Singular Band Behavior of the Extended Emery Model for High-$T_c$ Superconductors

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The three band structure of the extended Emery model for the copper-oxide layered materials is analyzed for all the values of the effective tight-binding parameters. The model is characterized by the Cu-O site energy splitting, the Cu-O first neighbor hopping and the O-O second neighbor hopping. For the sufficiently large O-O hoppings, the two bands can come together at one point on the diagonal of the square Brillouin zone, but they cannot cross. The range of the parameters for which the band touching occurs is determined. The model relates the band touching at the bottom of the two bands to the appearance of the extended, one-dimensional-like van Hove singularity at the lower edge of the density of states. With $1 + \delta$ holes ($\delta$ small) the extended van Hove singularity can thus occur close to the Fermi level only if the latter cuts two bands. The topology of the Fermi surfaces observed by ARPES in the high-$T_c$ superconductors eliminates such possibility. The Fermi surfaces in LSCO, Bi2212 and Y123 are then fitted with the one of the three bands at the Fermi level. The agreement is excellent considering in particular the fact that the fits use only two parameters. The departure of the measured band structure from the three band prediction found on the small energy scales away from the Fermi level is attributed to the effects of the fluctuations not included into the energy scales which define the three band structure.

1. INTRODUCTION

ARPES measurements of YBa$_2$Cu$_3$O$_{6.95}$ (Y123) [3], YBa$_2$Cu$_4$O$_8$ (Y124) [4], Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi2212) [4,5] and La$_2$-Sr$_x$CuO$_4$ (LSCO) [10,11] Fermi surfaces provide interesting information about the qualitative properties of the electron system in the high $T_c$ materials. At least roughly, the electrons behave as fermions with large Fermi surfaces which pass through the vicinity of the hyperbolic van Hove points of the Brioullin zone (BZ), in agreement with some early theoretical conjectures [12,13]. Additionally, the Fermi surface is unusually flat along one of the high symmetry directions passing through the hyperbolic van Hove point. This corresponds to the increase of the strength of the logarithmic van Hove singularity in the electron density of states. Related to it is the early theoretical proposal of the extended (one-dimensional) van Hove singularities [3,4,7,11], which are stronger than logarithmic.

The experimentally obtained $k$-dependance of the conducting band is usually fitted throughout the BZ with the Fourier series involving only the first and second harmonics in the symmetry allowed combinations $\Gamma$. Such fits use six independent parameters and they suggest in particular that the direct oxygen-oxygen hopping is small, but not negligible with respect to the direct copper-oxygen hopping of the electrons. The former procedure is unjustly called “tight-binding” fits.

Actually, the proper tight-binding calculation with one copper state and two oxygen states per unit cell leads to the three band structure which involves the first and higher harmonics in non-linear way. Only when the site energy splitting between copper and oxygen is by far the largest energy in the problem, the tight-binding structure of the conduction band becomes an additive combination of low order Fourier harmonics. Here, we will point out that the topology of the measured Fermi surfaces, especially those of the weakly doped LSCO, suggests that the site energy splitting between copper and oxygen is not large. The analysis of the electric field gradients in the high-$T_c$ superconductors led to the same conclusion. Therefore we carefully examined the tight-binding band structure characterized with the Cu-O site energy splitting, the Cu-O hopping and the O-O hopping, for all the ratios of these three parameters. The agreement with the experiments turns out to be remarkably good, although our fits use small number of parameters, presumably because the non-linear dependence of the band structure on the first harmonics is properly taken into account.

The observation of the shadow bands in Bi2212 [4,5,12,13] opens the possibility that two of three tight-binding bands are present at the Fermi level. The range of parameters for which this can occur is determined here. In the three band model this is accompanied by the appearance of the extended van Hove singularities. It will turn out, however, that the topologies of these two tight-binding Fermi surfaces and the observed Fermi surfaces cannot be reconciled, suggesting that the shadow band in Bi2212 is the result of spin or of structure induced doubling of the BZ. This also means that in the three band model the extended van Hove singularities cannot occur close to the Fermi level, but the usual logarithmic singularities are expected to be strongly enhanced.

Surprisingly enough, the simple three band tight-binding model [18] has not been examined in sufficient
detail before. The previous attempts were focused on the correlation effects in the high-$T_c$ oxides [19-23], examining the restricted range of the tight-binding parameters. It was concluded in particular that two lower bands can touch each other in the neighborhood of the Fermi level when the Cu-O site energy splitting and the oxygen-oxygen hopping are both positive [24]. Here we point out that such touching can occur for any relative sign of these parameters and even when the splitting vanishes. Small, doping dependant values of the renormalized Cu-O splitting are suggested by our comparison of the three band model with the ARPES data in the full range of the tight-binding parameters. This emphasizes the need for the correlation theory which leads to small, doping dependant values of the Cu-O splitting. It is interesting to note in this respect that the standard (the O-O hopping neglected) slave-boson mean field theory does lead to the effective Cu-O splittings which are small and even change sign for resolvable values of the bare tight-binding parameters [27]. The extensions of those results to the finite O-O hopping is therefore being carried out and will be presented in separate paper.

II. GENERAL

Here we examine the usual, nonmagnetic, undistorted CuO$_2$ square unit cell with $d_{x^2-y^2}$ ionic wave function associated to the Cu site, whereas the oxygen sites on the x and y axes are associated to the $p_x$ and $p_y$ states respectively. The phases of the wave functions are chosen as in Fig. 1, $\Delta$ is the splitting between oxygen and copper site energies, $\Delta = \varepsilon_p - \varepsilon_d$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{Schematic representation of the CuO$_2$ plane defining the band parameters and the choice of the phases of the ionic wave functions.}
\end{figure}

The hole picture is used here so that $\Delta > 0$ corresponds to the usually quoted values of $\varepsilon_p - \varepsilon_d$ [19-23]. The hybridisations between Cu and O and between two neighbouring oxygens are introduced through the hopping integrals $t$ and $t'$ respectively. This simple picture covers the noninteracting holes (electrons) in the CuO$_2$ plane, but also the case of the very large interaction $U_d$ on the copper site, if the latter is treated by the mean-field slave boson approximation [19] or by the appropriate Hartree-Fock [24]. Both approximations lead to the renormalisation of the bare values of $\Delta$ and $t$, whereas $t'$ is not affected by correlations. The Bloch states are built in the usual tight-binding way from $d_{x^2-y^2}$, $p_x$ and $p_y$ states in each unit cell and the band energies $\varepsilon_i(k)$ are found by diagonalisation of 3x3 hermitean matrix. This leads to the secular equation of the third order

$$\varepsilon^3 + 3p\varepsilon + 2q = 0$$  \quad (1)

where

$$p = -[\alpha + \beta(\eta^2 + \xi^2) + \gamma\eta^2\xi^2],$$  \quad (2)

$$q = a + b(\eta^2 + \xi^2) + c\eta^2\xi^2,$$  \quad (3)

with

$$a = \frac{1}{27}\Delta^3, \quad b = \frac{2}{3}t^2\Delta, \quad c = -\frac{16}{3}t'[t'\Delta + 3t'^2],$$

$$\alpha = \frac{1}{9}\Delta^2, \quad \beta = \frac{4}{3}t^2, \quad \gamma = \frac{16}{3}t'^2,$$  \quad (4)

and

$$\eta = \sin\frac{k_x}{2}, \quad \xi = \sin\frac{k_y}{2}. \quad (5)$$

$\varepsilon$ is the energy measured with respect to $\bar{\varepsilon} = (\varepsilon_d + 2\varepsilon_p)/3$. The hermiticity of 3x3 tight-binding matrix ensures that three roots $\varepsilon_i(k)$ of Eq. (1) are real. It should be noted that Eq. (1) is invariant on the simultaneous replacement $\Delta \rightarrow -\Delta$, $t' \rightarrow -t'$ and $\varepsilon \rightarrow -\varepsilon$, irrespectively of the sign of $t$. This means that the band structure $\varepsilon_i(k)$ for $\Delta < 0, t' < 0$ or for $\Delta > 0, t' < 0$ can be obtained from the $\varepsilon_i(k)$ for $\Delta > 0, t' > 0$ or for $\Delta < 0, t' > 0$ respectively by the reflection on the k plane. We shall therefore, without the loss of generality, carry out the theoretical discussion for $t, t' > 0$ and for both signs of $\Delta$, although $t' < 0$ will also suit the experimental situation, as discussed in Section III. It can be finally noted that the band structure in the electron language, appropriate for the ARPES analysis is obtained from the band structure in the hole language used here by the reflection on the k plane.

III. SMALL $T'$

It is instructive to start the discussion of the features of the energy bands by introducing $t'$ as a small quantity. The well known results for $t' = 0$ are shown in Fig. 1. For $\Delta > 0$ lower band $\varepsilon_L$ is splitted from the intermediate and the upper band $\varepsilon_I, \varepsilon_U$ by $\Delta$ and the latter two bands,
$\varepsilon_L$ being dispersionless, are degenerate at the $\Gamma$ point. For $\Delta < 0$, the dispersionless band joins the lower band coinciding with it at the $\Gamma$ point. The lowest band $\varepsilon_L$ is half filled in the stoechiometric crystal, and the Fermi energy $\varepsilon_F^L$ coincides with the van Hove singularities at $\varepsilon_x^L$, for any value of $t$ and $\Delta$.

The main qualitative effect of $t'$ is the change in the number of the states below the van Hove singularity at $\varepsilon_x^L$, the value of which remains itself unaffected by $t'$. For $\Delta < 0$ or $\Delta > 0$ the number of the states below $\varepsilon_x^L$ is increased or decreased respectively. In both cases the Fermi level $\varepsilon_F^0$ of the half-filled band is removed from the van Hove singularity at $\varepsilon_x^L$. The quantitative discussion is based on Fig. 3.

For $\Delta < 0$ the $\varepsilon_x^L$ equienergetic straight line is bent towards the $\Gamma$ point and all the states between this line and the finite $t'$ curve are transferred from below $\varepsilon_x^L$ to the energies above it. The number of the transferred states can be determined for small $t'$ by expanding in terms of the small departure of the $\varepsilon_x^L$ equienergetic curve for $t' \neq 0$ from the straight line and by calculating the surface between the straight line and this curve. Thus obtained number of the transferred states $\delta_c$ is

$$
\delta_c = -\frac{4t'}{\pi^2t} \text{sign}\Delta, \quad t' < |\Delta| < t, \quad (8a)
$$

and

$$
\delta_c = -\frac{8t'}{\pi^2\Delta}, \quad t'|\Delta| < t^2 < \Delta^2. \quad (8b)
$$

The energy $\varepsilon^0$ which divides the number of the states in the band in two halves can be calculated in the same spirit by finding the equienergetic curve which encompasses the same number of states below and above the straight line, as shown in Fig. 3. For the two regimes considered above

$$
(\varepsilon^0 - \varepsilon_x^L) \ln \frac{|\varepsilon^0 - \varepsilon_x^L|}{4t} = 2t'\text{sign}\Delta, \quad (9a)
$$

and

$$
\frac{\Delta(\varepsilon^0 - \varepsilon_x^L)}{t^2} \ln \frac{\Delta(\varepsilon^0 - \varepsilon_x^L)}{t^2} = \frac{16t'}{\Delta}. \quad (9b)
$$

Note that $\varepsilon^0$ coincides with the Fermi level when the band $\varepsilon_L$ is half filled, and then $\delta_c$ is the critical hole doping which brings the Fermi level to $\varepsilon_x^L$.

The number of the states $\delta$ between the two close energies $\varepsilon$ and $\varepsilon^0$ can be determined by similar reasoning as

$$
\varepsilon - \varepsilon^0 = \frac{\pi^2t\delta}{2 \ln \frac{|\varepsilon - \varepsilon_x^L|}{4t}} \text{sign}\Delta, \quad (10a)
$$

and

$$
\varepsilon - \varepsilon^0 = \frac{\pi^2t\delta}{8\Delta \ln \frac{\Delta(\varepsilon_x^L - \varepsilon^0)}{\varepsilon^0 - \varepsilon_x^L}}. \quad (10b)
$$

Obviously, Eq. (10) also defines the position of the Fermi level at $\varepsilon = \varepsilon_F$, if $\delta$ is taken to be the doping of the CuO$_2$ plane.

In two considered limits Eqs. (10) can be used to determine the density of states $d\delta/d\varepsilon$ for $\varepsilon$ between $\varepsilon_x^L$ and $\varepsilon^0$

$$
n_L(\varepsilon) = \frac{2}{\pi^2t} \frac{1 + 2t'}{t} \ln \frac{|\varepsilon - \varepsilon_x^L|}{4t}, \quad (11a)
$$
and

\[ n_L(\varepsilon) = \frac{|\Delta|}{2\pi^2t^2}(1 + 4t')\ln \frac{\Delta(\varepsilon - \varepsilon_0^L)}{t^2}, \]  

(11b)

or vice versa, Eqs.(11a) and (11b) can be used to derive Eq.(10). The density of states between \( \varepsilon \) and \( \varepsilon_0^L \) is given by

\[ n_L(\varepsilon) = \frac{2|\Delta|}{\pi^2t} \frac{1}{\sqrt{t^2 - 32t'\varepsilon}} K\left[ \frac{8(2^{1/2}|\Delta| - 4t't^2 - 2\varepsilon\Delta^2)}{t^3\sqrt{t^2 - 32t'\varepsilon}} \right], \]

where the first term in Eq. (12a) is omitted and \( K(x) \) is the complete elliptic integral of the first kind. For \( t'|\Delta| < t^2 < \Delta^2 \), Eq.(12b) reproduces the result (11b).

**IV. BAND DEGENERACY**

The main aim of the discussion which follows is to consider the degeneracies of the three bands \( \varepsilon_i \), at a given \( k \), which are caused by inclu- 

ding the oxygen-oxygen hopping \( t' \) into the dispersions in non-perturbative way. It is clear from Fig. 3 that such effects can occur only when the dispersions related to \( t \) and \( t' \) are at least of the same order of magnitude, i.e. for the sufficiently large \( t' \).

The large \( t' \) is also related to the qualitative modification of the dispersion within each band itself, e.g. the bending of the \( \varepsilon_i^L \) equienergetic line, instead of being small, as in Fig 3, becomes large, obviously changing the symmetry properties of the equienergetic surfaces all over the BZ. This is related to the fact that the O-O overlap induces the hopping along the diagonal of the Cu-O unit cell, unlike the Cu-O overlap, associated with the propagation along the cell’s main axes, i.e. the additional propagation axes are rotated by \( \pi/4 \) with respect to the original ones.

As well known, the quantity proper to the study of the degeneracy of the spectrum \( \varepsilon_i \), at a given \( k \) is

\[ D = q^2 + p^3, \]  

(13)

known as the discriminant of the third order Eq.(1). The hermiticity of the problem, i.e. of 3x3 tight-binding matrix, which makes the roots \( \varepsilon_i \) real, ensures that

\[ D \leq 0 \]  

(14)

For \( D < 0 \), all the roots \( \varepsilon_i \) are real and different, whereas \( D = 0 \), with \( p^3 = -q^2 \neq 0 \) implies that two roots are degenerate. For \( p = q = 0 \), all three roots coincide. Together with the inequality (14), this means that the zero of \( D \) at a given point \( k \) of the BZ is also the maximum of \( D \). Therefore, instead of the direct calculation of the zeroes of \( D \), which is the third order polinomial in \( \eta^2 \) and \( \xi^2 \), it is possible to find the optima of \( D \) with respect to \( \eta \) and \( \xi \), and to determine which of those, if any, are the zeros of \( D \). In carrying out this procedure, it is convenient to use the polar coordinates instead of \( \eta \) and \( \xi \) of Eq.(1)

\[ \eta = \rho \sin \varphi, \xi = \rho \cos \varphi. \]  

(15)

The zero of the derivative of \( D \) with respect to \( \varphi \) is easily found to be

\[
\frac{\partial D}{\partial \varphi} = \rho^4 \sin 4\varphi [c(a + b\rho^2 + cp^4 \sin^2 2\varphi) - \frac{3\gamma}{2}(a + \beta \rho^2 + \gamma \rho^4 \sin^2 2\varphi)^2] = 0. \]  

(16)

The advantage of this representation is that, besides separating out immediately the trivial solution at \( \rho = 0 \), which corresponds to the degeneracy at the \( \Gamma \) point, it also exhibits other possible band degeneracies at \( \varphi = 0, \pi/4 \), i.e. on the \( \Gamma X \) and \( \Gamma M \) axes of the BZ.

The nature of the third maximum, associated with the zero of the square braces in Eq.(16) is best understood for \( t = 0, \) when this zero occurs for

\[ \rho^2 \sin 2\varphi = \frac{|\Delta|}{2t'}. \]  

(17)

This is easily recognized as the condition that the pure oxygen band crosses the dispersionless copper level, as shown in Fig. 4. Consequently, \( D_0 = D(t = 0) = 0 \) on the line (17).

**FIG. 4.** Energy structure bands when \( t = 0 \), separated in two oxygen bands and the dispersionless copper level, energy in units \( t' \).
In the next step the change $\Delta D$ is calculated to the leading order in $t$. On the line \([17]\)

$$\Delta D = -\frac{32}{27} t^2 (\rho^2 - \frac{\Delta}{2t'})$$  \(18\)

It follows that $\Delta D < 0$ in all the points on the crossing line (17) except for $\Delta > 0$ in the single point on the $\Gamma M$ diagonal

$$\varphi_3 = \frac{\pi}{4}, \quad \rho^3 = \frac{\Delta}{2t'}$$  \(19\)

where $\Delta D = 0$, i.e. $D = D_0 + \Delta D = 0$. The band degeneracy associated with the third maximum of D occurs on the $\Gamma M$ diagonal and it is possible only for the same sign of $\Delta$ and $t'$. The variation of $\Delta D$ in the vicinity of the line (17) is weak with respect to the variation of $D_0 < 0$, i.e. $D = D_0 + \Delta D < 0$ in the vicinity of the line (17). Therefore, small $t$ removes the degeneracy of two bands, except at the point (19), rather than displacing slightly the crossing line (17) to the new position. In other words, small $t$ introduces the anticrossing of the oxygen band and the former copper level, excepting the single point (19) for $\Delta > 0$, as exemplified in Fig.5a and 5b.

\[
\begin{array}{c}
\text{FIG. 5. Band anticrossing when } t'/t = 3 \text{ and } \\
\text{or } \Delta/t = -5 \text{ (a) and touching for } \\
\text{or } t'/t = 3 \text{ and } \Delta/t = 5 \text{ (b), energy in units } t.
\end{array}
\]

Turning back to the first, $\varphi_1 = 0$ maximum of $D$, on the $\Gamma X$ line, we note that for $t = 0$ it corresponds to the degeneracy of two oxygen bands, symmetric by reflection on the $k$ plane, while the dispersionless copper level is decoupled from the oxygen bands. When the copper is removed, the natural BZ corresponds to one oxygen per unit cell, i.e. it is rotated for $\varphi/4$ with respect to the original one and increased by $\sqrt{2}$. In this zone two bands unfold into one continuous oxygen band and the dispersionless $\Gamma X$ line becomes analogous to the dispersionless straight line in Fig.5 for $t = 0$. The corresponding singularity in the density of states is therefore logarithmic \([13, 20]\).

For $t \neq 0$, the degeneracy on the $\Gamma X$ line is removed, except in the $\Gamma$ point, as shown e.g. in Fig.5b, with the consequences further discussed in Sec.5.

A. Lower critical value of $t'$. The previous discussion shows that for finite $t, t'$ the degeneracies of the bands at a given $k$ point can occur only on the $\Gamma M$ line. Setting $\eta = \xi$ in the equation $D(\eta, \xi) = 0$ simplifies considerably further discussion. To this effect, it is convenient to distinguish between $\Delta > 0$ and $\Delta < 0$, as already suggested by Eq.(18) and start with the limit of small $|\Delta|$. The solution of the equation $D = 0$ is particularly simple around $\Delta = 0$ at the $M$ point of the BZ. By increasing $t'$ from zero, the dispersionless oxygen level $\epsilon_L$ of Fig.2 bends towards the lower band $\epsilon_I$ and these two bands touch at the $M$ point. It can be shown analytically that, for $|\Delta|$ small, the degeneracy at the $M$ point occurs for

$$\frac{t'}{t} = 0.5 + 0.167 \frac{\Delta}{t},$$  \(20\)

i.e. for $\Delta > 0$ the oxygen level must bend more to cross the gap $\Delta$ than for $\Delta < 0$, when there is no gap to cross. Eq.(20) shows that the band touching occurs not only for $\Delta > 0$, as already known [21], but also for $\Delta < 0$. This is allowed by the solution $\varphi_2 = \pi/4$ of the Eq.(18), although the solutions $\varphi_3 = \pi/4, \rho_3$, given by Eq.(19), is not a zero of $D$ when $\Delta < 0$. The full curve $t'_{cr}/t$ versus $\Delta/t$ is obtained numerically in Fig.6. The limit of the large $\Delta/t$ in Fig.5 is transparent: it corresponds to the situation when the pure oxygen band touches the flat copper level at the $M$ point of the BZ. According to the Eq.(17), this occurs for $4t'_{cr} = \Delta$. In Fig.7a and 7b, the full three band structures, obtained by solving Eq.(11) numerically, are displayed for $\Delta/t = \pm 0.5$ when $t'/t = t'_{cr}/2t = 0.64$ and 0.39 respectively.

\[
\begin{array}{c}
\text{FIG. 6. For } t' \text{ increasing from the lower critical value } t'_{cr} \text{ to the upper critical value } t'_{cr}, \text{ the band touching that starts at the } \Gamma \text{ point moves along the } \Gamma M \text{ line towards the } \Gamma \text{ point. Limiting behaviors for small and large } \Delta/t \text{ described in the text are completed numerically (red dots). } \Delta \text{ and } t' \text{ in units } t.
\end{array}
\]
\[ \Delta/2t = -1 \] of Fig. 8d.

### B. Upper critical value of \( t' \)

It is further interesting to investigate what happens for \( t' > t'_{\text{cr}} \) for the fixed value of \( \Delta/t > 0 \) in Fig. 4. Some representative band structures are shown in Fig. 7 for \( \Delta/t = 1 \). It appears that the bands \( \varepsilon_I \) and \( \varepsilon_L \) touch at a point which moves from the M point towards the \( \Gamma \) point as \( t' \) increases from \( t'_{\text{cr}} \). For \( t'/t \gg 1 \), the regime of the Eq. (17), (18) and (19) is reached, i.e. the touching of the bands occurs at \( \rho^2 = \Delta/2t' < 1 \).

![Fig. 7. Illustration of the touching of the two lower bands when \( t' \) and \( \Delta \) are of the same sign for \( \Delta/t = 1 \). The touching point moves from M point (a) towards \( \Gamma \) point (b), when the value of \( t' \) is increased from its critical value \( t'_{\text{cr}} \). Energy in units \( t \).](image1)

The situation is more complicated for \( \Delta < 0 \). It is illustrated in Fig. 8 for \( \Delta/t = -1 \). As \( t'/t \) increases beyond \( t'_{\text{cr}}/t \), the point of the coincidence moves towards the \( \Gamma \) point, reaching and leaving it for

\[
\frac{t'_{\text{cr}}}{t} = -\frac{2t}{\Delta}. \tag{21}
\]

For this value of parameters \( \varepsilon_I \) is again dispersionless as it was before for \( t = 0 \) in Fig. 4. The corresponding dispersions of the bands \( \varepsilon_L \) and \( \varepsilon_U \) are given by

\[
\varepsilon_{L,U} = -\frac{\Delta}{2} \left[ 1 \pm \sqrt{1 + \frac{16t^2}{\Delta^2} \left( \eta^2 + \xi^2 + 16\eta^2\xi^2 \right)} \right]. \tag{22}
\]

For \( t' > t'_{\text{cr}} \), \( \varepsilon_I \) starts to bend towards \( \varepsilon_U \) and, according to the Eq. (19), reaches the anticrossing with this band at \( \rho^2 \) given approximately by Eq. (17). This anticrossing is more pronounced for \( \Delta/2t = -5 \) of Fig. 8b, than for

![Fig. 8. Illustration of the touching of the two lower bands when \( t' \) and \( \Delta \) are of the opposite sign for \( \Delta/t = -1 \). The touching point of the two lower bands moves from M point (a) towards \( \Gamma \) point when the value of \( t' \) is increased from \( t'_{\text{cr}} \) to \( \tilde{t'}_{\text{cr}} \) at which the intermediate band becomes flat (c). With further increment of \( t' \) this band bends upwards (d). Energy in units \( t \).](image2)

The discussion is completed by showing in Fig. 9a, the band touching of Fig. 8b with better resolution, the equienergetic surfaces of the bands \( \varepsilon_L \) and \( \varepsilon_I \) when they touch in the Fig. 8d and the full dispersion of the bands \( \varepsilon_L \) and \( \varepsilon_I \) in Figs. 8c and d. The topology of the bands on Fig. 8b for \( \Delta < 0 \) shows striking similarity to the one found before for the bands that touch at \( \Delta > 0 \), i.e. the observation of such topology cannot be used to select the
ε can be obtained in the closed form those two (cf. Fig.6) because then the electron spectrum be studied explicitly on the borderline ∆ = 0 between ∆ = 0 limit.

In Sec.VI that the experimental spectra are close to the Eq.(23) and (24) are useful also because it will turn out low order harmonics tight-binding approximation the spectrum is built from sign of ∆.

The features described above for ∆ = 0 can

\[ \varepsilon_L = -4t' \sqrt{\frac{n^2 \xi^2}{4t'^2} (\eta^2 + \xi^2) + \frac{t'^2}{t' \eta^2 \xi^2} + \frac{\eta^2 \xi^2}{4t'^2} (\eta^2 + \xi^2)} , \]  
\[ \varepsilon_I = -2t^2 \frac{\eta^2 \xi^2}{t' \eta^2 \xi^2} + \frac{t'^2}{4t'^2} (\eta^2 + \xi^2) , \]  
\[ \varepsilon_U = 4t' \sqrt{\frac{n^2 \xi^2}{4t'^2} (\eta^2 + \xi^2) + \frac{t'^2}{t' \eta^2 \xi^2} + \frac{\eta^2 \xi^2}{4t'^2} (\eta^2 + \xi^2)} . \]

for \( t' \gg t \) and similarly for \( t' \ll t \).

Eqs.\([34],[23]\) and \([23]\) illustrate the fact that in the tight-binding approximation the spectrum is built from low order harmonics \( n^2, \xi^2 \) of the Eq.\([3]\) in nonlinear way. Eq.\([23]\) and \([24]\) are useful also because it will turn out in Sec.VI that the experimental spectra are close to the \( \Delta = 0 \) limit.

FIG. 9. The band touching of Fig.8d with better resolution (a), the equienergetic surfaces of the bands \( \varepsilon_L \) and \( \varepsilon_I \) when they touch (b) and the full dispersion of the bands \( \varepsilon_L \) and \( \varepsilon_I \) (c and d). Energy in units \( t \).

**V. EXTENDED VAN HOVE SINGULARITIES**

Inspection of Figs.\([3],[4,\dot{5}]\) shows that the degeneracy of the bands \( \varepsilon_L \) and \( \varepsilon_I \) at the point \( \mathbf{M} \), for \( t' = t'_{cr} \) is accompanied in the band \( \varepsilon_L \) with the absence of the dispersion on the line between \( \Gamma \) and \( \mathbf{M} \) points. It appears that the dispersion depends only on the component of the wavevector perpendicular to the \( \Gamma \mathbf{M} \) line, in a quadratic way, i.e. the dispersion is one-dimensional on whole \( \Gamma \mathbf{M} \) line. As a result, an "extended" van Hove singularity is found in the density of states \([3],[4,\dot{5}]\) of the lowest band

\[ n_L(\varepsilon) \approx \frac{B}{\sqrt{\varepsilon - \varepsilon_{L}^M}} . \]  

When the degeneracy between the \( \Gamma \) and \( \mathbf{M} \) points is lifted by changing slightly \( t' \) from \( t'_{cr} \), the usual step singularity at \( \varepsilon_L^M \) and the logarithmic singularity at \( \varepsilon_I^M \) are recovered in \( n_L(\varepsilon) \), lying close to each other in energy, i.e. enhancing each other. The described coalescence of these two singularities can be explicitly found in Eq.\([12]\), but it occurs there for \( -8t' = \Delta \), when, unfortunately, the expansion in terms of \( |\Delta| \gg t, t' \) is only qualitatively correct.

Similar extended van Hove singularities are associated with the absence of the dispersion on the \( \Gamma \mathbf{X} \) line in the band \( \varepsilon_I \) for any finite values of \( t \) and \( t' \). For \( t = 0 \) however, as already explained below Eq.\([15]\), the copper level is decoupled from the oxygen band structure and the usual step singularity \( \varepsilon_I^M \) and the logarithmic singularity \( \varepsilon_I^M \) are recovered in \( n_L(\varepsilon) \), lying close to each other in energy, i.e. enhancing each other. The described coalescence of these two singularities can be explicitly found in Eq.\([12]\), but it occurs there for \( -8t' = \Delta \), when, unfortunately, the expansion in terms of \( |\Delta| \gg t, t' \) is only qualitatively correct.

It is apparent here that in the three band model with \( 1 + \delta \) holes, the Fermi level falls far from the extended van Hove singularity in the \( \varepsilon_I \) band. On the other hand, when the extended van Hove singularity \( \varepsilon_I^M \) occurs for \( t' = t'_{cr} \) in the \( \varepsilon_L \) band, the Fermi level crosses necessarily two bands, \( \varepsilon_L \) and \( \varepsilon_I \). This fact makes the discussion of the main band and the shadow bands, observed in some of the high-\( T_c \) superconductors \([2],[3],[5]\), quite relevant. The rest of this paper is devoted to the analysis of the empirical band structure. As already mentioned, it will turn out that the observed dispersions of the main band and the shadow band cannot be reconciled with \( \varepsilon_L(\mathbf{k}) \) and \( \varepsilon_I(\mathbf{k}) \), i.e. the extended van Hove singularities of the three band model do not occur close to the Fermi level.
VI. EXPERIMENTS

The previous discussion provided the complete description of the three band structure. Although it was carried out for \( t' > 0 \) and arbitrary sign of \( \Delta \), the symmetry properties (cf Sec.I) extend it to the entire range of the parameters. In this section, we shall compare these results with the experimental data obtained by the ARPES measurements.

The first step is to determine the position of the Fermi level \( \varepsilon_F \) for the doping \( \delta \) in the calculated band structure, then to find the corresponding Fermi surface and finally to compare it with the empirical data. Since the discussion was carried out in the hole picture, \( 1 + \delta \) holes by varying appropriately the tight-binding parameters. In this section, we shall compare these results with the experimental data obtained by the ARPES measurements.

Using in particular the regime separation summarized in Fig.11, all the regimes of the parameters are examined in this way, comparing the topology of the obtained Fermi surfaces with the corresponding experimental data. The bending of the Fermi surfaces towards the \( \Gamma \) point requires that \( \Delta \) and \( t' \) have the opposite signs for all the considered materials. This is already apparent in the small \( t' \) limit of Sec.III and generalizes to arbitrary \( t' \). The values of the parameters vary among different materials as will be discussed below. It is also appropriate to point out that all the experimentally obtained Fermi surfaces are fitted here with only two different parameters, e.g. with \( t/2t' \) and \( \Delta/2t' \). Two more parameters, e.g. \( t \) and \( \bar{\varepsilon} = (\varepsilon_d + 2\varepsilon_p)/3 \) are needed to fit the conducting band(s) away from \( \varepsilon_F \).

A. \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \)

The recent ARPES measurements in LSCO \([10,11]\) give the evolution of the Fermi surface in the large range of dopings \( \delta \). The two parameters fit of those data are shown in Fig.10. Two sets of fitting parameters, given in Fig.11, one characterized by \( t' > 0, \Delta < 0 \) and the other by \( t' < 0, \Delta > 0 \), fit the data equally well. It follows that the rigid band model is completely inadequate to describe the evolution of the Fermi surface with \( \delta \), because in both sets \( \Delta/2t' \) and \( t/2t' \) undergo large variations with \( \delta \).

It is further important to note in Fig.11 that for both sets of parameters \( \Delta/2t' \) and \( t/2t' \) are small for small \( \delta \). This is best understood by noting that for \( \Delta = 0, t = 0 \) the Fermi surface of the half-filled (\( \delta = 0 \)) band coincides with \( k_x \), \( k_y \) axes of the BZ, which in the qualitative terms corresponds to the Figs.10a–e. As already explained in Sections II and V, the energetic degeneracy of the \( \Gamma \) line in the pure \( (t = 0) \) oxygen model is related to the logarithmic rather than to the extended van Hove singularities.
larity in the density of states.

FIG. 11. Two sets of the fitting parameters with $\Delta > 0$, $t' < 0$ (a) and $\Delta < 0$, $t' > 0$ (b) in units $2t'$, that fit the experimentally obtained Fermi surfaces [10,11] of LSCO, shown on Figs. 11a-e, equally well. For $\delta = 0.05$ and $\delta = 0.1$ on the Fig. 11a, $\Delta/2t'$ and $t/2t'$ have the same values.

The full band structure with $\Delta$ and $t$ small, but finite is shown in the Fig. 12 for $\Delta < 0$, $t' > 0$. In particular Figs. 12e and d illustrate that weak dispersion is introduced by $t$ in the conducting band $\varepsilon_{L}$ along the $\Gamma\mathbf{X}$ line, i.e. the van Hove singularity at $\mathbf{X}$, although enhanced, is logarithmic. Fig. 12 also shows that for the values of the parameters found in the case $\Delta < 0$, $t' < 0$ the band $\varepsilon_{I}$ is rather far from the Fermi level. For $\Delta > 0$, $t' > 0$, this holds independently on the values of the parameters.

FIG. 12. Calculated three band structure obtained for the parameters of Fig. 11, energy in units $t$.

The usual $t' = 0$ mean field slave boson theory with large $U$, other interactions absent, allows small and even negative values of $\Delta$ [24], but large variations of $\Delta$ and $t$ with the doping $\delta$ are not obtained this way. The slave boson calculations with finite $t'$ are under way for this reason and also because the previous results with finite $t'$ do not cover the range of parameters which appeared to be relevant here.

B. $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$

As interesting feature of the ARPES results in Bi2212 taken in the normal state is the appearance of two Fermi surfaces in the BZ [4–6, 8, 9]. There are points in the 2d $k$ space in which two Fermi lines cross or touch. In the three band model such points can occur only on the $\Gamma\mathbf{M}$ line, as shown in Figs. 13a and b, whereas the experimental crossing or touching points fall quite far from this line. It is therefore more appropriate to interpret two observed Fermi lines as belonging to the main band of the same topology as the one found in LSCO, and to the shadow band obtained by the $(\pi, \pi)$ shift of the main band. It is likely that this shift is produced by AF or by structural $(\pi, \pi)$ superlattice. The values of parameters which fit the main band are $\Delta/2t' = -0.0625$ and $t/2t' = -0.1$, i.e. Bi2212 has even smaller values of $\Delta$ and $t$ than LSCO with $\delta \approx 0.05$. However, the number of holes $1 + \delta$ below Fermi level corresponds to $\delta \approx 0.25$. Similar conclusion holds also for $\Delta < 0$, $t' > 0$.

In addition to the Fermi surfaces the ARPES measurements in Bi2212 provide the information about the states filled with electrons, i.e. about the empty hole states [16]. When the fit is extended to the energies away from the $\varepsilon_{F}$, $\bar{\varepsilon}$ and $t$ are determined. The best fits to those measurements are shown in Fig. 13c. The idea underlying these fits is that the Fermi liquid theory applies to the effects of magnetic, structural or superconducting fluctuations, beyond the mean field slave boson theory. The latter gives only the basic band structure, which was discussed here. The Fermi liquid renormalisation of this structure by fluctuations presumably vanish at $\varepsilon_{F}$, i.e. the band theory is accurate at $\varepsilon_{F}$ [27], as it is implicit from the fits of the Fermi surfaces, given in Figs. 11 and 13. The departures of the experimental data from such fits are thus to be associated with the fluctuation effects.
away from $\varepsilon_F$.

![Diagram](image1.png)

**FIG. 13.** Experiments in Bi2212 [4] for the Fermi surface (a) and band structure (b) (green dots), the three band model fits (solid) and the full three band structure (c) obtained for the parameters $\Delta/2t' = -0.0625$, $t/2t' = -0.1$, $\bar{\varepsilon} = 0.44\text{eV}$ and $t = 0.08\text{eV}$.

The most prominent fluctuation effect defined this way is the flattening of the measured dispersion along the XM line, compared to the band model prediction (Fig. 13b). This flattening is understood here as the precursor of the gap opening around the X point, which is observed e.g. on doping Bi2212 with Dy [28]. The precursor is not expected to be a simple pseudogap, which occurs only when the adiabatic approximation can be applied to the relevant fluctuations. Due to the small velocity of electrons, the adiabatic approximation fails in the van Hove singularity, and the band states are conserved at the Fermi level, although a part of them can be transferred to the pseudogap wings. This theoretical prediction, which justifies the description of the Fermi surface by the band theory, is borne out by the recent high resolution ARPES measurements along the $\Gamma X$ line [29]. Those data show empirically that the states close to $\varepsilon_F$ in the vicinity of the X point are shared between the peak at $\varepsilon_F$ and the pseudogap wings. The calculations of the detailed $k$ dependences and the comparison with the experiments is currently under way.

**C. YBa$_2$Cu$_3$O$_6.95$**

There are two planes per unit cell of Y123 which result in dimerisation of the CuO$_2$ bands along the axis perpendicular to the planes. In addition, the CuO chains of Y123 are conducting, which complicates further the analysis of the observed band structure. It is however reasonable to assume that the lowest of the CuO$_2$ bands undergoes only the dispersionless dimerisation shift towards lower energies.

The fit of the lowest band measured in Y123 [12] with the three band model, shown in Fig. 14, proceeds similarly to the cases of LSCO and Bi2212. The Fermi surface fit leads to $\Delta/2t' = -0.0625$, $t/2t' = -0.1$ i.e. to the values characteristic for Bi2212. It is interesting to note that the band flattening observed in Bi2212 along the XM line does not occur in Y123. If not a problem of the experimental resolution, this suggests that the nature of fluctuations which affect the vicinity of the X point in the electron spectrum differs considerably between Bi2212 and Y123 and opens an interesting question which requires further investigation.

![Diagram](image2.png)

**FIG. 14.** Experimentally measured structure of the lowest band of Y123 [1] (green dots) and the three band model fits (solid) with parameters $\Delta/2t' = -0.0625$, $t/2t' = -0.1$, $\bar{\varepsilon} = 0.58\text{eV}$ and $t = 0.08\text{eV}$.

**VII. CONCLUSION**

In contrast to the most of the many body theories of the high-$T_c$ superconductors, which are attempting to construct the electron band structure starting from a given set of bare band and interaction parameters, this paper assumes that the resulting average band structure can be described with a few effective near-neighbor tight-binding parameters. After the detailed analysis, which encompasses the rich structure of the three band model, it appears that the single band at the Fermi level describes the Fermi surfaces in LSCO, Bi2212 and Y123 remarkably well. Only two parameters are used in those fits, compared to the usual, at least four parameter fits of the Fermi surfaces. The improvement is obtained by the use of the effective tight-binding band structure which is non-linear in low order harmonics in contrast to the Fourier fits. This indicates that the average band structure arises from the (large) short range correlations. The departure of the predicted band behavior, measured in the vicinity the Fermi level, is used to determine the effects of the fluctuations on the small energy scales not included in the average band structure. This way the desired results of the many body theories are defined more clearly, they should end up with the effective tight-binding parameters in the energy range between 1eV and 0.1eV, and with the additional fluctuation effects on the
energy scales of the order of 0.1eV to 0.01eV. The corresponding space scales of the correlations involved into the average band structure and into departures from it are related in analogous way. Large energy scales alone describe the Fermi surface, what implies that the Fermi liquid theory is the good starting point in the calculation of the fluctuation effects.

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