Role of strong correlation in the recent ARPES experiments for cuprate superconductors

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Motivated by recent photoemission experiments on cuprates, the low-lying excitations of a strongly correlated superconducting state are studied numerically. It is observed that along the nodal direction these low-lying one-particle excitations show a linear momentum dependence for a wide range of excitation energies and, thus, they do not present a kink-like structure. The nodal Fermi velocity \(v_F\), as well as other observables, are systematically evaluated directly from the calculated dispersions, and they are found to compare well with experiments. It is argued that the parameter dependence of \(v_F\) is quantitatively explained by a simple picture of a renormalized Fermi velocity.

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Since the discovery of the copper-based high-\(T_c\) superconductors \(^1\), there have been extensive studies, both experimentally and theoretically, to understand the origin of the superconductivity as well as the unusual normal state properties \(^2\). This vast effort has proved that among the many experimental techniques angle-resolved photoemission spectroscopy (ARPES) is one of the most powerful tools, since it can provide important microscopic information of the electronic structure of these materials \(^3\). One of the recent key findings by ARPES experiments concerns the low-lying electronic excitations in the \((0,0)\) to \((\pi,\pi)\) direction (nodal direction) of the Brillouin zone: (i) the low-lying dispersion shows a kink at an energy in the range 50–80 meV from the Fermi level \(^4\) \(^5\), and (ii) the nodal Fermi velocity shows almost no doping dependence within the experimental error bars \((\sim 1.8 \pm 0.4 \text{ eV}\cdot\text{Å})\) for a wide range of hole concentrations \(x\) \((0 < x \lesssim 0.2–0.3)\) \(^6\). To explain the peculiar feature (i), the idea that electrons could be strongly coupled to the higher degrees of freedom, such as phonons and magnetic fluctuations, has been introduced \(^7\). This can naturally explain the appearance of a new energy scale. There are already theoretical studies in this direction \(^8\). However, the kink structure origin is still under debate. Regarding feature (ii), there have been no consensus on its origin. We believe that before studying more complicated models it is important to understand to what extend a purely electronic model alone can explain these features observed experimentally. This is precisely the main purpose of this work.

In this paper, using a variational Monte Carlo (MC) method, the low-lying excitations of a strongly correlated superconducting state with \(d\)-wave pairing symmetry are studied numerically. It is observed that the low energy one-particle excitations in the nodal direction show a linear momentum dependence, instead of a kink-like structure. Our detailed and systematic calculations for the nodal Fermi velocity \(v_F\), as well as a coupling strength \(\lambda\) defined below, reveals that in spite of not having a kink-structure in \(\varepsilon(k)\) nevertheless the doping dependence of \(v_F\) and \(\lambda\) are in good agreement with experiments. Moreover, it is shown that the doping dependence of \(v_F\) can be understood quantitatively as a renormalized Fermi velocity.

As a canonical model for the cuprates, here we consider the two dimensional (2D) \(t-J\) model on a square lattice described by the following Hamiltonian \(^9\):

\[
H = J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - n_i n_j / 4) - t \sum_{\langle i,j \rangle} \left( c_{i,\uparrow}^\dagger c_{j,\downarrow} + c_{i,\downarrow} c_{j,\uparrow}^\dagger + \text{H.c.} \right)
- t' \sum_{\langle i,j \rangle} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.} \right).
\]

Here \(c_{i,\sigma}^\dagger\) is the creation operator of a spin \(\sigma(=\uparrow, \downarrow)\) electron at site \(i\), and \(n_i = n_{i,\uparrow} + n_{i,\downarrow}\) and \(\mathbf{S}_i = \frac{1}{2} \sum_{\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} \theta_{\alpha\beta} c_{i,\beta}\) are the electron density and spin operators. \((i,j)\) \((\langle i,j \rangle)\) runs over the (next) nearest neighboring sites, and no double occupancy is allowed on each site. This model has been studied extensively and found to show a \(d\)-wave superconducting regime in its phase diagram \(^10\) \(^11\).

It is well known that a Gutzwiller projected BCS wave function with \(d\)-wave singlet pairing provides a satisfactory variational state for the 2D \(t-J\) model over a wide range of parameters \(^11\). Here we use a slightly more complex variational wave function \(^12\) defined by \(\mid \Psi_{\text{var}}^{(N)} \rangle = \hat{P}_N \hat{P}_G \hat{P}_J \mid |BCS\rangle\), where \(|BCS\rangle\) is the BCS ground state wave function, \(|BCS\rangle = \Pi_{\hat{P}_G} \left[ 1 + f_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{-\mathbf{k}} \right] \mid |0\rangle\), \(c_{\mathbf{k},\sigma}^\dagger\) the Fourier transform of \(c_{i,\sigma}^\dagger\), \(\hat{P}_N\) the projection operator onto the subspace of \(N\) electrons, \(\hat{P}_G = \Pi_{\hat{P}_G} (1 - n_{\alpha,\sigma} n_{\beta,\sigma})\) the Gutzwiller projection operator, \(\hat{P}_J = \exp \left( \sum_{\alpha,\beta} \alpha^\dagger \beta n_{\alpha,\sigma} n_{\beta,\sigma} \right)\) a Jastrow factor, and \(f_{\mathbf{k}} = \Delta_{\mathbf{k}} / (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}})\) with \(\Delta_{\mathbf{k}} = \Delta_{\text{var}} \cos k_x - \cos k_y\), \(\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu_{\text{var}}\), \(\varepsilon_{\mathbf{k}} = -2 \cos k_x + \cos k_y - 4 t_{\text{var}} \cos k_x \cos k_y\), and \(\xi_{\mathbf{k}} = -\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}\).
The variational parameters, all the independent pairs of $\alpha^2_{\text{var}}$, $\Delta_{\text{var}}$, $\mu_{\text{var}}$, and $t_{\text{var}}$, are determined by minimizing the variational energy: $E(\psi^{(N)}_{\text{var}}) = \langle \psi^{(N)}_{\text{var}} | H | \psi^{(N)}_{\text{var}} \rangle / | \psi^{(N)}_{\text{var}} \rangle | \psi^{(N)}_{\text{var}} \rangle$ for $N$ even [19]. In this case $\psi^{(N)}_{\text{var}}$ is a spin singlet and has a well-defined total momentum zero. Hereafter, the wave function with the optimized parameters is denoted by $| \psi^{(N)} \rangle$, and $E^{(N)} = E(\psi^{(N)}_{\text{var}})$. Also the energy unit ($t$) and the lattice constant ($a$) are both set to be one.

A single hole added to $| \psi^{(N)} \rangle$ is naturally described by $| \psi^{(N-1)}_{\text{var}} \rangle = \tilde{P}_{N-1} \tilde{P}_{G} \tilde{P}_{J} \gamma^L_{k_F} | \text{BCS} \rangle$, where $\gamma^L_{k_F}$ is the creation operator of the standard Bogoliubov quasiparticle with momentum $k$ and $s=\uparrow$ [13]. The state with a single added electron, $| \psi^{(N+1)}_{\text{var}} \rangle$, is described in a similar way replacing $\tilde{P}_{N-1}$ by $\tilde{P}_{N+1}$. Note that these states have sharply defined $k$, total spin 1/2, and z-component of total spin 1/2. The use of these states is partially motivated by the diagonalization of $H$ on small clusters — effort that indicated that the low-lying single-particle excitations are well described by a renormalized Bogoliubov quasiparticle state [16] — and partially on the recent proposal of a similar state [17]. The variational energies for these $(N \pm 1)$-electron states are denoted by $E^{(N \pm 1)}_{\text{var}}$. The single-particle excited states dispersion is thereby evaluated using $\varepsilon(k) = E^{(N)} - E^{(N-1)}_{k} (E^{(N+1)}_{k} - E^{(N)})$ for the one-electron removal (addition) spectrum [2].

In Fig. 1(a), as a typical example, the calculated dispersion $\varepsilon(k)$ in the nodal direction is shown for the 2D $t$-$J$ model with $J/t = 0.3$ and $t'/t = -0.2$, at $x=0.099$. (a): Full dispersion for $L=162$ (triangles) and 242 (circles). The one-electron removal (addition) spectrum is denoted by open (solid) symbols. The dashed (long dashed) line is a fitting curve of branch A (B) for the $L=242$ data, using up to 3rd order polynomials. The estimated Fermi momentum and energy are indicated by $k_F$ and $E_F$, respectively. (b): Same as (a) but focusing on the excitations near $E_F$. In addition to the data for $L=162$ (open triangles) and 242 (open squares), results for $L = 1250$ (solid squares and circles) are also plotted. Dotted lines are a guide to the eye.

Let us refer to branch A as the main dispersion and to branch B as the “shadow” dispersion, since branch A (branch B) consists of all the one-electron removal (additional) states inside $k_{NF}^x$, and all the one-electron additional (removal) states outside $k_{NF}^x$. Here, $k_{NF}$ is the nodal Fermi point of $| \text{BCS} \rangle$ with the optimized parameters. Although this assignment is quite natural, we also calculated the quasi-particle weight directly and found that branch A has substantially more weight than branch B. The energy difference between $k = (0, 0)$ and $k = (\pi, \pi)$ in each branch naturally defines the bandwidth $W = \varepsilon(\pi, \pi) - \varepsilon(0, 0)$. Next, we fit the data in each branch using up to third-order polynomials. As shown in Fig. 1(b), the fitting is highly satisfactory. The intersection of the fitting curves provides the Fermi energy $E_F$ and the nodal Fermi point $k_F$ [18]. From these fitting curves, we obtain the nodal Fermi velocity $v_F$ at $k_F$.

The satisfactory fitting of the dispersions $\varepsilon(k)$ in the nodal direction already indicates that $\varepsilon(k)$ is a smooth function of $k$ and, therefore, it suggests that the state used here does not have the kink structure observed experimentally. To study this in more detail, we calculated the nodal dispersion $\varepsilon(k)$ on a cluster with $L=1250$, where the number of allowed k-points in the nodal direction is 50 and, thus, the momentum resolution $\delta k$ is about 0.18/a [19]. The results are presented in Fig. 1(b). It is fairly clear that the dispersions in both branches are almost linear around $E_F$, and no kink-like structure is seen. If there were a kink structure in the dispersion, as observed experimentally, it would not be possible to fit the data for both one-electron removal and additional spectra using the same straight line. Comparing the data for $L = 1250$ and those for smaller systems shown in Fig. 1(b), it is apparent that the size dependence of the dispersion is small, and therefore we can safely estimate quantities such as $v_F$ using the smaller systems.

Figure 2 summarizes the $x$ dependence of various quantities for the 2D $t$-$J$ model with $J/t = 0.3$ and $t'/t = -0.2$, which is a typical parameter set for the cuprates [2]. Fig. 2 (a) shows that $v_F$ is weakly dependent on $x$ up to about $x=0.1$—0.2 — with $v_F \sim 0.8$—1.0 $t$ — and then
increases with further increasing $x$. If $t \sim 500$ meV and $a \sim 4$ Å are used, the calculated value of this nearly $x$-independent $v_F$ corresponds to approximately 1.6–2.0 eV-Å, which is compatible with ARPES data within the experimental error bars. The present results are also consistent with recent reports by Paramekanti, et al. [20, 21], including the overall increasing behavior of $v_F$ as a function of $x$. [22].

In Fig. 2 (b) and (c), the calculated bandwidth $W$ and the nodal Fermi momentum $|k_F|$ are shown, respectively. Although $k_F$ approximately follows the result for free electrons (with $t'$), $W$ has a stronger $x$ dependence. It should be emphasized that this non-trivial dependence of $W$ is caused by strong correlations, which are imposed in the wave function by the Gutzwiller projection $P_G$. From Fig. 2 (b), it is expected that the effective mass in the nodal direction monotonically increases with decreasing $x$, but it is finite even at $x \to 0$

Now we show that the $x$ dependence of $v_F$ is understood quantitatively by a simple picture of a renormalized Fermi velocity. Since $k_F$ is similar to the free electrons results (with $t'$), a natural procedure to follow is to calculate a renormalized Fermi velocity $v_F^*$ from the value of the free electrons $v_F^0$ at $k_F$. In Fig. 2 (d), $v_F^* = \gamma v_F^0$ is plotted, where $\gamma = W/W_0$ is a renormalization constant and $W_0 = 8t$ is the free electrons bandwidth. Clearly, $v_F^*$ can now reproduce $v_F$ for almost all the doping range studied. To support this argument, systematic calculations are done for various model parameters, and the results are shown in Fig. 3 (a)–(d). It is apparent from the figures that $v_F^*$ can indeed explain the $x$ dependence of $v_F$ quantitatively for a wide hole-doping range. The main features of the $J$ and $t'$ dependences are as follows: (i) $v_F^*$ increases with $J$ [Fig. 3(a) and (b)], and (ii) the increasing tendency of $v_F^*$ with $x$ weakens with $|t'|$ [Fig. 3 (b)–(d)]. These dependences can be explained by the renormalized velocity picture as well. While $v_F^*$ does not depend on $J$ [Fig. 3(f)] and, thus, neither does $v_F^0$ [Fig. 3(g)], $W$ does depend on $J$ and becomes larger with $J$ [Fig. 3(c)]. Therefore $v_F^*$ increases with increasing $J$. In contrast, $t'$ does affect the value of $v_F^0$, and has a decreasing trend with increasing $x$ [Fig. 3(g)]. Thus, $v_F^0$ shows a reduced tendency to increase with $x$. Moreover, this decreasing trend can cancel the increasing behavior of $W$ with $x$ and, as a consequence, $v_F^*$ can present a rather weak $x$ dependence over a wide hole-doping range, as in Fig. 3(d), which agrees qualitatively with the calculated dependence of $v_F^*$. For comparison with experiments, we also show $E_F$ for various $t'$ in Fig. 3 (h). The $x$ dependence of $E_F$ seems to be stronger for large $|t'|$ than for small $|t'|$, a trend that has been seen in experiments [23].

FIG. 2: (a) Nodal Fermi velocity $v_F$, (b) bandwidth $W$, (c) nodal Fermi momentum $|k_F|$ (solid symbols), and (d) renormalized Fermi velocity $v_F^*$ (solid symbols) (see text) for the 2D $t$-$J$ model with $J/t=0.3$ and $t'/t=-0.2$ at different $x$. For comparison, in (c) the free-electrons nodal Fermi points (crosses) are also shown. In (d) the Fermi velocity for the free electrons $v_F^0$ (crosses) and $v_F$ (open symbols) are also plotted.

FIG. 3: (a)–(d): $x$ dependence of the nodal Fermi velocity $v_F$ (open marks) and the renormalized Fermi velocity $v_F^*$ (crosses) for the 2D $t$-$J$ model. The parameters used are indicated in the figures. (e)–(h): $x$ dependence of $W$ (e), $k_F$ (f), the nodal Fermi velocity of the free electrons at $k_F$ (g), and $E_F$ (h) for the different parameters indicated in (f).
As observed in Fig. 4 (a), the calculated function MC simulation using \( \Psi_k^{(N+1)} \) is to interest the accuracy of our estimate of \( v_F \) for the 2D \( t-J \) model. To this end, we have carried out a fixed-node approximation Green function MC method with fixed node approximation (solid symbols). For comparison, the variational estimates shown in Fig. 2 (a) are also provided (open symbols). (b) \( x \) dependence of \( \lambda \) for \( J/t=0.3 \) (open marks) and 0.5 (solid marks) with different \( t'/t \).

Finally, we show in Fig. 4 (b) a coupling strength defined as \( \lambda = v_F^0 / v_F - 1 \) which is the first derivative of the real part of the single-hole self energy \( \Sigma' \) at \( E_F \) \( \lambda = -\partial \Sigma'(\omega) / \partial \omega |_{\omega=E_F} \) if the momentum dependence of \( \Sigma' \) is assumed weak. It is interesting to note that \( \lambda \) seems to be determined largely by \( J \), not by \( t' \), for a wide range of \( x \), and becomes weakly depending on \( J \) and \( t' \) for \( x \gtrsim 0.3 \). This monotonically decreasing behavior with \( x \) as well as the value of \( \lambda \) are in good agreement with experimental estimates.

In conclusion, the low-lying one-particle excitations of a strongly correlated superconducting state was studied. It was found that the dispersion \( \varepsilon(k) \) in the nodal direction shows a linear dependence for a wide range of excitations around \( E_F \) \( (\sim 1.0-1.5\varepsilon) \) and, thus, does not present a kink-like structure. Systematic estimations are made for the nodal Fermi velocity \( v_F \) directly from the calculated \( \varepsilon(k) \). The \( x \) dependence of \( v_F \) as well as \( \lambda \) are in good agreement with experiments. It is shown that the model parameter dependence of \( v_F \) is quantitatively explained by a simple picture of the renormalized Fermi velocity. Our results suggest that the kink structure observed experimentally is caused by other degrees of freedom not included in our study. Although the calculated \( \varepsilon(k) \) in the nodal direction has no kink, the estimated \( v_F \) as well as the coupling strength \( \lambda \) compare well with ARPES experiments. These results lead us to the speculation that a major part of the low energy physics for the cuprates can still be described mainly by a purely electronic \( t-J \)-like model. The "universal" Fermi velocity found in experiments turns out to be explained here by a rather accidental compensation of two effects: the bandwidth \( W \) decreases with decreasing doping \( x \) due to correlation, while the bare Fermi velocity instead increases and further changes with \( t'/t \). Therefore this effect might be less significant from the theoretical point of view, contrary to what was previously assumed. Our results indicate that more accurate experiments should eventually detect a "non-universal" and weakly doping dependent Fermi velocity.

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