Intrasublattice Hopping and $T_c^{\max}$ in the Cuprates

In a recent Letter [1], it was shown that the critical temperature at optimum doping $T_c^{\max}$ is determined by $t_- = t_2 - 2t_3$, where t_i is the hopping between ith nearest neighbors (including the effect of three-site terms $\langle t^{3s}\rangle_{AF}$) in a generalized t-J model. While we believe that the result is correct and important, some assumptions, crucial for the physics of the cuprates, should be corrected.

The authors assumed that holes introduced by doping fill a rigid quasiparticle band with dispersion $\epsilon_k = \hat{t}_+(\cos\times k_x + \cos k_y)^2 - \hat{t}_-(\cos k_x - \cos k_y)^2$, where $\hat{t}_+ = t_+ + J/2, \hat{t}_- = t_-$. This is not valid for realistic (small) J/t_1, for which the antiferromagnetic background is strongly distorted, as described by the "string" picture [2]. The intrasublattice hoppings are strongly renormalized. We have calculated the dispersion of a hole using the self-consistent Born approximation [3]. For the "bare" t-J model with $t_1 = 0.4, J = 0.12$ (other $t_i = 0$), the above equations give $\hat{t}_+ = 0.06, \hat{t}_- = 0$, and the Van-Hove singularities would be reached for doping $\delta_{vH} = 0$ [1]. We find that ϵ_k with $\hat{t}_+ = 0.06$, but $\hat{t}_- = -0.0102$ accurately reproduces the resulting dispersion. For these values, $\delta_{vH} = 0.374$, which lies beyond the overdoped region of any high-T_c material. A negative t_- (which corresponds to the systems with higher T_c) increases the difference between $\epsilon_{(\pi,0)}$ and $\epsilon_{(\pi/2,\pi/2)}$ and moves δ_{vH} further towards 0.5. This is probably the reason why Dagotto *et al.* introduce a positive t_2 leading to positive t_- in their antiferromagnetic Van Hove (AFVH) scenario [4]. Specifically, using the same low-energy reduction procedure from the three-band model (H_{3b}) as Feiner *et al.* [1,5], taking $\Delta = 3, U_d = 8, U_{pd} = 1 U_p = 4, t_{pp} = 0.5$ in units of t_{pd}, without corrections due to apical O atoms, we obtain $t_1 \sim 0.4, t_2 = 0.035, t_3 = 0.089$. Taking (as always in this work) $J = 0.12$, the self-consistent Born approximation (SCBA) gives a quasiparticle band which can be reasonably well described by $\epsilon_k + \hat{t}_5 \cos 2k_x \cos 2k_y$ with $\hat{t}_+ = 0.066, \hat{t}_- = -0.058, \hat{t}_5 = -0.009$. Neglecting $\hat{t}_5, \delta_{vH} = 0.499$ results. However, if one takes the noninteracting band defined by $\epsilon_k + 2t_1(\cos k_x + \cos k_y)$ with $\hat{t}_\pm = t_\pm$, and band filling satisfying Luttinger theorem, the van Hove points [now at $k = (\pi, 0)$ and equivalent wave vectors] are reached at the more reasonable doping $\delta_{vH}^{ni} = 0.28$. Corrections due to t^{3s} practically do not modify the critical dopings. Neglecting them, we obtain $t_2 = -0.03, t_3 = 0.057$, the SCBA gives $\hat{t}_+ = 0.064$, $\hat{t}_- = -0.052, \hat{t}_5 = -0.006$, and then $\delta_{vH} = 0.499$, $\delta_{vH}^{ni} = 0.30$. This is important since for other three-band parameters [5], and particularly using a mapping in terms of nonorthogonal singlets, or numerical fitting of the energy levels, t^{3s} changes sign [6].

For moderate apical corrections, $t_2 = 0.075, t_3 = 0.69$, the SCBA dispersion is reasonably well reproduced with $\hat{t}_+ = 0.065, \hat{t}_- = -0.036, \hat{t}_5 = -0.009$, leading to $\delta_{vH} = 0.48$, while $\delta_{vH}^{ni} = 0.12$. Thus, contrary to the strongly renormalized one-hole results, the noninteracting values δ_{vH}^{ni} agree with the tendencies pointed out in Ref. [1]. In fact, recent angle-resolved photoemission experiments show that $\epsilon_{(\pi,0)}$ moves strongly with doping and that the Fermi surfaces of optimally doped superconductors (for reasons still unclear) are very similar to those predicted by the local-density approximation [7]. A negative t_- shifts δ_{vH}^{ni} from the underdoped to the optimally doped region. Qualitatively, the effect of the apical O p_z and Cu $d_{3z^2-r^2}$ orbitals in shifting the Van Hove singularities is already clear from the Hartree-Fock solution of the multiband model [8].

We also argue that the model with up and down spin quasiparticles moving in opposite sublattices and with nearest-neighbor attraction $V \sim J/2$ (AFVH picture [4]), for realistic J/t_1, does not reproduce even qualitatively the pairing interaction of t-J-like models. The AFVH model leads to equal amounts of singlet and triplet pairs. In one dimension, it is clear from the continuum limit theory that $K_\rho > 1$ (superconducting correlations dominate) as soon as $V > 0$, while numerical calculations in the t-J model, even in the presence of a staggered magnetic field $h = J/2$, require $J > 0.4t_1$ to show pairing [9]. We have diagonalized the t-J model with $t_1 = 0.4, J = 0.125$, together with the corresponding AFVH model [4], in a 4×4 cluster with $\delta = 0.25$. We find that the behavior of the singlet d-wave pairing correlation functions is quite different. At the largest distance $(2\sqrt{2})$, the AFVH value is 0.114, while the corresponding t-J result is more than 10 times smaller. The effect of the spin-flip part of t^{3s} on the pairing mechanism cannot be disregarded [6].

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