ETH
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Solid State Theory
Exercise 3

FS 10
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Exercise 3.1 6-Orbital tight-binding model
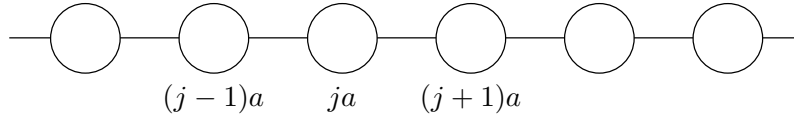

$(j-1)a$ ja $(j+1)a$

Figure 1: One-dimensional chain of atom cores.

In this exercise we want to calculate the band structure of (fictitious) one-dimensional sodium in the tight-binding approximation. The (single-particle) Hamiltonian of the system is given by

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m} + \sum_j \frac{-Ze^2}{|\mathbf{r} - \mathbf{r}_j|}, \tag{1}$$

with $Z = 11$ for Na and $\mathbf{r}_j = (x, y, ja)$ and the lattice constant a.

a) As a starting point for the tight-binding approximation, a formulation in terms of Wannier functions is more practicable. We define the Wannier function $w_n(x, y; z - ja)$ of atom j in band n by

$$\Psi_{n,k}(x, y; z) = \frac{1}{\sqrt{N}} \sum_j e^{ikja} w_n(x, y; z - ja). \tag{2}$$

Note that the potential is periodic in the z-direction only. The different bands originate from the atomic orbitals. Since Na has 11 electrons we need to consider the 6 orbitals $n = (1s, 2s, 2p_x, 2p_y, 2p_z, 3s)$. Show that within the tight-binding approximation taking only nearest-neighbor hopping into account, the hamiltonian can be written as

$$\mathcal{H} = \sum_n \mathcal{H}_n + \sum_{n \neq n'} \mathcal{H}_{n,n'}, \tag{3}$$

$$\mathcal{H}_n = \sum_j \varepsilon_n c_{n,j}^\dagger c_{n,j} + (t_n c_{n,j+1}^\dagger c_{n,j} + \text{h.c.}), \tag{4}$$

$$\mathcal{H}_{n,n'} = \sum_j t_{n,n'} c_{n,j+1}^\dagger c_{n',j} + t_{n',n} c_{n,j}^\dagger c_{n',j+1}, \tag{5}$$

where we have omitted spin indices. Define t_n and $t_{n,n'}$.

b) Approximate the Wannier functions by atomic (hydrogen) states. Use symmetry arguments to determine whether the t_n and $t_{n,n'}$ are positive, negative, or zero.
Remarks: Choose the phase of the Wannier functions equal on each atomic site. The (relative) signs and whether the hopping elements are finite follows directly from

the symmetry of the wave functions and the Hamiltonian, except for those elements containing two p_z orbitals or one p_z and one s orbital. In these cases determine the sign of the matrix elements using the fact that the state lower in energy (in a space spanned only by those orbitals) is the one with the least nodes in the total wave function. Alternatively, you can argue that the major contribution to the matrix element originates in the area between the lattice sites.

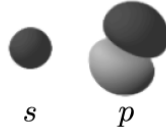*Attention:* It may turn out that for some $t_{n,n'} \neq t_{n',n}$!

s p

Figure 2: Polar plots of hydrogen s and p orbitals.

c) Make the Ansatz $t_n(a) = t_n \exp(-a/a_n)$, $t_{n,n'}(a) = t_{n,n'} \exp(-a/a_{n,n'})$ with a the lattice constant and a_n, $a_{n,n'}$ characteristic length-scales of the order of the atomic radius. Calculate the resulting band structure for some ratios of a, a_n and $a_{n,n'}$.
   Remark: For simplicity, choose $t_n \equiv t_1$, $t_{n,n'} \equiv t_2$ etc. If, on the other hand, you want more challenge, you can actually calculate the matrix elements using hydrogen wave functions. Be aware, however, that this is a very ambiguous choice and can not be considered a better approximation to the "real" band structure (keywords: screening, interaction).

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

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