Possible explanation for the absence of bilayer splitting in YBCO

H. Monien, N. Elstner and A. J. Millis
Physikalisches Institut, Universität Bonn, Nussallee 12, D-53115 Bonn, Germany
(October 18, 2018)

It has been claimed that the absence of the bilayer splitting in the high-temperature superconductor YBCO is a strong experimental indication that there are no coherent quasiparticles present in the CuO planes. We study a pair of strongly correlated planes which are connected by a hopping transfer integral $t_{\perp}$ in the limit of large in-plane coordination number. The effect of the correlation is incorporated in a dynamical mean-field theory, where the Weiss field is determined by a two-site Hubbard Hamiltonian. We have solved this problem by numerical techniques and present results for the spectral function $\rho$ for relevant parameters of the model. For small $t_{\perp}$ we find the coherent hoping between planes to be proportional to the in-plane quasiparticle renormalisation.

PACS: 71.10.-w,71.10.Ay,71.10.Fd,71.28.+d,71.30.+h,74.25.Jb,74.72.-h

The transport properties of the high temperature superconductors show an unusual behavior in many respects. Anderson has emphasized the difference between the transport properties in a CuO plane and perpendicular to the CuO plane stressing in particular the optical conductivity, in the $c$-direction perpendicular to the CuO plane. Also photoemission experiments in YBCO show only a small if any splitting of the bonding and antibonding CuO plane bands due to coherent hopping between the CuO planes. This is even more surprising in view of the relatively large value of the bare hopping matrix element, $t_{\perp} \approx 0.3$ eV compared to $t_{||} \approx 1$ eV, estimated from bandstructure calculations. The experimental data have been interpreted as a signal for the absence of coherent quasiholes in the CuO plane.

The question of how interactions affect the coherent transport between the planes has been studied mostly on one dimensionally strongly correlated systems because in that case it is clear that the excitations above the ground state are spinons and holons as in the original proposal by Anderson. Two coupled chains (ladders) have been recently studied in detail by many groups with numerical and analytic techniques. The result was that the hopping matrix element $t_{\perp}$ is a relevant perturbation for physically relevant values of the Luttinger liquid exponents and that the transport between the chains is coherent. Recently it has been claimed from an exact diagonalization study that for longer range interactions in the chains the coherent hopping between the chains can be reduced to zero for a finite value of the bare hopping matrix element $t_{\perp}$.

The problem of two coupled CuO planes is clearly more difficult since at this point the ground state and the excitation spectrum even for a single plane of the two dimensional Hubbard model away from half filling are not known. The problem has been studied with numerical techniques like Quantum Monte Carlo (QMC) and the fluctuation exchange approximation (FLEX) approximation. The subtle features of the dynamics of the quasiparticles in the coupled planes can currently not be resolved in the QMC due to finite size effects although the results for one plane look encouraging. The FLEX calculations are able to resolve the dynamics and yield surprisingly good results when compared to the QMC calculation but this approximation is uncontrolled in the regime where the interaction is large.

In this paper we present a calculation of the spectral function and the reduction of the coherent hopping in an approximation where the local correlations are taken into account exactly. We are in particular interested in the dynamics of the quasiparticles. We consider a model of two strongly correlated planes. We neglect the Coulomb interaction between the two planes. The motion of the holes in each plane is described by a Hubbard Hamiltonian.

$$H_a = -t \sum_{<ij>,\sigma} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

(1)

where $t$ is the hopping matrix element between two nearest neighbors $i$ and $j$, $\mu$ is the chemical potential, $c_{i\sigma}^\dagger$ is the electron creation operator on site $i$ with spin $\sigma$ in plane $a \ (a = 1, 2)$ and $n_{i\sigma}$ is the electron number operator for spin $\sigma$ at site $i$ in plane $a$, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. We denote the electron creation and annihilation operators in plane 1 by $c_{1i}^\dagger$ and $c_{1i}$ respectively and in plane 2 by $c_{2i}^\dagger$ and $c_{2i}$. The two planes are coupled by the hopping

$$H_{\text{hopping}} = t_{\perp} \sum_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \left( \sum_{j\perp} c_{j\downarrow} c_{j\uparrow} \right),$$

(2)

where $t_{\perp}$ is the hopping matrix element between the planes. The result was that the coherent hopping between the planes is zero for a finite value of $t_{\perp}$.
The Hamiltonian is diagonal in the bonding - antibonding representation. The full Green’s function can be obtained from the Dyson equation

$$G^{-1}(k, \omega) = G_0^{-1}(k, \omega) - \Sigma(k, \omega)$$

We are now in the position to derive the dynamical mean field equations for the coupled planes. In the limit of large coordination number the self energy becomes local and therefore k-independent. The only k-dependence of the Green’s function is left in the free electron dispersion $\epsilon_k$. This k-dependence can be absorbed in the density of states $D(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k)$, which of course depends on the type of lattice in which the electrons are moving. For the hypercubic lattice $D(\epsilon) = \exp(-(\epsilon/\sqrt{2t})^2)/\sqrt{2\pi}$. The full local Green’s function is therefore given by:

$$G(\omega) = \int d\epsilon_k D(\epsilon_k) (G_0^{-1}(\epsilon, \omega) - \Sigma(\omega))^{-1}$$

In the dynamical mean field approach $G_0^{-1}(\tau)$ plays the role of a Weiss field. The main point of this approach is that the local self energy of the full problem is determined by the local impurity model in our case a two impurity model. It has the action

$$S = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma \bar{\psi}_\sigma(\tau) G_0^{-1}(\tau - \tau') \psi_\sigma(\tau')$$

$$+ U \sum_{a=1,2} \int_0^\beta d\tau \bar{\psi}_{a\sigma}(\tau) \psi_{a\sigma}(\tau)$$

where $\bar{\psi}_\sigma = (\bar{\psi}_{1\sigma}, \bar{\psi}_{2\sigma})$ is a spinor of Grassmann variables. We only consider the paramagnetic state. The Weiss field $G_0^{-1}(\omega)$ is therefore diagonal in spin space. Using Eq. 4 we obtain the full local Green’s function in the bonding, anti-bonding basis:

$$G(\omega) = \begin{bmatrix} \hat{D}_+(\omega) & 0 \\ 0 & \hat{D}_-(\omega) \end{bmatrix}$$

where $\hat{D}_k(\omega) = \hat{D}(\omega - \Sigma(\omega) \pm (t_\perp - \Sigma(\omega)))$ is the Green’s function of the anti-bonding and bonding band respectively and

$$\hat{D}(\omega) = \int d\epsilon \frac{D(\epsilon)}{\epsilon - \omega}$$

is the Hilbert transform of the density of states $D(\epsilon)$.

We solve the two impurity model, Eq. 4, using the "iterated perturbation theory" (IPT) which has been shown to yield qualitative agreement with QMC and exact diagonalization approaches for interaction strength up to $U/t \sim 4$. The self energy is approximated by the first two terms of a perturbation expansion in the interaction $U$. However these two terms are calculated with the local Green’s function $G_0$ which is then determined selfconsistently. For doping levels away from half filling we used an extension of the IPT due to Kajueter and Kotliar.
In Fig. 2 the spectral functions of the bonding and antibonding band are shown as a function of frequency for a $U = 4$, a bilayer hopping of $t_\perp = 0.3$ and a filling of $n = 0.4375$. All energies are measured in units of the in-plane hopping matrix element $t$. For each band the lower and upper Hubbard band can be clearly identified. The quasiparticle peak close to $\omega = 0$ for each band is slightly shifted away from zero as expected from the noninteracting limit. The first interesting observation is that the spectral weight in the lower and the upper Hubbard band is not symmetric anymore even at half filling. The spectral density of the upper Hubbard band of the bonding band and the lower Hubbard band of the anti-bonding band are suppressed. With increasing hopping between the planes the quasiparticle peaks move further apart and the features associated with the Hubbard bands become less and less pronounced. For very large values of $t_\perp$ the noninteracting density of states of the two bands is recovered. The small features in the spectral function which are associated with the formation of so called shadow bands as obtained in the FLEX calculation can not be found in our calculation, because the finite momentum antiferromagnetic fluctuations are missing from our calculation. However the redistribution of weight from the Hubbard bands to the quasiparticle peak and vice versa has not been resolved in the FLEX perhaps because it is inherently a weak coupling approach. At half filling both bands are filled up to $\omega = 0$. The self energy of the bonding and antibonding propagator is given by $\Sigma_\parallel(\omega) + \Sigma_\perp(\omega)$. For small values of $t_\perp$ the quasiparticle peak is strongly reduced.

Next we discuss the reduction of the coherent hopping between the planes. There are two measures of coherent hopping: one is $\Delta E$, the splitting in frequency between the quasiparticle peaks in the bonding and anti-bonding bands; the other is $\Delta K = 2(t_\perp - \Sigma_\perp(\omega = 0))$, the splitting in momentum space between the bonding and antibonding bands at the Fermi surface. We consider $\Delta E/2t_\perp$ first. Its $t_\perp$ dependence is shown in Fig. 3. In the noninteracting case $\Delta E$ assumes the value $2t_\perp$. For small $t_\perp$ the ratio $\Delta E/2t_\perp$ is clearly reduced from the noninteracting value of 1. However unless one drives the system through the Mott transition at very large values of $U$ where the planes themselves are insulating the reduction factor is nonzero. In the $t_\perp \to 0$ limit the reduction factor can be analytically related to the reduction of the bandwidth in the plane. The off-diagonal part of the self-energy $\Sigma_\perp$ is proportional to $t_\perp^3$ for small $t_\perp$. The position of the quasiparticle-peak is given by the zeros of $\Delta E/2t_\perp$ in the complex plane. For small $t_\perp$ and doping not too far from half filling the position of the pole is given by the zero of $\omega - \text{Re } \Sigma_\parallel(\omega) = t_\perp + O(t_\perp^3) = 0$. The selfenergy does not depend on the momentum. The reduction of the bandwidth is therefore solely given by $(1 - \partial \Sigma_\parallel(\omega)/\partial \omega)^{-1}$ which is the same as the reduction of the bandwidth due to interaction in a single plane. Interestingly the coherent hopping is seen to be enhanced for larger values of $t_\perp$. This effect can be understood in terms of a level repulsion of the two site Hubbard model in the regime where $t_\perp \gg U \gg t$. For very large values of $t_\perp$ the splitting asymptotically approaches the value $2t_\perp$ as one would expect from the noninteracting system.

In Fig. 4 we plotted the spectral density $A(\epsilon_k, \omega)$ at zero temperature as function of frequency for parameter values $t_\perp = 0.3$ and $U = 4$. The wavevector dependence is only implicitly contained via $\epsilon_k$, because of the local nature of dynamical mean field theory. For $\epsilon_k$ close to zero we observe one sharp peak associated with the bond-
different values of $\epsilon$ self energy away from tions which manifest themself in a rapid increase of the comes broader. The broadening is due to strong correla-

ing band just below the Fermi level as one would expect (The bonding band actually crosses the Fermi level at $\epsilon_k \approx 0.15$). When going to lower energies this maximum moves downwards in the spectrum and very rapidly be-

ing out an error in our early analysis. We acknowledge
the hospitality of Lucent Technology, the Aspen Center
of Physics and the Johns Hopkins University were part
of this work was carried out. This work was supported
in part by the ISI foundation under grant ERBCHRC-

\[ \Delta K/2t_\perp \approx 1.1. \]

In conclusion we have studied the problem of two cou-
pled planes in the dynamical mean field theory in the
paramagnetic state as a function of interaction, doping
and interplane hopping matrix elements. Within our ap-
proximation the coherent hopping between the planes is
strongly reduced due to the interaction however it stays
nonzero as long as the planes stay in the paramagnetic
phase. It is still an open question if short range antifer-
romagnetic correlations which are completely neglected
in our approach can suppress the coherence between cou-
pled planes even further. For intermediate values of the
interplane coupling the coherent hopping motion of the
quasiparticles between planes is increased by the inter-
action. The spectral weight in the Hubbard bands is
redistributed in an unsymmetric way even at half filling.
Our approach can be easily extended to include more realistic density of states. It is interesting to examine
the stability of other groundstates like for example the
antiferromagnetic groundstate.

We would like to acknowledge useful discussions on this
problem with A. J. Ruckenstein, A. Georges, G. Kotliar,
J. Schmalian, D. Poilblanc, J. R. Schrieffer and D. Voll-
hardt. We are particular indebted to G. Uhrig for point-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4}
\caption{Single particle spectral function $A(\epsilon_k, \omega)$ vs. $\omega$ for
different values of $\epsilon_k$. The parameters are $t_\perp = 0.3$, $U = 4$ and
$n = 0.4375$.}
\end{figure}

\begin{thebibliography}{99}
\bibitem{Anderson1991} P. W. Anderson, Phys. Rev. Lett. 67, 3844 (1991) and
Science 256, 1526 (1992)
\bibitem{Homes1994} see e.g. C. C. Homes, T. Timusk, R. Liang, D. A. Bonn,
and W. N. Hardy, Phys. Rev. Lett., 71, 1645 (1993)
\bibitem{Shen1995} Z. X. Shen, Phys. Rep. 253, 1 (1995)
\bibitem{Ding1996} H. Ding et al., Phys. Rev. Lett, 76, 1533 (1996)
\bibitem{Pickett1989} W. Pickett, Rev. Mod. Phys. 61, 43 (1989)
\bibitem{Strong1992} S. P. Strong and A. J. Millis, Phys. Rev. Lett. 69, 2419
(1992)
\bibitem{Clarke1994} D. G. Clarke, S. P. Strong and P. W. Anderson, Phys. Rev.
Lett. 72, 3218 (1994)
\bibitem{Rice1993} T. M. Rice, S. Gopal and M. Sigrist, Europhys. Lett. 23,
445 (1993) and Phys. Rev. B49, 8901 (1994)
\bibitem{Noack1995} R. M. Noack, S. R. White and D. J. Scalapino, Phys. Rev.
Lett. 73, 882 (1994) and Europhys. Lett. 30, 163 (1995)
\bibitem{Dagotto1996} E. Dagotto and T. M. Rice, Science 271, 89 (96)
\bibitem{Tsunetsugu1997} H. Tsunetsugu and M. Imada, cond-mat 9705268
\bibitem{Capponi1996} S. Capponi, D. Poilblanc and F. Mila, Phys. Rev. B54,
17547 (1996)
\bibitem{Scalettar1994} R. T. Scalettar, J. W. Cannon, D. J. Scalapino, R. L. Sugar,
Phys. Rev. B50, 13419 (1994)
\bibitem{Putz1996} R. Putz, A. Preuss, A. Muramatsu and W. Hanke, Phys.
Rev. B53, 5133 (1996)
\bibitem{Grabowski1997} S. Grabowski, J. Schmalian, M. Langer and K. H. Benne-
mann, Phys. Rev. B55, 2784 (1997)
\bibitem{Dahm1997} T. Dahm, T. Manske and L. Tewordt, Zeitschrift für Physik
102, 323 (1997)
\bibitem{Pruschke1995} T. Pruschke, M. Jarell and J. K. Freericks, Adv. Phys.
44, 187 (1995)
\bibitem{Georges1996} A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg,
Rev. Mod. Phys. 68, 13 (1996)
\bibitem{Muller1989} E. Müller-Hartmann, Zeitschrift für Physik 74, 507 (1989)
\bibitem{Metzner1990} W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324
(1989)
\bibitem{Georges1992} A. Georges and G. Kotliar, Phys. Rev. B45, 6479 (1992)
\bibitem{Kajueter1996} H. Kajueter and G. Kotliar, Phys. Rev. Lett. 77, 131 (1996)
\end{thebibliography}