Institute of Theoretical Physics
University of Cologne
Winter semester 2022/23

Prof. Dr. Simon Trebst
Lasse Gresista

Solid State Theory

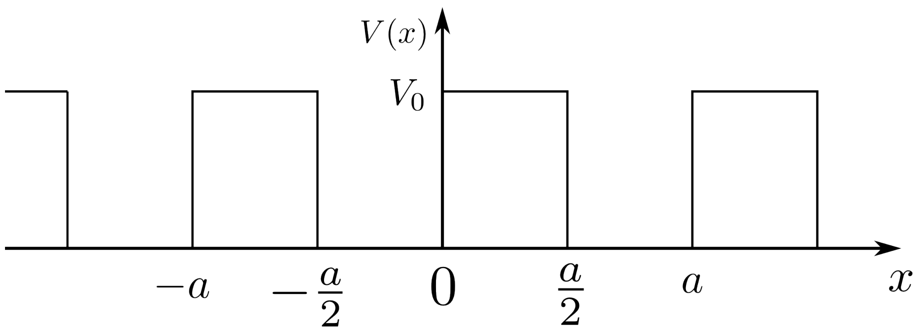
Exercise sheet 4

This exercise sheet will be discussed on Friday, December 16th 2022.
via mail (gresista@thp.uni-koeln.de) by 10:00 AM on Thursday December 15th 2022.

Kronig-Penney model

Consider a periodic rectangular potential with periodicty a and strength V_0 as shown in the figure:

$$V(x) = \begin{cases} V_0 & x \in (na, na + \frac{a}{2}) \\ 0 & x \in (na - \frac{a}{2}, na) \end{cases} \quad (n \in \mathbb{Z}) \tag{1}$$



We want to solve the Schroedinger equation

$$\left(-\frac{\hbar^2 \partial_x^2}{2m} + V(x)\right) \Psi(x) = E\,\Psi(x) \tag{2}$$

to see that we obtain energy gaps in the electronic band structure. Bloch's theorem

$$\Psi(x) = e^{ikx} u(x), \text{ where } u(x) = u(x+a) \tag{3}$$

says that it is sufficient to solve problem only in one period of the potential, for example $x \in [-a/2, a/2]$

Exact solution

a) Show that the ansatz

$$\Psi_I(x) = Ae^{i\alpha x} + Be^{-i\alpha x} \quad (0 < x < a/2) \tag{4}$$

$$\Psi_{II}(x) = Ce^{i\beta x} + De^{-i\beta x} \quad (-a/2 < x < 0) \tag{5}$$

where $\alpha = \frac{\sqrt{2mE}}{\hbar}$ and $\beta = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ solves the Schroedinger equation in the respective range.

To make sure that the solution is in accordance with Bloch's theorem and boundary conditions of continuity and continuity of probability current, it has to satisfy

$$\begin{aligned}\Psi_I(0) &= \Psi_{II}(0)\\ \Psi'_{II}(0) &= \Psi'_{II}(0)\\ u_I(a/2) &= u_{II}(-a/2)\\ u'_I(a/2) &= u'_{II}(-a/2)\end{aligned}$$

Write this in the form (you may use an algebra software like Mathematica or SymPy)

$$\boldsymbol{M}(E,k)\begin{pmatrix}A\\B\\C\\D\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\end{pmatrix}. \tag{6}$$

For this system of linear equations to have a non trivial solution, the determinant of $\boldsymbol{M}$ has to be zero:

$$\det\boldsymbol{M}(E,k)\overset{!}{=}0 \tag{7}$$

b) Show that Eq. (7) is equivalent to (again, you may use a computer)

$$\cos(ak)=\cos(\frac{a\,\alpha}{2})\,\cos(\frac{a\,\beta}{2})-\frac{\alpha^2+\beta^2}{2\,\alpha\beta}\sin(\frac{a\,\alpha}{2})\,\sin(\frac{a\,\beta}{2}). \tag{8}$$

As this equation can not be solved analytically for $E(k)$, visualize the possible solutions for different values of k in the first Brillouin zone.

Perturbation theory for a periodic potential (★)

Consider a single electron in a weak periodic potential with the Hamiltonian $H=H_0+H_1$, where H_0 is the free Hamiltonian

$$H_0=\frac{p^2}{2m} \tag{9}$$

and H_1 is defined via

$$\langle x|\,H_1\,|x'\rangle=V(x)\delta(x-x')\quad V(x+a)=V(x). \tag{10}$$

We want to consider the effect of the periodic potential using standard perturbation theory with H_1 as the perturbation. As a starting point, we consider the eigenstates $|k\rangle$ and energies $\epsilon_k^{(0)}$ of the unperturbed Hamiltonian

$$H_0\,|k\rangle=\epsilon_k^{(0)}\,|k\rangle=\frac{\hbar^2k^2}{2m}\,|k\rangle\,. \tag{11}$$

In order for these eigenstates to be normalizable, we consider a finite system $x\in[0,L]$ with periodic boundary conditions, resulting in a discrete set of $|k\rangle$ with $\langle x|\,k\rangle=\frac{1}{\sqrt{L}}e^{ikx}$.

a) Show that the matrix elements of the periodic potential in momentum space are given by

$$\langle k|\,H_1\,|k'\rangle=\sum_{G_n}V_{G_n}\delta_{k-k',G_n}\ , \tag{12}$$

where V_{G_n} are the Fourier components of the potential $V(x)$ with the reciprocal lattice vectors $G_n=\frac{2\pi}{a}n$ ($n\in Z$). What does this imply for interactions between different momenta?
Hint: Insert $1=\int_0^L dx\,|x\rangle\,\langle x|$ and the Fourier expansion $V(x)=\sum_{G_n}e^{iG_nx}V_{G_n}$.

b) Now apply perturbation theory: Show that, up to second order, the energy is given by

$$\epsilon_k = \epsilon_k^{(0)} + V_{G_0} + \sum_{G_n \neq G_0} \frac{|V_{G_n}|^2}{\epsilon_k^{(0)} - \epsilon_{k-G_n}^{(0)}} \ . \tag{13}$$

What is the effect of the linear correction? For which k is the second correction the strongest?
Hint: The general formula for non-degenerate, time-independent second order perturbation theory is

$$\epsilon_k = \epsilon_k^0 + \langle k| H_1 |k\rangle + \sum_{k' \neq k} \frac{| \langle k| H_1 |k'\rangle |^2}{\epsilon_k^{(0)} - \epsilon_{k'}^{(0)}} \tag{14}$$

c) At the edges of the (emerging) Brillouin zones at $k_m = \frac{\pi}{a} m$ $(m \in Z)$, second-order pertubation theory breaks down, because the zero order energies of $k = k_m$ and $k' = k_m - G_m$ are degenerate. To remedy this, use degenerate perturbation theory to show that the shift in energy at these momenta is given by

$$\epsilon_{k_m}^{\pm} = V_{G_0} \pm |V_{G_m}|. \tag{15}$$

What does this imply for the band structure?
Hint: In degenerate perturbation theory the energy shift is given by the eigenvalues of the two dimensional Hamilton matrix of H_1 in the degenerate subspace spanned by $|k\rangle$ and $|k'\rangle$.

d) Now consider the periodic potential of the Kronig-Penney model defined in the previous exercise. Calculate the first order energy correction and use Eq. 15 to show that the band gap

$$\Delta_m = \begin{cases} \frac{2V_0}{\pi m} & m \text{ odd} \\ 0 & m \text{ even} \end{cases} \tag{16}$$

opens at the Brillouin zone boundaries.
Hint: The Fourier components of the potential are given by $V_{G_n} = \frac{1}{a} \int_0^a V(x) e^{iG_n x}$

e) Sketch the result in the reduced zone scheme.