Intrasublattice Hopping in the Extended t-J Model and $T_c^{\max}$ in the Cuprates

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It is shown that BCS-like scenarios for high-T_c superconductivity based on the extended t-J model yield a characteristic prediction for $T_c^{\max}$, the critical temperature at optimum doping. A pivotal role is played by $t_- \equiv t' - 2t''$ (t' is the next-nearest-neighbor hopping, t'' is the third-neighbor hopping). Because t_- determines the shape of the Fermi surface and the nature of saddle points, it strongly affects $T_c^{\max}$. Owing to symmetry, structural differences outside the CuO_2 planes are described exclusively by t_-. This explains semiquantitatively the actual variation of $T_c^{\max}$ among the various cuprates, with estimated parameters that are consistent with the observed Fermi surfaces. [S0031-9007(96)00506-6]

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The recent observation by angle-resolved photoelectron spectroscopy [1] of very flat quasiparticle dispersion ("extended saddle points") near the Fermi surface in some (but not all) high-T_c cuprates has revived interest in the possible role of Van Hove singularities in the density of states (DOS) [2]. While the anomalous flatness is probably due to strong correlation effects [3,4], the resulting enhancement of the Van Hove singularities can lead to T_c's well over 100 K even in a conventional BCS-like theory, as shown explicitly, for example, by Dagotto, Nazarenko, and Moreo (DNM) [5] for their antiferromagnetic Van Hove (AFVH) scenario. In this Letter we show that such theories necessarily entail a very specific prediction for the *variation in maximum critical temperature* among the various cuprates. Specifically, it is shown that the crystal structure outside the CuO_2 planes affects the dispersion of in-plane quasiparticles, influencing the location and the nature of saddle points, and that this, in turn, can have a large effect on $T_c^{\max}$, the critical temperature at optimum doping $\delta^{\max}$. This provides an explicit mechanism for the role played by the "chemistry" in determining $T_c^{\max}$ via its effect on the electronic structure, where previous work had established a semiempirical correlation [6,7]. We further predict that only the "higher-T_c" ($T_c^{\max} \gtrsim 90$ K) hole-doped compounds have extended saddle points, in contrast to the "lower-T_c" ($T_c^{\max} \approx 30$ K) La_2CuO_4 group and the electron-doped cuprates.

The low-energy physics of the CuO_2 planes can be described by the two-dimensional extended (i.e., augmented by small additional terms) t-J model [8]. For our analysis it will be essential that this effective single-band model is not phenomenological, but can be rigorously *derived* from chemically realistic multiband models [9–11]. These derivations identify unambiguously the terms that arise in addition to nearest-neighbor hopping t and exchange J (namely, next-nearest-neighbor hopping t', third-neighbor hopping t'', and three-site spin-dependent hopping terms t'_{3s}, t''_{3s}), and moreover permit the single-band parameters to be calculated from those of the multiband model. At half filling the extended t-J model reduces to the Heisenberg model, which accurately describes the antiferromagnetism of the undoped cuprates. Particles doped into the antiferromagnet get strongly dressed, forming magnetic polarons which show up in the spectral function as a sharp quasiparticle peak at the low-energy side of a featureless incoherent background [3]. Recent work [4] has shown that these fermionic quasiparticles persist at finite doping with fairly uniform weight over most of the Brillouin zone (BZ) and little change in dispersion, supporting a rigid-band picture. The polarons move effectively *within one magnetic sublattice* to avoid distortion of the antiferromagnetic background, as demonstrated by their dispersion

$$\varepsilon(\mathbf{k}) = \hat{t}_+(\cos k_x + \cos k_y)^2 - \hat{t}_-(\cos k_x - \cos k_y)^2, \tag{1}$$

where $\hat{t}_\pm = \hat{t}' \pm 2\hat{t}''$, and the *effective* polaron hopping parameters $\hat{t}'$ and $\hat{t}''$ can be calculated from the parameters of the extended t-J model [see Eq. (3) below] [12].

Although $|\hat{t}_-| \ll \hat{t}_+$ ($\hat{t}_+ > 0$) so that the overall bandwidth is determined by $\hat{t}_+$ (which is of order J; see below), $\hat{t}_-$ is a crucial parameter because it has a major effect on the location of the saddle points and the shape of the Fermi surface, as shown in Fig. 1. If $\hat{t}_- > 0$, the saddle points are at $P \equiv (\pm\pi/2, \pm\pi/2)$, the minima at X and Y. If $\hat{t}_- < 0$, the saddle points are at $S \equiv (\pm k_S, 0), (0, \pm k_S)$ where $k_S = \pi - \arccos[(1 + \hat{t}_-/\hat{t}_+)/(1 - \hat{t}_-/\hat{t}_+)]$, the minima at P, while X and Y are secondary maxima. In the latter case one has the peculiarity that the straight lines through the saddle points are exact energy contours, so that at appropriate doping [$\delta = 2k_S(\pi - k_S)/\pi^2$] the Fermi surface shows perfect nesting, consisting of one large and four small squares. For k_S close to π (i.e., $|\hat{t}_-|$ small) there is very little dispersion over the small squares [$E_X - E_S \approx 4\hat{t}_-^2/\hat{t}_+ \approx$

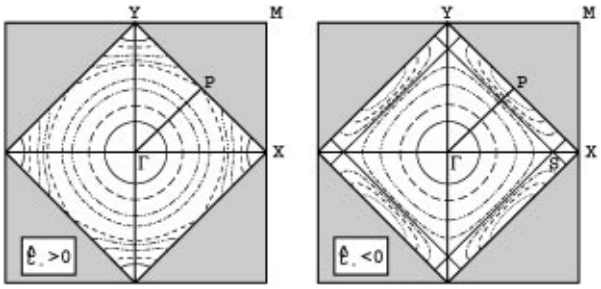

FIG. 1. Energy contours in the BZ for $\hat{t}_-/\hat{t}_+ = \pm 0.1$. The plots correspond to hole doping; for electron doping the outer part of the BZ is relevant.

$6(\hat{t}_-/\hat{t}_+)^2 J \lesssim 15$ meV], which will therefore look like "extended saddle points" [1] in experiments with finite energy resolution. Although the resulting Van Hove singularity is formally still logarithmic, it is much higher and narrower than for positive $\hat{t}_-$.

One thus expects $\hat{t}_-$ to be a relevant parameter in *any* BCS-like theory based upon these magnetic polarons. Here we investigate this explicitly, following DNM, for the case of a *static* attractive nearest-neighbor interaction $H_{\rm int} = -V \sum_{\langle ij \rangle} n_i n_j$. Such an interaction is actually provided in the *t-J* model by the exchange term because of the extra magnetic bond in the system when two polarons are on neighboring sites ($V \approx 0.585J$, as proposed by DNM), or, equivalently, by the dominant term of the static approximation to the (actually somewhat longer-range) interaction generated by spin fluctuations [13]. Straightforward application of BCS pairing theory assuming a *d*-wave [14] order parameter $\Delta(\mathbf{k}) = \Delta_0 (\cos k_x - \cos k_y)$ leads in the familiar way to a self-consistent equation determining T_c,

$$\frac{k_B T_c}{V/4} = \frac{1}{N} \sum_{\mathbf{k}} \frac{(\cos k_x - \cos k_y)^2}{|\varepsilon(\mathbf{k}) - \mu|/2k_B T_c} \times \tanh\left(\frac{|\varepsilon(\mathbf{k}) - \mu|}{2k_B T_c}\right). \quad (2)$$

Solving this self-consistently for a given chemical potential μ in conjunction with the equation determining the number of carriers, and then varying μ yields T_c as a function of doping.

We have investigated how the resulting, approximately parabolic, T_c vs δ curves vary with the model parameters. Figure 2(a) shows that $T_c^{\max}$ is surprisingly sensitive to even a small nonzero $\hat{t}_-$. The asymmetry with respect to the sign of $\hat{t}_-$ is due not only to the different nature (ordinary or extended) of the saddle points, but also to the *d*-wave weight function $(\cos k_x - \cos k_y)^2$ in Eq. (2), which enhances the effect of the Van Hove singularity when the responsible saddle points are close to *X*, *Y*, i.e., if $\hat{t}_- < 0$, but suppresses it when they are at *P*, i.e., if $\hat{t}_- > 0$. As a result, when $\hat{t}_-$ is negative $T_c^{\max}$ first increases with $|\hat{t}_-|$ as the extended saddle points develop, whereas $T_c^{\max}$ decreases rather rapidly with positive $\hat{t}_-$. Also, for $\hat{t}_- < 0$ the maximum T_c is always reached when the Fermi surface passes through the saddle points, so that $\delta^{\max}$ is nearly independent of V. In contrast, for $\hat{t}_- > 0$ the optimum location of the Fermi surface is a compromise between high DOS and not too small weight function, which depends on the value of $T_c^{\max}$ itself so that $\delta^{\max}$ depends quite strongly on V. The above distinction becomes less pronounced for $V \gtrsim \hat{t}_+$ when the BZ integral in Eq. (2) is no longer constrained to the vicinity of the Fermi surface by $|\varepsilon(\mathbf{k}) - \mu| \lesssim 2k_B T_c$ because T_c gets large.

Let us now turn to the calculation of $\hat{t}_+$ and $\hat{t}_-$ for the cuprates. We start from the five-band model [6,7], which includes in addition to the copper $3d_{x^2-y^2} \equiv d_x$ and oxygen $2p_x$ and $2p_y$ σ orbitals of the familiar three-band *d-p* model [15] also the copper $3d_{3z^2-r^2} \equiv d_z$ orbital and the $2p_z$ orbital on the apical oxygen. Parameter estimates have converged towards a "standard" set of in-plane parameters [16], with only $\varepsilon_{\rm apex}$, the energy of the apex orbital, varying considerably from compound to compound because of the variation of Madelung potentials [6]. To this model we apply the cell-perturbation method [10] as summarized below (details on its application to the five-band model will be published elsewhere [11]). After transformation of the in-plane oxygen orbitals into Wannier orbitals *b* and *a* (transforming locally like b_1 and a_1), the Hamiltonian is divided into intracell and intercell terms. The intracell part is diagonalized exactly, yielding *n*-hole cell eigenstates, and the whole Hamiltonian is rewritten in terms of Hubbard operators acting on these cell states. Reduction to an effective single-band model is now achieved by retaining in each cell only the lowest zero-hole state $|0\rangle$, one-hole state $|g_\sigma\rangle$, and two-hole state $|S\rangle$ (the generalized Zhang-Rice singlet [17]), and accounting for the effect of the omitted cell states by second-order perturbation theory. In the three-band case the largest second-order terms come from the [Emery-Reiter (ER)] triplet $|T\rangle = |d_x b\rangle$ [18]. The result is a *generalized* single-band Hubbard model with $U_{\rm eff}$ of the order of the charge-transfer energy, which is electron-hole

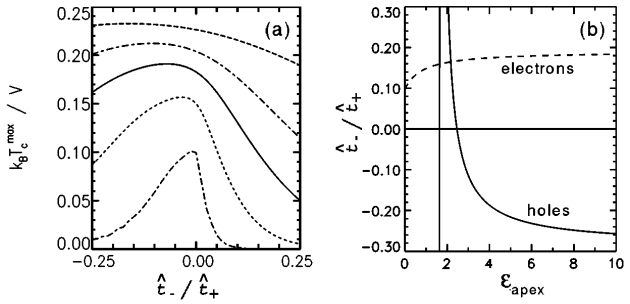

FIG. 2. (a) Maximum critical temperature $T_c^{\max}$ in units of the interaction V vs ratio of intrasublattice hopping parameters $\hat{t}_-/\hat{t}_+$. Curves are for $V/\hat{t}_+ = 0.05$, 0.15, 0.30, 0.50, and 1.00 from bottom to top. The full curve corresponds to realistic cuprate parameters. (b) Ratio $\hat{t}_-/\hat{t}_+$ vs $\varepsilon_{\rm apex}$; other parameters: standard cuprate set [16].

asymmetric ($t_{ij}^{hh} \neq t_{ij}^{ee} \neq t_{ij}^{eh}$) and contains additional interaction terms, e.g., (super)exchange $J_{\rm SB}$.

The new aspect introduced by the a_1-symmetry orbitals d_z and p_z is the presence of two-hole states of B_1 ($= b_1 \times a_1$) symmetry. The lowest of these (denoted by $|B\rangle$) is generally below the ER triplet, its wave function and energy depending sensitively on $\varepsilon_{\rm apex}$. Yet the single-band description remains valid [11], and the B_1 states only generate additional second-order hopping terms, of which the most important are those for *doped holes* (i.e., ZR singlets) arising from the process $|S, g, g\rangle \rightarrow |g, B, g\rangle \rightarrow |g, g, S\rangle$. Since the relevant first-order hopping parameter corresponds to a hole hop between an a_1- and a b_1-symmetry orbital, it has the opposite sign for horizontal and vertical hops and is zero for diagonal hops. Thus, by symmetry alone, the second-order contribution to t vanishes while the contributions to t' and t'' have opposite sign, $t'^{(2)\,hh}(B) = -2\,t''^{(2)\,hh}(B)$, the factor 2 accounting for the two paths to a next-nearest-neighbor cell, so that $t_{+}^{(2)\,hh}(B) = 0$, but $t_{-}^{(2)\,hh}(B) \neq 0$. The corresponding parameter $t_{-}^{(2)\,ee}(B)$ for *doped electrons*, arising from the process $|0, g, g\rangle \rightarrow |0, B, 0\rangle \rightarrow |g, g, 0\rangle$ is much smaller because of the much larger energy denominator involved. Note that the (three-site) hopping terms similarly produced by the ER triplet satisfy $t_{3s}^{\prime\,(2)}(T) = +2\,t_{3s}^{\prime\prime\,(2)}(T)$ because the ER triplet has A_1 ($= b_1 \times b_1$) symmetry.

For the cuprates $U_{\rm eff} \gg t^{eh}$, and, as with the ordinary Hubbard model, the effective single-band Hubbard model may be further mapped onto an extended t-J model, describing either a hole-doped or an electron-doped system, where t, t', etc., are the appropriate (hh or ee) hopping parameters [19] and $J = J_{\rm SB} + J_{\rm ZR}$, where $J_{\rm ZR} = 4(t_{01}^{eh})^2/U_{\rm eff}$. Fixing the AF magnetic background one finds for the effective intrasublattice hopping parameters relevant to the polaron dispersion (1),

$$\begin{aligned} \hat{t}_{+} &= t_{+}^{(1)} + \langle t_{3s,+}^{(2)}(T)\rangle_{\rm AF} + J_{\rm ZR} + \tfrac{1}{2}J\,, \\ \hat{t}_{-} &= t_{-}^{(1)} + t_{-}^{(2)}(B) = t_{-}\,, \end{aligned} \tag{3}$$

where $t_{\pm}^{(1)}$ correspond to first-order farther-neighbor hopping produced by the Wannier transformation of the in-plane oxygen orbitals, $\langle\cdots\rangle_{\rm AF}$ denotes the expectation value in the antiferromagnetic background, $J_{\rm ZR}$ comes from the three-site terms arising as in the reduction of the ordinary Hubbard model, and $\frac{1}{2}J$ from quantum fluctuations restoring spin order after intersublattice hops [3,4]. It follows that, *because of symmetry*, differences between the various cuprates (reflected mainly in $\varepsilon_{\rm apex}$) affect *only* $\hat{t}_{-} = t_{-}$ and not $\hat{t}_{+}$. Figure 2(b) shows the dependence of $\hat{t}_{-}/\hat{t}_{+}$ on $\varepsilon_{\rm apex}$ with standard cuprate values for the other parameters [16]. One notes that this ratio is *positive* for electrons and *negative* for holes unless the apex level falls significantly below the in-plane oxygen level (just before the single-band description finally breaks down). There is no conflict with the earlier arguments for the significance of t' having the opposite sign for holes and electrons [20], as they assumed $t'' = 0$. However, both the present symmetry-based derivation and the above analysis of the dispersion (1) indicate that it is more appropriate to consider t_{-} rather than t' as the relevant parameter differentiating between the cuprates.

Combining the above results yields $T_c^{\rm max}$ as a function of $V/\hat{t}_{+}$ and $\varepsilon_{\rm apex}$ (through $\hat{t}_{-}$). Clearly, if the interaction V is of in-plane nature, as in the AFVH scenario where $V \propto J$, the dependence on $\varepsilon_{\rm apex}$ amounts directly to the variation of $T_c^{\rm max}$ between different compounds. The crucial question is whether this accounts for (i) the much higher critical temperatures in hole-doped than in electron-doped cuprates, and (ii) the trend observed in the hole-doped systems [6,7] that a stronger coupling of the apical oxygens to the CuO_2 planes generally leads to a lower $T_c^{\rm max}$. Qualitatively it certainly does, as Fig. 2(a) in combination with Fig. 2(b) shows, ascribing (i) to the generally opposite signs of $\hat{t}_{-}$, and (ii) to the fact that a decrease in $\varepsilon_{\rm apex}$ raises $\hat{t}_{-}$, which generally decreases $T_c^{\rm max}$. Quantitatively, for $V \approx 0.5J$ (the AFVH assumption) the values of $T_{\rm c}^{\rm max}$ are too large if one uses J as calculated by the cell-perturbation method [which overestimates J, mainly because it does not include (ferromagnetic) direct exchange [10]], but their magnitude is, perhaps somewhat fortuitously, about right if one uses (as did DNM) the experimental value of J instead. (Note that V will also be reduced because of the decrease in spin-spin correlation upon doping and by effective nearest-neighbor Coulomb repulsion [21].) This is shown in Fig. 3, where we have plotted *calculated* versus *observed* $T_c^{\rm max}$ for those representative cuprate compounds for which the parameters can be reliably computed from the data compiled in Ref. [6]. Most importantly, Fig. 3 shows that the overall trend in $T_c^{\rm max}$ is very robust, as we have further verified by making similar plots for different values of V, and remaining discrepancies may well be due to uncertainties in the structural parameters.

We also see from Fig. 3 that $\hat{t}_{-} > 0$ for the lower-T_c ($T_c^{\rm max} \approx 30$ K) La_2CuO_4 group, but $\hat{t}_{-} < 0$ for the higher-T_c ($T_c^{\rm max} \gtrsim 90$ K) compounds. This agrees with the observed Fermi surfaces and, in particular, with only the higher-T_c group having extended saddle points (corroborating that the Van Hove singularities *do play a role* in high-T_c superconductivity). The calculation also gives $\delta^{\rm max} \approx 0.25$ for the higher-T_c compounds, but $\delta^{\rm max} \approx 0.15$ for the La_2CuO_4 group, in remarkable agreement with experiment. Finally, we note from Fig. 3 that there is also a clear correlation between the observed $T_c^{\rm max}$'s and the calculated $\hat{t}_{-}/\hat{t}_{+}$ values themselves. Clearly, the magnitude of $\hat{t}_{-}/\hat{t}_{+}$ and not just its sign *is* important, and it would be interesting to see if a less simplified scenario, including, for example, a dynamic instead of a static interaction [22] and/or doping dependence of the dispersion (e.g., due to the changing spin-spin correlations [23]), could even more convincingly reproduce the observed variation of $T_c^{\rm max}$.

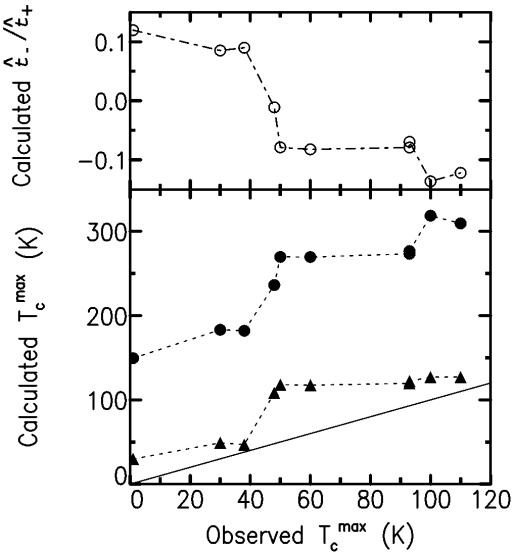

FIG. 3. Ratio $\hat{t}_-/\hat{t}_+$ and calculated maximum critical temperature $T_c^{\max}$ for $V = 0.5J$ (dots: J calculated by cell-perturbation method; triangles: experimental J) versus experimental $T_c^{\max}$ for various cuprates. Compounds included are $La_2SrCu_2O_6$ ($T_c^{\max} = 0$ K), $La_{1.85}Ba_{0.15}CuO_4$ ($T_c^{\max} = 30$ K), $La_{1.85}Sr_{0.15}CuO_4$ ($T_c^{\max} = 38$ K), $(Ba_{0.67}Eu_{0.33})_2(Eu_{0.67}Ce_{0.33})_2Cu_3O_{8.78}$ ($T_c^{\max} = 48$ K), $Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.11}$ ($T_c^{\max} = 50$ K), $YBa_2Cu_3O_{6.5}$ ($T_c^{\max} = 60$ K), $YBa_2Cu_3O_7$ ($T_c^{\max} = 93$ K), $Bi_2Sr_2Ca_{0.9}Y_{0.1}Cu_2O_{8.24}$ ($T_c^{\max} = 93$ K), $TlBa_2CaCu_2O_7$ ($T_c^{\max} = 100$ K), $Pb_{0.5}Tl_{0.5}Sr_2CaCu_2O_7$ ($T_c^{\max} = 110$ K). The straight line corresponds to perfect correlation.

In conclusion, we have shown that in the extended t-J model the intrasublattice parameter $t_- \equiv t' - 2t''$ governs the topology of the Fermi surface, and, in particular, the presence or absence of extended saddle points. As a consequence t_- strongly affects $T_c^{\max}$ in BCS-like scenarios for high-T_c superconductivity. When the extended t-J model is derived from a five-band model which includes orbitals outside the CuO_2 planes, the structural differences between the various cuprates are reflected precisely in t_-, whereas all other single-band parameters are completely determined by the CuO_2 planes and are therefore virtually identical for all compounds. While estimated parameters are consistent with the observed Fermi surfaces, the simplest quasiparticle scenario, which assumes a static interaction and doping-independent dispersion, explains semiquantitatively both that $T_c^{\max}$ is much larger for hole-doped than for electron-doped cuprates together with the trend in $T_c^{\max}$ among the hole-doped cuprates.

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