The compound with chemical formula La_2CuO_4 has the 3D structure with body-centered tetragonal conventional cell shown in Fig. 1. Note that it comprises a stack of LaO and CuO_2 planes.

1. *On Fig. 1, indicate the primitive vectors and basis of a primitive cell in the 3D crystal.*

The electronic configurations of the neutral atoms making up this structure are

$$\text{La}: \quad (\text{Xe})\ 5d^1\ 6s^2\,, \qquad \text{Cu}: \quad (\text{Ar})\ 3d^{10}\ 4s\,, \qquad \text{O}: \quad 1s^2\ 2s^2\ 2p^4\,.$$

2. *According to an LCAO calculation, is this compound insulating or metallic?*

The LCAO calculation shows that the La and oxygen in the LaO planes are in the configurations La^{3+} and O^{2-} corresponding to fully occupied shells. Bands resulting from these orbitals are at energy levels well below those of the Cu($3d$) and O($2p$) bands of the oxygens in the CuO_2 planes. It is thus the latter that constitute the valence or conduction levels of the crystal. It therefore suffices to consider the electronic structure of the CuO_2 plane.

3. *Specify the primitive cell of the CuO_2 plane, along with its reciprocal lattice and first Brillouin zone.*

We shall assume that the last occupied band corresponds to one orbital per Cu site of atomic energy E_0. The band is calculated using the LCAO approximation, only taking into account nearest-neighbour hopping integrals t_0 and t_1.

4. *Find the eigenergies $E(k_x,k_y)$ and plot the constant energy curves in the first Brillouin zone. What is the curve corresponding to an occupancy of one electron per unit cell?*

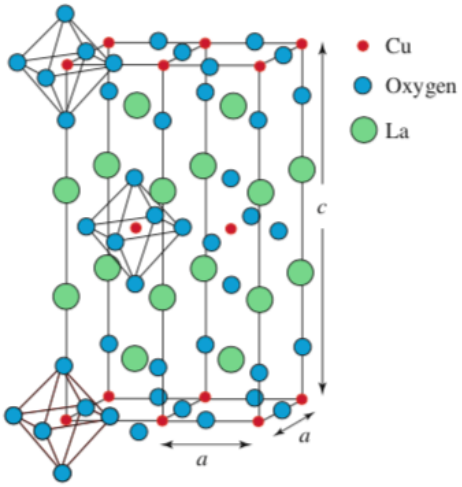

Fig. 1 Crystal structure of La_2CuO_4, showing body-centered tetragonal conventional cell

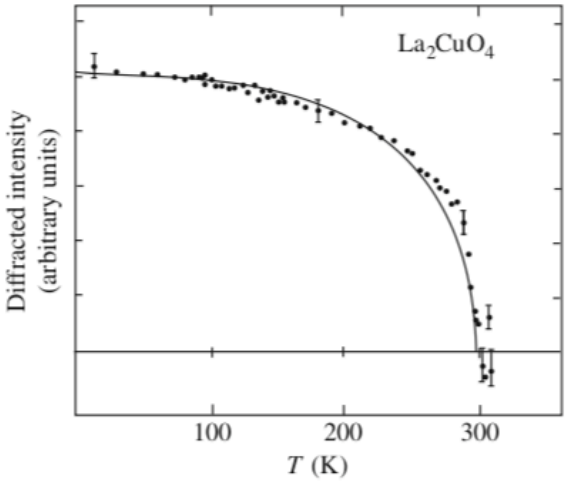

Fig. 2 Temperature dependence of the intensity of the neutron diffraction peak at $(\pi/a,\pi/a)$. Adapted from Yamada, K., Kudo, E., Endoh, Y., Hikada, Y., Oda, M., Suzuki, M., Murakami, T.: Solid State Commun. **64**, 753 (1987)

Conductivity measurements show that La_2CuO_4 is insulating. Moreover, neutron diffraction produces Bragg peaks at the four points $(\pm\pi/a,\pm\pi/a)$ of the plane below 300 K. The intensity of these peaks increases at low temperatures and saturates at $T = 0$ K, as shown in Fig. 2. X-ray diffraction only picks up the Bragg spots corresponding to the reciprocal lattice found in question 3.

5. *What can you deduce about the ground state of the electronic system of the CuO_2 plane? Specify the primitive cell of the real lattice of the CuO_2 plane for $T <$ 300 K.*

6. is optional, but you should try

A fraction of the La^{3+} is replaced by Sr, which has the ionic form Sr^{2+} in the crystal. In the compound $La_{1.85}Sr_{0.15}CuO_4$ it is observed that the spots at the four points $(\pm\pi/a,\pm\pi/a)$ of the plane disappear in a neutron diffraction experiment. Moreover, this compound is superconducting with a critical temperature of 40 K.

6. *What conclusions can be drawn from these observations? According to the LCAO approximation, what should be the Fermi surface of this metal?*