Institute of Theoretical Physics
University of Cologne
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Prof. Dr. Simon Trebst
Henry F. Legg
Based on problem sets by Peter Bröcker

Solid State Theory

Exercise sheet 4

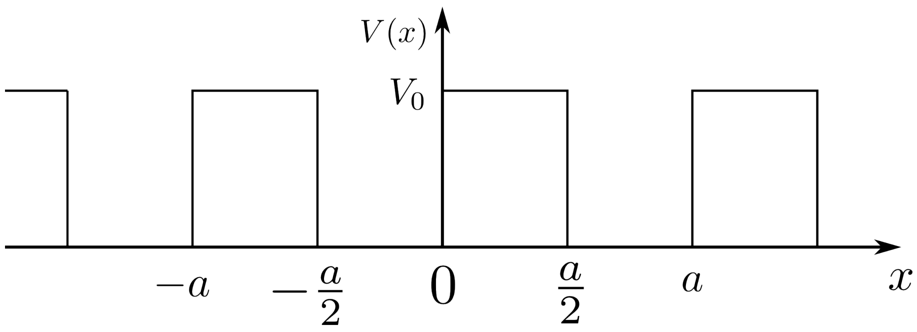
This exercise sheet will be discussed on Friday, December 7th 2018.
You should hand in your solution of the exercise marked with (★)
in the mail box by 16:00 on Thursday December 6th 2018.

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

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. 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

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

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

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

b) Show that Eq. (7) is equivalent to (you may use a computer e.g. Mathematica)

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

This equation can not be solved analytically for $E(k)$ but visualize the possible solutions.

Perturbation theory (★)

We start from the eigenstates of the free Hamiltonian:

$$H_0\,|p\rangle = E_p\,|p\rangle = \frac{\hbar^2 k^2}{2m}\,|p\rangle \tag{9}$$

$\langle x|\,p\rangle = e^{ipx}/\sqrt{2\pi}$ and treat the effect of the periodic potential H_1 with matrix elements $\langle x|\,H_1\,|x'\rangle = V(x)\delta_{x,x'}$ in perturbation theory.

a) Show that the matrix elements of the periodic potential in momentum space are given – up to an arbitary phase – by

$$\langle p|\,H_1\,|p'\rangle = V_0 \sum_{m=-\infty}^{\infty} \frac{e^{i\pi m}-1}{2\pi m}\delta_{p-p',\frac{2\pi\,m}{a}}. \tag{10}$$

b) Now apply pertubation theory: Show that first order gives an overall energy shift $\langle p|\,H_1\,|p\rangle = V_0/2$ and that second order is dominated by terms

$$p = -p' = \pm\frac{\pi m}{a}, \tag{11}$$

the edges of the (emerging) Brillouin zones.

c) Show that the band gap Δ_m at $p = \pm\frac{\pi m}{a}$ is given by

$$\Delta_m = \begin{cases} \frac{2\,V_0}{\pi m} & m \text{ odd} \\ 0 & m \text{ even} \end{cases}. \tag{12}$$

Hint: You will need to use degenerate pertubation theory.

d) Sketch the result in the reduced zone scheme.