Difference between microscopic and effective overlaps in the copper-oxide planes of high-Tc superconductors

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We investigate parametrizations required to reproduce observed Fermi surfaces of overdoped and slightly underdoped LSCO in two different models. One is the standard three-band saddle-point slave boson (SB). The other is a model of CuO4 'molecules' randomly tiled in the plane, emphasizing the distinction between the local overlap, always the full (bare) one, and the effective overlap, connected with the reduced bandwidth due to the random tiling (RT). We conclude this distinction is physically significant for underdoped, but not for overdoped LSCO. This is consistent with the observed open Fermi surfaces being due to correlation effects.

1. Introduction

The nature of the normal state of high-T_c superconductors is still an open question. Within ARPES, the discussion has initially centered on line shapes [1], but with improved resolution and material preparation, has moved to pseudogap behavior [2] and Fermi surface evolution [3].

The present work investigates, does the recently observed [3] change of shape of the Fermi surface in $La_{2-x}Sr_xCuO_4$ with doping by itself require invoking correlations. In particular: is there a sign that the local electronic environment is different than the 'effective' one-particle picture which can reproduce these shapes.

2. Model

We start from a metallic state and three bands, and assume that the principal effect of the infinite on-site repulsion is in charge correlations. This regime was first described by the SB model at the saddle-point [4], by renormalizing the copper-oxygen overlap t. Physically, the local overlap is not always renormalized, because when an electron of one spin is on a site, the other may not be near. This distinction between local and long-range behavior is lost at the saddle-point.

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The RT model [5] keeps the distinction, by first hybridizing the electron within a single CuO_4 'molecule' through the bare overlap, and then producing an effective band by randomly tiling these molecules in the plane. It satisfies the Pauli principle for the original electrons exactly. The price paid is that the one-particle formulation is achieved by assuming that the down-spins do not hop at all. The fact that they do is simulated by annealment. We cannot justify this microscopically; however, the assumption, that the two spins see each other as static [6], is implicit at the SB saddle-point as well [7].

3. Results

To face measurements, we include the oxygen-oxygen overlap t' in the RT model in the simplest local approximation, just adding the t' terms to a CuO_4 'tile'. This underestimates the tendency of t' to rotate the Fermi surface, strenghtening our conclusion. The implementation of the slave-boson model with t' [8] follows the literature.

In fig. 1, we compare the RT and SB input parameters needed to fit observed Fermi surfaces [3]. Both models can fit all the data equally well at all dopings. The fit was sensitive to t', while less was gained by varying t and the bare copper-oxygen splitting Δ_{pd}, so they were kept fixed.

Overdoped samples ($x > 0.2$) require a rather

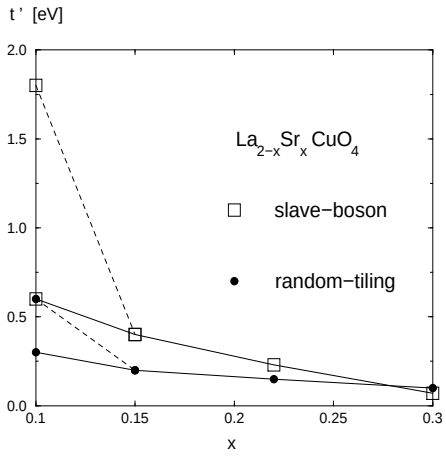

Figure 1. Full lines: values of t' which fit Fermi surfaces within error bars. Dotted lines: changes in t' required for 'perfect' fits. For all points, $t = 1$ eV, $\Delta_{pd} = 3$ eV.

small value of $t' \sim 0.1$ eV, and the two models nearly agree. For the underdoped ($x = 0.1$) sample, the discrepancy is a factor of two (0.6 eV for SB, 0.3 eV for RT). It is known [9] that such, fairly large, values of t' are required to rotate the Fermi surface in the SB model.

At $x \geq 0.15$, the fits are 'too good', passing near data points, not merely within error bars. However, if the same 'perfect' fits are required at $x = 0.1$, t' needs to be much larger, increasing the discrepancy factor to three.

4. Discussion

Fourier series being efficient in fitting smooth curves, the mere fact that a dispersion with more than nearest neighbors fits a 2D Fermi surface is hardly significant. A credible phenomenology needs to be both sensibly constrained, and require little variation in the input parameters. Cases where it breaks down should also be understood. The fits in this work were constrained by modelling, with only the bare parameters put in. Also, only t' varied with the data, which amounts to 'freezing' the lattice. Although technically no more than fits within error bars are required, it is significant that the data overtax both models at underdoping, as evident by drastically increased t' when pushed to overfit.

The RT model treats the data more sparsely, with a range in t' (full lines) of 0.2 eV, *vs.* 0.55 eV for the SB model. This, and the quantitatively different tendency to breakdown at $x = 0.1$, leads us to conclude that the distinction between local and effective overlap is physically relevant for the underdoped and, probably, optimally doped samples, but not for $x > 0.2$. We find open Fermi surfaces at $x = 0.1$ and 0.15 as the result of correlations, at a reasonably low bare t'. This corresponds to one of the regimes where an extended vH singularity can be obtained in the copper bonding band [10]. The 0.2 eV variation of t', still remaining in the RT model, could be due to our 'local' approximation in including it, lattice evolution, and spin correlations [11].

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REFERENCES

1. Y. Chang *et al.*, Phys. Rev. **B39** (1989) 7313.
2. J.C. Campuzano *et al.*, Physica **B259–261** (1999) 517.
3. A. Ino *et al.*, J. Phys. Soc. Japan **68** (1999) 1496.
4. G. Kotliar, P.A. Lee, and N. Read, Physica **C153–155** (1988) 538.
5. D.K. Sunko and S. Barišić, Europhys. Lett. **36** (1996) 607. *Erratum:* **37** (1997) 313.
6. M.C. Gutzwiller, Phys. Rev. **137** (1965) A1726.
7. G. Kotliar and A.E. Ruckenstein, Phys. Rev. Lett. **57** (1986) 1362.
8. E. Tutiš, PhD thesis, U. of Zagreb, 1994.
9. Qimiao Si, Yuyao Zha, K. Levin and J.P. Lu, Phys. Rev. **B47** (1993) 9055.
10. I. Mrkonjić and S. Barišić, in *Contributions to the 2nd meeting of the Croatian Physical Society*, I. Batistić *et al.*, eds., Zagreb 1999, p. 26 (in Croatian).
11. C. Kim *et al.*, Phys. Rev. Lett. **80** (1998) 4245.