Institute of Theoretical Physics
University of Cologne
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Based on problem sets by Peter Bröcker

Solid State Theory

Exercise sheet 6

This exercise sheet will be discussed on Friday, January 18th 2019.
You should hand in your solution of the exercise marked with (★)
in the mail box or email by 16:00 on Thursday January 17th 2019.

Exercise sheets online at `www.thp.uni-koeln.de/trebst/Lectures/2018-SolidState.shtml`

1 The Kronig-Penney model revisited

In this exercise, we return to the **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 is known as the **Wannier** basis. You can download the accompanying IPython notebook.

1.1 Numerical solution

On a previous sheet we already analytically solved 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 Kronig-Penney Hamiltonian is given as follows:

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

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

$$V_j = \begin{cases} V_j & j\,a < x < j\,a + w \\ 0 & \text{else}\,. \end{cases} \tag{2}$$

To solve the Schrödinger equation and obtain the wavefunctions ψ, we discretise space with a step size h.

a) Show that we can rewrite the discretised Hamiltonian as

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

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

b) Study the accompanying IPython notebook and use it to calculate the wavefunctions.

c) How are the boundary conditions taken care of in the simulation?

As seen in previous sheets, an alternative route is to make use of Bloch's theorem. It states that the wavefunction in a system with discrete translational invariance can be written as:

$$\psi(x) = \exp{(ik\,x)} u_{k,n}(x), \tag{4}$$

where the functions u are periodic in the lattice.

d) As above, insert the wavefunction in Bloch form into the Schr´odinger equation and derive the discretized version of the equation.

e) Using the supplied notebook perform the calculation and study the results for various strengths of the interaction.

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 in terms of Bloch functions is as follows:

$$w_n(r - an) = \frac{1}{\sqrt{N}} \sum_k \exp(-ikan)\psi_{nk}(r). \tag{5}$$

It is, however, not always guaranteed that the resulting functions are localized around the centers of the potentials. In particular, each of the Bloch function carries a phase that might interfere or be influenced by other terms. In a worst case scenario, this phase may cause the wavefunctions to be superposed in such a way that does not 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 ϕ_k for the reciprocal lattice vector k as

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

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.

a) Read through the source code to understand how Bloch functions are created from the simple wave function.

b) Choose a different band for which to calculate the Wannier basis.

c) Check for orthogonality, i.e. verify that you have a set of orthonormal basis vectors.

2 Tight binding in second quantisation (★)

Solving a tight binding model becomes particularly easy if the formulation of second quantisation 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. **However there is no need to use the IPython notebook for this particular exercise.**
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

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

a) Fourier transforming the creation/annihilation operators to show that each term of the form $c_i^{\dagger} c_j$ contributes $c_k^{\dagger} c_k e^{ik\,(r_n - r_m)}$.

b) Use this to solve for the energy spectrum of the tight binding chain.

Square lattice

Tight binding is applicable regardless of the dimensionality of the problem. Only the phase factor $c_k^{\dagger} c_k e^{ik\,(r_n - r_m)}$ changes such that each term is now determined by a scalar product $c_k^{\dagger} c_k e^{i\mathbf{k}\cdot(\mathbf{r}_n - \mathbf{r}_m)}$. Our first example is easily extended to two dimensions:

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

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

c) 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

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

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.

d) Rewrite the Hamiltonian using these new operators.

e) Continue by transforming the Hamiltonian into Fourier space and rewrite the result in the form of a vector-matrix-vector product.

f) Solve for the energy spectrum by diagonalizing this matrix.

Honeycomb lattice

As our final example we take the honeycomb lattice. This is the lattice upon which carbon atoms are placed to form graphene. The basis vectors are given by

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

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

$$\delta_1 = (1, 0) \ . \tag{11}$$

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

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

g) 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 δ_1, δ_2, and δ_3.

h) Set up the Hamiltonian matrix and solve for the dispersion relation as a function of k.

i) Now switch to the notebook or another computer programme (e.g. Mathematica) and compute the spectrum along the following path in the Brillouin zone:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \to \mathbf{K}_1 = \frac{2\pi}{3}\begin{pmatrix} 1 \\ 1/\sqrt{3} \end{pmatrix} \to \mathbf{K}_2 = \frac{2\pi}{3}\begin{pmatrix} 1 \\ -1/\sqrt{3} \end{pmatrix} \to \Gamma \tag{13}$$

Do you observe any special features along this path?