Problem 1. The material $La_{2-x}Sr_xCuO_4$ has a layered crystal structure that consists of two-dimensional square lattices of CuO_2 planes (shown in Fig. 1) separated by layers of $La_{2-x}Sr_xO_2$. You may assume that La has valence 3+, Sr valence 2+, and O valence 2−; the electrons from these cations are donated uniformly to the widely separated CuO_2 layers, which thus have a two-dimensional electronic structure. Neutral atomic Cu has the configuration $[Ar]4s^23d^9$. In this compound, four of the Cu d levels are completely filled, and there is a partially filled band formed from $d_{x^2-y^2}$ orbitals. You may assume the Cu $4s$ levels are unoccupied, and the O $2p$ levels are fully occupied. Electronic dispersion perpendicular to the planes may be neglected.

The band structure in the independent particle approximation is well described by a tight-binding model incorporating a single orbital (per unit cell) of $d_{x^2-y^2}$ symmetry centered on the Cu atom, with nonzero Hamiltonian matrix elements t between nearest neighbor orbitals in the x and y directions, and matrix elements t' between second neighbors across the diagonals.

1(a) Show that in this approximation the energy dispersion of an electron is

$$E(k) = 2t[\cos(k_x a) + \cos(k_y a)] + 4t' \cos(k_x a)\cos(k_y a).$$

Solution. The band energy in the tight-binding description is given by (4.57) in the lecture notes,

$$E(k) = \epsilon_0 + t\sum_{\boldsymbol{\rho}} e^{-i\mathbf{k}\cdot\boldsymbol{\rho}}.$$

In the two-dimensional CuO_2 plane, the four nearest neighbors to the origin are located at

$$\boldsymbol{\rho} \in a\{(1,0,0),\ (0,1,0),\ (-1,0,0),\ (0,-1,0)\}, \tag{1}$$

and the four second-nearest neighbors are located at

$$\boldsymbol{\rho}' \in a\{(1,1,0),\ (-1,1,0),\ (1,-1,0),\ (-1,-1,0)\}. \tag{2}$$

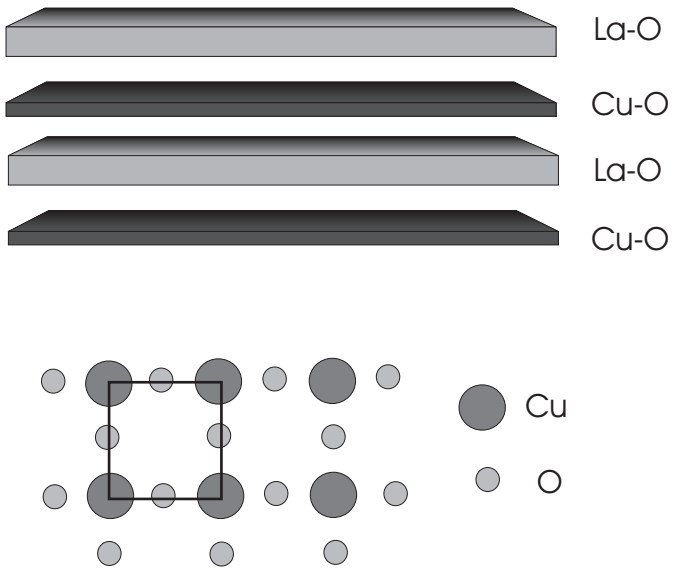

Figure 1: Schematic drawing of the layered crystal structure of $La_{2-x}Sr_xCuO_4$, and a drawing of the a single two-dimensional CuO_2 plane. The square is a primitive unit cell, with primitive lattice vectors $a(1,0,0)$ and $a(0,1,0)$.

So, assuming $\epsilon_0 = 0$, the band energy is

$$\begin{aligned}
E(k) &= t\sum_{\boldsymbol{\rho}} e^{-i\mathbf{k}\cdot\boldsymbol{\rho}} + t'\sum_{\boldsymbol{\rho}'} e^{-i\mathbf{k}\cdot\boldsymbol{\rho}'} \\
&= t\left(e^{-iak_x} + e^{-iak_y} + e^{iak_x} + e^{iak_y}\right) + t'\left(e^{-ia(k_x+k_y)} + e^{ia(k_x-k_y)} + e^{-ia(k_x-k_y)} + e^{ia(k_x+k_y)}\right) \\
&= t\left(e^{-iak_x} + e^{iak_x} + e^{-iak_y} + e^{iak_y}\right) + t'\left(e^{-iak_x}e^{-iak_y} + e^{iak_x}e^{-iak_y} + e^{-iak_x}e^{iak_y} + e^{iak_x}e^{iak_y}\right) \\
&= t\left[\left(e^{-iak_x} + e^{iak_x}\right) + \left(e^{-iak_y} + e^{iak_y}\right)\right] + t'\left(e^{-iak_x} + e^{iak_x}\right)\left(e^{-iak_y} + e^{iak_y}\right) \\
&= t\left[2\cos(k_x a) + 2\cos(k_y a)\right] + t'\left[2\cos(k_x a)\right]\left[2\cos(k_y a)\right] \\
&= 2t[\cos(k_x a) + \cos(k_y a)] + 4t'\cos(k_x a)\cos(k_y a) \qquad (3)
\end{aligned}$$

as we wanted to show. □

1(b) What do you expect to be the signs of t and t'? Explain your reasoning.

Solution. The signs of t and t' are expected to be negative because the Coulomb potential ΔU between the two electrons at any two sites is negative [**?** , pp. 78–79]. We see that t depends on ΔU by Ashcroft & Mermin (10.18), and we see that t has the same sign as ΔU by (4.56) in the lecture notes:

$$t = \int d\mathbf{r}\, \psi^*(\mathbf{r} - \rho)\Delta U \psi(\mathbf{r}).$$

1(c) For the case that $|t'/t| = 0$, sketch the Fermi surface for Sr concentrations of $x = 0$, $x \approx 0.2$, and $x \approx 0.5$.

Solution. As x increases, the partially-filled band of Cu becomes more empty. When $x = 0$, the band is mostly full. When $x = 0.5$, it is half full. Fig. 2 (left) shows the Fermi surface in the reduced zone scheme for $x = 0$ (blue line), $x \approx 0.2$ (gold line), and $x \approx 0.5$ (green line) when $t' = 0$ [**?** , p. 231]. The figures were created in Mathematica by plotting Eq. (3) and choosing appropriate contours.

1(d) How do these contours change qualitatively if $|t'/t| \sim 0.1$? (Choose the signs of t and t' that you proposed in 1(b).)

Solution. For t and t' both negative, the contributions from t' will distort the contours by pulling their ends toward the corners of the frame. This happens because, in general, the Fermi surface is stretched toward the positions of the nearest neighbors (for $t < 0$) given by Eq. (1). There is a nearest neighbor at the center of each edge of the frame. When we also consider $t' < 0$ contributions from the next-nearest neighbors, which are located in the corners of the frame by Eq. (2), the Fermi surface is pulled toward those ions as well. The effect is not too large since $|t'|$ is small compared to $|t|$. Fig. 2 (right) shows the Fermi surface in the reduced zone scheme for $x = 0$ (blue line), $x \approx 0.2$ (gold line), and $x \approx 0.5$ (green line) when $t' = 0.1t$.

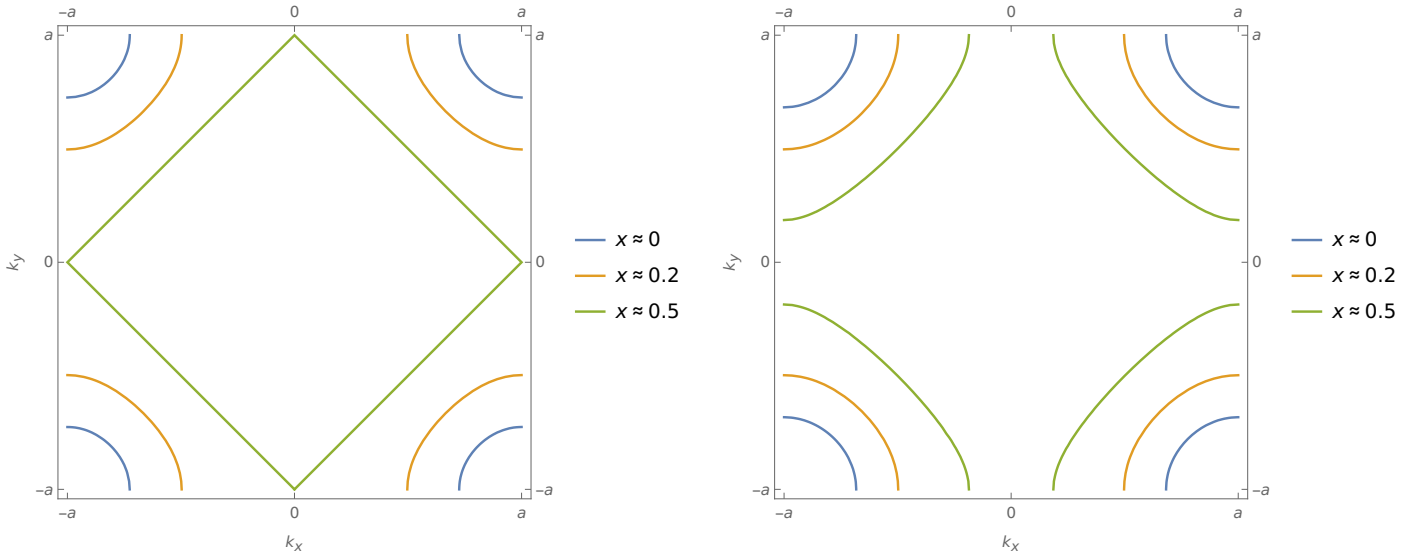

Figure 2: Fermi surfaces for $t' = 0$ (left) and $|t'/t| = 0.1$ (right) for $x = 0$ (blue line), $x \approx 0.2$ (gold line), and $x \approx 0.5$ (green line).

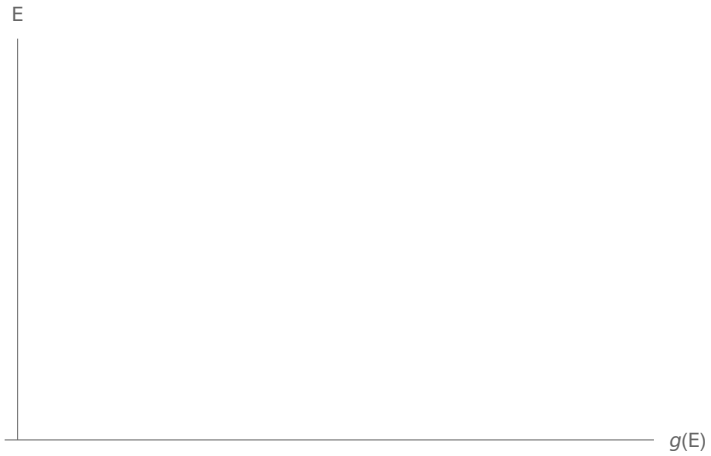

Figure 3: Density of states $g(E)$ for the dispersion shown in Fig. 2 (right).

1(e) Assuming the dispersion of 1(d), sketch the electronic density of states in energy, paying particular attention to the behavior near the edges of the band and at a saddle point in the middle of the band.

Solution. Our sketch of $g(E)$ is based on Fig. 4.2 in the course lecture notes, and is shown in Fig. 3. The logarithmic singularity in the middle represents the saddle point. Near the edges, the curve flattens out.

1(f) What would the independent electron model predict for the temperature dependence of the low-temperature electronic specific heat when the chemical potential is exactly at the saddle point near the middle of the band?

Solution. By (2.15) in the lecture notes, the electronic specific heat is given by

$$c_v = \int dE\, E g(E) \frac{df(E)}{dT},$$

where $f(E)$ is the Fermi distribution. At low temperature, the chemical potential is approximately equal to the specific heat. The saddle points are located at the positions of the nearest neighbors, given by Eq. (1). Since the lattice is periodic, we can choose $\boldsymbol{\rho} = (a, 0, 0)$ without loss of generality.

1(g) La_2CuO_4 is an antiferromagnetic insulator. Suggest, and discuss, reason(s) why the ground state differs from that predicted by the band structure in the independent particle approximation. Your answer should include a qualitative explanation of both the magnetic and the insulating behavior.