Enhancement of Pairing Correlation by $t'$ in the Two-Dimensional Extended $t-J$ Model

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We investigate the effects of the next-nearest-neighbor ($t'$) and the third-nearest-neighbor ($t''$) hopping terms on superconductivity correlation in the 2D hole-doped extended $t-J$ model based on the variational Monte-Carlo, mean-field calculation, and exact diagonalization method. Despite of the diversity of the methods employed, the results all point to a consistent conclusion: While the $d$-wave SC correlation is slightly suppressed by $t'$ and $t''$ in underdoped regions, it is greatly enhanced in the optimal and overdoped regions. The optimal $T_c$ is a result upon balance of these two opposite trends.

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Right after the discovery of high temperature superconductors, the two-dimensional (2D) $t-J$ model has been proposed to provide the mechanism of superconductivity (SC) [1]. This idea quickly gained momentum when variational calculations showed that the doping dependence of pairing correlation [2, 3] and the phase diagram of antiferromagnetic (AFM) phase and SC [4] seem to agree with experimental results fairly well. However, recently calculations [5] beyond the variational method have challenged the notion that pure 2D $t-J$ model has high values of $T_c$. In fact they found highest $T_{c,max}$ for different mono-layer cuprates strongly correlates with $t'/t$ [6, 7].

The trial wave function (TWF) used in this study is

$$|\Psi\rangle = P_G \prod_k (u_k + v_k c^\dagger_{k,\uparrow} c_{-k,\downarrow}) |0\rangle$$

with $u_k/v_k = \Delta_k/(\epsilon_k + \sqrt{\epsilon_k^2 + \Delta_k^2})$, $\epsilon_k = -2t(\cos k_x + \cos k_y) - 4t'' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) - \mu$, and $\Delta_k = 2\Delta(\cos k_x - \cos k_y)$. Here the projection operator $P_G$ enforces the constraint of one electron per site. In addition to $\Delta$ and $\mu$, we have included two important variational parameters $t'_n$ and $t''_n$ which determine the Fermi surface topology.

The d-wave pair-pair correlation $P_d(R)$ is defined as

$$P_d(R) = \frac{1}{N^2} \langle \sum_{\mu \neq \nu} \Delta_{R_\mu} \Delta_{R_\nu} \rangle$$

where $\Delta_{R_\mu} = c_{R_\mu,\uparrow} c^\dagger_{R_\mu,\downarrow} + c_{R_\mu,\downarrow} c^\dagger_{R_\mu,\uparrow} - c_{R_\mu,\uparrow} c_{R_\mu,\downarrow} - c_{R_\mu,\downarrow} c_{R_\mu,\uparrow}$. The long range part of $P_d(R)$ is flat plateau for nonzero $\Delta$, and we define $t^\text{ave}_d$ as the averaged value of the $|R| > 2$ part of $P_d(R)$ to estimate the strength of SC of the system.
Fig. 1 shows the variational Monte Carlo (VMC) results of $P_d^{\text{ave}}$ for several $t'$ and $t''$ for different hole densities $\delta$ with $J/t = 0.3$ in a $12 \times 12$ lattice. $P_d^{\text{ave}}$ for the $t-J$ model (open circles) has the “dome-like” shape which is similar to the experimental results of $T_c$ versus doping. However, this could be an artifact of the variational study which, we believe, overestimates the order parameters and will be largely suppressed when we go beyond variational calculation as shown in our previous study. The most surprising result is that when $t'$ is included, $P_d^{\text{ave}}$ changes dramatically. For the overdoped regime, $P_d^{\text{ave}}$ is greatly enhanced by almost one order of magnitude for $t'/t = -0.3$ and $t''/t = 0.15$. The SC region extends to $\delta \sim 0.4$ and the peak of the superconducting dome is at $\delta = 0.3$ and the magnitude of the maximal $P_d^{\text{ave}}$ is about 2.5 times larger than for $t' = t'' = 0$. In the underdoped region, $P_d^{\text{ave}}$ is almost unchanged or very slightly suppressed. Another thing to note is that beyond the value of $t'/t = -0.3 \sim -0.4$ $P_d^{\text{ave}}$ is no longer enhanced.

Fig. 2 plots the maximal possible value of $P_d^{\text{ave}}$ for all doping density as a function of $t'$. The maximal $P_d^{\text{ave}}$ is proportional to $t'$ in the range $0 \geq t' \geq -0.3 \sim -0.4$. Beyond these values pairing is no longer enhanced. Coincidentally these values are about the same value of $t'/t$ for mercury cuprates as estimated by Pavarini et al. but much larger than what was reported in Ref. 3. Among all the cuprate series, mercury cuprate maintains the record of having highest $T_c$ for almost a decade.

The above result resolves the discrepancy between previous density-matrix-renormalization-group (DMRG) studies and the band structure calculation. As DMRG studies were concerned with underdoped region while the highest $T_c$ examined by the band structure calculation certainly depends on optimal and overdoped regions.

The different effects of $t'$ and $t''$ on $P_d^{\text{ave}}$ between overdoped and underdoped regions are related to the shape of Fermi surface. Fig. 3 shows the relations of $P_d^{\text{ave}}$ and $\text{n}(\pi,0)$ versus $t'$ for $\delta = 0.31$ and 0.083. For the overdoped case ($\delta = 0.31$), as $-t'$ increases up to 0.3, $\text{n}(\pi,0)$ increases from less than 0.4 to larger than 1 and $P_d^{\text{ave}}$ also increases sharply from less than 0.01 to larger than 0.04. Since $d$-wave SC gap is largest at $k = (\pi,0)$, occupation of this $k$ states by electrons enhances $P_d^{\text{ave}}$. On the other hand for the underdoped case, $\text{n}(\pi,0)$ is almost unchanged because the occupation $\text{n}(\pi,0)$ is already quite large (> 0.9) for $t' = t'' = 0$ and the effect of Fermi surface becomes unimportant. The slight suppression of $P_d^{\text{ave}}$ may be due to the destructive interference mechanism of the pair-hopping as suggested by Martins et al.

The decrease of $P_d^{\text{ave}}$ for $-t' \geq 0.4$ in the overdoped regime such as $\delta = 0.31$ is also likely the consequence of the change of the Fermi surface. $\text{n}(\pi,0)$ is al-
most saturated at $-t' = 0.4$ and remains unchanged for larger $-t'$. It is not difficult to recognize that as $-t'$ becomes much larger than $t$, electrons will occupy in separate regions around $k = (\pm \pi, 0)$ and $k = (0, \pm \pi)$. Hence the Fermi surface becomes disjoint pieces. Although at $-t'/t = 0.4$, the Fermi surface is still connected but this tendency is already observed. The density of states begins to decrease and this is probably the reason for the suppression of pairing beyond $-t'/t' \geq 0.4$.

Fig. 4 shows the Fermi surface and optimal parameters $\Delta$ and $t'_o$ as a function of doping density for a $12 \times 12$ lattice with $J/t = 0.3$, $t' = -0.3$ and $t'' = 0$. In (a-d) the white region denotes $n(k) \geq 1.2$ and dark region for $n(k) \leq 0.5$. The density with maximal $P^d_{av}$ is near $\delta_{opt} = 0.31$ as shown by the solid square in Fig. 4. The shapes of the Fermi surfaces are very different for $\delta > \delta_{opt}$ and $\delta < \delta_{opt}$ cases. Fig. 4(e) shows that in the region $0.2 < \delta < 0.3$ although $\Delta$ becomes smaller, $-t'_o$ is still quite large and pairing is further enhanced. Doping beyond $\delta > 0.3$, $-t'_o$ begins to decrease quickly. This gives very low electron occupation at $\delta = 0$ as shown in Fig. 4(c) and (d), then the pairing is reduced. This result shows that the enhancement of pairing by including $t'$ is not due to larger $\Delta$ but from the deformation of the Fermi surface instead.

Although we have emphasized the particular correlation between d-wave SC gap and electron occupation at $k = (\pi, 0)$ as the reason for enhancement of pairing, another familiar effect may also have played a role. It is well known that $t''$ will shift the van Hove singularity in density of states, but it is always around $k = (\pi, 0)$.

The results of slave-boson MF calculation in Fig. 5 show similar behavior for the overdoped regime that indeed $t''$ enhances $T_c$. Including $t''$ pushes the superconducting regime to even larger doping density $\delta$ by occupying the momenta around $(\pi, 0)$. A similar effect of $t''$ can also be seen in Fig. 1 by comparing the $(t', t'') = (-0.3, 0)$ (full squares) and $(-0.3, 0.15)$ (open triangles) curves. Since the slave-boson method is not quite reliable quantitatively in the underdoped regime, we did not show the values of $T_c$ in Fig. 5. However, if we do take the values literally, the values achieved for $T_{c,max}$ are not as greatly enhanced by $t'$ as for the VMC result shown in Fig. 2. Similar results are reported by the interlayer tunneling model.

Fig. 6 shows the pair-pair correlation for the longest distance $R = 1.3$ for 20-site lattices obtained by the ED method. Pairing correlations for 2 and 4 holes are suppressed by $t'$ and $t''$, but enhanced for the overdoped 6- and 8-hole cases. The non-monotonic behavior of the overdoped cases is due to the level crossing of this system. If we focus on the $s-$like symmetry states, $P^d_{av}$ will vary monotonically in the region $0 \geq t' \geq -0.3$. The result of ED method is quite consistent with the variational and MF results that the enhancement of $P^d_{av}$ by $t''$ occurs for larger hole densities.

In summary, in the optimal and overdoped regions, SC is greatly enhanced because of the deformation of the Fermi surface at these doping densities. $n(k = (\pi, 0))$ is enhanced by including $t'$ and $t''$. The occupation of $(\pi, 0)$ by electrons is important for the enhancement. The maximum enhancement of pairing correlation seems to be reached for $-t'/t = 0.3 \sim 0.4$. On the other hand, $P^d_{av}$ is not enhanced for the underdoped regime as $n(k = (\pi, 0))$ is hardly affected by including $t'$. It is well accepted that the physics on the overdoped side is apparently much simpler in that experiments on the cuprates and theory for the t-J model indicate that the overdoped materials are very close to ordinary Fermi liquids, whence ‘Fermi-
FIG. 6: $P_d(R = (1, 3))$ for versus $t'$ ($t'' = -t'/2$) for different $2$ (open circle), $4$ (full circle), and $6$ (open triangle) holes in 20 sites. The dash line shows $P_d$ for the same symmetry of the 8-hole case.

surface-based’ arguments like ours are much more reliable than in the underdoped region. Our result shows that the extended $t - J$ model naturally predicts the strong correlation [10] between $t'/t$ and $T_{c,max}$ observed in experiments for monolayer cuprates. In addition it also indicates that further increase of $t'$ beyond what mercury cuprates have most likely will not enhance $T_{c,max}$.

Although we have consistent results from VMC, ED methods and slave-boson MF calculations, the optimal doping density, $\delta_{opt}$, in Fig.1 is around 0.3 instead of 0.17 obtained in the experiments and in the VMC results without including $t'$. But this is actually not a drawback. As argued in References [10, 11, 12, 13, 14], VMC is expected to overestimate the values of the variational parameters $\Delta$ which is related to the exchange energy $J$. Hence the pairing correlation is definitely much larger than that of a real ground state. From our previous experiences the $\delta_{opt}$ seems to be always shifted to a smaller value when we improve the variational wave functions. Thus in the future work going beyond VMC calculations, we believe there is a better chance that we will have $\delta_{opt}$ closer to the experimental value. We also expect interlayer coupling will be important in getting the correct $\delta_{opt}$. Now $t'$ is shown to be important in enhancing pairing and it is also present in all high $T_c$ cuprates, the debate [15] about pairing robustness in the 2D $t - J$ model without $t'$ becomes somewhat irrelevant. The agreement of $\delta_{opt}$ between $t - J$ VMC and experiments looks fortuitous.

One of the consequences of our results is that the shape of the Fermi surface plays an important role for high temperature superconductors in the optimal and overdoped regions. Fig. 6 (b) and (c) show that the Fermi surface changes from hole-like to electron-like once the maximum pairing is reached and the pairing is reduced as doping increases. This is consistent with the ARPES results for $La_{2-x}Sr_xCuO_4$ [15]. It may also be related to the recent experiment [23] which shows that the low-temperature Hall coefficient for the $Bi_2Sr_{1.5}La_{0.45}CuO_6$ system exhibits a sharp change at the optimal doping density. Clearly this issue deserves more detailed study in the future.

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