

Frankfurt, Dec. 9, 2009

Theoretikum zur Einführung in die Theoretische Festkörperphysik
WS 2009/10

Exercise Set 8

(Due date: Tuesday, December 15, 2009)

Exercise 17 (Scattering from a delta function potential) (10 points)

We consider scattering from a one-dimensional potential $V(x) = g\delta(x)$ with $g \neq 0$ where $\delta(x)$ is the Dirac delta function.

- Which continuity conditions do the wave functions and their derivatives at $x = 0$ have to fulfil?
- A plane wave with energy $E > 0$ coming in from the left is described by the wave function

$$\psi^L(x) = \begin{cases} e^{ikx} + r(k)e^{-ikx}, & \text{for } x < 0 \\ t(k)e^{ikx}, & \text{for } x > 0 \end{cases}$$

with $k = \sqrt{2mE}/\hbar$. Determine the complex amplitudes $r(k)$ and $t(k)$ by evaluating the continuity conditions from a) and calculate from that the transmission coefficient T as a function of E . Does the result for T depend on the sign of g ?

Exercise 18 (Kronig Penney model) (25 points)

The physical reason for the existence of energy bands is the periodic arrangement of the atoms in the crystal on the one hand and the quantum mechanical tunneling process on the other. The Kronig Penney model allows to demonstrate this in a simple one-dimensional example. The model assumes a periodic arrangement of delta function potentials in one dimension:

$$V(x) = g \sum_{n=-\infty}^{\infty} \delta(x - na),$$

where a is the lattice constant and the coupling constant $g > 0$ is fixed.

- In the regions $B_n = \{x | na < x < (n+1)a\}$, $n \in \mathbb{Z}$ the solution shows an oscillatory behaviour. Formulate a suitable *ansatz* for the wave function.

- b) Use the continuity conditions for ψ and ψ' at $x = n\mathbf{a}$ for deriving an equation for the possible energy eigenvalues E .
- c) Use the periodicity of the problem $V(x) = V(x + \mathbf{a})$ for showing that $\psi(x)$ and $\psi(x + \mathbf{a})$ differ only by a phase factor.
- d) Use the Bloch theorem and the periodic boundary conditions for simplification of the problem. Show that the periodic boundary conditions lead to a discretization of the possible k values where k is an additional wave number that arises from the periodicity of the potential. Show also that the application of the Bloch theorem reduces the number of quantities to be determined to two.
- e) Show that the disappearance of the coefficient matrix leads to the condition

$$\cos k\mathbf{a} = \cos k_\epsilon \mathbf{a} + \frac{mg}{\hbar k_\epsilon} \sin k_\epsilon \mathbf{a}, \quad k_\epsilon = \frac{\sqrt{2m\epsilon}}{\hbar}$$

for the possible electron energies.

- f) Plot your result in a way that shows that the energy axis is separated into allowed and forbidden regions, corresponding to energy bands and band gaps.
- g) Show the discrete energy values that correspond to a given k ($-\pi/\mathbf{a} < k < \pi/\mathbf{a}$) graphically.
- h) Discuss the shape of the energy bands for $g\mathbf{a} \rightarrow \infty$, $g\mathbf{a} \rightarrow 0$ and for fixed g and \mathbf{a} .