-t'' plane shown in Fig. 3. The solid lines are DMRG scans as discussed above. The blue parts of these scans denote parameter ranges with d-wave pairing and the red parts without pairing. By connecting the transition points on these scans, we have mapped out an approximate boundary of the pairing phase, as indicated by the green dotted line.

It is clear from Fig. 3 that $t' > 0$ and $t'' < 0$ enhance pairing, while $t' < 0$ and $t'' > 0$ suppress it. This is true when t' [27] or t'' acts individually, as can be seen from the $t' = 0$ and

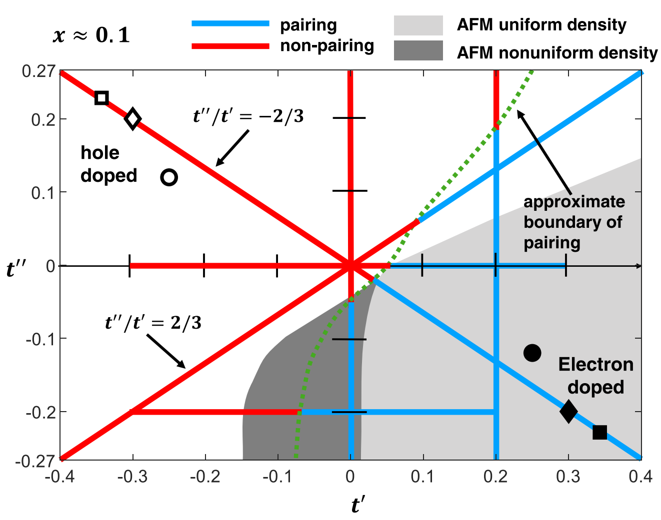

FIG. 3. Approximate phase diagram in the t'-t'' plane at doping $x \approx 0.1$. The lines are "scans" with the blue/red color denoting the parameter range with/without pairing. The dotted green line shows the extrapolated pairing phase boundary based on the scans. The light/dark gray regions have AFM order with uniform/nonuniform hole density, while the white background is striped. Square [33], diamond [31,32], and circle [2] markers indicate the (t', t'') values proposed in several studies with solid markers for electron-doped systems and hollow markers for hole-doped systems.

$t'' = 0$ axis. When they act together, the effect appears to be largely additive since the approximate pairing phase boundary is roughly orthogonal to the $t''/t' = -2/3$ line. In other words, one always has a decrease of pairing strength when starting from a point in the pairing phase (within the range shown in Fig. 3) and decreasing t' or increasing t''.

The region with superconductivity largely has coexisting AFM order with uniform density, as indicated by the light gray area. This supports the idea that charge stripes (either with or without π phase shift of AFM order) compete with pairing and the absence of stripes supports good pair mobility and superconducting phase coherence. We also note that the longer range hoppings t' and t'' will in principle lead to longer range next-nearest J' and third nearest neighbor J'' exchange couplings. For example, if one assumes that the exchange coupling $J = 0.4$ arises from a Hubbard model with $t = 1$ and $U = 10$, then for $t' = 0.3$, one would have $J' \approx (t'/t)^2 J = 0.036$. This longer range exchange coupling has a negligible effect on the AFM order and as we have discussed one will have a phase with coexisting d-wave superconducting and AFM order arising from electron doping. However, as Jiang and Kivelson [29] have discussed, for a larger value of $J' = J/2$ and corresponding $t' = t/\sqrt{2}$, they find that a d-wave superconductor arises from electron doping a spin-liquid state. The parameters $t' = 0.3$, $t'' = -0.2$, associated with an electron-doped system and marked by the open diamond in Fig. 3, correspond to a state which is deep inside the pairing phase. Alternatively, the parameters $t' = -0.3$, $t'' = 0.2$, associated with a hole-doped system and marked by the solid diamond in Fig. 3, correspond to a state which is far away from the pairing phase boundary. We have tried numerous ways to obtain a phase in the hole-doped region which is superconducting, but the only way seems to be to apply an unphysical large pairing field throughout the system, and its removal leads to the disappearance of pairing within a few DMRG sweeps. These results indicate a fundamental flaw in the model for a reliable description of the doping dependence of pairing in the cuprates.

Discussion. If the t-t'-t''-J model is not sufficient to describe superconductivity in the cuprates, it is natural to look at less renormalized models. One can think of these models as devised in successive steps starting with all electron calculations, constructing a three-band model, reducing it to a single-band Hubbard model and from there, in the large U limit, to a t-t'-t''-J model. Apparently, somewhere in this process the correct modeling of the pairing for the hole-doped system is lost. It may be that the restriction of no double occupancy is too severe and a single band Hubbard model will turn out to be adequate. However, another possibility may stem from the reduction of the three-band charge-transfer model to a single-band Mott-Hubbard model, and in particular this reduction on the hole-doped side. In the case of electron doping, this reduction is fairly simple: the doped electrons dominantly occupy the coppers sites, and so it is reasonable to integrate out the oxygens. However, on the hole-doped side, the doped holes tend to go onto both the Cu and its surrounding O(p_x, p_y) orbitals [39], and conceptually the reduction to a one band model proceeds through the Zhang-Rice singlet picture [34]. Although there is evidence from simulation [40–42] and experiments [43–45] that support the Zhang-Rice singlet picture, it may also be that a more careful treatment of the reduction could introduce new terms beyond extended hoppings, which are necessary to get the pairing behavior right. It may also be that the required terms are complicated or very extended, and it would be better to go back to a three-band model.

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