HW 5 SSP 601- 2017.
here is a very realistic calculation which uses the concepts of lattice, reciprocal space, Brillouin zone and tight-binding approximation. Go over the solution and fill up every step and every detail in the provided solution. No computer algebra calculation i s allowed.

Problem 3: Band Structure of $YBa_2Cu_3O_7$[2]

In 1986, a family of oxides was found that proved to be superconducting with much higher critical temperatures than metals and alloys. The compounds in this oxide family all contain planes of copper and oxygen with Cu atoms at the nodes of a square lattice (see Fig. P3.1). Some members of this family also contain copper–oxygen chains.

An example is $YBa_2Cu_3O_7$. The real structure is shown in Fig. P3.2 (left). The simplification used in this problem is shown in Fig. P3.2 (right). The primitive cell of this compound contains two copper–oxygen planes (levels 2 and 3) and one family of chains, e.g., level 1.

The aim here is to investigate the band structure of $YBa_2Cu_3O_7$ in a simplified way using the tight-binding approximation (LCAO). 3.1 examines an isolated copper–oxygen chain. 3.2 then looks at an isolated copper–oxygen plane and two

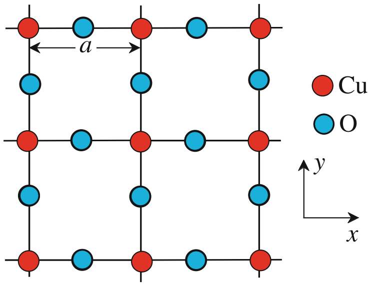

Fig. P3.1 CuO_2 square lattice

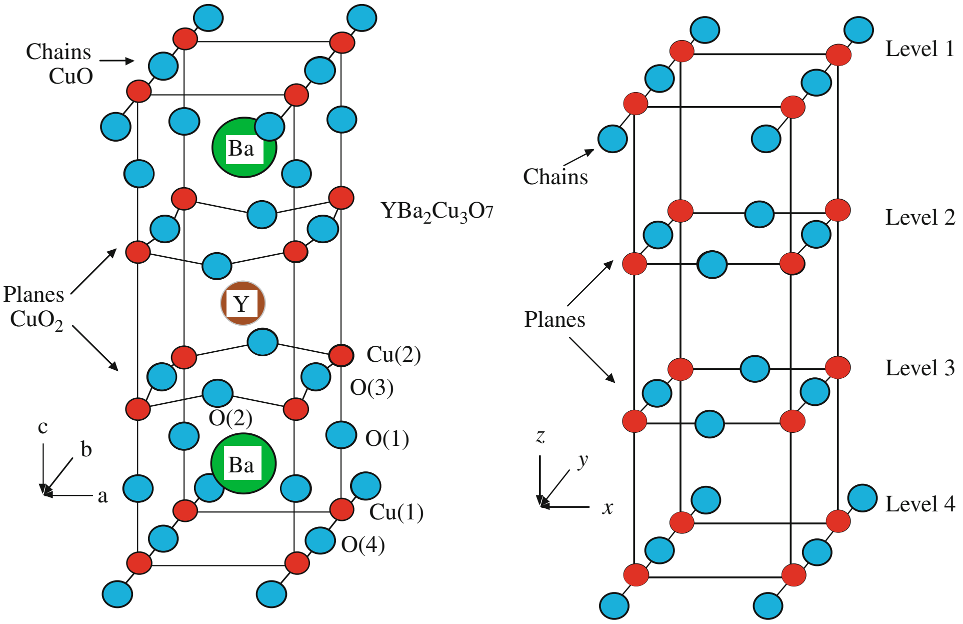

Fig. P3.2 Real structure of $YBCO_7$ (*left*) and simplified structure used in this problem (*right*)

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[2] This problem has been designed with C. Hermann and T. Jolicœur.

coupled planes, while 3.3 deals with the coupling between a plane and the nearest chains. Finally, 3.4 compares the results obtained in this way with a more detailed calculation and experimental data concerning $YBa_2Cu_3O_7$.

Throughout this exercise, we only take into account those orbitals with energy levels close to the Fermi level of the solid, i.e., the $3d$ orbitals of copper and the $2p$ orbitals of oxygen. To simplify, we assume that, within the basis, these atomic orbitals combine to form one atomic orbital per Bravais lattice point. This orbital will be denoted by $\phi_1(\mathbf{r})$ for the chains (3.1) and $\phi_2(\mathbf{r})$ for the planes (3.2 and 3.3). These orbitals are assumed to be isotropic, real, and normalised. We apply the LCAO method to these orbitals. We also assume that the orbitals of two neighbouring sites barely overlap, and take them to be orthogonal for simplicity. There is no need to write down the relevant Hamiltonians explicitly. All the necessary matrix elements will be given.

Note: Questions 4 and 7 in 3.2 are not essential for tackling the neighbouring questions.

3.1: Isolated Copper–Oxygen Chain

Consider an isolated chain of copper and oxygen atoms. Let a be the Cu–Cu distance and $\mathbf{y}$ the unit vector along the chain.

1. *Using Fig. P3.3, specify the Bravais lattice and basis of a copper–oxygen chain.*
2. *What is the associated reciprocal lattice? Specify the corresponding first Brillouin zone.*
3. *Give the form of the Bloch functions in the tight-binding approximation.* Let k be the corresponding wave vector.
4. *Considering only nearest neighbours, calculate the dispersion relation $E_C(k)$. Express the result in terms of the matrix elements*

$$E_C^0 = \int d^3\mathbf{r}\phi_1(\mathbf{r})\hat{H}_C\phi_1(\mathbf{r})\,, \qquad V_{2\,\text{chain}} = V = -\int d^3\mathbf{r}\phi_1(\mathbf{r})\hat{H}_C\phi_1(\mathbf{r}+a\mathbf{y})\,,$$

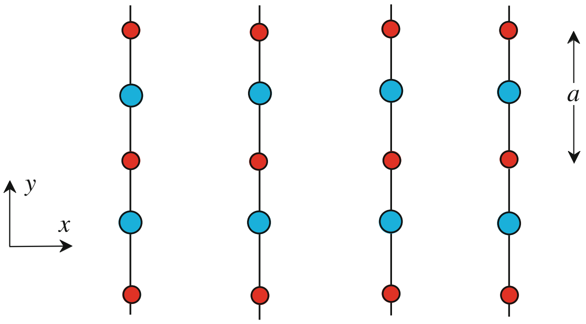

Fig. P3.3 Copper–oxygen chains

where $\mathbf{y}$ *is the unit vector along the chain and* $\hat{H}_C$ *is the Hamiltonian of an electron in the chain.*

5. *Plot the dispersion relation, assuming* $V > 0$. *If the electron occupation of this band is one electron per unit cell, what is the shape of the Fermi 'surface'? What happens if the electron occupation is very low? Give the effective mass* m^* *of the electrons in that case.*

3.2: Isolated Copper–Oxygen Plane

Consider an isolated copper–oxygen plane:

1. *From Fig. P3.1, specify the Bravais lattice and basis of a copper–oxygen plane. What is the associated reciprocal lattice. Specify also the corresponding first Brillouin zone.*

As in 3.1: consider one orbital per basis, denoted $\phi_2(\mathbf{r})$. Let $\hat{H}_P$ be the Hamiltonian of an electron in the plane.

2. *Give the form of the Bloch functions in the tight-binding approximation*. Let $\mathbf{k}$ be the corresponding wave vector. *Calculate the dispersion relation* $E_P(\mathbf{k})$, *considering only nearest neighbours. Use the matrix elements*

$$E_P^0 = \int d^3\mathbf{r}\phi_2(\mathbf{r})\hat{H}_P\phi_2(\mathbf{r})$$

   and

$$V_P = -\int d^3\mathbf{r}\phi_2(\mathbf{r})\hat{H}_P\phi_2(\mathbf{r}+a\mathbf{x}) = -\int d^3\mathbf{r}\phi_2(\mathbf{r})\hat{H}_P\phi_2(\mathbf{r}+a\mathbf{y}) \,,$$

   where $\mathbf{x},\mathbf{y}$ *are unit vectors along the x and y axes.*

3. *If the electron occupation of this band is one electron per unit cell, what is the shape of the Fermi 'surface'? If the number of electrons is* $1 \pm \delta$ *with* $\delta \ll 1$, *sketch the Fermi surface in the Brillouin zone. What happens if the band is almost empty?*

Now, and only for this question, consider second nearest neighbours in the plane using the matrix element

$$V_P' = \int d^3\mathbf{r}\phi_2(\mathbf{r})\hat{H}_P\phi_2(\mathbf{r} \pm a\mathbf{x} \pm a\mathbf{y}) \,,$$

where the notation ± indicates that the four matrix elements are equal by symmetry. Assume that $V_P' > 0$.

4. *For one electron per unit cell, what is the new value of the energy for those values of* $\mathbf{k}$ *that corresponded to the Fermi surface in the last question? Deduce the approximate position of the new Fermi surface in the region* $0 \le k_x, k_y \le \pi/a$.

In the compound $\mathrm{YBa_2Cu_3O_7}$, the planes are in fact coupled into pairs [levels 2 and 3 are coupled in Fig. P3.2 (right)]. We treat the case of an isolated double plane. This complicates the square lattice basis considered above. We now consider that there are two orbitals per site of this basis, one for each plane. These are $\phi_2(\mathbf{r})$ and $\phi_2(\mathbf{r}+c\mathbf{z})$, where $\mathbf{z}$ is the vector joining the two planes. Use the following LCAO function:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_j \exp(\mathrm{i}\mathbf{k}\cdot\mathbf{R}_j)\Big[A_k\phi_2(\mathbf{r}-\mathbf{R}_j) + B_k\phi_2(\mathbf{r}+c\mathbf{z}-\mathbf{R}_j)\Big] ,$$

where the sites $\mathbf{R}_j$ run over the points of the Bravais lattice of the plane $z = 0$ with j as index. The coefficients A_k and B_k are adjustable parameters.

5. *Show that the LCAO function satisfies Bloch's theorem. The Hamiltonian of an electron in the double plane is denoted by* $\hat{H}_{\mathrm{DP}}$.

Project Schrödinger's equation $\hat{H}_{\mathrm{DP}}|\Psi_{\mathbf{k}}\rangle = E(\mathbf{k})|\Psi_{\mathbf{k}}\rangle$ onto the functions $\phi_2(\mathbf{r})$ and $\phi_2(\mathbf{r}+c\mathbf{z})$. Simplify the problem by neglecting overlaps between distinct sites, i.e., assume that the orbitals $\phi_2(\mathbf{r})$ and $\phi_2(\mathbf{r}+c\mathbf{z})$ are orthogonal.

6. *Derive a homogeneous linear system of equations in which the unknowns are the coefficients* A_k *and* B_k*. Specify the coefficients of the system in the form of matrix elements of* $\hat{H}_{\mathrm{DP}}$*. Assume that the matrix elements involving only the orbitals of a given plane are the same as those of* $\hat{H}_{\mathrm{P}}$ *introduced in question 2. For matrix elements involving orbitals from both planes, keep only the one involving the same site, viz.,*

$$\int \mathrm{d}^3\mathbf{r}\,\phi_2(\mathbf{r}-\mathbf{R}_n)\hat{H}_{\mathrm{DP}}\phi_2(\mathbf{r}+c\mathbf{z}-\mathbf{R}_n) = T\ .$$

7. *How many bands are there? Give their dispersion* $E(\mathbf{k})$ *as a function of* $E_{\mathrm{P}}(\mathbf{k})$ *and* T*. Plot the result for* $0 \le k_x = k_y \le \pi/a$*. Assuming* T *small, and when there are two electrons per unit cell, one from each plane, locate the Fermi energy on the band diagram* $E(\mathbf{k})$ *for the given direction. Deduce the shape of the Fermi surface in the region* $0 \le k_x, k_y \le \pi/a$*, with the help of question 3.*

3.3: Chain and Plane

In $\mathrm{YBa_2Cu_3O_7}$, there are also copper–oxygen chains, as discussed in 3.1 and shown in Fig. P3.2 (right). Consider now a plane coupled with a lattice of chains. To describe the combined $\mathrm{CuO_2}$ plane in level 2 and Cu–O chains in level 1, use the same Bravais lattice as in 3.2, but consider two orbitals per primitive cell, viz., $\phi_1(\mathbf{r})$ of the chain and $\phi_2(\mathbf{r})$ of the associated plane.

1. Start by examining the lattice of Cu–O chains in level 1 using the tight-binding approximation. These chains are barely coupled together in $YBa_2Cu_3O_7$ and we may completely neglect matrix elements involving different chains. *Using 3.1, give the dispersion* $E_{CL}(\mathbf{k})$. *Plot this function for* $\mathbf{k} = (0, k_y)$ *and* $-\pi/a \leq k_y \leq +\pi/a$. *Plot the constant energy curves of* $E_{CL}(\mathbf{k})$ *in the region* $-\pi/a \leq k_x, k_y \leq +\pi/a$. *With one electron per unit cell in this band, sketch the Fermi 'surface'.*

2. Now investigate the coupled problem of the plane and the chains using the wave function

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_j \exp(\mathrm{i}\mathbf{k}\cdot\mathbf{R}_j)\Big[C_k\phi_1(\mathbf{r}-\mathbf{R}_j) + D_k\phi_2(\mathbf{r}+c\mathbf{z}-\mathbf{R}_j)\Big] .$$

   The one-electron Hamiltonian is now $\hat{H}_{PC}$. Assume that the matrix elements within a given plane are the same as those of $\hat{H}_P$ (see question 2 of 3.2: *Isolated Copper–Oxygen Plane*) and that, in the chain lattice, they are the same as those of $\hat{H}_C$ (see question 4 of 3.1 and question 1 of 3.3). *Using the arguments in 3.2, show that there are two bands* $E_\pm(\mathbf{k})$ *and express them in terms of* $E_P(\mathbf{k})$, $E_{CL}(\mathbf{k})$, *and the matrix element*

$$T' = \int \mathrm{d}^3\mathbf{r}\phi_1(\mathbf{r}-\mathbf{R}_n)\hat{H}_{PC}\phi_2(\mathbf{r}+c\mathbf{z}-\mathbf{R}_n) .$$

3. Assume that $T' = 0$ and that there are two electrons per unit cell, one per unit cell of the plane and one per unit cell of the chain lattice. Assume also that $E_P^0 = E_C^0$. *Plot the Fermi surface of the ensemble in the square* $0 \leq k_x, k_y \leq +\pi/a$.

4. Now consider the case $T' \neq 0$, still with $E_P^0 = E_C^0$. This coupling is only important where the Fermi surfaces of the plane and the chains used to intersect. *By examining the neighbourhood of the point* $\mathbf{k} = (\pi/2a, \pi/2a)$, *make a qualitative sketch of the Fermi surface for the electron occupation of question 3 in* 3.3: *Chain and Plane, then for an occupation number close to this. What simple remark can be made about the wave functions at the edge of the region* $0 \leq k_x, k_y \leq +\pi/a$? This may be important for explaining the Josephson effect in $YBa_2Cu_3O_7$ [see Combescot, R., Leyronas, X.: Phys. Rev. Lett. **75**, 3732 (1995)].

3.4: Realistic Models of $YBa_2Cu_3O_7$

1. In fact the structure of $YBa_2Cu_3O_7$ comprises two weakly coupled planes (levels 2 and 3) and a chain lattice (level 1 coupled to 2) in the primitive cell. Each isolated CuO_2 plane is described by the dispersion obtained in question 7 of 3.2. This system is more weakly coupled to the chains by $T' \ll T$ in question 4 of 3.3. Figure P3.4 (left) shows the results of a more detailed calculation. *Give a qualitative interpretation of the different parts of the Fermi surface.*

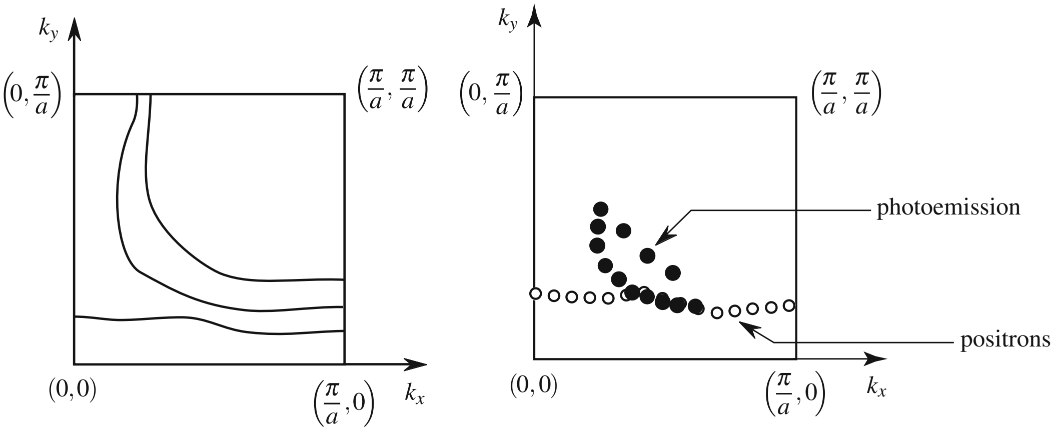

Fig. P3.4 *Left:* Fermi surface obtained from a detailed calculation, adapted from results of Yu, J., et al.: Phys. Lett. A **122**, 203 (1987) *Right*: Data taken by photoemission and positron annihilation adapted from Pickett, W.E., et al.: Science **255**, 46 (1992)

2. In Fig. P3.4 (right), black points represent photoemission measurements of the band structure and white points correspond to results obtained by another technique using positron annihilation. *What parts of the band structure are these techniques able to reveal?*

Solution

Isolated Copper–Oxygen Chain

1. The Bravais lattice of a chain is the set of points $\mathbf{R}_n = na\mathbf{y}$, where $n \in \mathbb{Z}$ and $\mathbf{y}$ is a unit vector along the chain axis. The basis then comprises one copper atom at $\mathbf{R}_0 = \mathbf{0}$ and one oxygen atom at $a\mathbf{y}/2$.
2. The reciprocal lattice is then $\mathbf{K}_p = (2\pi/a)p\,\mathbf{y}$, where $p \in \mathbb{Z}$. The first Brillouin zone is the interval $[-\pi/a, +\pi/a]$.
3. Using the notation adopted in this book, we have

$$\psi_k(\mathbf{r}) = \frac{1}{\sqrt{N_n}} \sum_\ell e^{ik\ell a} \phi_1(\mathbf{r} - \ell a\mathbf{y}) ,$$

   where N_n is the number of unit cells.
4. We obtain

$$E_C(k) = E_C^0 - 2V \cos ka .$$

5. Restricting to the first Brillouin zone, this relation is shown in Fig. P3.5. The function $E_C(k)$ is symmetric under

$$k \longrightarrow \frac{\pi}{a} - k , \qquad E_C(k) \longrightarrow 2E_C^0 - E_C(k) .$$

   So half the states are in the sub-interval $[-\pi/2a, +\pi/2a]$. One electron per unit cell corresponds to a half-filled band, and the Fermi energy is then E_C^0. The Fermi 'surface' reduces to the two points $k = +\pi/2a$ and $k = -\pi/2a$. If the occupation is very low, only the bottom of the band close to $k \approx 0$ is occupied. Then

$$E_C(k) \simeq E_C^0 - 2V\left(1 - \frac{1}{2}k^2a^2\right) , \qquad \text{whence} \quad m^* = \frac{\hbar^2}{2Va^2} .$$

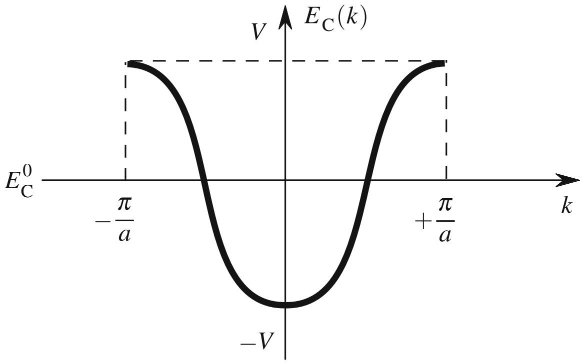

Fig. P3.5 Dispersion relation of the chain obtained in question 4, identical to the one given in Chap. 1

Isolated Copper–Oxygen Plane

1. The Bravais lattice is square: $\mathbf{R}_{n,m} = na\mathbf{x} + ma\mathbf{y}$, $n, m \in \mathbb{Z}$. The basis can be taken as CuO_2 with Cu at $(0,0)$ and two oxygens at $a\mathbf{x}/2$ and $a\mathbf{y}/2$. The reciprocal lattice is square: $\mathbf{K}_{p,q} = (2\pi/a)p\mathbf{x} + (2\pi/a)q\mathbf{y}$, $p, q \in \mathbb{Z}$. The first Brillouin zone is then the square

$$\left(\left[-\frac{\pi}{a}, +\frac{\pi}{a}\right] \text{ along } k_x\right) \times \left(\left[-\frac{\pi}{a}, +\frac{\pi}{a}\right] \text{ along } k_y\right) .$$

2. We have

$$\psi_{\mathbf{k}}^{\text{plane}}(\mathbf{r}) = \frac{1}{\sqrt{N_n}} \sum_j \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_j} \phi_2(\mathbf{r} - \mathbf{R}_j) ,$$

where N_n is the number of unit cells and j indexes the sites of the Bravais lattice. Further,

$$E_{\mathrm{P}}(\mathbf{k}) \left\langle \psi_{\mathbf{k}}^{\text{plane}} | \hat{H}_{\mathrm{P}} | \psi_{\mathbf{k}}^{\text{plane}} \right\rangle = \frac{1}{N_n} \sum_{i,j} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)} \int \mathrm{d}^3\mathbf{r} \phi_2(\mathbf{r} - \mathbf{R}_i) \hat{H}_{\mathrm{P}} \phi_2(\mathbf{r} - \mathbf{R}_j) .$$

The diagonal terms are all equal to E_{P}^0. A given site $\mathbf{R}_i$ has four nearest neighbours: $\mathbf{R}_i + a\mathbf{x}$, $\mathbf{R}_i - a\mathbf{x}$, $\mathbf{R}_i + a\mathbf{y}$, and $\mathbf{R}_i - a\mathbf{y}$. For just these cases, we have a nonzero matrix element equal to $-V_{\mathrm{P}}$. Hence,

$$E_{\mathrm{P}}(\mathbf{k}) = E_{\mathrm{P}}^0 - V_{\mathrm{P}} \left(\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot a\mathbf{x}} + \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot a\mathbf{x}} + \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot a\mathbf{y}} + \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot a\mathbf{y}} \right) ,$$

and

$$\boxed{E_{\mathrm{P}}(\mathbf{k}) = E_{\mathrm{P}}^0 - 2V_{\mathrm{P}}(\cos k_x a + \cos k_y a)} .$$

3. The constant energy terms have the form

$$\boxed{\cos k_x a + \cos k_y a = C} .$$

We have the symmetry

$$k_x \longrightarrow \frac{\pi}{a} - k_x , \qquad k_y \longrightarrow \frac{\pi}{a} - k_y , \qquad C \longrightarrow -C .$$

The half-filled state thus corresponds to $C = 0$, which reduces to

$$\boxed{|k_x| + |k_y| = \frac{\pi}{a}} .$$

The Fermi 'surface' comprises four straight-line segments [see Fig. P3.6 (center)]. The general shape of the constant energy curves has been given in Chap. 3, Fig. 3.7. If the number of electrons is $1 + \delta$, the immediately adjacent states

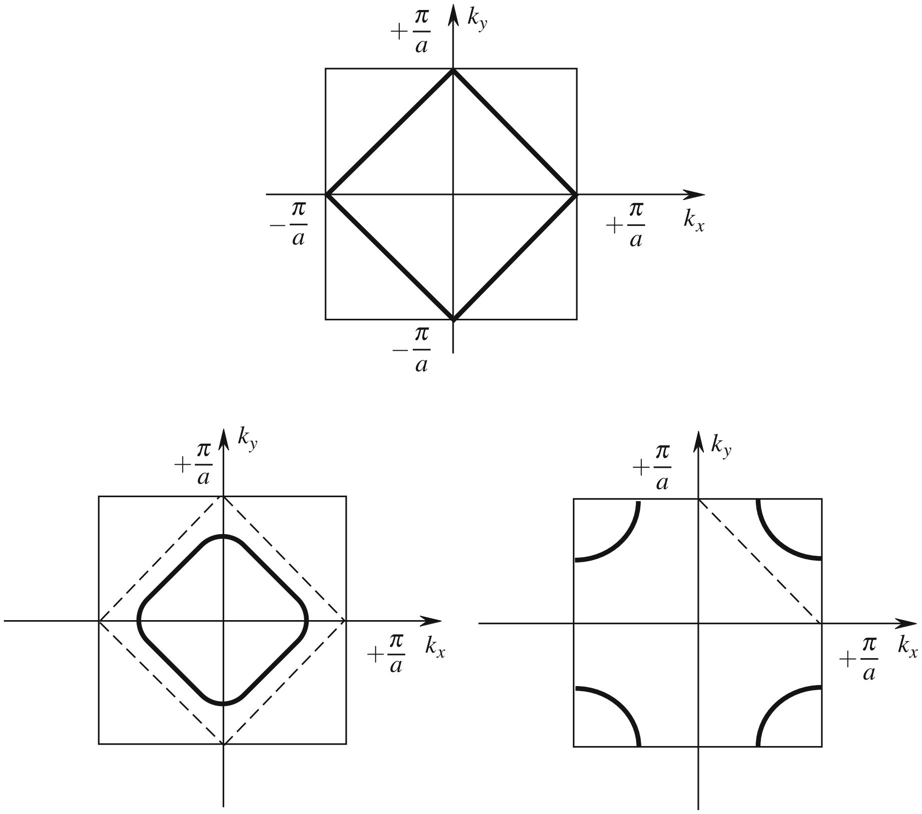

Fig. P3.6 Fermi surface calculations for a 2D square lattice with nearest neighbour hopping, for one electron per unit cell (*center*), $(1+\delta)$ electron per unit cell (*right*) and for $(1-\delta)$ electron per unit cell (*left*)

are filled [see Fig. P3.6 (right)] and if the number is $1-\delta$ the surface becomes connected [see Fig. P3.6 (left)]. If the band is almost empty, $\mathbf{k} \approx 0$ and $E_{\mathrm{P}}(\mathbf{k})$ has almost circular level curves as seen in Fig. 3.7.

4. In the calculation for question 2, for each site $\mathbf{R}_i$, we take into account second neighbours, viz., $\mathbf{R}_i \pm a\mathbf{x} \pm a\mathbf{y}$. This produces an extra term in $\langle \psi_{\mathbf{k}}^{\text{plane}} | \hat{H}_{\mathrm{P}} | \psi_{\mathbf{k}}^{\text{plane}} \rangle$ equal to

$$+V'_{\mathrm{P}}\left[\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(a\mathbf{x}+a\mathbf{y})} + \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(a\mathbf{x}-a\mathbf{y})} + \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(a\mathbf{x}-a\mathbf{y})} + \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(a\mathbf{x}+a\mathbf{y})}\right],$$

and then

$$E'_{\mathrm{P}}(\mathbf{k}) = E^0_{\mathrm{P}} + 2V_{\mathrm{P}}(\cos k_x a + \cos k_y a) + 4V'_{\mathrm{P}} \cos k_x a \cos k_y a \,.$$

In the region $0 \le k_x, k_y \le \pi/a$, the Fermi surface of question 3 is $k_x + k_y = \pi/a$. With second nearest neighbours, the energy on this straight line is equal to

$$E'_{\mathrm{P}} = E^0_{\mathrm{P}} - 4V'_{\mathrm{P}} \cos^2 k_x a \,.$$

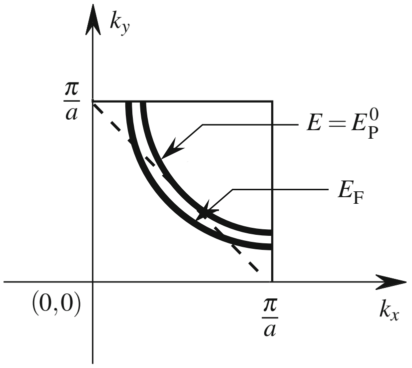

Fig. P3.7 Fermi surface taking into account second nearest neighbour contributions

When $V'_P > 0$, this energy remains unchanged at the center of the square, but is always reduced for the other values of k_x. The constant energy curve E_P^0 thus moves toward the corner of the Brillouin zone. For the half-filled band, the new Fermi surface takes the form shown in Fig. P3.7. (Note that it divides the Brillouin zone into two equal areas.)

5. If $\mathbf{r}$ is translated to $\mathbf{r}+\mathbf{R}_0$ for $\mathbf{R}_0$ in the Bravais lattice, the dummy sum changes by

$$\mathbf{R}_j \to \mathbf{R}_j + \mathbf{R}_0 \, , \qquad \psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_0) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_0}\psi_{\mathbf{k}}(\mathbf{r}) \, .$$

6. First project onto $\phi_2(\mathbf{r})$ to obtain

$$\langle \phi_2 | E(\mathbf{k}) | \psi_{\mathbf{k}} \rangle = E(\mathbf{k}) A_k \, ,$$

since we neglect non-local overlaps. Then we have

$$\langle \phi_2 | \hat{H}_{\mathrm{DP}} | \psi_k \rangle = A_k \sum_j \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_j} \int \mathrm{d}^3 r \phi_2(\mathbf{r}) \hat{H}_{\mathrm{DP}} \phi_2(\mathbf{r}-\mathbf{R}_j)$$
$$+ B_k \sum_j \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_j} \int \mathrm{d}^3 \mathbf{r} \phi_2(\mathbf{r}) \hat{H}_{\mathrm{DP}} \phi_2(\mathbf{r}+c\mathbf{z}-\mathbf{R}_j) \, .$$

The first sum only involves matrix elements within a plane. These are equal to the matrix elements of H_{P}. This first sum is thus equal to $E_{\mathrm{P}}(\mathbf{k})$ as obtained in question 2. In the second sum, only the term $\mathbf{R}_j = \mathbf{0}$ is nonzero and equal to T. Therefore,

$$\langle \phi_2 | \hat{H}_{\mathrm{DP}} | \psi_k \rangle = E_{\mathrm{P}}(\mathbf{k}) A_k + T B_k = E(\mathbf{k}) A_k \, .$$

As the two planes enter the expression for $\psi_k(r)$ in a symmetric way, the projection onto $\phi_2(\mathbf{r}+c\mathbf{z})$ leads in a similar manner to

$$\left\langle \phi_2(\mathbf{r}+c\mathbf{z}) | E(\mathbf{k}) | \psi_{\mathbf{k}} \right\rangle = T A_k + E_{\mathrm{P}}(\mathbf{k}) B_k = E(\mathbf{k}) B_k \, .$$

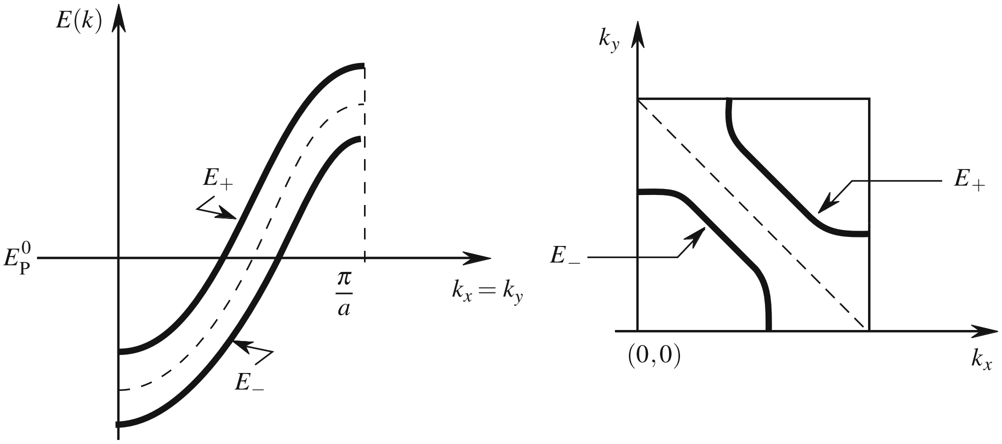

Fig. P3.8 Two bands obtained in the tight-binding approximation for a bilayer of CuO_2 planes. Dispersion relation of the two bands obtained in the direction $k_x = k_y$ (*left*). Fermi surface obtained for one electron per CuO_2 unit cell per plane (*right*)

The coefficients A_k and B_k thus satisfy the system

$$\boxed{\begin{cases} A_k E_{\mathrm{P}}(\mathbf{k}) + B_k T = A_k E(\mathbf{k}) \\ A_k T + B_k E_{\mathrm{P}}(\mathbf{k}) = B_k E(\mathbf{k}) \end{cases}} .$$

7. There are eigenstates if the determinant of this system is zero:

$$\begin{vmatrix} E_{\mathrm{P}}(\mathbf{k}) - E(\mathbf{k}) & T \\ T & E_{\mathrm{P}}(\mathbf{k}) - E(\mathbf{k}) \end{vmatrix} = 0 .$$

There are two solutions, hence two bands of dispersion

$$\boxed{E_{\pm}(\mathbf{k}) = E_{\mathrm{P}}(\mathbf{k}) \pm T} .$$

Along $k_x = k_y$, $E_{\mathrm{P}}(\mathbf{k}) = E_{\mathrm{P}}^0 - 4V_{\mathrm{P}} \cos k_x$. The two bands $E_{\pm}$ are related to one another by translation [see Fig. P3.8 (left)]. By symmetry, the Fermi energy for one electron per plane remains equal to E_{P}^0. This Fermi energy cuts the surface E_+ at a level curve of question 3 with occupation $1 - \delta$, but cuts the surface E_- at a level curve with occupation $1 + \delta$. The Fermi surface thus comprises two arcs [Fig. P3.8 (right)].

Chain and Plane

1. Use the LCAO function

$$\psi_{\mathbf{k}}^{\mathrm{CL}}(\mathbf{r}) = \frac{1}{\sqrt{N_{\mathrm{CL}}}} \sum_j \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_j} \phi_1(\mathbf{r} - \mathbf{R}_j) .$$

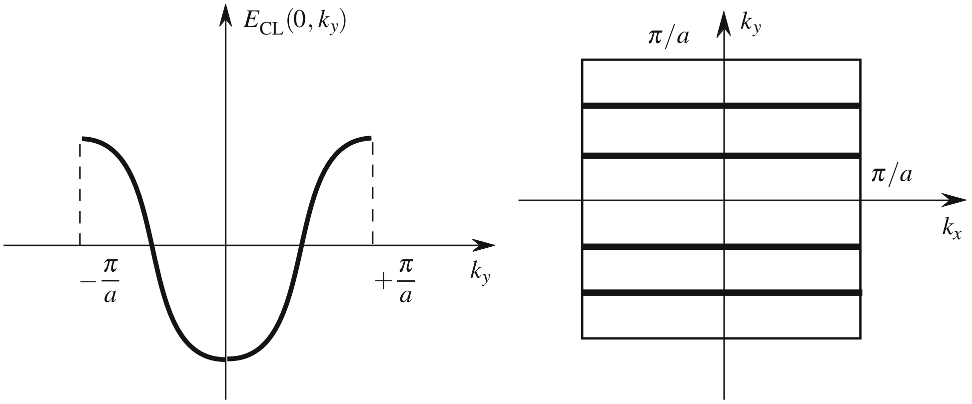

Fig. P3.9 Band structure for a lattice of chains: Dispersion relation $E_{\mathrm{CL}}(\mathbf{k})$ (*left*) and constant energy level curves in the region $-\pi/a \le k_x, k_y \le +\pi/a$ (*right*)

Only the matrix elements of $\hat{H}_{\mathrm{C}}$ come in when calculating $E_{\mathrm{CL}}(\mathbf{k})$ (see question 3 of 3.1), because there is no coupling between chains. As a consequence,

$$E_{\mathrm{CL}}(\mathbf{k}) = E_{\mathrm{C}}(k_y)\,,$$

as shown in Fig. P3.9 (left). The constant energy curves of $E_{\mathrm{CL}}(k_x, k_y)$ are thus straight lines at fixed k_y [see Fig. P3.9 (right)]. According to question 5 of 3.1, with one electron per unit cell, the Fermi surface thus comprises two straight lines $k_y = +\pi/2a$ and $k_y = -\pi/2a$, as shown in Fig. P3.10.

2. Project $\hat{H}_{\mathrm{PC}}|\Psi_{\mathbf{k}}\rangle = E(\mathbf{k})|\Psi_{\mathbf{k}}\rangle$ onto $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r}+c\mathbf{z})$. The calculation is similar to the one in question 6 of 3.2. For $\phi_1(\mathbf{r})$, we obtain

$$C_k E_{\mathrm{CL}}(\mathbf{k}) + D_k T' = C_k E(\mathbf{k})\,,$$

and with $\phi_2(\mathbf{r}+c\mathbf{z})$, we obtain

$$C_k T' + D_k E_{\mathrm{P}}(\mathbf{k}) = D_k E(\mathbf{k})\,.$$

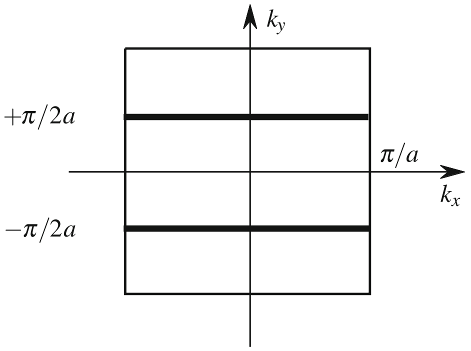

Fig. P3.10 Fermi surface of the chains for one electron per unit cell

Setting the determinant equal to zero, this yields two bands:

$$E_{\pm}(\mathbf{k}) = \frac{1}{2}\left\{E_{\mathrm{P}}(\mathbf{k}) + E_{\mathrm{CL}}(\mathbf{k}) \pm \sqrt{\left[E_{\mathrm{P}}(\mathbf{k}) - E_{\mathrm{CL}}(\mathbf{k})\right]^2 + 4T'^2}\right\} .$$

3. Since $E_{\mathrm{P}}^0 = E_{\mathrm{C}}^0$, the plane and chain bands are filled equally. The Fermi surface then comprises the surfaces of these two ensembles [see Fig. P3.11 (left)].
4. The surfaces intersect in $(\pi/2a, \pi/2a)$ when $T' = 0$. If $T' \neq 0$, the result of question 2 above shows that the equality $E_{\mathrm{P}} = E_{\mathrm{CL}}$ no longer holds for E_+ and E_-: the levels repel one another. Level crossing disappears and we obtain the qualitative result shown in Fig. P3.11 (right). At the edge of the Brillouin zone, the Bloch states correspond to states completely within the plane or completely within the chains.

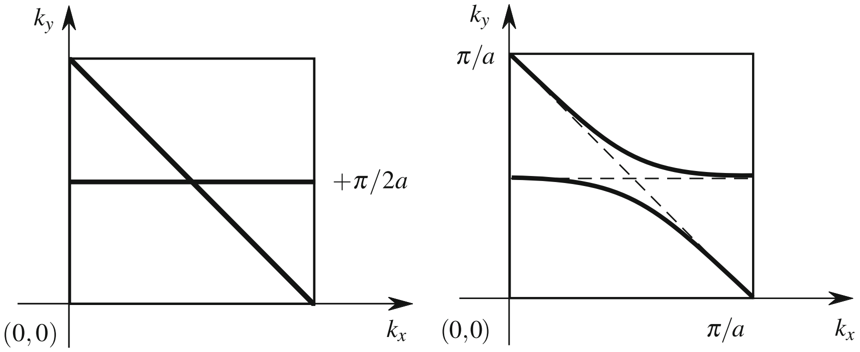

Fig. P3.11 Chain and plane Fermi surface for different hopping T' between chain and plane (*left*) $T' = 0$, (*right*) $T' \neq 0$

Realistic Models of $YBa_2Cu_3O_7$

1. A system of two planes with $V_{\mathrm{P}}' \neq 0$ will have a Fermi surface made up of two segments in $[0, \pi/a]^2$, as shown in Fig. P3.12 (left). If there is a chain lattice as

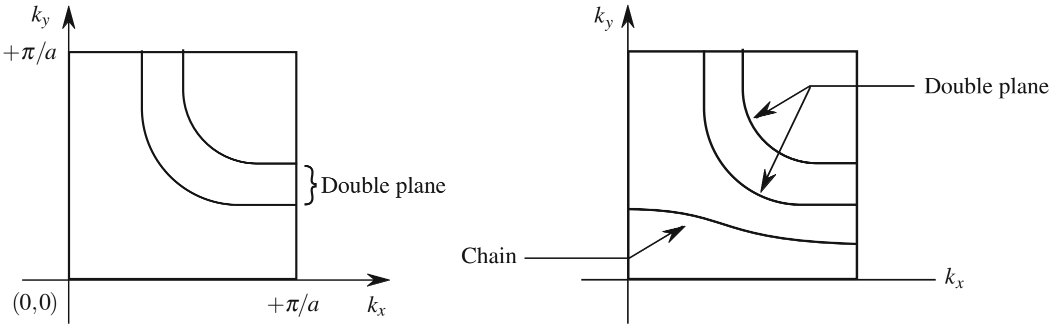

Fig. P3.12 Fermi surfaces for the bilayer of CuO_2 planes (*left*) and for the bilayer coupled to a CuO chain (*right*) well, it will also give a branch that will avoid crossing the branches of the double plane by the hybridisation phenomenon of questions 3 and 4 of 3.3. This gives Fig. P3.12 (right), which agrees with Fig. P3.4 (left).

2. The dispersion points due to photoemission [see Fig. P3.4 (right)] coincide with contributions coming from double planes. In contrast, positron annihilation sees the chain contribution. A single technique was not enough initially to investigate the whole Fermi surface. It has since been viewed by higher resolution ARPES experiments, and matches the results of a full calculation illustrated in Fig. P3.13.

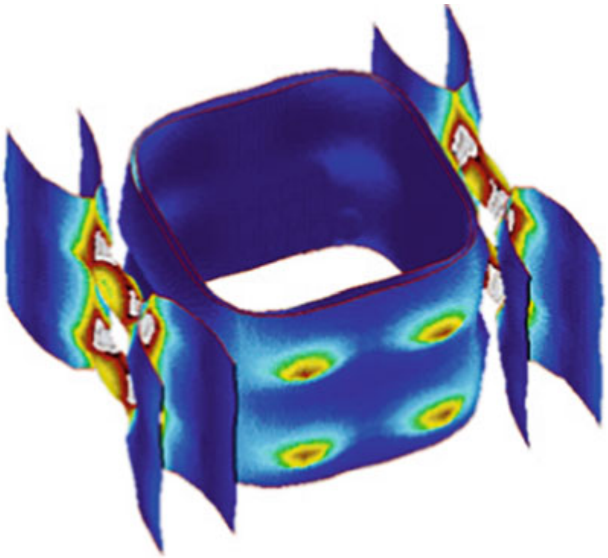

Fig. P3.13 Full calculation of the 3D band structure. Surfaces due to double planes are very close together, while those due to chains are widely spaced. The Fermi surface is almost cylindrical, because the hopping integrals between cells are very small in the *c* direction. Image courtesy of O. Andersen and I. Mazin from results published in Andersen, O.K., Liechtenstein, A.I., Rodriguez, O., Mazin, I.I., Jepsen, O., Antropov, V.P., Gunnarsson, O., Gopalan, S.: Physica C **185–189**, 147–155 (1991)