Abstract

The superconducting phase of the 2D one-band Hubbard model is studied within the FLEX approximation and by using an Eliashberg theory. We investigate the doping dependence of $T_c$, of the gap function $\Delta(\mathbf{k}, \omega)$ and of the effective pairing interaction. Thus we find that $T_c$ becomes maximal for 13% doping. In overdoped systems $T_c$ decreases due to the weakening of the antiferromagnetic correlations, while in the underdoped systems due to the decreasing quasi particle lifetimes. Furthermore, we find shadow states below $T_c$ which affect the electronic excitation spectrum and lead to fine structure in photoemission experiments.
There is still no definite understanding of the pairing interaction in the High-T\textsubscript{c} superconductors. However, improved experimental techniques like phase sensitive measurements of the superconducting order parameter\cite{1} and angular resolved photoemission (ARPES)\cite{2} have revealed important new structures in the electronic excitation spectrum that might help to clarify the nature of superconductivity in the cuprates. The observation of shadows of the Fermi surface (FS) in the normal state by Aebi \textit{et al.}\cite{3} and the strong evidence for a $d_{x^2-y^2}$ pairing symmetry\cite{1,2} indicate that there might be a strong interdependence between the occurrence of high transition temperatures and antiferromagnetic spin fluctuations. Furthermore, the interesting dip structures in ARPES spectra of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) found for the first time by Dessau \textit{et al.}\cite{4} and confirmed by other measurements\cite{2,5,6} is currently debated and could be a further fingerprint of the pairing mechanism.

From a theoretical point of view the two dimensional one-band Hubbard Hamiltonian serves as a basic model to describe the highly correlated electrons within the CuO$_2$ planes. The first important steps to investigate the superconducting properties of the cuprates within this approach was done simultaneously by Monthoux \textit{et al.}\cite{7} and Pao \textit{et al.}\cite{8}, who found a $d_{x^2-y^2}$ pairing state for low temperatures within a pertubative ansatz, namely the fluctuation exchange approximation (FLEX). Despite these interesting results the superconducting excitation spectrum and in particular its doping dependence are far from being understood. Moreover, it is still unclear if this microscopic approach can explain the observed optimal doping concentration in the High-T\textsubscript{c} superconductors.

In this article we present new results for the doping dependence of the superconducting state of the Hubbard Hamiltonian. We discuss the resulting phase diagram and find that $T_c$ becomes maximal for a doping concentration of 13 %. By determining the excitation spectrum directly on the real frequency axis we demonstrate that shadow bands as proposed by Kampf and Schrieffer\cite{9} for the normal phase are also present below $T_c$. We show that they have an important impact on the pairing mechanism, on $T_c$ and on the gap function $\Delta(k,\omega)$. In addition, they cause observable effects in the spectral density of states and are responsible for fine structures in ARPES experiments.
Our theory is based on a strong coupling Eliashberg approach for the one-band Hubbard Hamiltonian with nearest neighbor hopping integral \( t = 0.25 \text{ eV} \), bare dispersion \( \varepsilon_0(k) = (-2t[\cos(k_x) + \cos(k_y)] - \mu) \) with chemical potential \( \mu \) and local Coulomb repulsion \( U = 4t \). The superconducting state is treated in the Nambu formalism, where the Greens function \( \hat{G}(k, \omega) \) is a \( 2 \times 2 \) matrix that can be expanded in terms of Pauli matrices. The corresponding expansion coefficients of the diagonal electronic self energy are \( \omega(1 - Z(k, \omega)) \) and \( \chi(k, \omega) \), whereas \( \phi(k, \omega) = \Delta(k, \omega)Z(k, \omega) \) is the coefficient of the anomalous off-diagonal self energy that vanishes above \( T_c \) and \( \Delta(k, \omega) \) is the gap function. These three functions were calculated self consistently by using a newly developed numerical method for treating the FLEX equations directly on the real frequency axis. The calculations were performed on a \((64 \times 64)\) square lattice in momentum space and by using 4096 equally spaced energy points in the interval \([-30t, 30t]\) leading to a low energy resolution of \(0.014t \approx 4 \text{ meV}\).

In the Fig. 1(a) we present the doping dependence of \( T_c \), where \( x \) is the doping concentration and \( n = 1 - x \) the occupation number per site. Note that the order parameter was found to have a \( d_{x^2-y^2} \) symmetry for all doping values. For large \( x \), \( T_c \) increases up to \( T_c = 79 \text{ K} \) at \( x = 0.13 \), whereas below the optimal doping \( T_c \) starts to decrease for \( x < 0.13 \). Consequently, three different doping regimes with qualitatively different behavior occur within the Hubbard model: The underdoped \((x < 0.13)\), the optimally doped and the overdoped \((x > 0.13)\) compounds. In the following we will demonstrate \((i)\) that the optimally doped systems are characterized by a constructive interference of superconducting and antiferromagnetic excitations, resulting from the comparable time scales of both phenomena, \((ii)\) that the suppression of \( T_c \) in the overdoped systems is due to the increasing weakening of the effective pairing interaction, and \((iii)\) that in the underdoped systems the dynamical character of the spin fluctuations becomes less pronounced causing \( T_c \) to decrease. Here the rather stiff arrangement of antiferromagnetically correlated spins and their interplay with the \( d \)-wave pairing state enhances the formation of shadow states, i.e. states resulting from the coupling of wave vectors \( k \) at the FS and its shadow at \( k + Q \ (Q = (\pi, \pi)) \).

Important information about the origin of the doping dependence of \( T_c \) and the optimal
doping can be obtained from the effective interaction $V_s(k, \omega)$ below $T_c$. In Fig. 1 (b) we compare $V_s(k, \omega)$ with $V_n(k, \omega)$ that was obtained at the same temperature, but with $\phi \equiv 0$, for $\omega = 0$ and $k$ points near $Q$ where $V_s(k, 0)$ is maximal. For non-optimal doping we find that the interaction and in turn the antiferromagnetic correlations increase only slightly below $T_c$, whereas for compounds close to $x = 0.13$ an enhancement up to 40% occurs with respect to the normal state. It is interesting that this happens although our calculation yields that $V_s(k, \omega)$ increases continuously for decreasing doping even below the optimal doping. The enhancement of the pairing interaction is consistent with the interesting doping dependence of $\Delta_0 \equiv \Delta(T = 0) = \phi(T = 0)/Z(T = 0)$. The superconducting gap has a maximum slightly above the optimal doping and decreases sharply in the underdoped compounds, because the quasi particle scattering increases for smaller doping due to the strong antiferromagnetic correlations via $Z$, whereas $\phi$ does not change significantly for $x \leq 0.13$. In addition the $2\Delta_0$ curve intersects the $\tau^{-1}$ curve at $x = 0.13$, where $\tau$ is the lifetime of the quasi particle, and $\tau^{-1} \equiv \text{Im} \Sigma(k, 0)$ with FS-momentum $k$ and self energy $\Sigma(k, 0) = \omega(1 - Z(k, \omega)) + \chi(k, \omega)$ at $T_c$. In Fig. 1 (b) one sees that $\tau^{-1}$ increases monotonously with decreasing doping and saturates for small and large values of $x$ as observed in transport measurements. Therefore the occurrence of an optimal doping in our results is related to an interference of the typical lifetime of the Cooper pairs $\sim \Delta_0^{-1}$ and the lifetime $\tau$ of the quasi particles: First $T_c$ increases for decreasing doping, since $V_s(k, \omega)$ increases and since $\tau$ is large enough to guarantee an effective Cooper pair formation. Then below the optimal doping, $T_c$ decreases again even so $V_s(k, \omega)$ continues to increase, since $\tau$ becomes too small and there are no well defined quasi particles during the pairing process. Notice, that there are also remarkable variations of the ratio $2\Delta_0/k_B T_c$ upon doping shown in Fig. 1(c). The deviations of $2\Delta_0/k_B T_c$ from the BCS value demonstrate the qualitative new changes of the superconducting state for decreasing temperatures, which are mostly pronounced at the optimal doping, where a strong increase of the pairing interaction occurs.

The interdependence of dynamical antiferromagnetism and superconductivity leads not only to an optimal doping, but also to a different behavior of the gap function $\Delta(k, \omega)$ in
*overdoped* and *underdoped* compounds. In Fig. 2 we plot $\Delta(k, \omega)$ for different frequencies along a path in the Brillouin zone as indicated in the insets. By comparing our results with the ansatz $\Delta_d \sim \cos(k_x) - \cos(k_y)$ one sees deviations from the simple $d$-wave behavior. These are mostly pronounced for small frequencies and in particular for underdoped systems, where the gap function is enhanced and largest at the FS and at its shadow. By transforming our results for $\Delta(k, \omega)$ to real coordinate space, we find that this corresponds to a pairing dominated by nearest-neighbor interactions in the case of $x = 0.16$. However, the appearance of higher harmonics in $\Delta(k, \omega)$ for $x = 0.09$ indicates that pairing processes between more distant antiferromagnetically correlated spins come into play. This results from the increasing stiffness of the nearest-neighbor spin correlations, which do not contribute any longer as strongly to the spin fluctuation mediated pairing interaction.

Further insight into the effect of the short range antiferromagnetic order on the excitations can be obtained by investigating the frequency dependence of the quasi particle decay. This is dominated by the coupling of states at the FS and its shadow. By inverting the matrix Greens function $\hat{G}(k, \omega)$ one can define an effective electronic self energy that includes the off-diagonal contributions and is equal to $\Sigma(k, \omega)$ in the normal state:\textsuperscript{11}

$$\Sigma_\phi(k, \omega) = \omega(1 - Z(k, \omega)) + \chi(k, \omega) + \frac{(\phi(k, \omega))^2}{\omega Z(k, \omega) + (\varepsilon_0(k) - \mu) + \chi(k, \omega)}.$$  \textsuperscript{(1)}

In Fig. 3 we compare the imaginary part of $\Sigma_\phi(k, \omega)$ at the FS and at its shadow for an overdoped and an underdoped compound above and below $T_c$. In the normal state we find for $x = 0.16$ that $\text{Im } \Sigma_\phi(k, \omega)$ is linear in $\omega$ down to energies $\omega \approx 8 \text{ meV} \approx 80 K$, which is consistent with the marginal Fermi-liquid (MFL) theory.\textsuperscript{13} For $x = 0.09$ we find besides an overall increase of the scattering rates a minimum (III) at the shadow at the FS that is a precursor of the singular behavior of $\Sigma_\phi(k, \omega)$ in the antiferromagnetic state. Thus the underdoped compounds are clearly not in agreement with the properties of an MFL. Below $T_c$ and for $x = 0.16$ a sharp minimum (I) becomes visible at the Fermi energy ($\omega = 0$) when $k$ is close to the FS which is the analogue of the corresponding $\delta$-function in the BCS theory.\textsuperscript{14} Thus minimum I shifts well below the Fermi energy when $k$ approaches the...
shadow of the FS. Furthermore, its intensity decreases and becomes almost equal to the additional minimum (II) at $\omega \approx +50$ meV in Fig 3(a) and (b). Note that minimum II vanishes for $k$ points away from the FS and its shadow (not shown) and is purely caused by the opening of the superconducting gap and a related shift of spectral weight in the effective interaction. Hence, this dip reflects the enhancement of the antiferromagnetic coupling below $T_c$ as already discussed in the context of Fig. 1(b). A similar feedback effect between spin fluctuations and $d$-wave pairing state occurs in the underdoped system. Here, the strongly enhanced scattering rates and the smaller superconducting gap lead to a rather small minimum I at the FS with respect to $x = 0.16$ and to a much weaker minimum II above the Fermi energy, whose energy shifts to the Fermi level for decreasing doping. However and more interestingly, the remarkable enhancement of minimum III shows that it is not a simple superposition of the precursor of the antiferromagnetic singularity and the superconducting singularity, but caused by a real interdependence between both phenomena.

To demonstrate that the interplay between dynamical antiferromagnetism that causes shadow states in the cuprates and superconductivity has not only consequences for the doping dependence of $T_c$, but can also be observed in ARPES experiments we extended previous results for the spectral density of states $\rho(k, \omega)$ to analyze what happens when $k$ crosses the shadow of the FS. In Fig. 4 we plot $\rho(k, \omega)$ for $k$ close to the shadow of the FS in the neighborhood of the $(\pi, 0)$ point. For the overdoped system one sees that the maximum II in $\Sigma_\phi(k, \omega)$ of Fig. 3 leads to a corresponding dip in $\rho(k, \omega)$ at $\omega \approx +60$ meV, where spectral weight is suppressed with respect to the normal state. This dip-structure agrees well with the experimental finding of an anomalous dip structure at the shadow of the FS which is mostly pronounced near the $(\pi, 0)$ point with energy $\omega_{exp} \approx 70$ meV. In the normal state of the underdoped system the small satellites below the Fermi level, which are separated from the main band above the Fermi energy, are the shadow states. They become visible below $x = 0.13$ and increase with decreasing doping. Below $T_c$ the dip structure as discussed for $x = 0.16$ shifts to smaller energies leading to a transfer of spectral weight below the Fermi level. Note that a first experimental indication for this anomalous transfer of
spectral weight was recently obtained by Dessau et al.\textsuperscript{4}.

Summarizing, we presented new results for the superconducting properties and the phase diagram of the 2D Hubbard model (Fig. 5). In particular, we obtained an \textit{optimal doping} as a result of the constructive interference between magnetic correlations and \textit{d}-wave pairing state. Furthermore, we demonstrated for the first time that shadow states exists below $T_c$ which are related to dip structures and to an anomalous transfer of spectral weight at the shadow of the FS in the spectral density of states. These were observed in photoemission experiments indicating the importance of spin fluctuations for the formation of superconductivity in the cuprates.
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18 Although we believe that our model dispersion captures the important physical mechanism
of the dip phenomenon, for a comparison with the experiments one has to perform a particle hole transformation and to exchange momenta $k$ and $k + Q$. An even better agreement with the photoemission experiment might be obtained by using the observed topology of the FS in the Bi2212 system.
FIGURES

FIG. 1. Doping dependence of the superconducting state: (a) $T_c$ obtained from $\Delta(T = T_c) = 0$. (b) Enhancement of the effective interaction $\max(V_s(k, 0))/\max(V_n(k, 0))$, $2\Delta_0$ and inverse quasi particle lifetime $\tau^{-1}$. (c) Ratio $2\Delta_0/k_B T_c$.

FIG. 2. Superconducting gap function $\Delta(k, \omega)$ for different frequencies and along different paths in the Brillouin zone (see inset). Note that $\Delta(k, \omega)$ is normalized by $\Delta(k = (\pi, 0), \omega)$ and that for comparison we plot the simple $d$-wave gap function $\Delta_d \sim \cos(k_x) - \cos(k_y)$.

FIG. 3. $\text{Im} \Sigma(\phi(k, \omega))$ at the Fermi surface and at its shadow. Note, the results $T = T_c$ refer to the normal state.

FIG. 4. Density of states $\rho(k, \omega)$ along a path in the Brillouin zone that crosses the shadow of the Fermi surface above and below $T_c$.

FIG. 5. Schematic phase diagram of the 2D Hubbard model, where the antiferromagnetic phase is only plotted for illustration although we get no magnetic phase transition in two dimension.
(a) \( x=0.16 \), \( T_c=75 \text{ K} \)

\[ k=(27,0)\pi/32 \]

(II) dip

(b) \( x=0.16 \), \( T_c=75 \text{ K} \)

\[ k=(32,6)\pi/32 \]

(II) dip

(c) \( x=0.09 \), \( T_c=65 \text{ K} \)

\[ k=(28,0)\pi/32 \]

(III)

(d) \( x=0.09 \), \( T_c=65 \text{ K} \)

\[ k=(32,4)\pi/32 \]

(II) dip
(a) $x=0.16$

$T_c=75$ K

$k=(32,6)\pi/32$

$k=(32,5)\pi/32$

$k=(32,4)\pi/32$

(b) $x=0.09$

$T_c=65$ K

$k=(32,5)\pi/32$

$dip$

$k=(32,4)\pi/32$

$k=(32,3)\pi/32$