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Advanced Quantum Mechanics - Problem Set 4

Winter Term 2023/24

Due Date: Hand in solutions to problems marked with * as a single pdf file using Moodle before the lecture on **Thursday, 09.11.2023, 15:15**. The problem set will be discussed in the tutorials on Monday 13.11.2023 and Wednesday 15.11.2023.

Website: https://home.uni-leipzig.de/stp/Quantum_Mechanics_2_WS2324.html

Moodle: https://moodle2.uni-leipzig.de/course/view.php?id=45746

*1. SSH model

4+2+3 Points

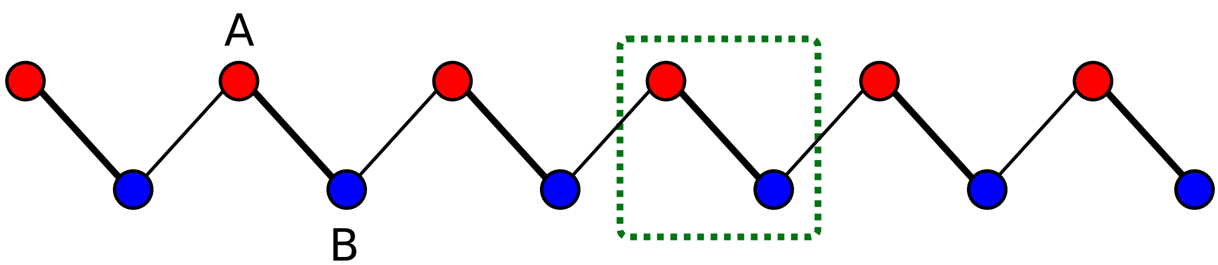

Figure 1: The SSH model. The red and blue circles symbolise different types of sites. The thin lines denote couplings with strength $t(1-\delta)$ whilst the thick lines are couplings with strength $t(1+\delta)$. The dashed square denotes a unit cell.

In this problem we consider the Su-Schrieffer-Heeger (SSH) model which describes spinless fermions hopping on a one-dimensional lattice with staggered hopping amplitudes (see the figure). The model contains two sub-lattices, A and B and has the following Hamiltonian

$$H = \sum_n t(1+\delta)|n,A\rangle\langle n,B| + t(1-\delta)|n+1,A\rangle\langle n,B| + \text{h.c.}.$$

Here h.c. stands for hermitian conjugate and $|n,A\rangle$ describes a state of site n, in sublattice A. t and δ are taken to be real parameters.

(a) By Fourier transforming, $|n\rangle = \frac{1}{\sqrt{N}}\sum_k e^{-ink}|k\rangle$, show that the Hamiltonian can be written as $H(k) = \boldsymbol{d}(k)\cdot\boldsymbol{\sigma}$, where $\boldsymbol{\sigma}$ is the vector of Pauli matrices, and $d_x(k) = t(1+\delta) + t(1-\delta)\cos(k)$, $d_y(k) = t(1-\delta)\sin(k)$, and $d_z(k) = 0$.

Hint: Write the wave function as a vector with two components describing the amplitudes on the A and B sublattices, respectively.

(b) Calculate the energy eigenvalues of the system.

(c) Plot your result from (b) for $\delta > 0$ and $\delta < 0$. What happens when $\delta = 0$?

2. Nearly free electron model

3+2+2+3 Points

Often it is sufficient to treat the periodic potential on a lattice as a small perturbation. For such problems it is useful to expand the periodic potential in a plane wave expansion which only contains waves with the periodicity of the reciprocal lattice, such that

$$U(\boldsymbol{x}) = \sum_{\boldsymbol{G}} U_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{x}},$$

where $\boldsymbol{G}$ is a reciprocal lattice vector which satisfies $e^{i\boldsymbol{G}\cdot\boldsymbol{R}} = 1$, with $\boldsymbol{R}$ denoting a point on the lattice. We moreover expand the wave functions in terms of a set of plane waves which satisfy the periodic boundary conditions of the problem

$$\psi(\boldsymbol{x}) = \sum_{\boldsymbol{k}} c_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}.$$

(a) Using the expansions above, show that the Schrödinger equation

$$\left[\frac{-\hbar^2\nabla^2}{2m} + U(\boldsymbol{x})\right]\psi(\boldsymbol{x}) = E\psi(\boldsymbol{x}),$$

can be written as

$$\left(\frac{\hbar^2 k^2}{2m} - E\right) c_{\boldsymbol{k}} + \sum_{\boldsymbol{G}} U_{\boldsymbol{G}} c_{\boldsymbol{k}-\boldsymbol{G}} = 0.$$

(b) Perform the shift $\boldsymbol{q} = \boldsymbol{k} + \boldsymbol{K}$, where $\boldsymbol{K}$ is a reciprocal lattice vector which ensures that we can always find a $\boldsymbol{q}$ which lies in the first Brillouin zone[1], and show that the Schrödinger equation now gives

$$\left(\frac{\hbar^2}{2m}(\boldsymbol{q} - \boldsymbol{K})^2 - E\right) c_{\boldsymbol{q}-\boldsymbol{K}} + \sum_{\boldsymbol{G}} U_{\boldsymbol{G}-\boldsymbol{K}} c_{\boldsymbol{q}-\boldsymbol{G}} = 0.$$

(c) Consider for concreteness a one-dimensional chain, but in the simple case where only the leading Fourier component contributes to the potential

$$U(x) = 2U_0 \cos\frac{2\pi x}{a}.$$

Explain how your result in (b) can be used to calculate the energy of the system.

(d) Suppose now that U_0 is very small. Near $q = \pi/a$ the Schrödinger equation reduces to

$$\begin{pmatrix} \frac{\hbar^2}{2m}\left(q - \frac{2\pi}{a}\right)^2 - E & U_0 \\ U_0 & \frac{\hbar^2 q^2}{2m} - E \end{pmatrix} \begin{pmatrix} c_1 \\ c_0 \end{pmatrix} = 0.$$

Calculate and plot the energy eigenvalues. What happens at $q = \pi/a$?

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[1] As an example of a Brillouin zone consider the simple cubic lattice with sides of length a. The lattice vectors can be written as $\boldsymbol{R}_1 = a\hat{\boldsymbol{x}}$, $\boldsymbol{R}_2 = a\hat{\boldsymbol{y}}$, and $\boldsymbol{R}_3 = a\hat{\boldsymbol{z}}$. In reciprocal space the basis vectors become $\boldsymbol{b_1} = \frac{2\pi}{a}\hat{\boldsymbol{x}}$, $\boldsymbol{b_2} = \frac{2\pi}{a}\hat{\boldsymbol{y}}$, and $\boldsymbol{b_3} = \frac{2\pi}{a}\hat{\boldsymbol{z}}$. In this case the first Brillouin zone is the region $-\pi/a \leq k_i < \pi/a$ (where $i = x, y, z$). The reziprocal lattice vectors can be written as $\boldsymbol{K} = \sum_i n_i \boldsymbol{b}_i$ (where $n_i \in \mathbb{Z}$). Therefore, for arbitrary $\boldsymbol{k}$ it is possible to find $\boldsymbol{q} = \boldsymbol{k} + \boldsymbol{K}$ so that $\boldsymbol{q}$ lies in the first Brilloin zone.