Electronic structure of strongly correlated d-wave superconductors

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We study the electronic structure of a strongly correlated d-wave superconducting state. Combining a renormalized mean field theory with direct calculation of matrix elements, we obtain explicit analytical results for the nodal Fermi velocity, \(v_F\), the Fermi wave vector, \(k_F\), and the momentum distribution, \(n_k\), as a function of hole doping in a Gutzwiller projected d-wave superconductor. We calculate the energy dispersion, \(E_k\), and spectral weight of the Gutzwiller-Bogoliubov quasiparticles, and find that the spectral weight associated with the quasiparticle excitation at the antinodal point shows a non monotonic behavior as a function of doping. Results are compared to angle resolved photoemission spectroscopy (ARPES) of the high temperature superconductors.

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Recent progress in angle resolved photoemission spectroscopy (ARPES) of the high temperature superconductors has led to considerable interest in the electronic structure of a strongly correlated d-wave superconducting state\textsuperscript{1,2}. Experiments show a variety of interesting phenomena and it is generally agreed that strong electronic correlations play a dominant role in explaining some of the universal spectral features. Hence it would be desirable to obtain, e.g., for comparison with experimental results, explicit analytical results from a simple model of a strongly correlated d-wave superconductor.

Thus motivated, we consider in this paper, the electronic structure of a Gutzwiller projected superconductor, defined by the ground state wave function, \(\exp(iS)\langle \Psi_0 | P_G | \Psi_0 \rangle\). The projection operator, \(P_G \equiv \prod_i (1 - n_i u_{i\uparrow})\), acting on a BCS wave function, \(|\Psi_0\rangle\), eliminates states with double occupancies in \(|\Psi\rangle\). The operator, \(\exp(iS)\), allows for a systematic calculation of corrections to the fully projected state, \(|\Psi\rangle\). Gutzwiller projected states, \(|\Psi\rangle\), were initially proposed as variational states to describe superconductivity in the proximity of a Mott insulating phase\textsuperscript{3,4}. They have been used recently for numerical investigations of the electronic structure of the high temperature superconductors. Paramekanti \textit{et al.}, used Variational Monte Carlo (VMC) to study some spectral properties of a Gutzwiller projected d-wave superconductor\textsuperscript{5}. Yunoki \textit{et al.}, extended the VMC technique to the direct calculation of excited states in Jastrow-Gutzwiller wave functions\textsuperscript{6}. The VMC technique also allows to study the coexistence of superconductivity with antiferromagnetism\textsuperscript{3}, and the quasiparticle current renormalization\textsuperscript{10}. In this paper, we will follow an alternate route and use a combination of renormalized mean field theory (RMFT)\textsuperscript{6,11} and direct calculation of matrix elements\textsuperscript{4,11} to examine the electronic structure of a Gutzwiller projected d-wave superconductor. Though Gutzwiller projection is only an approximate method to treat the effects of strong correlations, the advantage lies in its directness and clarity. Explicit analytical expressions derived in this paper can be used to evaluate directly the successes as well the limitations of this approach. Using RMFT, we determine the energy dispersion, \(E_k\), of the Gutzwiller-Bogoliubov quasiparticles, and the nodal Fermi velocity, \(v_F\). We show that \(v_F\) stays finite as the (Mott) insulating phase is approached. We calculate the spectral weight associated with the d-wave quasiparticles, and the momentum distribution, \(n_k\), by a direct evaluation of the relevant matrix elements\textsuperscript{11}. We find that the quasiparticle weight associated with the antinodal excitation exhibits a non monotonic behavior as a function of doping.

We consider the one band Hubbard model,

\[ H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \]

where the hopping integrals, \(t_{ij}\), connect sites \(i\) and \(j\). We will restrict our attention to nearest \((t)\), and next nearest \((t' = -t/4)\) neighbor hopping. We choose an onsite repulsion \(U = 12t\); i.e., we work in the strong coupling regime \(U \gg t, t'\). In this limit, a unitary transformation, \(\exp(is)\), yields an effective Hamiltonian, \(H_{\text{eff}} = \exp(-is)H \exp(is)\), which is block diagonal and does not mix states between the lower and upper Hubbard bands\textsuperscript{3,12}. To \(O(t^2/U)\), it corresponds to the \(t - J\) Hamiltonian with the correlated hopping term (three-site term), for which the Gutzwiller wave function \(P_G|\Psi_0\rangle\) has been established as an excellent variational ground state\textsuperscript{12}. Retransformation of the trial wave function, \(\exp(is)P_G|\Psi_0\rangle\), then provides a systematic way to study the Hubbard model using Gutzwiller projected states.

Two steps are necessary to obtain explicit analytic expressions for the low energy properties in the strong coupling regime. The first is the Gutzwiller renormalization procedure, where the effects of the projection...
$P_G$ are taken into account by appropriate renormalization factors, following Hilbert space counting arguments: 
\[ \langle \Psi_0 | P_G H_{\text{eff}} P_G | \Psi_0 \rangle \approx \langle \Psi_0 | H_{\text{eff}} | \Psi_0 \rangle \]

The next step is the realization that $H_{\text{eff}}$ allows for two types of molecular-fields: the hopping amplitude, $\xi \equiv \sum_i \langle \epsilon_i \sigma_i c_{i\uparrow} c_{i\downarrow} \rangle_0$, and the singlet pairing amplitude, $\Delta \equiv \langle \epsilon_i c_{i\uparrow} c_{i\downarrow} - \epsilon_i c_{i\uparrow} c_{i\downarrow} \rangle_0$, where $r$ connects nearest (nn) or next nearest neighboring (nnn) sites; $\langle \ldots \rangle_0$ denotes the expectation value with respect to $|\Psi_0\rangle$.

This decoupling scheme of the renormalized Hamiltonian (RMFT) leads to a BCS ground state $|\Psi_0\rangle = \prod_i (u_k + v_k c_{k\uparrow} c_{k\downarrow}) |0\rangle$, with $v_k^2 = (1 - \zeta_k/E_k)/2$ and $u_k^2 = 1 - v_k^2$. The corresponding gap equations are $\xi = -1/L \sum_k \cos(kr) \zeta_k/E_k$ and $\Delta = 1/L \sum_k \cos(kr) \Delta_k/E_k$, together with the condition $x = 1/L \sum_k \zeta_k/E_k$ for the hole-doping concentration $\delta$. Solving the gap equations, we find that a d-wave pairing state is most stable for $x \leq 0.4$. In this case, $\Delta \equiv |\Delta_x| = |\Delta_y|$ with $\Delta_x = -\Delta_y$, $\xi \equiv \xi_x = \xi_y$, and $\xi' \equiv \xi_x - y$. The dispersion relation of the Gutzwiller-Bogoliubov quasiparticle is given by, $E_k = \sqrt{\xi^2 + \Delta^2}$, where,

\[ \zeta_k = - \left( 2g t + J \frac{\xi}{4} x_1 + J' \frac{\xi'}{4} x_2 \right) (\cos k_x + \cos k_y) - \left( 2g t' + J'' \frac{\xi'}{4} x_1 + J' \frac{\xi}{4} x_2 \right) 2 \cos k_x \cos k_y - x D \sum_{\tau \neq \tau'} \frac{t_\tau t_{\tau'}}{U} \cos [k(\tau - \tau')] - \mu, \]  

\[ \Delta_k = J \frac{\Delta}{4} \left[ 3g t_\tau + \left( 1 - 3 + x^2 \right) g_3 \right] (\cos k_x - \cos k_y). \]

In Eq. 1 and Eq. 2, the Gutzwiller factors corresponding to the kinetic, superexchange and the three-site term are $g_1 = 2x/(1 + x^2)$, $g_2 = 4/(1 + x^2)$ and $g_3 = 4x/(1 + x^2)$ respectively. The last sum in Eq. 1 is a sum over all pairs of neighboring sites $\tau$ and $\tau'$, where $t_\tau$ and $t_{\tau'}$ are the nn and nnn hopping terms. We define, $J = 4t^2/U$, $J' = 4t' t/U$, and $J'' = 4t''^2/U$ and abbreviate, $x_1 = 3g t_\tau + \left( 1 - 3 + x^2 \right) g_3$, $x_2 = 4(3 - x) g_3$, and $x D = \left( 1 - x^2 \right) g_3$ in Eq. 1.

Fig. 1(a) shows the doping dependence of the mean field field hopping parameters, $\xi$ and $\xi'$, and the d-wave mean field pairing, $\Delta$, obtained by solving the RMFT gap equations. Since $g_1, g_3, x_2, x D$ and $\xi'$ vanish as $x \to 0$, the dispersion relation, $\zeta_k \to -(11/4) J \xi (\cos k_x + \cos k_y)$ in the limit of zero doping.

The d-wave order parameter $\Delta$ decreases nearly linearly with doping and vanishes around $x \approx 0.4$, for our choice of parameters. This is in agreement with previous studies [17]. Note that we retain all terms of $O(t^2/U)$ in the effective Hamiltonian, $H_{\text{eff}}$, including the three-site term, which suppresses d-wave pairing in the overdoped regime.

The doping dependence of the superconducting (SC) gap, $|\Delta_k|$ at $k = (\pi, 0)$, is shown in Fig. 1(b). The doping dependence resembles experimental observations quite well. However, the gap is overestimated by a factor of about 2 [see scaling factor $\alpha = 1/2$ in Fig. 1(b)] within mean field theory which neglects additional off site correlations as well as dynamical effects due to the motion of holes [13]. The SC gap is not identical to the true SC order parameter, $\Phi \equiv \langle c_{i\uparrow} c_{i\downarrow} - c_{i\uparrow} c_{i\downarrow} \rangle$. Here, $\tau$ is a neighboring site and $\langle \ldots \rangle$ represents the expectation value calculated with the transformed wave function, $\exp(iS) P_G |\Psi_0\rangle$. Calculating $\Phi$ to $O(\xi/U)$, we find, $\Phi \approx g t_\tau + (t/U) g_3 \left( 6 - x \right) \Delta_\xi$, where we set $t_\tau \approx 0$, for simplicity. As shown in Fig. 1(b), $\Phi$ vanishes as $x \to 0$, as it should.

We now consider the nature of the low lying excitations, the quasiparticles created at the nodal point, $k_F$. The nodal dispersion around $k_F$ is characterized by the velocity, $v_F$, which directly influences a number of experimentally accessible quantities. Within RMFT, $v_F$ is directly obtained by calculating the gradient of $\zeta_k$ along the direction, $(0,0) \to (\pi, \pi)$. The result is presented in Fig. 2(a) (for $t = 0.3, 0.4, 0.5$ eV and $a_0 = 4A$) and is well approximated by the formula,

\[ v_F/a_0 \approx \sqrt{2} \sin k_F \left[ 2g t \left( 2t^2 \cos k_F \right) + x D \left( \frac{\pi}{4} \right) \right]. \]

In the above equation, we set $J', J''$, and $x_D$ to zero for simplicity. As seen in Fig. 2, $v_F$ increases with $x$, but remains finite as $x \to 0$. As can be inferred from Eq. 3, the energy scale of the nodal velocity at $x = 0$ is determined by $J$, i.e., $v_F/(a_0 J) \approx \sqrt{2} \sin(k_F/2) \approx 1.5$ (for $\xi \approx 0.38$ and $k_F \approx \frac{\pi}{2}$). The observed doping dependence stems from the effects of Gutzwiller projection $P_G$. As $x$ increases, holes gain kinetic energy by direct hopping, $v_\xi$, $g t_\tau$ increases with doping; but $g_3$ decreases, leading to the doping dependence of $v_F$ seen in Fig. 2.

Our results agree with the numerical VMC results of Paramekanti et al., who extract $v_F$ from the discontinuity of the first moment of the spectral function in the repulsive $U$ Hubbard model [3], and those of Yunoki et al., who

![FIG. 1](color online) (a) Doping dependence of the dimensionless mean field parameters $\xi$, $\xi'$, $\Delta$; (b) Doping dependence of (solid) the SC order parameter, $\Phi$, and (dashed) the SC gap, $|\Delta_k|$, at $k = (\pi, 0)$ for $t = 300$ meV. The RMFT SC gap is scaled by a factor $\alpha = 1/2$ for comparison with experimental data (red circles, Bi2212 [1]).
obtain \( v_F \) from the quasiparticle dispersion in the \( t-J \) model. A comparison to ARPES data \( \text{[10]} \), presented in Fig. 2(a), shows good agreement. The doping dependence of \( v_F \) in the severely underdoped regime remains to be settled experimentally. While some groups report a nearly constant Fermi velocity (see data for LSCO in Fig. 2), others observe an increase with doping (see data for YBCO and Bi2212 in Fig. 2). Within RMFT, we also verify that the nodal properties remain essentially unchanged when \( \Delta \) is set to 0; i.e., the doping dependence of \( v_F \) results from the vicinity of the state to a Mott insulator, rather than the occurrence of superconductivity itself.

We now calculate the spectral weight of the Gutzwiller-Bogoliubov quasiparticle (QP). The variational excited state in a projected superconductor is given by \( \exp(iS) |\Psi^-\rangle = \exp(iS) P_{\gamma,k-}\Psi_0\rangle \), where the corresponding Bogoliubov QP operator is defined by \( \gamma_{\downarrow,\mathbf{k}}^\dagger = u_{\mathbf{k}} c_{\mathbf{k}\downarrow} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow} \). In ARPES, the spectral weight corresponding to this excitation is determined by the matrix element \( M_k^- = \langle \Psi_k^- | \gamma_{\downarrow,\mathbf{k}}^\dagger | \Psi_0\rangle \), where, \( N_k^c \) and \( N_k^G \) are the norms of \( |\Psi_k^-\rangle \) and \( |\Psi_0\rangle \). Here, \( c_{\mathbf{k},\sigma} = \exp(-iS) c_{\mathbf{k},\sigma} \exp(iS) \). Using the Gutzwiller renormalization scheme we find, \( M_k^- \approx Z_k v_0 + O(t/U)^2 \) and,

\[
Z_k \approx g_t + \frac{g_3}{U} \left( 1 - \frac{x - x_0}{2 \xi_k^0} + \frac{3 - x}{L} \sum_{k'} v_{k}^2 v_{k'}^0 \right),
\]

for the QP renormalization \( |21\rangle \), with \( \xi_k^0 = 2t (\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y \). Here, \( v_0 = v_{\pi}^2 \) is the momentum distribution in the unprojected wave function \( |\Psi_0\rangle \). The renormalization, \( Z_k \), of the nodal QP weight is plotted as a solid line in Fig. 2(b), and agrees well with VMC results \( |3\rangle \). The dashed lines correspond to results without \( t/U \)-corrections. The dotted line, \( Z_k = x \), is the result from slave boson mean field theory (SBMFT).

As a qualitative comparison with ARPES we show the energy dispersion, \( \omega = -E_k \), of the Gutzwiller-Bogoliubov QP along the directions, \((0,0) \rightarrow (\pi,0)\), \((\pi,0) \rightarrow (\pi,\pi)\), and \((\pi,\pi) \rightarrow (0,0)\) for different \( x \) in Fig. 3. We emphasize that our calculations describe the low energy sector, and do not seek to explain the “kink” at higher energies \( |14\rangle \).

The spectral weight of the coherent peak, measured in ARPES, is related to the QP weight, \( M_k^- \approx Z_k v_0^0 \); it is shown in Fig. 3(b). As seen in the figure, the QP spectral weight is severely modified by Gutzwiller projection. It decreases with doping, and vanishes at half filling. This causes a shift of spectral weight to an incoherent background as seen in the momentum distribution function, \( \langle n_{k\sigma} \rangle \approx Z_k v_k^2 + n_k^0 + O(t/U)^2 \). While the first term corresponds to the coherent QP weight, the second gives the distribution of the incoherent part. We get,

\[
n_{k\sigma} \approx \frac{(1-x)^2}{2(1+x)} \sum \frac{t}{2U} \cos(k\tau) \left[ \frac{(1-x)^3}{1+x} + \frac{3g_s + 1}{2} \right. \left. - \frac{3 + x}{2} \right] |\Delta_k|^2 + \left( \frac{3g_s - 1}{2} - \frac{3 - x}{2} \right) \xi_k^2 ,
\]

which is a smooth function of \( k \). Results are shown in Fig. 3(c). The incoherent weight is spread over the entire Brillouin zone, and overlies the coherent part from the Gutzwiller-Bogoliubov quasiparticles. At half-filling, all weight becomes incoherent.

Finally, we consider the coherent QP weight, \( M_k^- \approx Z_k v_k^2 \), at the antinodal point, \( k = (\pi,0) \). As seen in Fig. 3(b) and Fig. 4, it exhibits a non monotonic behavior as a function of doping. Within our theory, this effect arises from a combination of the effects due to

\[
\text{FIG. 2: (color online) Doping dependence of (a) Fermi velocity, } v_F, \text{ and (b) renormalization, } Z_k, \text{ of the Gutzwiller-Bogoliubov nodal quasiparticle. RMFT results are compared with experiments in (a), data from Ref. [10] and VMC in (b), data from Ref. [3], respectively.}
\]

\[
\text{FIG. 3: (color online) (a) Energy dispersion, } \omega = -E_k, \text{ (b) quasiparticle weight, } Z_k v_k^0, \text{ and (c) momentum distribution, } \langle n_{k\sigma} \rangle, \text{ of the Gutzwiller-Bogoliubov quasiparticle for different doping } x; \text{ The energy dispersion in (a) is only shown when the corresponding quasiparticle weight is finite [see (b)]. The corresponding Fermi surface, } \zeta_k = 0, \text{ is shown in the inset of (a).}
\]
Gutzwiller projection and the topology change [see inset of Fig. 3(a)] of the underlying Fermi surface (FS). Fig. 3(a) illustrates this clearly. While the QP weight renormalization, $Z_k$, increases with increasing doping, $n_k^0 = v_k^2$, decreases due to the topology change, which occurs at $x \approx 0.15 - 0.20$ for our choice of hopping parameters ($t' = -t/4$). The change of the FS seems to be a generic feature of hole doped cuprates [22], although the exact doping concentration $x$, for which this occurs, is sensitive to the ratio between various hopping parameters. The combined effect of strong correlations and topology change leads to a maximum of the QP weight for the doping level, $x$, at which the underlying FS changes topology. This result should be tested by appropriate analyses of recent ARPES data [22]. Indications for such a behavior have already been published [23, 24]; Feng et al. [23] extracted the Superconducting Peak Ratio (SPR) for Bi2212 [23].

To summarize, we studied the electronic structure of a Gutzwiller projected $d$-wave superconductor. A systematic combination of renormalized mean field theory and direct evaluation of matrix elements was applied to the Hubbard model in the strong coupling limit. Our analytical results can be used to fit experimentally observed quantities as well as those obtained from numerical methods. The dispersion of the Gutzwiller projected superconductor is renormalized in the vicinity of the Mott insulator, but the nodal Fermi velocity stays finite as the insulating limit is approached. The spectral weight of the nodal quasiparticle increases with doping, whereas that of the antinodal excitation shows non monotonic behavior, when the underlying Fermi surface changes topology. Our results can be checked by experimental observations from ARPES of high temperature superconductors, thus providing a way to study the applicability of projected wave functions to these systems. The method we use is also amenable to other extensions such as coupling to the lattice, antiferromagnetism and long range interactions.

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