Fermi surface and ARPES of CuO_2 planes – violation of Luttinger's theorem?

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Abstract

We employ the dynamical cluster approach to the $2D$ Hubbard model in the intermediate coupling regime. For small to intermediate doping we observe strong deviations from conventional Fermi liquid behavior and evidence for a violation of Luttinger's theorem. Our spectra and Fermi surface data compare reasonably well with experiments on high-T_c compounds.

Key words: non-Fermi liquid; cuprates; ARPES; Fermi surface

1. Introduction

The rich phenomenology of high-T_c superconductors [1] has stimulated strong experimental and theoretical interest in the field of strongly correlated electron systems. Apart from the anomalously high transition temperatures, anomalous properties are found in a variety of dynamical quantities. Among the fundamental and controversial questions are whether the cuprates can be described as a Fermi liquid or not and what shape and volume a possible Fermi surface will have.

The standard model used to investigate the electronic properties of the high-T_c cuprates is the 2D Hubbard model [2]

$$H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} c^\dagger_{i\bar{\sigma}} c_{i\bar{\sigma}} \qquad (1)$$

in the intermediate coupling regime. This is the most complicated regime of the model, since both weak and strong coupling perturbative approaches fail. Exact diagonalization of small clusters suffers from strong finite-size effects and conventional Quantum Monte Carlo from a severe minus sign problem [3].

In this paper we use the recently developed dynamical cluster approximation (DCA) [4] to study the low-energy behavior of the $2D$ Hubbard model in the intermediate coupling regime. The DCA is a non-perturbative scheme going beyond conventional finite-size calculations. Its main assumption is that the single-particle self-energy $\Sigma(\mathbf{k}, z)$ is a slowly varying function of the momentum $\mathbf{k}$ and can be approximated by a constant within each of a set of cells centered at a corresponding set of cluster momenta $\mathbf{K}$ in the first Brillouin zone[4]. This prescription is sketched in

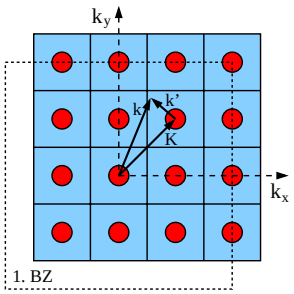

Fig. 1. The DCA coarse graining cells for a cluster size $N_c = 16$. Each cell is represented by a cluster $\mathbf{K}$-point (filled circles).

Fig. 1 for a cluster size $N_c = 16$. The set of cluster

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K-points is given by $K^n_\alpha = \pi(n_\alpha/2 - 1)$ with the spatial index $\alpha = x, y$ and $1 \leq n_\alpha \leq 4$. The self-energy is assumed to be constant within the shaded region around each **K**, i.e. $\Sigma(\mathbf{K} + \mathbf{k}', z) \approx \Sigma(\mathbf{K}, z)$.

Within this approximation one can set up a self-consistency cycle similar to the dynamical mean-field theory [5]. However, in contrast to the DMFT, where only local dynamics can be studied, the DCA includes non-local correlations with length scales that can be systematically varied with increasing cluster size. The resulting effective cluster problem we solve with the Hirsch-Fye impurity algorithm [6] modified to simulate an embedded cluster[7].

2. Results

For a proper description of the CuO_2 planes of the high-T_c cuprates within the Hubbard model (1) it is generally accepted that the tight-binding dispersion has the form

$$t_{\mathbf{k}} = -2t\,(\cos(k_x) + \cos(k_y)) \qquad (2)$$

$$-4t'\cos(k_x)\cos(k_y)$$

with a nearest neighbor hopping amplitude $t > 0$ and a next-nearest neighbor hopping amplitude t', which in principle can have any sign. From band structure calculations and the general form of the measured Fermi surface, especially in the overdoped regime, conventionally a negative t' is inferred[8].

In the following we use $t = 1/4$eV and $t' = -0.2t$ in accordance with typical values extracted from experiment and band structure calculations and choose $U = W = 2$eV. This value ensures that at half filling the system is a Mott insulator. We performed our simulations at a range of temperatures, but will present results for $T = 0.033$eV≈ 300K only, which is roughly room temperature. As cluster size we used 16 **k**-points in the irreducible part of the first Brillouin zone.

The single-particle spectra are plotted in Figs. 2 and 3 for dopings $\delta = 5\%$ and 20%, respectively. We use the standard notation for the high symmetry points in the first Brillouin zone. Peaks in the spectrum cross the Fermi energy along the $\Gamma \to M$ and $M \to X$ directions, indicated by the thick lines and arrows. Note that due to a finite, negative t' the Fermi surface is hole like for all dopings studied, in contrast to the case $t' = 0$, where a crossover from a hole-like Fermi surface at small doping to an electron-like at large doping is observed [9]. The imaginary part of the self energy at these crossing points is plotted versus frequency in panel (d) of Figs. 2 and 3.

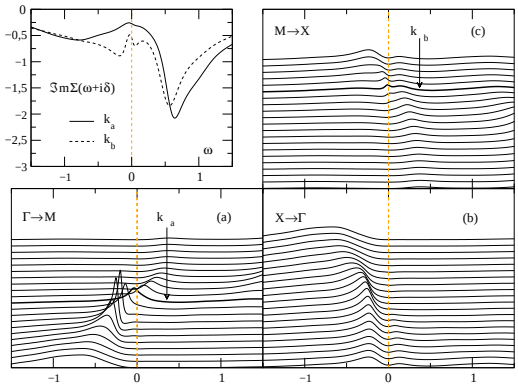

Fig. 2. (a)–(c) $A(\mathbf{k}, \omega)$ for $\delta = 5\%$ along symmetry directions. The thick lines indicate a peak crossing the Fermi energy. (d) the imaginary part of the self energy versus frequency at the Fermi surface crossing found in (a) and (c).

One very interesting feature of the spectra at low doping, Fig. 2, is that the peak near $(\pi/2, \pi/2)$ broadens dramatically before crossing the Fermi energy. Near X, on the other hand, one does not observe any dramatic change in the spectrum when crossing the Fermi energy. Note also that the spectra near the crossing points in Fig. 2 are strongly damped and one cannot truly speak of quasi-particles crossing the Fermi energy.

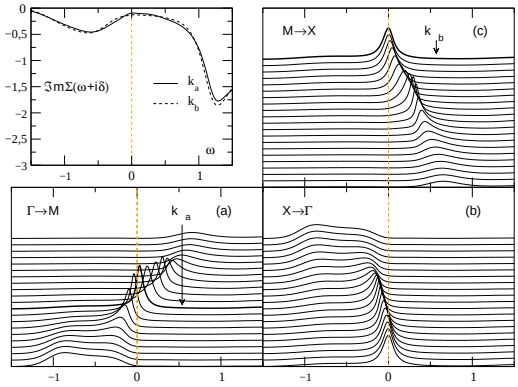

Fig. 3. (a)–(c) $A(\mathbf{k}, \omega)$ for $\delta = 20\%$, other parameters and symbols as in Fig. 2.

It is also quite instructive to look at the imaginary part of the self-energy at the crossing points (Fig. 2(d)). In particular at $\mathbf{k}_b$ close to $(\pi, 0)$, $\Im m\Sigma(\mathbf{k}_b, \omega)$ starts to develop an additional feature which eventually leads to the formation of a pseudo gap in the spectra along the $M \to X$ direction. In addition, one observes a rather large residual scattering rate for both momenta $\mathbf{k}_a$ and $\mathbf{k}_b$. This can either be taken as evidence for NFL behavior or as signal for the occurrence of a new very small low-energy scale[10]. Note that in the low-energy regime the self energy displays significant k-dependence. This clearly renders theories based on a

local approximation like the DMFA inadequate at least for small doping.

At high doping, Fig. 3, the peaks in the spectrum close to the Fermi energy are far sharper. Here it makes sense to speak of a conventional Fermi liquid and quasi particles.

The imaginary part of the self energy, shown in Fig. 3(d), has a broad maximum at $\omega = 0$ with a very small residual scattering rate and changes little as $\mathbf{k}$ moves along the Fermi surface. This weak dependence on $\mathbf{k}$ is an indication that approximations like the DMFA should be accurate here, i.e. that there is little effect of non-local correlations. All indications are that for this doping regime standard Fermi-liquid behavior has returned.

More direct evidence for NFL behavior can be seen in the shape of the Fermi surface. An analysis of the Fermi surface for the t-J model has been performed recently within a high-temperature expansion [11] and a physically motivated decoupling scheme [12]. The results have been considered as clear evidence for a violation of Luttinger's theorem and the possible formation of a non-Fermi liquid at small doping.

We map the Fermi surface from a constant energy plot of the single-particle spectra at the Fermi energy $A(\mathbf{k}, \omega = 0)$, which allows direct contact with ARPES experiments. The result for $\delta = 5\%, 10\%, 15\%$

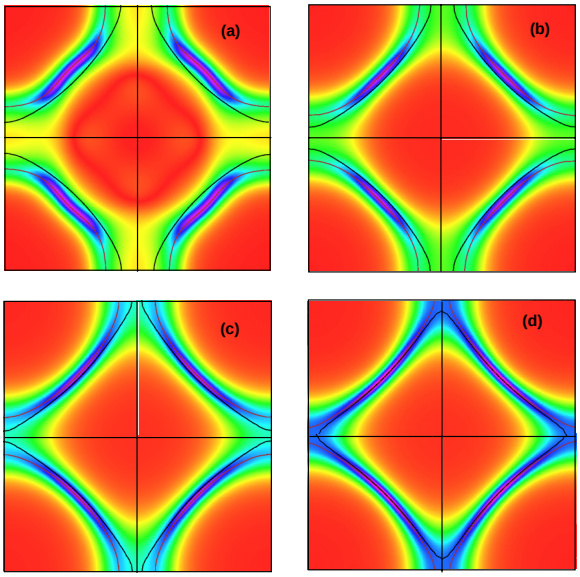

Fig. 4. Constant energy scans of $A(\mathbf{k}, \omega = 0)$ for $\delta = 5\%$ (a), 10% (b), 15% (c) and 20% (d). The violet (red) represents regions of high (low) electronic density. The Fermi surface for $U = 0$ is represented by a black line and the points where the real part of the denominator of the Green function vanishes by the solid red line indicates.

and 20% is shown in Fig. 4a-d. Regions of high density are colored in violet. The solid black lines represent the non-interacting Fermi surface. To distinguish between structures resulting from either quasiparticle excitations or incoherent background, we also plot the points where the real part of the denominator of the Green functions vanishes at zero frequency. These points which solve the quasi-particle equation $-\epsilon_{\mathbf{k}} - \Re e\Sigma(\mathbf{k}, \omega = 0) = 0$ are given by the solid red lines.

The Fermi surface resulting from our calculations is hole-like, centered around (π, π), and encloses a volume larger than the non-interacting Fermi surface for $\delta \geq 10\%$. This indicates a violation of Luttinger's theorem. In addition, the shape of the Fermi surface close to $(\pi/2, \pi/2)$, especially the clear shift above $(\pi/2, \pi/2)$ cannot be interpreted neither in terms of a simple tight-binding band structure nor a weak-coupling theory[13]. At least for $\delta = 5\%$ this structure rather is compatible with the notion of a small Fermi surface, i.e. pockets around $\mathbf{k} = (\pi/2, \pi/2)$ [11,12].

With increasing doping the structures around $(\pi/2, \pi/2)$ start to follow more or less the noninteracting Fermi surface again. This points towards a restoration of Luttinger's theorem. For $\delta = 20\%$, the Fermi surface has essentially the same volume and shape as the non-interacting surface, indicating a return to Fermi-liquid like behavior. Note, however, that at the X point the interacting Fermi surface is still hole-like, while the non-interacting already is closed around Γ. This feature, i.e. the tendency towards a hole-like Fermi surface of the interacting system even in the overdoped regime, is also in qualitative accordance with experiment [14].

3. Summary

The increasing precision and quality of experimental ARPES spectra in recent years has led to a number of new results on the single-particle dynamics of the high-T_c cuprates, both partially resolving long-standing issues and posing new questions and problems. Motivated by especially the interesting observations concerning the changes of Fermi surface topology with doping, we have studied the two-dimensional (2D) Hubbard model in the intermediate coupling regime (on-site correlation U equal to the bandwidth) at the temperature $T = 0.033$eV. To study the model in this most problematic parameter regime we used quantum Monte Carlo within the dynamical cluster approximation for a cluster of 16 $\mathbf{k}$-points in the irreducible part of the first Brillouin zone. Since this method allows for controlled and reliable calculations of low-energy features within a non-perturbative scheme and in the thermodynamic limit, fundamental problems in this field can be addressed. These include the single-particle

spectral properties at low energies, especially possible deviations from Luttinger's theorem or the formation of non Fermi liquid states, and the resulting topology of the Fermi surface.

From the constant energy scans of the spectrum at the Fermi energy we find that the there is clear evidence for a violation of Luttinger's theorem at small doping. For $\delta = 5\%$ the only sharp structures appear at $\mathbf{k} = (\pi/2, \pi/2)$ and strongly resemble the notion of a small Fermi surface, i.e. hole pockets.

Non Fermi liquid behavior is also evidenced by the spectra respectively the self-energy, which shows a rather large residual scattering rate and additional structures at $\omega = 0$.

With increasing doping the Fermi surface changes its topology around $(\pi/2, \pi/2)$, and beyond $\delta \approx 10\%$ one can infer a tendency towards restoration of Luttinger's theorem and conventional Fermi liquid behavior with the spectra showing well defined quasi-particle peaks around the Fermi energy.

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