

---

# Solid State Theory

## Problem set 6

---

Winter Term 2016

**Website:** <http://www.thp.uni-koeln.de/trebst/Lectures/2016-SolidState.shtml>

**Due date:** Discussed in class on **Thursday, January 26nd**.

If you turn in your solutions by Wednesday noon (Januar 25th), they will be graded.

Please submit your solutions to Henry Legg at [hlegg@uni-koeln.de](mailto:hlegg@uni-koeln.de).

## 1. The Kronig-Penney model revisited

In this exercise, we will once again turn to the famous **Kronig-Penney** model. Ultimately, our aim is to show that it is possible to choose a basis whose states are actually localized around the lattice sites instead of being delocalized over the entire solid. This will be referred as the **Wannier** basis. You can download an accompanying [IPython notebook](#).

### 1.1. Numerical solution

On a previous sheet, we already showed you how to analytically solve this model. In this exercise, we will tackle the problem using a technique called exact diagonalization. The basic idea that we take the Hamiltonian operator in its matrix form and diagonalize this matrix to find the eigenvalues and eigenvectors. As a reminder, the Hamiltonian is given as follows:

$$H = \frac{p^2}{2m} + \sum_j V_j(x), \quad (1)$$

where the  $V_i(x)$  are step functions of width  $w$  that have the form

$$V_j = \begin{cases} V_j & ja < x < ja + w \\ 0 & \text{else.} \end{cases} \quad (2)$$

To solve this Schrödinger equation and obtain the wavefunctions  $\psi$ , we simply discretize space with a step size  $h$  and rewrite the Hamiltonian as

$$-\psi_{i+1} - \psi_{i-1} + 2 \cdot \psi_i + \sum_j V_j(x_i) \cdot h^2 \psi_j = E \cdot h^2 \psi_i \quad (3)$$

Diagonalizing this matrix, we find the energies and the statevectors of the Kronig-Penney model for a fixed number of potential wells.

- Study the accompanying [IPython notebook](#) and use it to calculate the wavefunctions.

- How are the boundary conditions taken care of in the simulation?

An alternative route is to make use of Bloch's theorem. It states that the wavefunction in such a system with discrete translational invariance is given as

$$\psi(x) = \exp(ikx)u_{k,n}(x), \quad (4)$$

where the functions  $u$  are periodic in the lattice. We now insert this result for  $\psi(x)$  into our original equation and discretize that one as well.

- Insert the wavefunction in Bloch form into the Hamiltonian and derive the discretized version of the Hamiltonian just like above.
- Using the supplied notebook, perform this calculation for various strengths of the interaction on your own.

## 1.2. The Wannier basis

In a final step, we now use the results we obtained in the previous part of this exercise to perform a basis change to one where the eigenfunctions are almost perfectly localized around the respective atomic centers. This basis is called the **Wannier** basis. Its formal definition is as follows:

$$w_n(r-R) = \frac{1}{\sqrt{N}} \sum_k \exp(-ikR) \psi_{nk}(r) \quad (5)$$

It is, however, not always guaranteed that the resulting functions are localized around the centers of the potentials. In particular, each of the Bloch functions carries a phase that might interfere or be influenced by other devices. In a worst case scenario, this phase may cause the wavefunctions to be superposed in such a way that does concentrate most of the weight around one site. One possible way to gauge the phases and to get rid of the problem is to define a phase  $\phi_k$  for the reciprocal lattice vector  $k$  as

$$e^{i\phi_k} = \frac{\psi_{nk}(x_0)}{|\psi_{nk}(x_0)|} \quad (6)$$

The underlying idea of this choice of gauge is to choose the gauge such that the wavefunctions become real at the same point in time.

- Read through the source code to understand how Bloch functions are created from the simple wave function.
- Choose a different band for which to calculate the Wannier basis.
- Check for orthogonality, i.e. verify that you have a set of orthonormal basis vectors

## 2. Tight binding in second quantization

Solving a tight binding model becomes particularly easy if the formulation of second quantization is used. We will do this for a variety of lattices in this exercise. Setting up the Hamiltonian matrix becomes rather tedious when the lattice has a large number of atoms in the unit cell, which is why we provide you with an [IPython notebook](#) that contains routines to solve the tight binding problem for arbitrary lattices.

We start by recapitulating the essentials of the tight binding technique and solve a few simple models.

### Isotropic chain

Consider a one-dimensional chain described by a Hamiltonian

$$H = -t \sum_{i=1}^N \left( c_{i-1}^\dagger c_i + c_i^\dagger c_{i-1} \right) \quad (7)$$

whose dispersion we know to be  $E(k) = -2t \cos(k)$ .

1. Show that each term of the form  $c_i^\dagger c_j$  contributes  $c_k^\dagger c_k e^{ik(r_i - r_j)}$ .
2. Use this information to solve for the energy spectrum of the tight binding chain above.

### Square lattice

This method is applicable regardless of the dimensionality of the problem. Only the phase factor  $c_k^\dagger c_k e^{ik(r_i - r_j)}$  changes such that each term is now determined by a scalar product  $c_k^\dagger c_k e^{ik \cdot (r_i - r_j)}$ . Our first example is easily extended to two dimensions.

$$H = -t \sum_{\langle i,j \rangle} \left( c_i^\dagger c_j + c_j^\dagger c_i \right) \quad (8)$$

where the sum runs over all nearest neighbors  $i, j$ .

3. Proceed as previously to determine the energy spectrum of the square lattice.

### Diatomic chain

The number of bands that we find for a given Hamiltonian depends on the number of atoms per unit cell. If we change the hopping parameters to be alternating

$$H = -t \sum_{i=1}^{N/2} c_{2i-1}^\dagger c_{2i} - t' \sum_{i=1}^{N/2} c_{2i}^\dagger c_{2i+1} + \text{h.c.}, \quad (9)$$

we are dealing with two atoms  $A$  and  $B$ , per unit cell which will be described by two types of annihilation and creation operators that we may call  $a, a^\dagger$  and  $b, b^\dagger$ , respectively.

5. Rewrite the Hamiltonian using these new operators.

6. Continue by transforming the Hamiltonian into Fourier space and rewrite the result in the form of a vector-matrix-vector product.
7. Solve for the energy spectrum by diagonalizing this matrix.

### Honeycomb lattice

To facilitate solving such models, we provide you with an [IPython notebook](#). Let us discuss graphene as one final example. The basis vectors are given by

$$\mathbf{a}_1 = \frac{1}{2} \begin{pmatrix} 3 \\ \sqrt{3} \end{pmatrix}, \quad \mathbf{a}_2 = \frac{1}{2} \begin{pmatrix} -3 \\ \sqrt{3} \end{pmatrix} \quad (10)$$

The two atoms  $A$  and  $B$  in same the unit cell are connected by a vector

$$\delta_1 = (1, 0) . \quad (11)$$

Connecting one atom of species  $A$  to its remaining two neighbors in surrounding unit cells is achieved by the

$$\delta_2 = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \quad \delta_3 = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \quad (12)$$

8. Draw a quick sketch of one unit cell as defined above and its neighboring unit cells. Label the connecting vectors between atoms in the unit cell and its neighbors with  $\delta_1, \delta_2,$  and  $\delta_3$ .
9. Set up the Hamiltonian matrix and solve for the dispersion relation as a function of  $k$ .
10. Now switch to the notebook and compute the dispersion along the following path in the Brillouin zone:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \rightarrow \mathbf{K}_1 = \frac{2\pi}{3} \begin{pmatrix} 1 \\ 1/\sqrt{3} \end{pmatrix} \rightarrow \mathbf{K}_2 = \frac{2\pi}{3} \begin{pmatrix} 1 \\ -1/\sqrt{3} \end{pmatrix} \rightarrow \Gamma \quad (13)$$

Do you observe any special features along this path?

### bcc lattice

We now move on to add one more spatial dimension and study the *bcc* lattice. Its basis vectors are

$$\mathbf{a}_1 = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \quad \mathbf{a}_3 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} . \quad (14)$$

Every atom has 8 nearest neighbors, which are located at all combinations of  $\mathbf{v} = (\pm\frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2})$ .

11. Proceed as previously to calculate the dispersion relation for the *bcc* lattice.