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Effects of in-plane oxygens on the magnetic response in cuprates

G. Nikšić [a], O.S. Barišić [b], I. Kupčić [a], D.K. Sunko [a,*], S. Barišić [a]

[a] Department of Physics, Faculty of Science, University of Zagreb, Bijenička 32, 10000 Zagreb, Croatia
[b] Institute of Physics, Bijenička 46, 10000 Zagreb, Croatia

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ABSTRACT

A brief analysis of ARPES, Raman, and neutron data is used to show the importance of the oxygen degree of freedom for the metallic phase of cuprate high-T_c superconductors. It is based on published results and a number of new calculations, relevant to Raman and neutron scattering in the metallic underdoped and optimally doped regime. They are placed in the context of a recently developed theoretical understanding of the microscopic interplay between metallicity and local valence-bond fluctuations in the cuprates. It is argued that the oxygen degree of freedom is dominantly responsible for the metallicity in the normal state. The coexistence of metallic oxygen-dominated states with localized copper-dominated states is a key experimental constraint on the microscopic understanding of the normal-state pseudogap proposed here, especially of its strong k-dependence.

1. Introduction

The nature of the pseudogap (PG) state in high-T_c superconductors is generally taken to be the key to understanding their superconductivity (SC). There has been some controversy in the literature, whether the PG and SC gaps are essentially the same phenomenon, observed above and below T_c, or not. We adopt the so-called "two-gap" approach, in which the PG is taken to be distinct from the SC gap. We observe that the intrinsic PG energy scales are several times larger than the SC scale, which accounts for the need to understand it first, as the stage on which SC takes place. Our approach is neutral to SC, so we cannot determine yet, whether it is related to the same electronic interactions as the PG. We concentrate on correlations in the PG region, and try to understand them microscopically.

These correlations are nearly antiferromagnetic (AF) on coppers. Incommensurate AF, as stripes, corresponds to the dominant PG effect in k-space near the Fermi energy, but the same physical mechanisms are responsible for incoherent local valence-bond fluctuations, which draw spectral strength away from the coherent states. Experimentally, the latter may account for a large part of the spectral weight, so they would have to be called dominant, except for the importance of the pseudo-coherent states at the Fermi level.

The physical role of the oxygen degrees of freedom is the unifying feature of our understanding of the high-T_c cuprates, from optimal doping to still-metallic underdoping. We ascribe the generally observed crossover between the AF and PG regime to a metallization of the oxygen sites. Here we provide a cumulative overview of cuprate physics, with an emphasis on low-energy phenomenology, under the widely accepted assumption that the bare on-site repulsion U_d on the copper sites of the three-band (Emery) model is large.

2. ARPES

The chemical potential μ of all high-T_c cuprates [1], as measured by ARPES and also XPS, as well as of some analogous strongly correlated insulators [2], contradicts the Brinkman–Rice scenario, which relates the insulating behavior to a band-width collapse. It also contradicts the notion that the first doped holes go to the oxygen sites. In reality, wide bands are being continuously doped all the way to the insulating limit at half-filling, and the only jump in μ, observed when going from small hole to small electron doping, is about 0.8 eV, at least 2–3 times smaller than the value of the bare copper–oxygen splitting Δ_{pd}, as usually inferred from small-molecule and LDA ("local") calculations. This indicates that the effective interactions responsible for the PG are significantly renormalized relative to U_d. We do not mean that the LDA calculations are incorrect, but that they give the bare *intracell* overlaps, which are responsible for large-scale local hybridizations, important e.g. for the cohesion energy. We believe the residual metallicity very near half-filling is of a different nature than the PG state with Fermi arcs, because at extremely low hole doping the superexchange mechanism, which requires oxygens to be empty, may still be coherent [3]. Fermi arcs signify that the oxygens are sufficiently metallized to render superexchange

* Corresponding author. Tel.: +385 1 460 5575; fax: +385 1 468 0336.
E-mail address: dks@phy.hr (D.K. Sunko).

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incoherent. In particular, the chemical potential data mean that one cannot interpret the AF interactions in the metal as $J \sim t_{pd}^4/\Delta_{pd}^3$, because shifts across the charge-transfer gap Δ_{pd} are nowhere to be seen. As soon as the arcs appear, the *intercell* metallic states mediated by the bridging oxygens see a different regime, which is the principal interest of the present work. The physical scale of J is replaced by a renormalized repulsion, Eq. (1) of Ref. [4].

Band dispersions and spectral distributions obtained in ARPES can be understood in considerable detail, provided one accepts a significantly different parametrization than the one inferred from the above-mentioned local calculations [5]. In particular, the bare-band width $4|t_{pp}|$ of the oxygen band (t_{pp} is the O–O hopping) must exceed the observed copper–oxygen energy splitting Δ_{pd}, such that the effective copper level is found within the dispersive oxygen band. When hybridized with a relatively small effective Cu–O hopping t_{pd}, the open conduction band exhibits a strong "anticrossing" feature, where part of the Fermi surface around the vH points is weakly dispersive and copper-like, while the diagonal of the zone is strongly dispersive and oxygen-like. The small t_{pd} may well be the result of strong renormalizations, accompanying the large transfer of spectral weight to incoherent states. The effective parametrization is corroborated by the fact that LDA-derived dispersions lack 1-2 eV in the diagonal direction [6], precisely where the oxygen band is most dispersive. On the other hand, local calculations are corroborated in high-energy XPS experiments [7], so we presume that these reach an "undressing" scale, not probed by ARPES.

3. Raman and hall effect

The Raman response of the 2D copper–oxygen lattice encompasses several distinct symmetry modes. The A_{1g} mode couples to the long-wavelength variation of the total charge in the unit cell, while the B_{1g} mode is sensitive to the intracell oxygen–oxygen charge transfer. The latter breaks the X–Y symmetry and is dominant when the contribution of the vH singularities is important. The corresponding intracell micro-currents flow at low frequency back and forth along the two orthogonal t_{pd} bonds. The measured resonant B_{2g} Raman response is however of comparable intensity, which can only be reproduced by explicitly introducing the overlap t_{pp}. Nevertheless, a relative enhancement of the B_{1g} scattering was observed in overdoped lanthanates. This provides direct evidence of the importance of the O–O hopping in the cuprates [8].

A related, long-standing feature of interest has been the rapid rise of the effective Hall number n_H with doping [9,10]. A 10% change in the hole concentration, from 5% to 15%, results in a nearly 10-fold increase in n_H. This can be simply explained in the three-band model as approaching the vH singularity at incommensurate filling, where the Fermi surface changes topology from open (hole-like) to closed (particle-like). The Hall number is $n_H \sim n_{xx}n_{yy}/n_{xy}$, where the denominator is essentially a weighted curvature of the Fermi surface. At the vH filling, n_{xy} changes sign, meaning it is zero, so that n_H approaches a simple pole $\sim(\delta-\delta_{vH})^{-1}$ in the doping [8]. This is sufficient to account for the anomalous rise in n_H with doping, however the same fit again points to the absence of a large part of the spectral strength from the conductivity, because once the pole is fitted in the non-interacting three-band model, the n_H curve must be divided by a sizeable factor to conform with experiment.

It is common in the literature to fit ARPES and Hall effect data with a variant of the t–J model, with second- and third-neighbor hoppings t' and t'' added. An elementary trigonometric transformation shows [11] that the admixture of particle–hole (ph) symmetry breaking induced by t' is not of the order $|t'/t|$, but rather $|4t'/(t+2t')| \equiv \tau$, so that the values $-t'/t \sim 0.3$–0.4, imposed by realistic fits, give a range of 3–8 in the physically relevant ratio τ. In the cuprates, the oxygen levels are the physical reason for the ph symmetry breaking, so these values of t' indicate a breakdown of t–J physics, requiring one to take oxygens into account first, and coppers second, in conduction properties, as described in the next section. Once this is understood, one can interpret the t–t' dispersion as a simplified stand-in for the open band in the three-band model, which is convenient for modeling, and may serve as retroactive justification of the fits in the literature.

4. Theoretical background

A detailed microscopic understanding of the above phenomenological insights can be founded on two basic ideas. First, the copper on-site repulsion U_d is effectively infinite, and it is the only "bare" interaction kept in the Emery model. Second, metallicity is provided in zeroth order by the oxygen electrons, with excursions on the coppers as higher-order corrections. These ideas are embodied in a perturbation theory based on a slave-fermion decomposition of the d-electrons [4].

The vacuum is a translationally invariant Fermi sea of holes on oxygen sites. Correlations among them are due to intermittent visits to copper sites, where the Hubbard-U_d repulsion is replaced by the kinematic requirement that two holes cannot occupy the same copper site simultaneously, even if of opposite spins. While the theory is superficially similar to an expansion in the copper–oxygen overlap t_{pd}, the small parameter is in fact the copper occupation n_d^{HF} in the Cu–O Hartree–Fock state hybridized through the bare t_{pd}. Its renormalizations describe the actual physical situation near optimal doping, where the total $n_d \approx 0.5$, from the zeroth-order limit $n_d^{(0)} = 0$, while the "all coppers half-filled, doped holes on the oxygens" approach, typically implemented in the usual slave-boson setting, starts from $n_d^{(0)} = 1$. While the actual value of n_d appears to put both $n_d^{(0)}$ limits at equal distance from physical reality, each starting point emphasizes a different set of elementary propagators and correlators. In our approach, valence-bond fluctuations appear at lower order than spin (AF) correlations.

The first-order (triangular) vertices are counted by powers of the bare Cu–O hybridization $\alpha_k^{\pm} = |\sin k_x \pm \sin k_y|$ multiplied by the bare Cu–O overlap t_{pd}. The interesting objects appear in second and sixth order, as self-energy and vertex corrections of single-particle propagators, respectively. Significantly, the lower-order propagator renormalizations only indicate a local redistribution of strength away from the Fermi energy by incoherent valence-bond fluctuations, which in fact dominate the ARPES data, in spite of the attention usually focused on pseudo-coherence near the Fermi level. The AF correlations first appear through fourth-order square vertices, with internal slave-particle renormalizations. Both copper and oxygen can appear on the external lines of the squares. In this way a natural hierarchy is established, in which the dominant valence-bond fluctuations are local, while the secondary AF ones are extended. This justifies our previous inclusion of the AF correlations as dispersive bosons in an effective weak-coupling approach [5]; the principal correction required from the present point of view is a reduction of spectral weight at the Fermi energy, as already anticipated from the measurements.

5. Neutron scattering near Q_{AF} [12]

Neutron scattering near the AF momentum-transfer reveals the well-known "hourglass" shape of excitations in LBCO and