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A VALENCE-FLUCTUATION THEORY OF CUPRATE SUPERCONDUCTIVITY

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The concepts and formalism of valence-fluctuation theory are applied to an Anderson lattice model of the CuO_2 plane. Using a self-consistent variational treatment at the $(1/N)^1$ level, for a finite-U lattice, we find adequate pairing attraction for realistic Hamiltonian parameters. Several unconventional features of the cuprate phenomenology are explained, including the extremely short coherence length, large resistivity, and strong gap anisotropy.

Using valence-fluctuation concepts and formalism, we have developed a quantitative theory [1] of a specific pairing mechanism. This amounts to a highly refined version of the finite-U or "two-hole resonance" mechanism of Newns [2], although our formal treatment is quite different from his. We use a many-body variational formalism [3] in which all of the variational parameters are fully optimized. This provides a strong-coupling theory, valid in parameter regimes where perturbative expressions cannot be trusted. Our Anderson lattice model is based on the $2p\sigma$ - $3d(x^2-y^2)$ hybridization within a single CuO_2

plane. The Hamiltonian parameters are taken from an analysis [4] of photoemission and BIS data for CuO.

Application of this variational treatment at the mean-field or $(1/N)^0$ stage of approximation proved to be inadequate. There was a strong tendency towards magnetism, arising from a Gutzwiller form of hybridization renormalization. This and other evidence led us to extend our finite-U lattice treatment to formal order $(1/N)^1$. At this stage we encountered a new mechanism which is able, in an appropriate regime, to suppress the excess magnetic tendency and thereby now allow the Newns pairing tendency to dominate. This is also an advance in the state of the art for valence-fluctuation theory.

Our variational Ψ contains information equivalent to quasiparticle occupation numbers. We are therefore able to evaluate the Landau-Luttinger quasiparticle spectrum and the quasiparticle interaction by directly implementing the Landau recipes $E_{k\sigma} = \delta\langle H \rangle / \delta n_{qp}(k\sigma)$, $f(k\uparrow, k'\downarrow) = \delta^2\langle H \rangle / \delta n_{qp}(k\uparrow) \delta n_{qp}(k'\downarrow)$, for all k, k' in the Brillouin zone. This f is converted into a pairing interaction $V_{kk'}$ by analytic continuation in k and k' . The resulting $E_{k\sigma}$ and $V_{kk'}$ are then employed in the conventional BCS gap equation (without any k cutoff), to obtain the superconductivity.

Our quantitative study involved two stages. At first, we used an isotropic approximation for the in-plane band structure. Calculations at this stage were fully self-consistent (all parameters optimized). The second stage involved a more realistic (anisotropic) band structure, but was not fully self-consistent.

In the isotropic model, the pairing interaction is found numerically to be of the form $V_{kk'} \approx -a + bS_k S_{k'}$, where a and b are both positive and large (several eV), and $S_k = \sin(k\pi/2)$, for k in $(0,1)$. The strong k -dependence comes mainly from the k -dependence of the p - d hybridization. Due to the great strength of this interaction, it is very easy to obtain a T_C of several thousand Kelvin. A consequence is that when the charge-transfer energy Δ_{CT} is adjusted to bring T_C down to "only" around 100K, the pairing interaction at the Fermi surface $V(k_F, k_F)$ becomes strongly repulsive ($\sim +1$ eV). Some frustration

within the gap equation is evidently required in order to obtain such a "low" T_C . The quasiparticle interaction $f_{\uparrow\downarrow}$ at the Fermi surface is equal to this $V(k_F, k_F)$, so this $f_{\uparrow\downarrow}$ has the order of magnitude required to account for the large and linear resistivity, according to calculations of quasiparticle scattering [5]. This $f_{\uparrow\downarrow}$ is likewise a plausible source for other aspects of the marginal-Fermi-liquid phenomenology. (In the isotropic model, the forward-scattering sum rule constrains $f_{\uparrow\uparrow}$ to vanish at the Fermi surface.) It is also reassuring that the quasiparticle bandwidth is found to be about 1.5 eV. This is in good agreement with a value of 1.4 eV deduced from angle-resolved photoemission [6].

Given the present form of $V_{kk'}$, it follows that $\Delta_k \approx a' - b'S_k$, with a' and b' positive. Numerical solution of the gap equation confirms this. The general magnitude of Δ_k is very large (~ 0.1 eV), but there is also a node just above k_F . A consequence is that $\Delta(k_F)$ is positive but small, with the order of magnitude expected from the BCS theory. Because of the rough proportionality of $|\Delta_k|$ to $|E_k - \epsilon_F|$ over much of the Brillouin zone, the ratio function $\Delta_k/E_k^{\text{BCS}}$ is distributed fairly uniformly throughout the zone. The Fourier transform of this ratio function is the pair wavefunction, which is therefore short-ranged in r -space. This leads to an *extremely short* coherence length ξ_0 , around 5 lattice spacings (in-plane), in reasonable agreement with experiment. We consider the extremely short ξ to be a signature of the present mechanism, as well as the strongest evidence against a conventional phonon mechanism.

The isotropic gap equation gave $2\Delta_{k_F}(T=0)/k_B T_C = 1.6$, far below the BCS value of 3.5 and the cuprate experimental values of around 6. Also, our scaled $\Delta(T)$ curve ($\Delta = \Delta_{k_F}$) lies *below* the BCS form, whereas the experimental form is "more square" (flatter and then more abrupt) than BCS, and thus lies *above* this. Our results can be reconciled with experiment by assuming (a) the physical T_C is only around half of the value from the simple gap equation, due to the pair-breaking effect of the strong quasiparticle scattering, and (b) the apparent gap value Δ is enhanced by nearly a factor of two, due to strong gap anisotropy (see below).

We have explored anisotropy effects in a two-dimensional model, using a suitably warped (in-plane anisotropic) form for the band ϵ_k of 2p Bloch orbitals (the "conduction" band of valence-fluctuation theory). This warping is due to the combined effects of (a) p_x - p_y hybridization, and (b) $2p\sigma$ interaction with copper 4s and $3d(z^2-r^2/3)$ orbitals. The latter interactions greatly lower ϵ_k near the (1,0) point. One effect is to distort the Landau-Luttinger quasiparticle band spectrum, shifting the van Hove saddle point energy far below the middle of the band, and thus below the Fermi level. Another effect is to very strongly distort the gap (essentially, Δ_k evaluated around the Fermi surface). We find an s-like gap (full point-group symmetry of the crystal) which is nodeless, but which has a large maximum-to-minimum ratio $\Delta_{\max}/\Delta_{\min} \approx 4$. The gap maximum occurs at the Fermi surface point closest to $k = (1,0)$, i.e., near the Cu-O bond direction, in agreement with photoemission data [8]. Throughout a wide temperature interval ($T_c/4 \lesssim T < T_c$) this gap form should have consequences very similar to a d-wave gap. At the lowest temperatures ($T \lesssim T_c/4$), however, activated behavior is predicted. There is much experimental evidence for strong (d-like) gap anisotropy, and also some evidence for low-temperature activated behavior.

The tunnelling density of states for this gap form has been shown [8] to have a very prominent peak at the gap maximum, but only a weak feature (a mere shoulder) at the minimum. Typical experimental recipes for "the gap" should therefore be identifying $\Delta_{\max}$. (This considerably exceeds the average value, as needed above for the gap ratio.) It is significant that clear intra-gap features, consistent with $\Delta_{\max}/\Delta_{\min} \approx 4$, have been observed in SIN tunnelling in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ [9], and also in Tl-2212 and Tl-2223 [10].

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