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# POSSIBLE ELECTRONIC ENERGY STRUCTURE OF HIGH-$T_C$ CUPRATES

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## ABSTRACT

Possible electronic energy structure of the high-$T_c$ cuprates is reported within the framework of a simple algebraic Green's function analysis. The starting point is a two-band (d-p) restricted-hopping Hamiltonian in pseudospinor representation. The analysis leads to antiferromagnetic (AF) Mott-Hubbard or charge transfer (CT) normal (undoped) state, depending on bandwidth (~t) and levels separation (~U). In our so-called t-model pairing of electrons, doped cuprates present as CT- assisted superconductors with AF exchange energetically forbidden. Approximate numerical results from the analysis are consistent with experiment and corresponding results from some other theories.

Keywords: Two-band model, restricted hopping, electronic energy structure, algebraic Greens function, electronic levels separation, antiferromagnetic normal state, CT-assisted superconductivity

## 1. INTRODUCTION

A good theoretical understanding of the normal state characteristics of the new copper oxide compounds (cuprates), in which high-temperature (high-$T_c$) superconductivity (SC) was discovered [1,2], still poses a challenge. It remains a current issue because the normal state characteristics constitute the most realistic foundation for understanding the superconducting state, the latter an unsolved problem by itself.

Experimentally [3,4], the undoped (normal state) cuprates are found to be antiferromagnetic (AF) insulators (semi-conductors). The Cu (3d) ions have been closely asociated [5] with this order, there being some uncertainty about the role played by O(2p) ions in this regard. There is, nevertheless, a general consensus that the unusual superconductivity found in these systems resides in the crystallographic $CuO_2$ planes.

Ipso facto, and on account of difficulties in erecting an independent theory of the normal state, both AF and SC orders have been generally modelled [6-10] on a single Hamiltonian in which AF spin exchange (J) is expected to play a role in both phases. The insulating phase often turns out a Mott-Hubbard (MH) [11,12] system. The issue arises: does spin exchange in the normal state dictate spin exchange in the superconducting state? This point is yet not clarified but

high-$T_c$ theories based on spin exchange, or exchange-like [9] integrals, abound in the literature.

More recently, experimental [13] and theoretical [14] indications exist that the insulating cuprates are in charge transfer (CT) regime [15] rather than in the MH regime. Does this suggest that doped cuprates are CT superconductors? Charge transfer state in insulators or superconductors has, until recently, not been of much quantitative interest. It is, therefore, basic that the above issues be clarified. This is the problem briefly addressed in this paper.

## 2. NORMAL STATE HAMILTONIAN

We begin with the restricted-Hilbert-space hopping (transfer) Hamiltonian [16,17] for Cu (3d) and O(2p) electrons (holes), the so-called t-model [17]:

$$H = -\sum_{ij\sigma\bar{\sigma}} t_{ij}(1-n_{i\bar{\sigma}})c^{+}_{i\sigma}C_{j\sigma}(1-n_{i\bar{\sigma}}). \qquad (2.1)$$

In (2.1), i(j) = d,p labels electrons in Cu and O bands; $t_{ij}$ is the nearest-neighbour hopping integral; $C^{+}_{i\sigma}$ ($C_{i\sigma}$) is i-band creation (annihilation) operator for an electron with spin polarisation $\sigma$ (=↑or ↓), where $\sigma$ is the reverse of $\sigma$ , and vice versa; $n_{i\sigma} = C^{+}_{i\sigma}C_{i\sigma'}$ is the number operator.

It would appear, in (2.1), that double occupancy of O orbitals, as is known to obtain in the cuprates, has been prohibited. As (2.1) contains sum over spin variable ($\sigma$), however, we have in effect prohibited, in (2.1), double occupancy of any given spin site in all orbitals, be they of Cu or O. This is what is basic and physical. Doubly occupied orbitals would reveal, in such a model, degeneracy in spin energy while singly occupied orbitals would show no such degeneracy. As single spin per site is what forms the basis of the model Hamiltonian (2.1), we have incorporated no on-site interaction ($\tilde{U}$) as, in the sense [18] of the Hubbard model, no such ($\tilde{U}$)-term does exist presently. Thus, even for multiple orbital-occupancy, we have regarded each spin site as different.

It has been shown [17] that (2.1) can be transformed to the mean-field (MF) Bloch representation. For purposes of making the present paper self-contained, one expands (2.1) and employs single$^{t}$ -pair preserving mean-field (MF) (Gor'kov) decoupling [19]:

$$c^{+}_{1}c^{+}_{2}c_{3}c_{4} \rightarrow \langle c^{+}_{1}c^{+}_{2}\rangle c_{3}c_{4} + \langle c_{3}c_{4}\rangle c^{+}_{1}c^{+}_{2} - \langle c^{+}_{1}c^{+}_{2}\rangle\langle c_{3}c_{4}\rangle,$$

on the resulting terms. One recalls, however, that a sixth-order term in electron operators may be treated as third order in boson operators in the present pairing representation. Gor'kov decoupling of such a term would therefore follow

some terms in the light of the dominant realities of the physical model, one obtains (in k – space):

$$H = \sum_{ik\sigma} \in_{ik\sigma} c^{+}_{ik\sigma} c_{ik\sigma} - \sum_{ijk\sigma, i\neq j} t_{ij} c^{+}_{ik\sigma} c_{ik\sigma} + \sum_{ijk\sigma, i\neq j} ( \Delta_{iik} c^{+}_{ik\uparrow i} c^{+}_{ik\downarrow i} + h.c.). \quad (2.2)$$

The first term of (2.2) is the intraband hopping energy in which $t_{ij}$ is replaced by the Fourier transform ($\in_{ik\sigma}$), the second term is the band hybridization energy, and the third term is the opposite-spin pair interaction energy.

In (2.2), $\Delta_{iik}$ is the gap in energy spectrum for i-band and k is crystal wavevector for the electron with uperturbed kinetic energy ($\in_{ik\sigma}$) measured relative to the Fermi level, $E_F$. In (2.1) and (2.2), both spin and charge degrees of freedom (dof) are possibly accounted for via the transfer integral. For a system with all electrons in singlet pairs, as may obtain in antiferromagnetic and superconducting ordering, and bands (i,j) which, without prejudice, have equal probabilities of producing such pairs, we have, in (2.2), set terms like

$$\langle n_{i\bar{\sigma}} \rangle \sim \langle c_{i\bar{\sigma}} c_{i\sigma} \rangle,$$
$$\langle c_{ik\downarrow} c_{ik\uparrow} \rangle \sim \langle c_{jk\downarrow} c_{jk\uparrow} \rangle, i \neq j,$$

while regarding

$$t_{ij} >> t_{ii} (t_{jj}), i \neq j. \quad (2.3)$$

We have also conveniently neglected hybrid pair wavefunctions on the basis of (2.3). Under these conditions, the gap in energy is given in the form

$$\Delta_{iik} = -t_{ij} \langle c_{ik\downarrow} c_{jk\uparrow} \rangle \langle c_{ik\downarrow} c_{ik\uparrow} \rangle, i \neq j. \quad (2.4)$$

Observe that, except for the mixing term (second term of (2.2)), (2.2) has formal similarity with the Bardeen-Cooper-Schriefer (BCS)[20] and Suhl-Matthias-Walker [21] models in the MF approximation. Indeed, (2.2) has familiar aspects with the MF form of the Hamiltonian [10]. Our present emphasis (2.3) and the inclusion [17] of damping effects [12] lead to new insights about the normal state of the system.

In order to reveal these developments, let us write the kinetic (first) term of (2.2) in the matrix form

$$H_{kin} = \sum_{k\alpha} \alpha^{+}_{k\sigma} \frac{1}{4}((e_{\uparrow\downarrow} - e_{\downarrow\uparrow})\tau_{00} + (e_{\downarrow\uparrow} - e_{\uparrow\downarrow} + 2e'_{\uparrow\downarrow})\tau_{03}$$

$$+ (e'''_{\downarrow\uparrow} + e'''_{\uparrow\downarrow})\tau_{30} - (e_{\downarrow\uparrow} + e_{\uparrow\downarrow})\tau_{33})\alpha_{k\sigma}, \tag{2.5}$$

where we have defined the energy level-separations (and sums) by

$$\begin{aligned}
e_{\sigma\bar{\sigma}} &= \in_{pk\,\sigma} - \in_{dk\,\bar{\sigma}}, \\
e'_{\sigma\bar{\sigma}} &= \in_{dk\,\sigma} - \in_{dk\,\bar{\sigma}}, \\
e''_{\sigma\bar{\sigma}} &= \in_{pk\,\sigma} - \in_{pk\,\bar{\sigma}}, \\
e'''_{\sigma\bar{\sigma}} &= \in_{pk\,\sigma} + \in_{dk\,\bar{\sigma}}, \\
e''''_{\sigma\bar{\sigma}} &= \in_{dk\,\sigma} + \in_{dk\,\bar{\sigma}}.
\end{aligned} \tag{2.6}$$

The four-component spinor wavefunction is

$$\alpha^{+}_{k\sigma} = (c^{+}_{ik\uparrow} c_{ik\downarrow} c^{+}_{jk\uparrow} c_{jk\downarrow}), i \neq j, \tag{2.7}$$

and the corresponding Hermitian conjugate, $\alpha_{k\sigma}$; the 4 x 4 spin matrices are

$$\tau_{\nu\lambda} = \sigma_{\nu} \otimes \rho_{\lambda}, (\nu, \lambda = 0,1,2,3,), \tag{2.8}$$

where

$$\sigma_{\nu}, \rho_{\lambda} (\upsilon, \lambda = 1,2,3,)$$

are the Pauli (2 x 2) spin matrices and $\sigma_0, \rho_0$ the unit 2x2 matrices. The role of the operator $\otimes$ is examplified by

$$\tau_{31} = \sigma_3 \otimes \rho_1 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}$$

The mixing term and the pair-interaction, in (2.2), may now be written, respectively, as

$$H_{mix} = -\sum_{k\sigma} \alpha^{+}_{k\sigma} t \tau_3 \alpha_{k\sigma'} t = t_{ij} (i \neq j) \tag{2.9}$$

and

$$H_{int} = \sum_{k\sigma} \alpha^{+}{}_{k\sigma} (\epsilon_{sk}\ \tau_{10} + \epsilon_{ak}\ \tau_{13}) \alpha_{k\sigma'} \tag{2.10}$$

where $\epsilon_{sk}$ and $\epsilon_{ak}$ are, respectively, the symmetric and antisymmetric gap terms given by

$$\epsilon_{sk} = \frac{1}{2}(\Delta_{ddk} + \Delta_{ppk}); \epsilon_{ak} = \frac{1}{2}(\Delta_{ddk} - \Delta_{ppk}). \tag{2.11}$$

We argue [14] that the normal state of the cuprates is especially determined by levels-separations (and sums) given by (2.6) and the transfer integral (t). In this foray, the absence of terms in e'' in (2.5), (2.9), and (2.10), determines that

$$\epsilon_{pk\uparrow} = \epsilon_{pk\downarrow} = \epsilon_{pk\sigma} . \tag{2.12}$$

If we now associate this zero-energy separation of the p-band spins with the experimental and general belief [5] of non-AF ordering of this band, we may suggest that the wider the band levels-separation of up-spin and down-spin electrons the more likelihood of AF- order in that band. This permits the search for possible AF ordering of the bands by first equating to zero, in (2.5), (2.9), and (210), all terms that convey no obvious energy levels-separation. It prescribes that

$$e'''_{\uparrow\downarrow} + e'''_{\downarrow\uparrow} = 0. \tag{2.13}$$

By defining

$$U = -e'_{\uparrow\downarrow}, U' = e'''_{\downarrow\uparrow}, \tag{2.14}$$

in conjunction with (2.12) , one obtains the solutions for (2.13) as [16]:

$$\epsilon_{pk\sigma} = \epsilon_{dk\uparrow} = -\epsilon_{dk\downarrow} = -U/2. \tag{2.15}$$

The expected spin energy degeneracy of doubly occupied 0 orbitals and non-degeneracy of Cu orbitals are revealed in Eqn. (2.15). The new U-term is, by this equation, evidently k-dependent, as $\epsilon_{ik\sigma}$ are. Observe that (2.15) also satisfies

$$\epsilon'''_{\sigma\sigma} = 0,$$

as expected. These solutions are schematically illustrated in Fig. 1(a). Fig. 1(a) clearly exhibits correct assignments of single electron per Cu orbital and two electrons per 0 orbital, in the system. In addition, one must set, in (2.10), $e_{sk}=0$, which yields

$$\Delta_{ppk} = -\Delta_{ddk} = t. \tag{2.16}$$

The choice of U and t in the solutions (2.14) – (2.16) is advised by the need for due correspondence with the Mott-Hubbard picture of the insulating phase in strongly correlated fermion-systems. The parameter U is characterized, in sec. 3, as isomorphic to the Hubbard [12] interaction ( $\tilde{U}$ -term).

On the basis of the preceding argument, the Hamiltonian operator, representing the insulating (normal) state of the cuprates is, in the absence of band mixing (which assumption is reasonable in the highly atomic regine),

$$H = \tfrac{1}{4}((e_{\uparrow\downarrow} - e_{\downarrow\uparrow})\tau_{00} + (e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - U)\tau_{03} - (e_{\downarrow\uparrow} + e_{\uparrow\downarrow})\tau_{33}) + \epsilon_{ak}\,\tau_{13}. \tag{2.17}$$

It is then evident that (2.17) is determined solely by levels separations. The only source of uncertainty in this assertion is the last term in the bracket. Next, we enquire if this Hamiltonian adequately represents the normal state believed to be an AF [3,4] or CT [14] state.

## 3. NORMAL STATE ENERGY SPECTRUM

It is our belief that the normal state energy spectrum can serve as a preliminary indicator of the nature of the electronic structure, AF, CT, or both. In order to explore this, we define the thermal Green's function arising from (2.17), in the Matsubara representation

$$G_\sigma(k, iw_n) = (iw_n - H)^{-1}, \tag{3.1}$$

where

$$w_n = \pi\beta^{-1}(2n+1), n = 0, \pm1, \pm2, \ldots,$$

are Matsubara frequencies, in which $\beta^{-1} = k_B T$, with $k_B$ the Boltzmann constant and T, the temperature of the system. This leads to

$$G_\sigma(k,iw_n) = [(iw_n + \tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow}))\{ (iw_n + \tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow})) - \tfrac{1}{16}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2$$
$$- \epsilon^2_{ak} - \tfrac{1}{16}(e_{\downarrow\uparrow} + e_{\uparrow\downarrow})^2 \}\tau_{00} + \{\tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)((iw_n + \tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow}))^2$$
$$- \tfrac{1}{16}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2 - \epsilon^2_{ak} - \tfrac{1}{16}(e_{\downarrow\uparrow} + e_{\uparrow\downarrow})^2)$$
$$+ \tfrac{1}{2}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)\epsilon^2_{ak} + \tfrac{1}{32}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)(e_{\downarrow\uparrow} + e_{\uparrow\downarrow})^2 \}\tau_{03}$$
$$+ \{\epsilon_{ak}((iw_n + \tfrac{1}{4}(e_{\downarrow\uparrow} + e_{\uparrow\downarrow}))^2 - \tfrac{1}{16}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2 - \epsilon^2_{ak}$$
$$- \tfrac{1}{16}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow})^2) + \tfrac{1}{8}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2\,\epsilon_{ak} \}\tau_{13}$$
$$+ \{(-\tfrac{1}{4}(e_{\downarrow\uparrow} + e_{\uparrow\downarrow})((iw_n + \tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow}))^2$$
$$- \tfrac{1}{16}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2$$
$$- \epsilon^2_{ak} - \tfrac{1}{16}(e_{\downarrow\uparrow} + e_{\uparrow\downarrow}))^2) - \tfrac{1}{32}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2(e_{\downarrow\uparrow} + e_{\uparrow\downarrow})^2 \}\tau_{33}$$
$$+ \tfrac{1}{2}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)\{iw_n + \tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow}) \}\epsilon_{ak}\,\tau_{10}$$
$$- \tfrac{1}{8}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)(e_{\downarrow\uparrow} + e_{\uparrow\downarrow})\{iw_n + \tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow}) \}\tau_{30}]/B, \qquad (3.2)$$

where the denominator

$$B = ((iw_n + \tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow}))^2 - \tfrac{1}{16}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2 - \epsilon^2_{ak}$$
$$- \tfrac{1}{16}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow})^2)^2 - \tfrac{1}{4}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2\,\epsilon^2_{ak} \qquad (3.3)$$
$$- \tfrac{1}{64}(e_{\downarrow\uparrow} - e_{\uparrow\downarrow} - 2U)^2(e_{\downarrow\uparrow} + e_{\uparrow\downarrow})^2.$$

Using the level diagram (Fig. 1(a)), we may set

$$e_{\downarrow\uparrow} = \epsilon_{pk\sigma} - \epsilon_{dk\uparrow} = 0,$$
$$e_{\uparrow\downarrow} = \epsilon_{pk\sigma} - \epsilon_{dk\downarrow} = -U = -U_{dd}\,(\text{or} - U_{p\sigma d\downarrow}). \qquad (3.4)$$

These lead, in (3.3), to

$$B = ((iw_n + \frac{1}{4}U_{dd})^2 - \frac{1}{8}U^2_{dd} - t^2)^2 - \frac{1}{4}t^2U^2_{dd} - \frac{1}{64}U^4_{dd} \qquad (3.5)$$

The energy spectrum is realised by setting (3.5) to zero. It yields, ignoring, meanwhile, the $((U^2\ t^2))$ and $((U^4))$ terms, the interacting ground state energies

$$E_{dk\sigma} = -\frac{1}{4}U_{dd} \pm \frac{\sqrt{2}}{4}(U_{dd}^2 + 8t^2)^{\frac{1}{2}} = E_{k\pm}. \qquad (3.6)$$

In the low bandwidth ($U_{dd}$>>t) limit, which is analogous to the MH regime,

$$E_{dk\sigma} \sim \frac{1}{4}(-1 \pm \sqrt{2})U_{dd} \pm J, J = -\frac{t^2\sqrt{2}}{U_{dd}}. \qquad (3.7)$$

These spectra easily characterize an antiferromagnet of the Heisenberg type, with J the exchange constant. As is evident, the levels separation $U_{dd}$ performs the traditional role of the Hubbard U-term in conventional AF system. Observe that the AF ordering characterized here, is realised from $d_\uparrow$ - $d_\downarrow$ and $p_\uparrow$ -$d_\downarrow$ ($p_\downarrow$ - $d_\uparrow$) electrons. This explains the experimental realisation [3,4] of AF order only in the Cu(3d) subband in undoped cuprates. The question strongly arises: what are the $p_\uparrow$ -$p_\downarrow$ pairs, AF, CT, SC, or chiral [22] state ? The brief comment on Fig. 1 (b), suggests these to be any except AF states. This maps out the electronic spin energy structure of a typical $CuO_2$ - based system.

It is interesting presently to examine the other (high-bandwidth, $U_{dd}$<<t) limit. In this case

$$E_{k\pm} \approx (t - Q), Q = -\frac{U_{dd}^2}{16t} \qquad (3.8)$$

Apparently, an exchange term, t-Q, survives with small U, the latter otherwise related to band levels. We may take it that Q is an exchange constant in a new regime dominated by t. We propose that (3.8) is a CT spectrum with Q a charge transfer (exchange) constant. The shift from MH to CT regime was, indeed, envisaged [23], even in one dimension.
In order to buttress this point, let us freely set

$$e_{\uparrow\downarrow} + e_{\downarrow\uparrow} = 0. \qquad (3.9)$$

The solutions for this equation are given schematically in Fig. 1(b), for $e_{\downarrow\uparrow} = 0$.

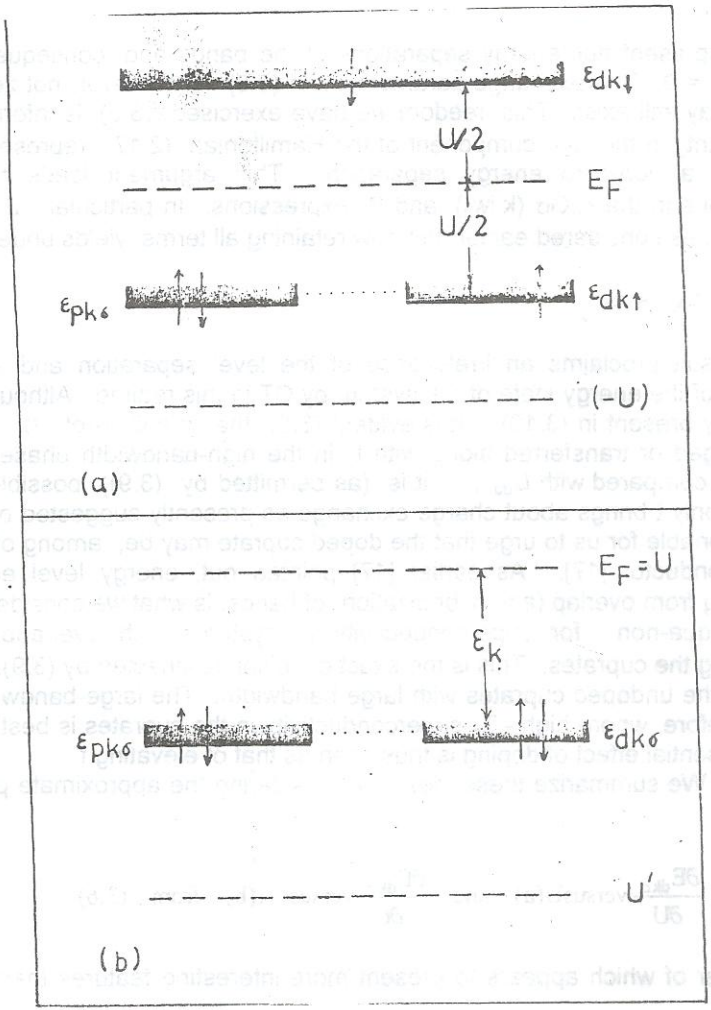


**FIG. 1:** Schematic representation of electronic energy levels, Eqns. (2.15) and (3.9), and levels-separations (U) for typical AF (a) and CT (b) states in undoped cuprates. [Fig. 1(a) inverted (to be appropriate to the hole picture) has an essential similarity with the levels proffered by Ref. [14], with particular regard to U in relation to $\epsilon_{pkv}$ and $\epsilon_{dkv}$. Fig. 1. (b) portends that, with zero levels-separation, two bands (subbands) otherwise AF – coupled, may only exchange charge there being no net AF transfers. On the basis of simple energetics, this is what is physical. Light is thus shed on the question of $P_\uparrow$-$P_\downarrow$ pairs raised in the text. It also illustrates the essential conditions for overlap that foreshadows singlet-pair superconductivity, which ordered state may (as we now know) allow charge and not spin exchange.

They represent null energy separations of the bands and, consequently, $U_{dd} = U_{pd} = Q = 0$. The exchange parameter, t, in (3.8) is, however, not zero and CT state may still exist. This freedom we have exercised (3.9), is informed by the uncertainty in the $\tau_{33}$ component of the Hamiltonian (2.17) representing, at all times, a non-zero energy separation. This argument leads to pleasant reductions in the $H,G\sigma(k,iw_n)$, and B expressions. In particular, B = O, for $e\downarrow\uparrow = 0$, as considered earlier, but now retaining all terms, yields under (3.9),

$$E_{k\pm} \approx \pm t. \qquad (3.10)$$

This result proclaims an irrelevance of the level separation and a complete control of the energy state of the system by CT in this regime. Although Q is not explicitly present in (3.10). It is evident (3.8) that it is Q (not J) that can be exchanged or transferred along with t in the high-bandwidth phase. For very large t compared with $U_{dd}$ , it is (as permitted by (3.9)) possible that Q = 0, and only t brings about charge exchange as presently suggested by (3.10). It is reasonable for us to urge that the doped cuprate may be, among others, a CT superconductor [17]. As earlier [17] pointed out, energy level equalisation, resulting from overlap (and hybridization) of bands, is what we consider [24] to be a sine-qua-non for superconductivity in systems with overlapping bands, including the cuprates. This is the exact condition re-enacted by (3.9), under $e_{\downarrow\uparrow} = 0$, in the undoped cuprates with large bandwidth. The large-bandwidth regime is, therefore, where high - $T_c$ superconductivity in the cuprates is best looked for. The essential effect of doping is thus seen as that of elevating t.

We summarize these ideas by considering the approximate plots (Fig.2) of

$$\frac{\partial E_{dk\sigma}}{\partial U} \text{ versus } U(a) \quad \text{and} \quad \frac{\partial E_{dk\sigma}}{\partial t} \text{ versus } t(b) \quad \text{from} \quad (3.6)$$

the latter of which appears to present more interesting features than (3.8) and (3.10).

The curves for the upper Hubbard band ($E_{k+}$) (continuous) and lower Hubbard band (Ek-) (broken) show saturation tendencies of the gradient functions, as indicated by the asymptotic behaviours. These occur at large $\pm$ U (a) and $\pm$t (b). About U(t)~ 0, these functions are poorly defined (in the present sketch) on account of our convenient units (indicated) for U and t which we thus pay for. The curves, nevertheless, simply summarize the behaviour of $E_{dk\sigma}$ in the insulating phase. They lead to the plausible possible conclusion that $E_{dk\sigma}$ is most stable at high $\pm U(\pm t)$. The high-bandwidth (~t) region is that expected to usher in CT and CT/SC regimes in the cuprates.

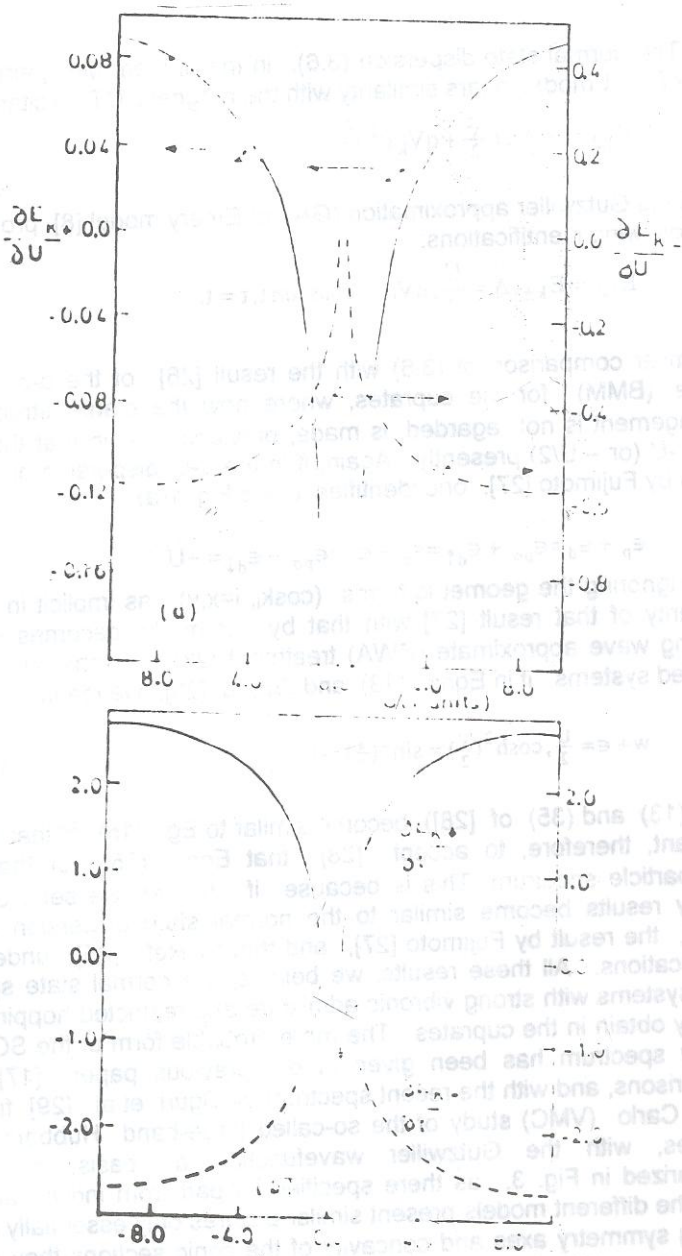


**FIG. 2** Approximate variation of electronic $\partial E_{dkv}/\partial u$ with U(a) and $\partial E_{dkv}/\partial t$ with t (b) in undoped cuprates, where $E_{jkv}$,u, and t are, respectively, the interaction spectrum, Cu($3d_{\downarrow}$) and O($2_{pv}$) levels-separation, and charge/spin transfer energy.

The normal state dispersion (3.6), in the present MF pairing approximation of the t-model, bears similarity with the magnetic/CT excitation energy [25]:

$$E_{1,2} = -\frac{\Delta}{2} \pm (\frac{\Delta^2}{2} + qV_k t^2)^{\frac{1}{2}} \tag{3.11}$$

from the Gutzwiller approximation (GA) of Emery model [8], provided one makes the following identifications:

$$E_{1,2} = E_{k\pm}, \Delta = \frac{U}{2}, qV_k = \cos tan\, t, t = t. \tag{3.12}$$

A similar comparison of (3.6) with the result [26] of the d-p breathing mode model (BMM) for the cuprates, where now the planar structure of $CuO_2$ arrangement is not regarded, is made, provided $\epsilon_G$ in that theory is identified with -U (or – U/2) presently. Again, if in the d-p dispersion of high-$T_c$ cuprates given by Fujimoto [27], one identifies, using Fig, 1(a):

$$\epsilon_p + \epsilon_d = \epsilon_{p\sigma} + \epsilon_{d\uparrow} = \epsilon_p - \epsilon_d = \epsilon_{p\sigma} - \epsilon_{d\downarrow} = -U \tag{3.13}$$

while ignoring the geometric terms ($\cos k_i$, i=x,y), as implicit in our model, the similarity of that result [27] with that by our model becomes evident. In the rotating wave approximate (RWA) treatment [28] of transitive electron-phonon coupled systems, if in Eqns. (13) and (35) of [28], we identify

$$w + \epsilon = \frac{U}{2}, \cosh^2(\frac{v}{2}) = \sin^2(\frac{k}{2}) = 1, \tag{3.14}$$

they ((13) and (35) of [28]) become similar to Eg. (15) of that theory. We are reluctant, therefore, to accept [28] that Eqn. (35) of that paper is SC quasiparticle spectrum. This is because if, further, we set their $\lambda$ = t, these energy results become similar to the normal state dispersion of the present model, the result by Fujimoto [27], and that by Ref. [25], under the specified identifications. All these results, we believe, are normal state spectra for two-band systems with strong vibronic admixture and restricted hopping of electrons, as may obtain in the cuprates. The more probable form of the SC quasiparticle energy spectrum has been given in our previous paper [17]. The above comparisons, and with the recent spectrum by Oguri et al. [29] from Variational Monte Carlo (VMC) study of the so-called three-band Hubbard model for the cuprates, with the Gutzwiller wavefunction as basis, are quantitatively summarized in Fig. 3, as there specified. Apart from individual details which differ, the different models present similar pictures only essentially differing in the rotating symmetry axes and concavity of the conic sections they represent. As can be seen (Fig. 3 (a)), only the BMM result is symmetric about the excitation energy (E) axis, as it does not contain an additive term to the square-root

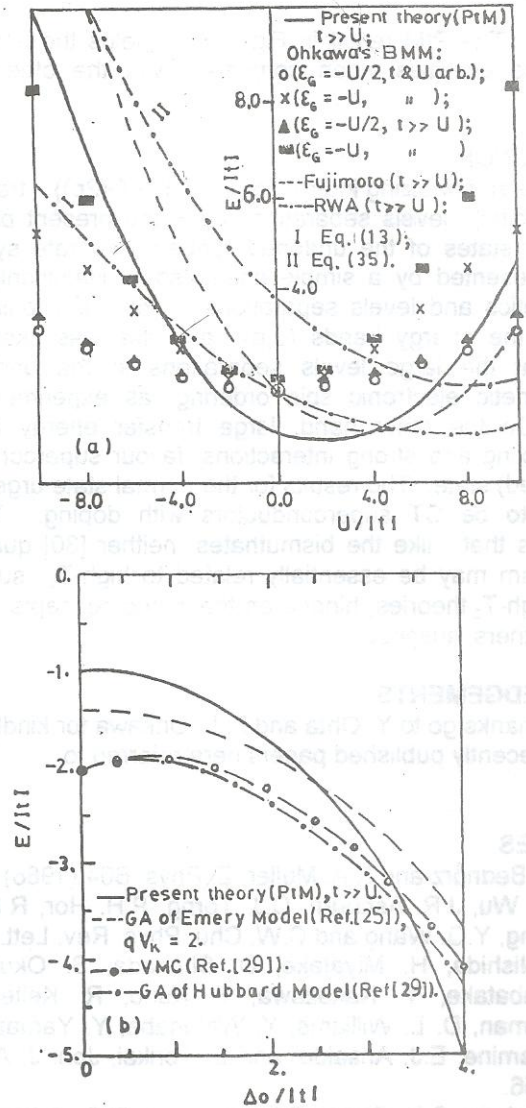


**FIG. 3**: (a) Comparison of normal state upper (antibonding) energy band in the present pairing t-model (PtM), for t>>U, the d-p breathing mode model (BMM) of Ohkawa (Ref. [26]), the d-p dispersion by Fujimoto (for t>>U), and the rotating wave approximate (RWA) d-p model applicable to the cuprates.

(b) The lower (bonding) band of the PtM (t>>U) compared with that of GA of the Emery model, the VMC result of Ref. [29] and GA of the three-band Hubbard model in the normal cuprates. Here the origin of E/|t| corresponds to $\Delta_o/|t| = U/(2|t|) = 0$.

energy term. The PtM result in Fig. (3b) yields the maximum and minimum bonding band energies when compared with the other three models there considered.

## 4. CONCLUSION

While emphasizing interband {Cu(3d) – O(2p)} transfer integral (t) and band (or orbital) levels separation (U), the present paper has isolated the possible pair states of the undoped (doped) cuprate system. The undoped system, represented by a simple pseudospm Hamiltonian, is dominated by electron kinetics and levels separations. This Hamiltonian revealed the level structure of the energy bands (d,p) and this was sketched. It was easily deduced that the large levels separations in the undoped system favour antiferromagnetic electronic spin ordering, as experimentally realised in the cuprates. On the other hand, large transfer energy integrals, that exhibit interband mixing and strong interactions, favour superconductive pairing in the excited (doped) state. The results for the normal state urge that the cuprates are most likely to be CT superconductors with doping. What appears to be reasonable is that, like the bismuthates, neither [30] quasi two-dimensionality nor magnetism may be essentially related to high-$T_c$ superconductivity in the cuprates. High-$T_c$ theories, hinged on these two concepts, for the cuprates, may be, among others, suspect.

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