Zeitschrift: Helvetica Physica Acta
Band: 65 (1992)
Heft: 2-3

Artikel: Single-particle spectrum for high-T_c superconductors : a numerical study
Autor: Dopf, G. / Wagner, J. / Dieterich, P.
DOI: https://doi.org/10.5169/seals-116469

Single-Particle Spectrum for High-T_c Superconductors: A Numerical Study.

G. Dopf[1,2], J. Wagner[1], P. Dieterich[1], A. Muramatsu[1,2], and W. Hanke[1]
[1]Physikalisches Institut, Universität Würzburg, 8700 Würzburg,
[2]HLRZ, KFA-Jülich, 5170 Jülich, Fed. Rep. of Germany

Quantum Monte Carlo data are used to calculate the spectral density $A(\vec{k},\omega)$ for the three-band Hubbard model in order to analyze the states near the Fermi energy. These states are related to the Zhang-Rice singlet and exhibit a band-like behavior for finite doping δ. At a hole concentration $\delta = 0.25$ we find both a good quantitative agreement for the Fermi velocity and the location of the Fermi surface, when compared with angle-resolved photoemission data. However, the imaginary part of the self-energy does not vanish close to the Fermi level, indicating that a non-Fermi liquid behavior sets in. This feature is absent for large doping ($\delta = 0.50$), where a Fermi liquid picture seems to be appropriate.

A central and controversial issue in the high-T_c cuprates concerns the nature of carriers near the Fermi surface. The most crucial experimental results until now stem from angle-resolved photoemission (ARPES) and inverse photoemission (ARIPES) measurements [1] that clearly show the existence of a dispersive band that crosses the Fermi surface. The topology of the Fermi surface is in general agreement with LDA-bandstructure calculations [2], however the Fermi velocity is quite different. This indicates that electronic correlations renormalize considerably the results obtained in the frame of a one-particle treatment. So far, strong correlation effects can be properly taken into account only by exact numerical methods.

In this article we study the dynamic properties of one-particle excitations in the three-band Hubbard model, which is the generic one to describe the CuO_2 planes in the high-T_c superconductors. The Hamiltonian of this model is as follows:

$$H = \sum_{\substack{i,j \\ \sigma}} \varepsilon_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{\substack{i,j \\ \sigma\sigma'}} U_{ij} n_{i\sigma} n_{j\sigma'},$$

where $c^\dagger_{i\sigma}$ creates a hole in the Cu-$3d_{x^2-y^2}$- and in the O-$2p_x$- or $2p_y$-orbital depending on the site i. ε_{ij} includes the on-site energies E_d (Cu) and E_p (O) with $\Delta = E_p - E_d$ and a Cu-O hopping t_{pd}, while U_{ij} describes the on-site Coulomb energies U_d and U_p and the inter-site Cu-O interaction U_{pd}.

Exact diagonalization methods are the natural framework for the calculation of dynamical properties. However, serious limitations are imposed on the system size. In particular, for a realistic model like the one discussed here, the largest size is 2×2 elementary cells (12 sites). This limitation is removed by using a QMC approach [3] complemented by a least-square fit in order to extract the dynamical information in the system [4]. In this article we have performed simulations for lattice sizes up to 48 sites (4×4 elementary cells).

The Matsubara thermodynamic Green's function is defined as

$$G_m(k,\tau) = \langle c_m(k,\tau) c^\dagger_m(k,0) \rangle,$$

where the index m corresponds either to the $d_{x^2-y^2}$- or the $p_{x,y}$-orbitals. To calculate the spectral density, we have to invert the spectral representation of the Green's function

$$G_m(k,\tau) = \int_{-\infty}^{\infty} d\omega A_m(k,\omega) \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}}.$$

This is essentially a Laplace transform, which is numerically extremely ill posed, if the data are noisy. In order to deal with this problem recent progress was made [4]. We follow closely the approach of White et al., applying a modified least-squares fit.

Using a parameter set $\Delta = 4$, $U_d = 6$ [5], which leads to a charge transfer gap in agreement with experimental values, we have checked the numerical accuracy of our QMC data for $A(k,\omega)$ in comparison with exact diagonalization results. The overall agreement between both curves is very good, especially near the Fermi surface [5].

Now we proceed to study a 48 site system (4×4 unit cells) in order to extract the dispersion of the low-lying excitations. As shown in [6] these excitations are correlated states, which are mainly of Zhang-Rice (ZR) [7] character. The result is plotted in Fig. (1) along the high-symmetry lines of the Brillouin zone. We can clearly see that the ZR states form a dispersive band, that crosses the Fermi energy.

In Fig. (1) also shows the ARPES and ARIPES data for the superconducting material $Bi_2Sr_2CaCu_2O_8$ [1]. For this material the doping is assumed to be approximately 20 %. The experimental electron-excitations are only given as error bars due to the finite experimental resolution. Compared to these data we find a very good agreement for the locus of the Fermi surface and, in addition, we can reproduce the Fermi velocity. Small differences are possibly due to marginal different doping concentrations in the simulation and the real material. This result shows that the three-band Hubbard model describes accurately the one-particle excitations of the cuprates. On the other hand the parameter set ($\Delta = 4, U_d = 6$) seems also to be a good starting point in order to investigate the superconducting behavior in these systems [5].

Additionally the relevance of fluctuations is clearly demonstrated by comparing our results with an ab initio LDA-bandstructure calculation for $Bi_2Sr_2CaCu_2O_8$ [2]. Although the LDA Fermi sur-

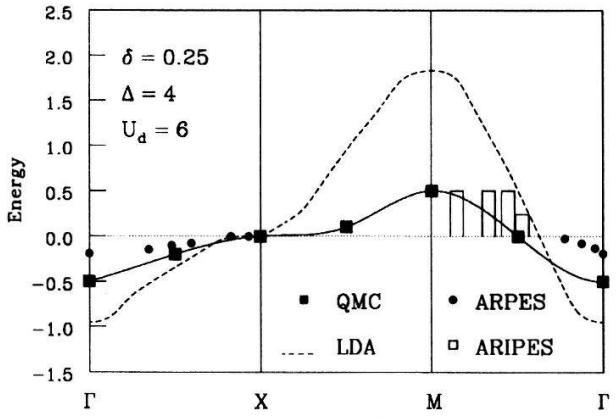

Figure 1: Comparison of the QMC-, LDA-bandstructure and experimental results.

face corresponds well to the experimental one, the Fermi velocity as well as the band-width are totally overestimated.

Finally we address the question whether the present system can be well described by a Fermi liquid picture. Fig. (2) shows the imaginary part of the self-energy obtained for a 2×2 (12 sites) system by exact diagonalization. For a doping concentration of 50 % $\mathrm{Im}\Sigma(k,\omega)$ vanishes for $k = (\pi, 0)$ in a broad region around the Fermi energy. This clearly indicates the existence of long-living quasiparticles and the Fermi liquid picture is appropriate. However, for a doping of $\delta = 0.25$, $\mathrm{Im}\Sigma(k,\omega)$ *does not vanish* on approaching the Fermi energy. Therefore the corresponding ZR state has a finite lifetime and the Fermi liquid picture with well defined quasiparticles at the Fermi energy breaks down. We suggest that at doping levels $\delta \lesssim 0.25$, which are relevant for the high-T_c cuprates, the system is better described as a Luttinger liquid [8]. A more quantitative characterization of this state needs a careful finite-size analysis of $\mathrm{Im}\Sigma(k,\omega)$. Such simulations are presently being carried out.

In the case of half-filling ($\delta = 0$) we find an enormous enhancement of $\mathrm{Im}\Sigma(k,\omega)$ at the Fermi energy. This is due to the fact that the system is an insulator for zero doping. The related gap was already observed in the single-particle excitation spectrum between the correlated states and the upper Hubbard band [5,6].

In summary, our numerical results show that the three-band Hubbard-model gives a very accurate description of the low-lying one-particle excitations in the high-T_c superconductors. We can reproduce the experimentally observed Fermi surface and Fermi velocity quantitatively. The Fermi liquid picture is supported by our data for heavily doped systems. However, at doping concentrations relevant for superconductivity, we find that the lifetime of the one-particle excitations remains finite on approaching the Fermi energy. Such a break-down of the Fermi liquid picture and the fact that the locus of the Fermi surface coincides with LDA calculations, suggest that at doping levels $\delta \lesssim 25\%$ the system is better described as a Luttinger-liquid.

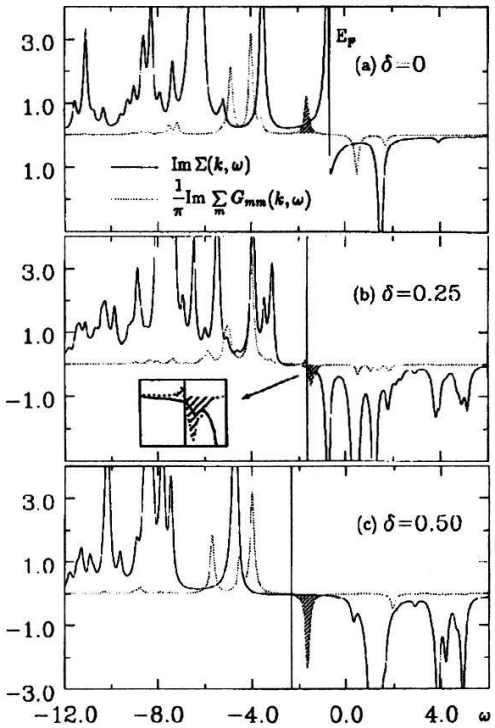

Figure 2: Imaginary part of the self-energy at $\vec{k} = (\pi, 0)$.

The numerical calculations were performed on the Cray Y-MP of the HLRZ Jülich. We thank the HLRZ for its support.

[1] G. Mante et al., Z. Phys. B **80**, 181 (1990).

[2] M. S. Hybertsen and L. F. Mattheiss, Phys. Rev. Lett. **60**, 1161 (1988).

[3] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D**24**, 2278 (1981); J. E. Hirsch, Phys. Rev. B**31**, 4403 (1985).

[4] S.R. White et al., Phys. Rev. Lett. **63**, 1523 (1989); R. Silver et al., Phys. Rev. Lett. **65**, 496 (1990); M. Jarrell and O. Biham, Phys. Rev. Lett. **63**, 2504 (1989).

[5] G. Dopf, A. Muramatsu and W. Hanke, Phys. Rev. B **41**, 9264 (1990), and to be published.

[6] J. Wagner, W. Hanke, and D.J. Scalapino, Phys. Rev. B **43**, 10517 (1991); P. Horsch et al., Physica C **162-164**, 783 (1989).

[7] F.C. Zhang and T.M. Rice, Phys. Rev. B **37**, 3759 (1988).

[8] P.W. Anderson, Phys. Rev. Lett. **65**, 2306 (1990).