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SUPERCONDUCTIVITY FROM VALENCE FLUCTUATIONS WITH FINITE U

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The finite- U pairing mechanism of Newns is found to be opposed by a magnetic tendency arising from Gutzwiller renormalization of the hybridization. This competition restricts superconductivity to the parameter regime $\Delta \gtrsim U$, and this also reproduces the parabolic rise and fall of T_c in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ with increasing x . Re-analysis of the photoemission data for CuO reveals that indeed $\Delta \gtrsim U$ for this compound, contrary to previous work.

Most of this study has been reported elsewhere in more detail.¹ We shall outline the main features, and then describe the main result of a new analysis of photoemission data for CuO. Contrary to previous analyses, this indicates that cuprate materials have parameters favorable for the present theory.

The conceptual picture of valence fluctuations or "heavy fermions" has *a priori* appeal, for a non-phononic theory of superconductivity, for two reasons. First, a variety of evidence suggests that oxygen 2p orbitals are somehow playing an important role, in addition to the copper 3d orbitals. This leads to a model Hamiltonian of the Anderson lattice form, which is the standard starting point for valence fluctuation (VF) theory. The other reason is that the VF picture immediately provides a normal Fermi liquid, with Landau quasiparticle states.² This permits much of the DCS theory to be taken over directly, and it may also serve to explain the normal state transport properties.³ This picture also provides some "heaviness" or enhancement of state density at ϵ_F , which seems to be required for a Fermi-liquid explanation of the magnetic susceptibility above T_c .

In the presumed VF phase of the superconducting cuprates above T_c , the 2p electrons provide Kondo screening of the copper local moments, thereby enabling the existence of a normal (nonmagnetic) Fermi liquid. This role of the 2p electrons is so different from that assumed in the Mott insulating "parent" compound,

and in the associated lightly-doped materials, that we expect these contrasting phases to be separated by a first order transition. This transition is presumably masked by sample inhomogeneities, leading to a range of doping with both phases present.

Pairing mechanisms within the framework of VF theory have been recognized from some time at the $(1/N)^1$ and $(1/N)^2$ orders of the $1/N$ expansion (which generally presumes that $U = \infty$); these mechanisms lead to p or d-wave pairing. We are focusing instead on the "two-hole resonance" mechanism of Newns,⁴ which arises already at the $(1/N)^0$ or "mean field" stage of approximation, and which gives s-wave pairing. This mechanism requires that U be finite ($U < \infty$), and we note that it has a simple diagrammatic interpretation.¹

Our method of analysis differs from that of Newns. We have extended our previous variational treatment² to the case of finite U . By analytic and numerical methods all of our variational parameters are fully optimized, i.e., they are fully self consistent. Our calculations therefore do not require any of the Hamiltonian parameters, or combinations of parameters, to be small; the calculations remain sensible throughout all of the Hamiltonian parameter space.

Our theory also differs physically in one major respect from that of Newns.⁴ At the "mean field" or $(1/N)^0$ level of approximation, it is well known that the Landau quasiparticles are described by a simple effective

hybridization model,² in which the 2p-3d hybridization interaction V_k is renormalized into $\tilde{V}_k = V_k \sqrt{q}$. News and co-workers have used the so-called mean field recipe, $q_{mf} = 1/n_f$, where n_f refers to the f-electron occupation number for a VF cerium compound. (For a cuprate, this n_f becomes the 3d hole number per Cu ion.) However, we have recently become convinced that the Gutzwiller form, $q_G = (1-n_f)/(1-n_f\sigma)$, is more correct. (This conclusion is based on a variety of evidence³: exactly-solvable test cases, combinatoric analysis, diagrammatic analysis, and the requirement of correct behavior as $U \rightarrow 0$.) We therefore use the Gutzwiller form, suitably generalized for the finite- U case.⁴

This difference in the renormalization has major consequences. The explicit spin dependence of the Gutzwiller q causes a strong tendency towards magnetism, and this effect opposes the News pairing mechanism. One result is that we do not find superconductivity unless Δ ($\equiv E(d^{10}\underline{L}) - E(d^9)$), the charge-transfer energy parameter of Sawatzky,⁶ is made considerably larger than the numerical values typically obtained from analyses of photoemission data.^{7,8} Instead of $\Delta \ll U$, as typically found, this theory requires that $\Delta \gtrsim U$, or in other words that $E(d^8) \sim E(d^9\underline{L}) \ll E(d^{10}\underline{L}^2)$. We recognize, of course, that this configuration-energy ordering may be considered heresy. Nevertheless, there is a further reward for this assumption. When we increase the doping level x of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, we find that T_c first increases, and then decreases and terminates, qualitatively following an inverted parabola, in qualitative agreement with the data of Torrance *et al.*⁹ This behavior results here from the competition between the pairing and magnetic tendencies. We consider this a significant success for the present theory.

Motivated by the foregoing, and by other arguments in Ref. 1, we have now carefully re-analyzed the CuO photoemission data of Sawatzky and co-workers.⁸ We have basically followed their method of analysis, but with several differences of detail. In particular, we have carefully calculated the intensity distribution for oxygen 2p electron removal, in addition to the 3d removal spec-

trum. This additional information demonstrates quite clearly that indeed $\Delta \gtrsim U$, as anticipated in Ref. 1. Besides supporting the present theory, this result has a number of implications which we shall discuss elsewhere, together with the details of this analysis. One of these implications is to refute the common assertion that the holes resulting from doping are accommodated almost entirely in oxygen 2p orbitals. We find¹ that these doping holes are shared between the 2p and 3d orbitals with quite similar probabilities.

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