Pseudogap and Central Peak in the Emery Model

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Abstract

The effect of antiferromagnetic (AF) correlations is studied in the framework of the three-band (Emery) model, with respect to experiments in BSCCO. We study the pseudogap regime with a central peak. Detailed dispersions of quasiparticle peaks show that one can simultaneously fit Fermi surfaces and ARPES leading-edge energy scales. The band parameter regime is a strong-coupling one: marked renormalization of the copper-oxygen overlap, making it smaller than the oxygen-oxygen overlap, while the copper-oxygen energy splitting is the largest of the three. The same regime was found previously in a zeroth-order fit of Fermi surfaces. The inclusion of AF correlations in a weak-coupling approach resolves the only qualitative discrepancy of the zeroth-order mean-field slave-boson calculation with experiment: it is argued that the observed large flat region of the dispersion around the vH point is due to the very non-dispersive central peak in the X-M direction. The sudden increase of the experimental one-particle dispersion in the X-M direction is explained by the quasiparticle strength shifting to the upper wing of the magnetic pseudogap, as one moves further away from the X (van Hove) point. Near it, the lower wing is predicted to be observed in the X-M direction, in addition to the narrow central peak, giving rise to a two-peaked structure below the Fermi level, as found experimentally.

Key words: strongly correlated electrons, pseudogap, ARPES, high temperature superconductors
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1. Introduction

To understand conducting electrons in high-\(T_c\) superconductors, one can try and separate the experimental situation into as many individually understandable pieces as possible. Simple calculations are then used to read experiment, rather than predict it, and so constrain the eventual complete theory. In this spirit, our main result here is that the narrow non-dispersive feature found in ARPES measurements in BSCCO along the \((\pi,0)-(\pi,\pi)\) (X-M) direction is antiadiabatic: the responsible fermionic excitation is much slower than the dominant perturbing boson, which imparts it with a \((\pi,\pi)\) momentum transfer.

This interpretation is obtained in the context of two other insights. First, the observed Fermi surface shapes in LSCO, YBCO and BSCCO are most efficiently fitted in a three band model, taking the oxygen degree of freedom explicitly into account [1]. This reduces the number of parameters needed from six (in a one-band model) to only three. Second, while the extended high ARPES background is not obtained here, we note it can be obtained by an explicit treatment of the on-site repulsion by slave-bosons with fluctuations, both in ARPES [2] and Raman spectra [3].

In this paper, we concentrate on the next piece of the puzzle. In BSCCO, the above-mentioned Fermi surface fit is not accompanied by a similarly successful fit of the dispersion. The experimental dispersion is very flat in the X-M direction, while the zeroth-order dispersion of the Cu-O resonant band, fitted to the Fermi surface, has a strong anisotropy at the X (vH) point. We show that the discrepancy is resolved by the intervention of a narrow antiadiabatic quasiparticle near the Fermi energy. The leading edge scale of the wide adiabatic

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Fig. 1. Log-intensity plot in the X–M direction, parameters of the best fit to the Fermi surface: $t = 0.4, t' = -1.6, \Delta_{pf} = 4.5, \mu = -0.04$ eV. Note the effective flattening near $E_f$ due to the central peak. The white line is the unperturbed band dispersion. Intensities are multiplied by a Fermi factor. Axes are the same as in Fig. 2.

2. Antiadiabatic regime

We calculate the one-loop contribution to the electron self-energy, extending a previous calculation [4] to a realistic dispersion, and electrons at arbitrary wavevectors. The dispersion accounts for the strong on-site repulsion through a mean-field renormalization of overlaps, so the parameter regime is $t < |t'| << \Delta_{pf}$, the effective Cu-O hopping, O-O hopping, and Cu-O energy splitting, respectively. The main feature of this work is that the perturbing paramagnon is faster than the electron around the vH point. Such an antiadiabatic regime always exists, because the electron velocity is zero there, but in our case, the large quasiparticle effective mass and short correlation length of paramagnons act in concert to extend the antiadiabatic quasi-particle to about 30% of the zone in the X–M direction. This requires a low, but not too low ‘bandhead’ of the paramagnons, we take 10 meV, appropriate for the superconducting state [5].

The corresponding intensities are shown in Fig. 1. The net effect on the dispersion around $E_f$ is as if one had cut out the rising part and replaced it horizontally. The lower wing turns upwards, following the unperturbed dispersion, but shifted by a pseudogap. The possible impact of the side wings on high Tc has recently been extensively analysed [7]. The antiadiabatic (horizontal) part has a maximum where it crosses the trace of the old dispersion. The valley separating the two peaks is due to the absence of explicit slave boson dynamics in the calculation [2].

Figure 2 shows the experimental intensities in the X–M direction [6]. We observe that the lower wing turns upward, and that the non-dispersive feature has a maximum where the lower wing ‘points’ at it. This unexpected correspondence of qualitative details with our calculation increases our confidence in the basic interpretation of the non-dispersive feature.

3. Discussion

The antiadiabatic quasiparticle is a very robust phenomenon, once the paramagnon anomaly increases at a sufficient rate out of its minimum at $(\pi, \pi)$, relative to the electron dispersion’s increase away from the vH point. This opens a ‘window’ in the BZ, where the fermions are slower than the bosons, so there is no adiabatic suppression of the quasiparticle strength. Then the relative strength of the central peak, and the energy scale at which the wings appear, may be adjusted through the paramagnon bandhead and coupling strength, respectively, without much fine-tuning.

As one moves away from the vH point in the Γ direction, the non-dispersive feature ‘melts’ with the lower wing into a single dispersion, both in our calculation and in experiment. However, while this is complete by $(0.9\pi/a, 0)$ in the calculation, the non-dispersive feature is observed up to $(0.6\pi/a, 0)$ [6], as also found in cuts along the Γ–M line [8]. We hope that a self-consistent calculation, allowing for charge and spin channels on equal footing, might resolve this issue.

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