ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Solid State Theory
Exercise 3

FS 2012
Prof. M. Sigrist

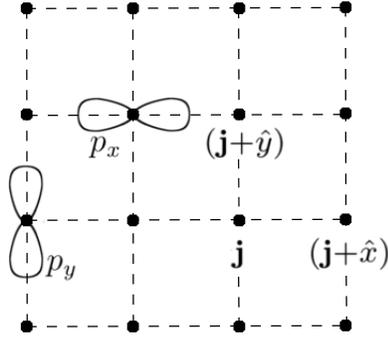## Exercise 3.1   Two-orbital tight-binding model in 2d

Figure 1: Two-dimensional lattice of atom cores with a sketch of the atomic orbitals.

We calculate the band structure of a two-dimensional model system within the tight-binding approximation. We consider atoms arranged in a square lattice configuration with lattice constant a. Each atom is described by a potential $V(\mathbf{r})$ giving rise to (Hydrogen-like) atomic orbitals. Here we focus on the p_x- and p_y-orbitals only. The (single-particle) Hamiltonian of the system is given by

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{j}} V(\mathbf{r} - \mathbf{R_j}) \tag{1}$$

with $\mathbf{j} = (j_x, j_y)$ and $\mathbf{R_j} = (j_x a, j_y a, 0)$ $(j_{x,y} \in \mathbb{Z})$.

a) As a starting point for the tight-binding approximation, we turn to the formulation in terms of Wannier functions. We define the Wannier function $w_\alpha(\mathbf{r} - \mathbf{R_j})$ of atom $\mathbf{j}$ in band α (with $\alpha = p_{x/y}$) by

$$\Psi_{\alpha,\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{j}} e^{i\mathbf{k}\cdot\mathbf{R_j}} w_\alpha(\mathbf{r} - \mathbf{R_j}), \tag{2}$$

where $\mathbf{k} = (k_x, k_y, 0)$ as the lattice is periodic in x- and y-direction. The different bands originate from the two different atomic orbitals p_x and p_y. The Hamiltonian can be written as the sum

$$\mathcal{H} = \sum_{\alpha} \mathcal{H}_\alpha + \sum_{\alpha \neq \alpha'} \mathcal{H}_{\alpha,\alpha'}, \tag{3}$$

where the first term includes all the intra-band effects whereas the second one couples the two bands. In a first step, we neglect inter-orbital coupling. Show that

within the tight-binding approximation taking only nearest-neighbor hopping into account, the Hamiltonian $\mathcal{H}_\alpha$ can be written as

$$\mathcal{H}_\alpha = \sum_{\mathbf{j}} \varepsilon_\alpha c_{\alpha\mathbf{j}}^\dagger c_{\alpha\mathbf{j}} + (t_\alpha^x c_{\alpha(\mathbf{j}+\hat{x})}^\dagger c_{\alpha\mathbf{j}} + t_\alpha^y c_{\alpha(\mathbf{j}+\hat{y})}^\dagger c_{\alpha\mathbf{j}} + \text{h.c.}). \tag{4}$$

where we have omitted spin indices. Define $t_\alpha^{x/y}$ in terms of the Wannier functions and determine relations between these coefficients.

b) Approximate the Wannier functions by atomic (hydrogen) states. Use symmetry arguments to determine whether the $t_\alpha^{x/y}$ are positive, negative, or zero. Calculate the resulting band structure and visualize both the band structure and the resulting Fermi surface.

c) Next we take into account the hybridization between different orbitals. For that purpose, we have to consider next-nearest neighbour hopping on the square diagonal. Show that the Hamiltonian part $\mathcal{H}_{\alpha,\alpha'}$ coupling the two bands can be written as

$$\mathcal{H}_{\alpha,\alpha'} = \sum_{\mathbf{j}} t_{\alpha\alpha'}^+ c_{\alpha(\mathbf{j}+\hat{x}+\hat{y})}^\dagger c_{\alpha'\mathbf{j}} + t_{\alpha\alpha'}^- c_{\alpha(\mathbf{j}+\hat{x}-\hat{y})}^\dagger c_{\alpha'\mathbf{j}} + \text{h.c.} \tag{5}$$

Define $t_{\alpha\alpha'}^\pm$ and determine the sign of $t_{\alpha\alpha'}^\pm$. Calculate the resulting band structure and visualize again both the band structure and the Fermi surface.

Exercise 3.2   Bloch Oscillations

In the quasi-classical description of a wave-packet peaked around some quasi-momentum $\hbar k$ the group velocity is given by

$$\dot{r} = \frac{1}{\hbar} \frac{\partial \varepsilon_k}{\partial k}, \tag{6}$$

while the change of the quasi-momentum is given by

$$\hbar \dot{k} = F_{\text{ext}}, \tag{7}$$

with F_{ext} the force due to applied external fields (in addition to the periodic potential).

a) We focus on the one-dimensional tight-binding model with the dispersion relation

$$\varepsilon_k = -2t \cos(ka), \tag{8}$$

where t is the nearest neighbor hopping constant and a the lattice constant (for simplicity we consider only one band). Show that a uniform electric field does not accelerate the electrons but lets them oscillate around some fixed position. This means that, for sufficiently large fields, all metals would behave like insulators. Why has this effect never been seen in normal metals? What would change if we considered semiconductor superlattices instead of metals?

b) We now add a small damping term to Eq. (7) and analyze the consequences. The rate of change of the quasi-momentum is thus given by

$$\hbar \dot{k} = F_{\text{ext}} - \frac{m\dot{r}}{\tau},\tag{9}$$

where τ is the relaxation time. Show that this damping can lead to a vanishing of the oscillations and thus to a stationary solution. What is the corresponding condition and how does the stationary solution look like? Calculate then analytically $k(t)$ for both situations to verify your considerations.

Office hour:
Monday, March 12th, 2012 - 13:00 to 15:00
HIT K 23.3
David Oehri