Solid State Theory
Exercise 4

FS 15
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Problem 4.1 Brillouin zone of simple crystals

Consider (a) a triangular lattice, (b) a honeycomb (graphene) lattice, and (c) the cubic lattice of sodium chloride, see Fig. 1. For each of them find the underlying Bravais lattice, the corresponding reciprocal lattice, and construct the first Brillouin zone. Denote the nearest neighbour distance as a in all lattices.

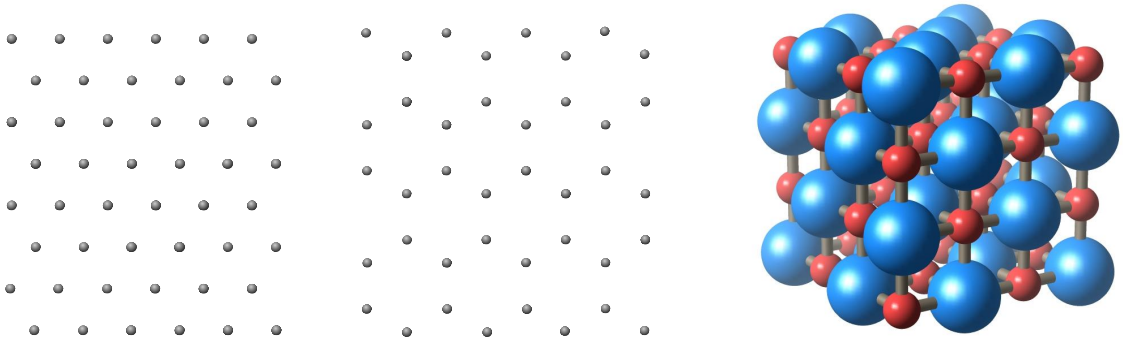

Figure 1: A triangular lattice, a honeycomb (graphene) lattice and the lattice of sodium chloride, respectively.

Problem 4.2 Two-orbital tight-binding model in 2d

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 $\mathbf{R_j} = (j_x a, j_y a, 0)$ $(j_{x,y} \in \mathbb{Z})$. For simplicity we suppress the spin index in all equations.
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 $\mathbf{k} = (k_x, k_y, 0)$, 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.

1. Show that within the tight-binding approximation, taking only nearest-neighbour hopping into account, the Hamiltonian $\mathcal{H}_{\alpha,\alpha'} = 0$ and $\mathcal{H}_\alpha$ 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 $\mathbf{R}_\mathbf{j}$. Define $t^{x,y}_\alpha$ in terms of the Wannier functions and determine the relations between these coefficients.

2. 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.

3. Now consider also the next-nearest neighbour hopping along the square diagonal. Such hopping leads to hybridization of the $p_{x,y}$ orbitals. 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. How does $\mathcal{H}_\alpha$ change after including the next-nearest neighbour hopping?

4. How does the band picture modify if we also consider p_z orbitals?

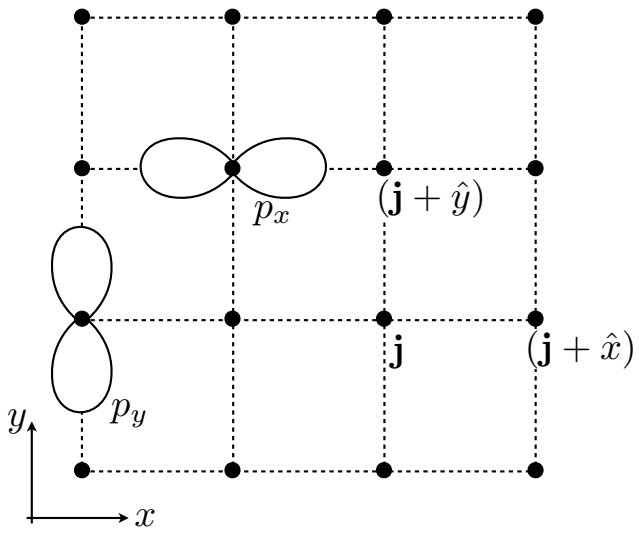

Figure 2: Two-dimensional lattice of atom cores with a sketch of the atomic orbitals.