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Metal–insulator transition and superconductivity in a $U_d = \infty$ extended Hubbard model

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Abstract. A $U_d = \infty$ extended Hubbard Hamiltonian (EHH) with a qualitatively accurate band structure, appropriate for a cubic lattice, is investigated. At half filling the system undergoes a metal–insulator transition at a critical value of the charge transfer gap. Doping beyond half filling produces rapid metallisation of the insulating state. For all dopings considered, the effective quasiparticle–quasiparticle interaction is only attractive in the d channel with $\sin k_x \sin k_y$ symmetry. The effective interaction in all symmetry channels is suppressed on doping.

1. Introduction

The development of a satisfactory many-body theoretical description of the properties of the high-T_c superconducting oxides still poses a serious theoretical challenge. Some features in common to all the cupric oxides are their quasi-two-dimensional structure, a strong on-site Cu repulsion U_d and copper orbitals strongly hybridised with their nearest-neighbour oxygen orbitals [1–3]. Direct O–O hopping which is also present is thought to be significantly weaker than the Cu–O hopping [4]. The set of O $2p_x$, O $2p_y$ and Cu $3d_{x^2-y^2}$ would seem therefore to represent a minimal but qualitatively sufficient manifold for a description of the electronic properties near the Fermi surface [1, 2]. Given the strong Cu–O mixing this leads to either a two- or three-band model effective Hamiltonian, depending on how direct O–O overlap is incorporated. At this point a reduction of these models to an effective one-band description remains controversial and this motivates further study of the properties of a multi-band model with a qualitatively realistic electronic structure.

We take as a starting point an extended Hubbard Hamiltonian (EHH), which can, in principle, accommodate all electronic effects. However, as the Coulomb repulsion on the Cu sites, U_d, is clearly the largest energy in the problem [4], we follow a procedure commonly used in treating the heavy fermion systems, and set U_d equal to infinity. The on-site repulsion on the O orbitals, which is unimportant in the doping regime we consider, and intersite Coulomb interactions, will be neglected in what follows. In the hole representation the $U_d = \infty$ EHH which we take to describe the Cu–O sheet is given by

$$H = \sum_{j,\sigma} E_d D^+_{j\sigma} D_{j\sigma} + \sum_{i,\sigma} E_p p^+_{i\sigma} p_{i\sigma} + \sum_{k,\sigma} 2V\gamma_k \left(D^+_{k\sigma} p_{k\sigma} + \text{HC}\right) \tag{1}$$

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when the additional operator constraint

$$\sum_{\sigma} D_{j\sigma}^{+} D_{j\sigma} \leq 1 \tag{2}$$

is imposed at all copper sites at all times. Here $D_{j\sigma}^{+}$ creates a hole on a Cu $3d_{x^2-y^2}$ orbital, while $p_{i\sigma}^{+}$ creates a hole in an O $2p_x$ or O $2p_y$ orbital. E_d and E_p are the site energies of the $3d_{x^2-y^2}$ orbital and the degenerate O $2p_x$ and O $2p_y$ orbitals respectively. V is the Cu–O hopping matrix element and $\gamma_k = [\sin^2(k_x/2) + \sin^2(k_y/2)]^{1/2}$ when lengths are measured in units of the Cu–Cu bond length. This model has been studied previously [5] and analytic results obtained in a regime of parameters such that V is much less than the charge transfer gap $2\Delta \equiv E_p - E_d$. In particular it was shown that at zero doping and for large enough Δ the model exhibits a metal–insulator transition from a heavy Fermi liquid to a charge transfer insulator. It is generally appreciated now that the type of superconducting instability allowed in the generic Hubbard models depends on both the band structure and filling factor. It is known that the $U_d = \infty$ Anderson lattice Hamiltonian with isotropic conduction band dispersion admits gauge boson mediated d-wave superconductivity to leading order in the residual interaction between the quasi-particles [6–8]. On the other hand in the one-band Hubbard model, onto which the two-band ALH can be mapped if $V \ll 2\Delta$ [9], it was shown within an RPA calculation [10] that Fermi surface nesting in a cubic lattice could drive either a d wave or extended s-wave pairing instability; but that at low carrier density p-state superconductivity was favoured. Similar conclusions were reached in a study of the one-band Hubbard model in the large-U limit [11]. However, the high-T_c oxides lie in a region of parameter space where $V \simeq \Delta$. It is the purpose of this work therefore to consider the EHH with a tight-binding parametrisation of the band structure, that allows for Fermi surface nesting, for arbitrary values of V and Δ. Given V and Δ inferred from experiment [4], this enables us to determine how close a given system is to the metal–insulator transition and to see how doping affects this transition. We also investigate the effect of varying Δ and doping on superconductivity within the model.

2. The metal–insulator transition

The constraint (2) is implemented by a slave boson method [12–14]. On writing $D_{j\sigma}^{+} = d_{j\sigma}^{+} b_j$, here $d_{j\sigma}^{+}$ is a fermion field creating the $3d^9$ state and b_j^{+} is a boson field creating the $3d^{10}$ state, (2) is transformed into a holonomic constraint

$$Q_j = b_j^{+} b_j + \sum_{\sigma} d_{j\sigma}^{+} d_{j\sigma} = 1 \tag{3}$$

which is then enforced by coupling it to the Hamiltonian with a Lagrange multiplier λ_j,

$$H \rightarrow H + \mathrm{i} \sum_{j} \lambda_j (Q_j - q_0 N). \tag{4}$$

To generate a consistent $1/N$ expansion, where N is the degeneracy of the d^9 level, q_0 is regarded formally as O(1). For our purposes it is most convenient to use a set of boson

coordinates in which the boson propagators are infrared finite. In this radial gauge [8] the Lagrange multiplier λ_j is promoted to a gauge field by absorbing the derivative, with respect to imaginary time, of the phase of the boson field $b_j = r_j \exp(i\theta_j)$. The grand canonical partition function can then be written as

$$Z = \int \mathrm{D}p^+ \,\mathrm{D}p \,\mathrm{D}d^+ \,\mathrm{D}d \,\mathrm{D}r \,\mathrm{D}\lambda \exp\left(-\int_0^\beta \mathrm{d}\tau \,\mathscr{L}(\tau)\right) \tag{5}$$

where

$$\mathscr{L}(\tau) = \sum_{i,\sigma} p_{i\sigma}^+ \left(\frac{\partial}{\partial\tau} + E_\mathrm{p} - \mu\right) p_{i\sigma} + \sum_{j,\sigma} d_{j\sigma}^+ \left(\frac{\partial}{\partial\tau} + E_\mathrm{d} - \mu\right) d_{j\sigma} + \sum_j r_j \frac{\partial}{\partial\tau} r_j$$
$$+ \sum_{k,q,\sigma} 2V\gamma_k \left(p_{k,\sigma} r_q d_{k+q,\sigma}^+ + \mathrm{HC}\right) + \mathrm{i}\sum_{j,\sigma} \lambda_j \left(r_j^2 + \sum_\sigma d_{j,\sigma}^+ d_{j\sigma} - q_0 N\right). \tag{6}$$

The stationary phase approximation to (5) is obtained on replacing the boson fields by c numbers:

$$Z_\mathrm{MF} = \int \mathrm{D}d^+ \,\mathrm{D}d \,\mathrm{D}p^+ \,\mathrm{D}p \exp\left(-\int_0^\beta \mathrm{d}\tau \,\mathscr{L}_\mathrm{MF}(\tau)\right) \tag{7}$$

where

$$\mathscr{L}_\mathrm{MF} = \sum_{i,\sigma} p_{i\sigma}^+ \left(\frac{\partial}{\partial\tau} + E_\mathrm{p} - \mu\right) p_{i\sigma} + \sum_{j,\sigma} d_{j\sigma}^+ \left(\frac{\partial}{\partial\tau} + \varepsilon_\mathrm{d} - \mu\right) d_{j\sigma}$$
$$+ \sum_{k,\sigma} 2s_0\gamma_k \left(p_{k\sigma} d_{k\sigma}^+ + \mathrm{HC}\right) + N_\mathrm{s}(\varepsilon_\mathrm{d} - E_\mathrm{d})\left(\frac{s_0^2}{V^2} - q_0 N\right). \tag{8}$$

$\varepsilon_\mathrm{d} \equiv E_\mathrm{d} + \mathrm{i}\langle\lambda_j\rangle$ is the renormalised d-level energy, $s_0 = V\langle r_j\rangle$, the renormalised hopping matrix element and N_s the number of unit cells. Varying the resultant effective action with respect to ε_d, s_0 and μ leads to the equations

$$-\mathrm{i}\langle\lambda_j\rangle = E_\mathrm{d} - \varepsilon_\mathrm{d} = -\frac{NV^2}{N_\mathrm{s}} \sum_k \frac{4\gamma_k^2}{E_k} f(E_k^{(-)}) \tag{9}$$

and

$$1 - \frac{s_0^2}{V^2} = \frac{N}{N_\mathrm{s}} \sum_k u_k^{(-)^2} f(E_k^{(-)}) \tag{10}$$

which determine ε_d and s_0, together with an equation

$$Nq_0(1 + x_h) = \frac{N}{N_\mathrm{s}} \sum_k f(E_k^{(-)}) \tag{11}$$

which positions the Fermi surface as demanded by Luttinger's theorem. In these expressions the function f is the Fermi distribution function, $E_k^{(\pm)} = \left((\varepsilon_\mathrm{p} + \varepsilon_\mathrm{d}) \pm E_k\right)/2$ the energies of the upper and lower hybridised bands respectively, with

$$E_k^2 = (\varepsilon_\mathrm{p} - \varepsilon_\mathrm{d})^2 + 16 s_0^2 \gamma_k^2.$$

The coherence factors $u_k^{(-)^2}$ ($v_k^{(-)^2}$) which determine the d (p) weight in the lower band are given by

$$u_k^{(-)^2} = 1 - v_k^{(-)^2} = \frac{4s_0^2\gamma_k^2}{(E_k^{(-)} - \varepsilon_d)^2 + 4s_0^2\gamma_k^2}$$

and x_h is the fraction of holes added on doping.

The set of equations [9–11] was solved numerically. Fixing V at 1.4 eV [4] the solutions were studied as a function of Δ and x_h. Of particular interest in this model is the quantity $|\langle b_j \rangle|^2 = \langle r_j \rangle^2 = m/m^*$ [15], the inverse of the quasiparticle mass enhancement, the magnitude of which determines the degree of itinerancy of the quasiparticles. When $\Delta \lesssim 3$ eV, the normal state is described by a Fermi liquid for all $x_h \geq 0$. However, as the charge transfer gap is increased further, $\langle r_j \rangle^2$ is renormalised downwards, and at finite doping there is a gradual change from a Fermi liquid with moderate mass enhancement to a heavy Fermi liquid in which charge fluctuations on the Cu sites are suppressed; see figure 1. At half filling $\langle r_j \rangle^2$ drops rapidly and vanishes for all $\Delta \geq \Delta_c = 3.25$ eV (figure 1), which signals a transition from a metallic to an insulating state—in this case a charge transfer insulator. The values of Δ at which this transition occurs is sensitive to V which is not known with precision, for example for $V = 1$ eV the critical value of Δ is 2.5 eV. We note from figure 1 that $\langle r_j \rangle^2$ is essentially doping independent for $\Delta \lesssim 3$ eV whereas doping produces a rapid metallisation† of the insulating state close to the transition point, as can be seen in both figures 1 and 2. These results are qualitatively the same as those obtained recently by Balseiro *et al* [16] who analysed a more complex finite-U_d EHH which also included an on-site Coulomb interaction on the oxygen sites as well as nearest-neighbour copper–oxygen repulsion.

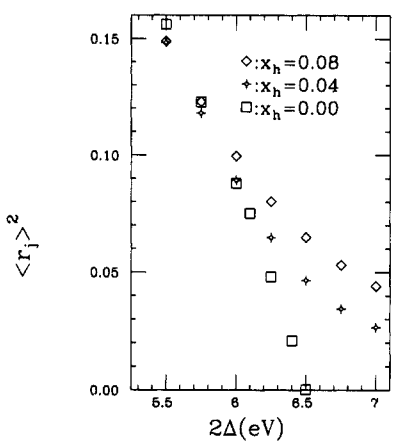

Figure 1. $\langle r_j \rangle^2 = m/m^*$ as function of charge transfer gap for various dopings.

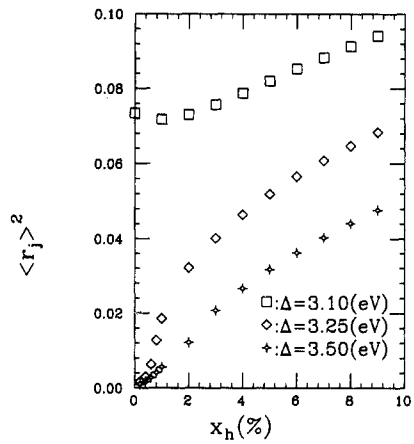

Figure 2. $\langle r_j \rangle^2 = m/m^*$ as function of doping for various values of the charge transfer gap Δ. Note in both figures 1 and 2 that $\langle r_j \rangle^2$ is essentially doping independent for $\Delta \lesssim 3$ eV, whereas doping produces rapid metallisation in the insulating state, in particular close to the transition.

† After this work was complete we received a preprint from C A R Sa de Melo and S Doniach (Stanford University) who have derived similar results within an isotropic model.

3. Superconducting instabilities

We now turn to consider the superconducting instabilities of the model, and study the behaviour of the coupling constants in various symmetry channels, both as a function of doping x_h and charge transfer gap Δ. To this end it will be necessary to include the fluctuations of the boson fields. We will limit the scope of the calculation to an effective free-boson theory giving $1/N$ corrections to the thermodynamics and the leading $(1/N)$ contribution to the quasiparticle–quasiparticle interaction.

The Lagrangian is given by

$$\mathscr{L} = \mathscr{L}_{\mathrm{MF}} + \mathscr{L}_{\mathrm{Gauss}} \tag{13}$$

where $\mathscr{L}_{\mathrm{MF}}$ is given by (8) and

$$\mathscr{L}_{\mathrm{Gauss}} = \frac{1}{2\beta} \sum_{q,\omega_\nu} \boldsymbol{\phi}^{\mathrm{T}}(-\boldsymbol{q}, -\mathrm{i}\omega_\nu) \mathbf{D}^{-1}(\boldsymbol{q}, \mathrm{i}\omega_\nu) \boldsymbol{\phi}(\boldsymbol{q}, \mathrm{i}\omega_\nu) \tag{14}$$

where

$$\boldsymbol{\phi}(\boldsymbol{q}, \mathrm{i}\omega_\nu) = \begin{pmatrix} r(\boldsymbol{q}, \mathrm{i}\omega_\nu) \\ \lambda(\boldsymbol{q}, \mathrm{i}\omega_\nu) \end{pmatrix} \tag{15}$$

and

$$\mathbf{D}^{-1}(\boldsymbol{q}, \mathrm{i}\omega_\nu) = \mathbf{D}_0^{-1} - \boldsymbol{\Pi}(\boldsymbol{q}, \mathrm{i}\omega_\nu). \tag{16}$$

The inverse bare boson propagator is given by

$$\mathbf{D}_0^{-1} = \frac{1}{V^2} \begin{pmatrix} 2(\varepsilon_{\mathrm{d}} - E_{\mathrm{d}}) & 2\mathrm{i}s_0 \\ 2\mathrm{i}s_0 & 0 \end{pmatrix}. \tag{17}$$

The elements of the self-energy matrix:

$$\Pi_{rr}(\boldsymbol{q}, \mathrm{i}\omega_\nu) = 8N \sum_{\boldsymbol{k}} \left[\tfrac{1}{2} \left(\gamma(\boldsymbol{k}+\boldsymbol{q}) v_{\boldsymbol{k}+\boldsymbol{q}}^{(-)} u_{\boldsymbol{k}}^{(-)} + \gamma(\boldsymbol{k}) u_{\boldsymbol{k}+\boldsymbol{q}}^{(-)} v_{\boldsymbol{k}}^{(-)} \right)^2 R_{11}(\boldsymbol{k}, \boldsymbol{q}, \mathrm{i}\omega_\nu) \right.$$
$$\left. + \left(\gamma(\boldsymbol{k}+\boldsymbol{q}) v_{\boldsymbol{k}}^{(-)} v_{\boldsymbol{k}+\boldsymbol{q}}^{(-)} - \gamma(\boldsymbol{k}) u_{\boldsymbol{k}}^{(-)} u_{\boldsymbol{k}+\boldsymbol{q}}^{(-)} \right)^2 R_{12}(\boldsymbol{k}, \boldsymbol{q}, \mathrm{i}\omega_\nu) \right] \tag{18a}$$

$$\Pi_{r\lambda}(\boldsymbol{q}, \mathrm{i}\omega_\nu) = \Pi_{\lambda r}(\boldsymbol{q}, \mathrm{i}\omega_\nu) = -8 s_0 \mathrm{i} N \sum_{\boldsymbol{k}} \left[\frac{\gamma^2(\boldsymbol{k}+\boldsymbol{q})}{E_{\boldsymbol{k}+\boldsymbol{q}}} u_{\boldsymbol{k}}^{(-)^2} R_{11}(\boldsymbol{k}, \boldsymbol{q}, \mathrm{i}\omega_\nu) \right.$$
$$\left. + \left(\frac{\gamma^2(\boldsymbol{k}+\boldsymbol{q})}{E_{\boldsymbol{k}+\boldsymbol{q}}} v_{\boldsymbol{k}}^{(-)^2} - \frac{\gamma^2(\boldsymbol{k})}{E_{\boldsymbol{k}}} u_{\boldsymbol{k}+\boldsymbol{q}}^{(-)^2} \right) R_{12}(\boldsymbol{k}, \boldsymbol{q}, \mathrm{i}\omega_\nu) \right] \tag{18b}$$

and

$$\Pi_{\lambda\lambda} = -N \sum_{\boldsymbol{k}} \left[u_{\boldsymbol{k}+\boldsymbol{q}}^{(-)^2} u_{\boldsymbol{k}}^{(-)^2} R_{11}(\boldsymbol{k}, \boldsymbol{q}, \mathrm{i}\omega_\nu) + 2 u_{\boldsymbol{k}+\boldsymbol{q}}^{(-)^2} v_{\boldsymbol{k}}^{(-)^2} R_{12}(\boldsymbol{k}, \boldsymbol{q}, \mathrm{i}\omega_\nu) \right] \tag{18c}$$

contain both intraband and interband contributions, where

$$R_{11}(\boldsymbol{k}, \boldsymbol{q}, \mathrm{i}\omega_\nu) = -\frac{f(E_{\boldsymbol{k}+\boldsymbol{q}}^{(-)}) - f(E_{\boldsymbol{k}}^{(-)})}{E_{\boldsymbol{k}+\boldsymbol{q}}^{(-)} - E_{\boldsymbol{k}}^{(-)} - \mathrm{i}\omega_\nu} \tag{19}$$

and

$$R_{12}(\boldsymbol{k},\boldsymbol{q},\mathrm{i}\omega_\nu) = -\tfrac{1}{2}\left(f(E^{(-)}_{k+q}) - f(E^{(+)}_{k})\right)\left(\frac{1}{E^{(-)}_{k+q} - E^{(+)}_{k} - \mathrm{i}\omega_\nu} + \frac{1}{E^{(-)}_{k+q} - E^{(+)}_{k} + \mathrm{i}\omega_\nu}\right) \tag{20}$$

ω_ν is a boson Matsubara frequency.

Retardation plays an important role in the pairing interaction and, as in the Eliashberg theory for the electron–phonon interaction [17], Fermi surface averaged spectral weights of the two-particle irreducible vertex $\Gamma(\boldsymbol{q},\omega)$ can be introduced:

$$F^i(\omega) \equiv \langle (1/\pi)\ \mathrm{Im}\,\Gamma(\boldsymbol{q},\omega)\rangle^i_{\mathrm{FS}}. \tag{21}$$

The average $\langle\ \rangle^i_{\mathrm{FS}}$ is defined by

$$\langle A\rangle^i_{\mathrm{FS}} = \frac{(1/(2\pi)^d)\int(\mathrm{d}S/|\boldsymbol{v}_k|)\int(\mathrm{d}S/|\boldsymbol{v}_{k'}|)g_i(\boldsymbol{k})A(\boldsymbol{k},\boldsymbol{k}')g_i(\boldsymbol{k}')}{\int(\mathrm{d}S/|\boldsymbol{v}_k|)g_i^2(\boldsymbol{k})} \tag{22}$$

where $\int \mathrm{d}S$ is an integration over the Fermi surface, $(1/(2\pi)^d)|\boldsymbol{v}_k|^{-1}$ the density of states and g_i a Fermi surface harmonic, see for example [18], as we model Cu–O sheets, cubic harmonics are used. The superconducting transition temperature can be determined from these spectral weights. Here, however, we only consider the one moment of $F^i(\omega)$

$$\lambda_i = 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}F^i(\omega) = \langle \mathrm{Re}\ \Gamma(\boldsymbol{q},0)\rangle^i_{\mathrm{FS}} \equiv \alpha_i/N \tag{23}$$

which measures the strength of the pairing interaction in a given channel; hence only the zero-frequency limit of the irreducible vertex is needed. We use a convention such that a negative α_i corresponds to an attractive interaction.

At leading order in $(1/N)$ the effective interaction between quasiparticles is mediated by the exchange of a single boson and $\Gamma(\boldsymbol{q},\omega=0)\equiv\Gamma(\boldsymbol{q})$ is given by

$$\begin{aligned}\Gamma(\boldsymbol{q}) = -4\big[&\gamma(\boldsymbol{k}_1)v^{(-)}_{k_1}v^{(-)}_{k_1+q} + \gamma(\boldsymbol{k}_1+\boldsymbol{q})v^{(-)}_{k_1+q}u^{(-)}_{k_1}\big]\big[\gamma(\boldsymbol{k}_2)v^{(-)}_{k_2}u^{(-)}_{k_2-q} + \gamma(\boldsymbol{k}_2-\boldsymbol{q})v^{(-)}_{k_2-q}u_{k_2}\big]D_{rr}(\boldsymbol{q})\\
&+ u^{(-)}_{k_1}u^{(-)}_{k_1+q}u^{(-)}_{k_2}u^{(-)}_{k_2-q}D_{\lambda\lambda}(\boldsymbol{q}) - 2\mathrm{i}u^{(-)}_{k_1}u^{(-)}_{k_1+q}\\
&\times\big[\gamma(\boldsymbol{k}_2)v^{(-)}_{k_2}u^{(-)}_{k_2-q} + \gamma(\boldsymbol{k}_2-\boldsymbol{q})u^{(-)}_{k_2}v^{(-)}_{k_2-q}\big]D_{r\lambda}(\boldsymbol{q})\\
&- 2\mathrm{i}u^{(-)}_{k_2}u^{(-)}_{k_2-q}\big[\gamma(\boldsymbol{k}_1)v^{(-)}_{k_1}u^{(-)}_{k_1+q} + \gamma(\boldsymbol{k}_1+\boldsymbol{q})u^{(-)}_{k_1}v^{(-)}_{k_1+q}\big]D_{\lambda r}(\boldsymbol{q}).\end{aligned} \tag{24}$$

Here the incoming momenta $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ (set equal to $\boldsymbol{k}$ and $-\boldsymbol{k}$) and the outgoing momenta $\boldsymbol{k}_1+\boldsymbol{q}$ and $\boldsymbol{k}_2-\boldsymbol{q}$ are all taken to lie on the Fermi surface, the momentum transfer $\boldsymbol{q}$ is carried by the bosons $D_{rr}(\boldsymbol{q}) = D^{(-)}_{\lambda\lambda}/\det\mathbf{D}^{-1}$, $D_{\lambda\lambda} = D^{-1}_{rr}/\det\mathbf{D}^{-1}$ and $D_{r\lambda} = D_{\lambda r} = -D^{-1}_{r\lambda}/\det\mathbf{D}^{-1}$.

We have determined the α_i by computing $\Gamma(\boldsymbol{q})$ numerically and considered its projection into different symmetry channels, for scattering on the Fermi surface. The results are shown in figures 3–6. For all dopings considered and over a wide range of values of the charge transfer gap the d channel $g_{xy} = \sin k_x \sin k_y$ was found to be attractive, as previously conjectured by Kotliar *et al* [5]. Whereas the effective interactions in the d channel $g_{x^2-y^2} = \cos k_x - \cos k_y$, the p channels $g_x = \sin k_x$ and $g_y = \sin k_y$ and the extended s wave $g_{x^2+y^2} = \cos k_x + \cos k_y$ are repulsive for all values

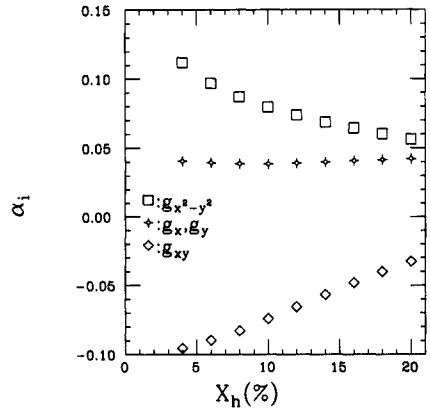

Figure 3. α_i, as defined in text, for various symmetry channels as a function of doping with $\Delta = 2$ eV. The variation with doping is dominated by the doping dependence of the quasiparticle density of states, at the Fermi level, which has a logarithmic singularity at half filling.

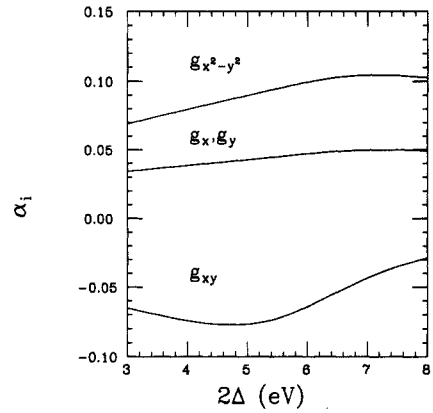

Figure 4. α_i as defined in text as a function of charge transfer gap for various symmetry channels, for $x_h = 0.10$.

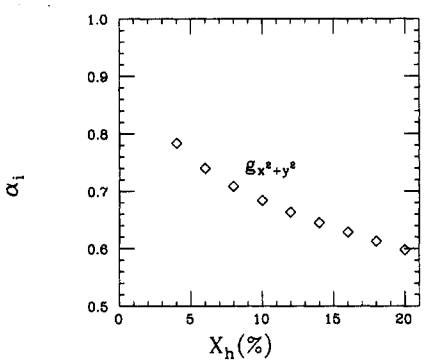

Figure 5. α_i for the extended s-wave channel as a function of doping with $\Delta = 2$ eV.

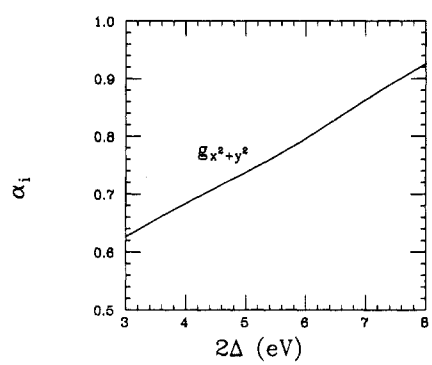

Figure 6. α_i for the extended s-wave channel as a function of charge transfer gap, for $x_h = 0.10$.

of the charge transfer gap considered. When the interband terms proportional to R_{12} (20) are neglected, only minor quantitative changes result, demonstrating that at least as far as superconducting instabilities are concerned an effective one-band model describes the physics.

It should be noted that $g_{x^2+y^2} = \cos k_x + \cos k_y$ is a constant on the Fermi surface for the band structure considered here and therefore within this model there is no distinction between isotropic and anisotropic s-wave superconductivity and the $g_{x^2+y^2}$ channel must be repulsive. Inclusion of direct O–O hopping, which destroys the perfect nesting of the Fermi surface, will not change this result. Similar considerations dictate that the effective interaction within the one-band Hubbard model studied in [10] must be repulsive in the extended s-wave channel.

The variation of α_i with x_h is in fact dominated by the doping dependence of the density of states at the Fermi surface which has a logarithmic singularity at half filling. As a result (see figures 3 and 5), the effective interaction in both repulsive and

attractive channels is suppressed with increasing doping. The system evolves smoothly from strong to weak coupling as the filling is increased.

Acknowledgments

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References

[1] Mattheiss L F 1987 *Phys. Rev. Lett.* **58** 1028
[2] Yu J, Freeman A J and Xu J H 1987 *Phys. Rev. Lett.* **58** 1035
[3] Pickett W E, Krakauer H, Papaconstantopoulos D A and Boyer L L 1987 *Phys. Rev.* B **35** 7252
[4] Mila F 1988 *Phys. Rev.* B **38** 11358
[5] Kotliar G, Lee P A and Read N 1988 *Physica* B + C **153–542** 538
[6] Auerbach A and Levin K 1986 *Phys. Rev. Lett.* **57** 877
[7] Lavagna M, Millis A J and Lee P A 1987 *Phys. Rev. Lett.* **58** 266
[8] Houghton A, Read N and Won H 1988 *Phys. Rev.* B **37** 3782
[9] Zhang F C and Rice T M 1988 *Phys. Rev.* B **37** 3759
[10] Scalapino D J, Loh E and Hirsch J E 1986 *Phys. Rev.* B **34** 8190
[11] Kotliar G and Liu J 1988 *Phys. Rev. Lett.* **61** 1784
[12] Barnes S E 1976 *J. Phys. F: Met. Phys.* **6** 1375
[13] Read N and Newns D 1983 *J. Phys. C: Solid State Phys.* **16** 3273
[14] Coleman P 1984 *Phys. Rev.* B **29** 3035
[15] Vollhardt D, Wölfle P and Anderson P W 1987 *Phys. Rev.* B **35** 6703
[16] Balseiro C A, Avignon M, Rojo A G and Alascio B 1989 *Phys. Rev. Lett.* **62** 2624
[17] Eliashberg G M 1960 *Zh. Eksp. Teor. Fiz.* **38** 966 (Engl. Transl. 1960 *Sov. Phys.–JETP* **11** 696)
[18] Allen P B and Mitrovic B 1982 *Solid State Physics* vol 37 (New York: Academic) p 1