Institute for Theoretical Physics
University of Cologne

Prof. Dr. Simon Trebst
Peter Bröcker

Solid State Theory

Problem set 4

Winter Term 2016

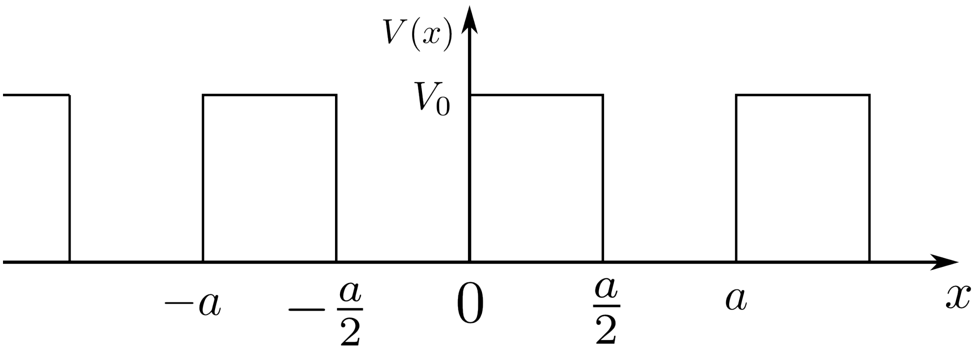
Website: http://www.thp.uni-koeln.de/trebst/Lectures/2016-SolidState.shtml
Due date: Discussed in class on **Thursday, December 8th**.

If you turn in your solutions by Wednesday noon (December 7th), they will be graded.
Please submit your solutions to Henry Legg at hlegg@uni-koeln.de.

1. 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. Blochs 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 $x \in [-a/2, a/2]$

1. **exact solution:** 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 Blochs theorem, 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:

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

Show that Eq. (7) is equivalent to

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

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

2. **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. Show that the matrix elements of the periodic potential in momentum space are given by

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

There is an overall energy shift $\langle p|\,H_1\,|p\rangle = V_0/2$. The rules of pertubation tell us that we have to connect degenerate enegy levels first. Show that that there are finite matrix elements only if

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

that is, at the corners of the (now emerging) Brillouin zones. Use degenerate perturbation theory to show that the band gap Δ_m at $p = \pm\frac{\pi m}{a}$ is given by

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

Sketch the result in the reduced zone scheme.