ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Solid State Theory
Exercise 3

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Exercise 3.1 Lifting the degeneracy of atomic states

Determine how the energy levels of the p, d and f orbitals of an atom lift due to a crystal field with cubic symmetry. Compute the corresponding eigenstates for the d orbitals. For this, consider the harmonic polynomials homogeneous of order 2.

Exercise 3.2 Two-orbital tight-binding model in 2d

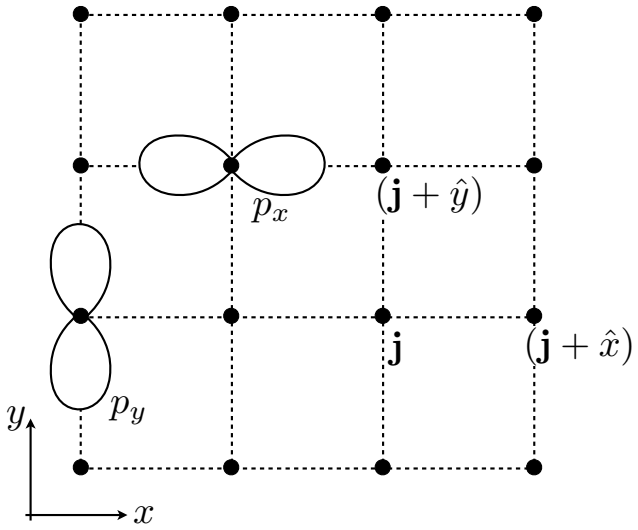

Figure 1: Two-dimensional lattice of atom cores with a sketch of the atomic orbitals.

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

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

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

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 $w_\alpha(\mathbf{r} - \mathbf{R}_\mathbf{j})$ of atom $\mathbf{j}$ in band α (with $\alpha = p_{x/y}$) by

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

where $\mathbf{k} = (k_x, k_y, 0)$, because 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

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

The operators $c^{\dagger}_{\alpha\mathbf{j}}$ and $c_{\alpha\mathbf{j}}$ create and annihilate, respectively, an electron in the band α at site $\mathbf{R}_{\mathbf{j}}$, where we have omitted spin indices.

Define $t^{x/y}_{\alpha}$ in terms of the Wannier functions and determine the relations between these coefficients.

b) Approximate the Wannier functions by atomic (hydrogen) states. Use symmetry arguments to determine whether the $t^{x/y}_{\alpha}$ 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

$$\mathcal{H}_{\alpha,\alpha'} = \sum_{\mathbf{j}} t^{+}_{\alpha\alpha'} c^{\dagger}_{\alpha(\mathbf{j}+\hat{x}+\hat{y})} c_{\alpha'\mathbf{j}} + t^{-}_{\alpha\alpha'} c^{\dagger}_{\alpha(\mathbf{j}+\hat{x}-\hat{y})} c_{\alpha'\mathbf{j}} + \text{h.c.} \tag{5}$$

Define $t^{\pm}_{\alpha\alpha'}$ and determine the sign of $t^{\pm}_{\alpha\alpha'}$. Calculate the resulting band structure and visualize again both the band structure and the Fermi surface.

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