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Condensed Matter Theory 1 — Exercise 7

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https://ilias.studium.kit.edu/goto.php?target=crs_2219528
To be discussed on: *Thursday 2023/12/14*

1. A tight-binding description of Sr_2RuO_4

In the tight-binding approximation, the dispersion $\epsilon_{n\vec{k}}$ is obtained by diagonalizing the matrix

$$\mathcal{H}_{mm'}(\vec{k}) = -\sum_{\vec{R}} t_{m,m'}(\vec{R}) e^{i\vec{k}\cdot\vec{R}}, \quad m, m' = 1, 2, \ldots, N \ . \tag{1}$$

The hopping amplitude $t_{mm'}(\vec{R})$ describes an electron hopping between the N distinct orbitals m and m', separated by the lattice vector $\vec{R}$.
In the case of Sr_2RuO_4, the relevant orbitals are the $N = 3$ so-called t_{2g} orbitals, i.e., d_{xy}, d_{yz}, and d_{xz}, see Fig. 1, of the Ruthenium (Ru) ions. The crystal structure is tetragonal but, for simplicity, consider only a two-dimensional sheet of Ruthenium ions which form a square lattice with lattice constant a. In the following, we use a notation where we label hopping from/to the d_{yz}-orbital with $m = x$, d_{xz} with $m = y$, and d_{xy} with $m = z$.

a) Consider only nearest neighbor hopping. Using symmetries such as the mirror with respect to the x-y-plane, argue that the hopping amplitude between distinct orbitals vanishes. Similarly, argue that the following hopping amplitudes are identical: $t_{y,y}(a\hat{x}) = t_{x,x}(a\hat{y}) = t_{z,z}(a\hat{x}) = t_{z,z}(a\hat{y}) \equiv t$ and $t_{y,y}(a\hat{y}) = t_{x,x}(a\hat{x}) \equiv t'$. Construct the matrix $\mathcal{H}^{(1)}(\vec{k})$ from Eq. (1) which takes into account the nearest neighbor hoppings.

b) Based on part **a)**, neglecting t' as we can assume $t \gg t'$, determine the Bloch energies $\varepsilon_{n\vec{k}}$ for the three bands $n = 1, 2, 3$. Identify each band index n with an orbital. Sketch the constant-energy surfaces for $\varepsilon_{n\vec{k}}/2t = -1/2, 0, 1/2$. Evaluate the four points $\vec{k}_0$ in the first Brillouin zone where the bands corresponding to d_{xz} and d_{yz} are degenerate for a given Fermi energy ε_F.

c) The degeneracy of the bands at $\vec{k}_0$ will be lifted by including next-nearest-neighbor hopping. The next-nearest-neighbor hopping matrix reads

$$\mathcal{H}^{(2)}(\vec{k}) = \begin{pmatrix} -4t_{xx}\cos(ak_x)\cos(ak_y) & 4t_{xy}\sin(ak_x)\sin(ak_y) & 0 \\ 4t_{xy}\sin(ak_x)\sin(ak_y) & -4t_{xx}\cos(ak_x)\cos(ak_y) & 0 \\ 0 & 0 & -4t_{zz}\cos(ak_x)\cos(ak_y) \end{pmatrix}, \tag{2}$$

where we used that $\cos(a(k_x + k_y)) - \cos(a(k_x - k_y)) = -2\sin(ak_x)\sin(ak_y)$ and $\cos(a(k_x + k_y)) + \cos(a(k_x - k_y)) = 2\cos(ak_x)\cos(ak_y)$. Convince yourself that indeed only the next-nearest-neighbor hoppings t_{xx}, t_{xy}, and t_{zz} are allowed by symmetry. Use a computer program such as Mathematica to diagonalize $\mathcal{H}(\vec{k}) = \mathcal{H}^{(1)}(\vec{k}) + \mathcal{H}^{(2)}(\vec{k})$.

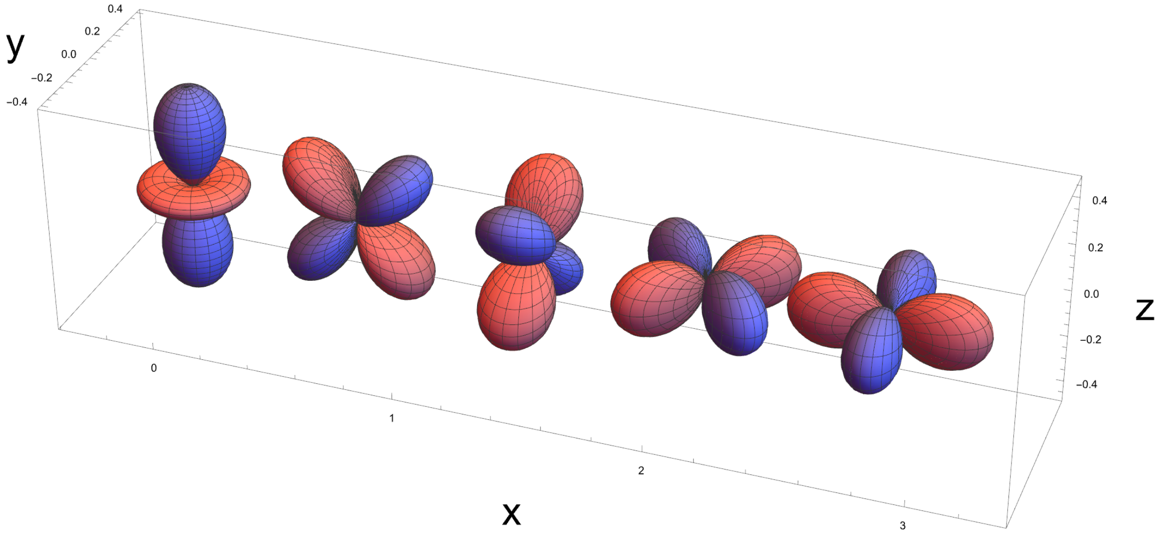

Figure 1: Sketches of the five d-orbitals, from left to right: d_{z^2}, d_{xz}, d_{yz}, d_{xy}, $d_{x^2-y^2}$. The color blue/red denotes the sign of the wave function. In particular, note that d_{xz} is antisymmetric under mirror operations with respect to the x-y-plane or the y-z-plane, and similar antisymmetric mirror planes exist for d_{yz} and d_{xy}.

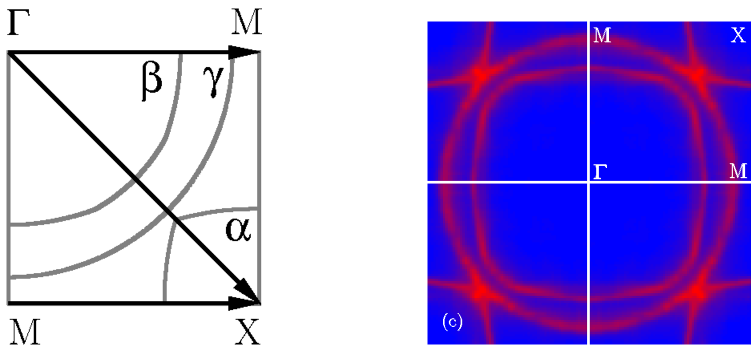

Figure 2: Theoretically (left) and experimentally (right) determined α, β and γ sheets of the Fermi surface of Sr_2RuO_4 (A. Damascelli *et al.*, Phys. Rev. Lett. **85** 5194, 2000).

Plot the Fermi surface for $\varepsilon_F = 0$ for various combinations of hopping amplitudes until you find a combination that qualitatively resembles the experimental result in Fig. 2. Which bands in the experimental result correspond to the hybridized d_{xz} and d_{yz} orbitals? Which band corresponds to the d_{xy} orbital?

2. Bloch oscillations

Consider an electron with charge $-e < 0$ in a one-dimensional tight-binding band. The dispersion is given as $\varepsilon_k = -2J\cos(ka)$, where $J > 0$ is the hopping amplitude in order to avoid confusion with the time t used below. Additionally, a constant electric field E is applied.

a) Solve the semiclassical equations of motion:

$$\hbar\dot{k} = -eE \quad \text{and} \quad \dot{x} = \frac{1}{\hbar}\partial_k\varepsilon_k \tag{3}$$

for the initial conditions $x(t=0) = x_0$ and $k(t=0) = k_0$. Plot $x(t)$ as a function of t and determine the amplitude x_a and period T of its Bloch oscillation.

b) Using the solutions $k(t)$ and $x(t)$ obtained in part **a)**, show that the energy $\mathcal{E} = \varepsilon_{k(t)} + eEx(t)$ is independent of time. Argue that the conservation of energy inhibits the electron to escape to $x \to \pm\infty$.

c) The probability $P(x)$ to find the electron at a certain position x is obtained by

$$P(x) = \frac{1}{T}\int_0^T dt\delta(x - x(t)) \tag{4}$$

where T is the time period of a Bloch oscillation and $x(t)$ is the semi-classical solution. Evaluate $P(x)$ for energy $\mathcal{E} = 0$ and express your result in terms of the amplitude x_a.

d) Consider now the quantum mechanical problem, i.e., the electron wavefunction with energy $\mathcal{E}$, $\Psi(x,t) = e^{-i\mathcal{E}t/\hbar}\psi_\mathcal{E}(x)$. Its Fourier transform $\psi_\mathcal{E}(k)$ with $\psi_\mathcal{E}(x) = \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi}\psi_\mathcal{E}(k)e^{ikx}$ obeys the stationary Schrödinger equation

$$\mathcal{E}\psi_\mathcal{E}(k) = (-2J\cos(ka) + eEi\partial_k)\psi_\mathcal{E}(k) \ . \tag{5}$$

Obtain the solution $\psi_\mathcal{E}(k)$ up to a normalization factor.

e) Show that if $\psi_\mathcal{E}(x)$ is an eigenfunction with energy $\mathcal{E}$ then $\psi_\mathcal{E}(x + na)$ with $n \in \mathbb{Z}$ is an eigenfunction with energy $\mathcal{E} + naeE$, i.e., $\psi_{\mathcal{E}+naeE}(x)$, giving rise to the *Wannier-Stark ladder.*
Hint: In order to show this, you do not need to evaluate the integral explicity since $i\partial_k = x$ *in position representation!*

f) Consider the wavefunction with energy $\mathcal{E} = 0$, i.e., $\psi_{\mathcal{E}=0}(x)$. Show that this wavefunction $\psi_0(x)$ with $x = na$, $n \in \mathbb{Z}$, is $\psi_0(na) \propto J_n(2J/eEa)$, i.e., proportional to the Bessel function

$$J_n(z) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\tau e^{in\tau - iz\sin\tau}. \tag{6}$$

With the help of Mathematica, plot the probability distribution $|\psi_0(na)|^2$ on the discrete lattice in the small-electric-field limit $2J/aeE \gg 1$, e.g. $2J/aeE = 100$. Compare the result with the semi-classical probability $P(x)$ from part (c).