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A VALENCE-FLUCTUATION MECHANISM WITH HIGHLY ANISOTROPIC S-WAVE PAIRING

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We have developed a fairly *ab initio* theory of cuprate superconductivity [1], based on the concept that the above- T_c state is a normal Fermi liquid with strong electronic correlations of the type found in valence-fluctuation (VF) and heavy-fermion materials. The ground-state-correlation aspect is found to provide a satisfactory source or mechanism for the pairing. In addition to the high T_c 's this explains many of the unusual features of cuprate superconductivity, as outlined below.

The many-body calculation proceeds by a variational approach, which is well suited for the strong-coupling aspect of this problem. Starting with the fiction of a normal ground state, our variational ground-state energy (fully optimized) is differentiated with respect to quasiparticle occupation numbers to generate the Landau quasiparticle energy spectrum $\epsilon_{k\sigma}$ and interaction $f(k\uparrow, k'\downarrow)$, for all k and k' in the Brillouin zone. The pair interaction $V_{kk'}$ is then obtained from this f by an analytic continuation. An Anderson-lattice form of model Hamiltonian is used (the usual three-band model, with a single $U = U_{dd}$), with input parameters taken from a careful reanalysis of the photoemission and inverse-photoemission data for CuO [2]. The claim of *ab initio* character for this theory is based on the use of a realistic model Hamiltonian, realistic input parameters, and a highly refined calculational technique. Our consistent $(1/N)^1$ level of approximation goes considerably beyond previous Anderson lattice treatments; this incorporates a new and previously unsuspected feature which arises specifically from the lattice aspect.

The various semi-quantitative results are quite encouraging: (a) We adjust one Hamiltonian parameter (the charge-transfer energy Δ_{CT}) to obtain a typical T_c ($\sim 100K$). The resulting Δ_{CT} is found to be reasonably close to the value deduced from photoemission data. (b) The quasiparticle ($pd\sigma$ antibonding) bandwidth (~ 1.6 eV) is close to a value (~ 1.4 eV) deduced from angle-resolved photoemission [3]. (c) The coherence length ξ is found to be extremely short, just a few lattice spacings, consistent with experiment. (d) The large $2\Delta/k_B T_c$ ratio (~ 6) emerges mainly as a consequence of strong gap anisotropy. [In a simpler in-plane-isotropic model, the large effect of a pair-breaking reduction of T_c is compensated by a very small value (1.75) for the "bare" gap ratio obtained from the simple gap equation.] (e) At the Fermi surface, the angle-averaged quasiparticle interaction $\langle f\uparrow\downarrow \rangle$ is found to be *large and repulsive*, $\approx +0.5$ eV. This *magnitude* is about the value required to account for the strong quasiparticle damping, and thus presumably also for the large normal-state resistivity, according to calculations of quasiparticle scattering [4]. (These calculations show that the linear behavior is due to the unusual band geometry, for ϵ_F close to the van Hove saddle point.) The *repulsive sign* leads to an expected Stoner enhancement factor of $\sim 2-3$, which is also consistent with available evidence.

Also significant are a number of results which are more qualitative in nature: (a) A clear proximity to a magnetic instability, at reduced hole-doping. (b) Evidence for a strong pair-breaking reduction of T_c , apparently due to quasiparticle damping from the above-mentioned quasiparticle scattering. (c) A highly anisotropic (although s-like) gap, which may or may not have nodes, perhaps depending on the material. (d) A simple argument for expecting a highly anomalous form of $H_{c2}(T)$, consistent with what has been observed [5]. (e) Qualitative explanations for major features of the T_c systematics (see below).

The net pair attraction is due to a very strong k dependence in the pair interaction $V_{kk'}$. For small k, k' (near the zone center Γ) this V is very attractive ($\sim$ several eV), while for large k, k' [near the zone corner (1,1)] this becomes very repulsive ($\sim$ several eV). The dominant effect is the strong attraction at small k 's. This leads to an s-like gap function, with the full point-group symmetry of the CuO₂ plane. The resulting gap function Δ_k is quite large (positive) at small k 's and also large (negative) at large k 's, with a single node line in between. (There is thus substantial pairing throughout the entire Brillouin zone.) The node line lies close to and mainly outside of the Fermi surface. Study of the gap anisotropy for a realistic band structure showed that the gap Δ (essentially, Δ_k on the Fermi surface) is largest in the direction of the Cu-O bonds, in agreement with experiment. Midway between the bond directions Δ is far smaller, and it may be either positive or negative. The negative case corresponds to intersection of the node line with the Fermi

surface, leading here to an 8-node gap form. The gap nodes in this case are expected to be closer to the (1,1) or 45° directions than to the (1,0) or bond directions.

There are several lines of evidence favoring this type of anisotropic-s gap (with or without nodes), as contrasted to the d-wave x^2-y^2 form: (a) Although gap nodes are confirmed in YBCO, there is evidence against such nodes in (Nd,Ce)CuO₄ [6]. This difference is reconciled most simply in the anisotropic-s scenario, which requires only a modest deformation of the node line. (b) Inner-gap features have been observed in tunnelling in at least five different cuprates. Some of the data even shows a non-monotonic or reentrant form [7], consistent with the 8-node gap form [8]. (c) Recently, more direct evidence for the 8-node form has been obtained from angle-resolved photoemission for Bi-2212 [9], and from thin-film tunnelling for YBCO [10].

Major aspects of the T_c systematics are rationalized, such as the strong dependence on the hole-doping "x". T_c is driven down on the low-doping side by the x dependence found in the numerical results [1], and on the high-doping side by local Madelung-potential changes induced by the doping. It is particularly noteworthy that this theory provides a qualitative explanation for the empirical dependence of T_c on the Madelung potential of the apical oxygens -- a correlation which is very strong [11] and which was quite unexpected. [The apical oxygen $2p_z$ orbitals interact strongly with the copper 4s orbitals, which in turn interact strongly with the planar oxygen Bloch orbitals near the (1,0) point, so that a Madelung effect on the $2p_z$ energy level is reflected in a shift of the charge-transfer energy difference, $\Delta_{CT} = \epsilon(3d) - \langle \epsilon_K(2p\sigma) \rangle$.] A corollary of this is that T_c also depends strongly on the number of apical oxygens per planar Cu ion; a reduction or elimination of apicals is generally quite beneficial, as can be seen in the data. We also argue that the apparent evidence for strong dependence of T_c on inter-plane coupling is an illusion, and is mainly a reflection of the effects just mentioned.

There is a considerable variety of evidence suggesting that the present mechanism is operating also in a number of other families of superconductors, especially the "exotic" superconductors of Uemura [12] and the "bad actors" of Anderson and Yu [13]. (The borocarbides also fit this general pattern, e.g. [14].) This evidence includes anomalously short coherence length, anomalously high resistivity, a highly anomalous form of $H_{c2}(T)$, and a number of features which we argue should help to justify an Anderson-lattice form of model Hamiltonian. These latter features include large U 's, "conduction" (non-d-like) bands, reduced dimensionality and/or clustering, ligand ions with electronegativity considerably different from the "localized" (d-like) ions or clusters, and large penetration depths (small carrier density and large effective mass).

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