Theory of Quantum Matter

Lecturer: Prof. Otfried Gühne (Mon 14:00, Fri 10:00, Room D120)
Exercises: Chau Nguyen (Fri 14:00, Room B030) **Sheet 4**

Hand in: Mon 12.11.2018 *(questions marked as ∗ are optional)*
Discussion date: Fri 16.11.2018

6. Electron in the Kronig–Penny potential

(a) (10pts) We start with considering the reflection of an electron with energy E on a δ-Dirac potential, $V(x) = S\delta(x)$ with $S > 0$. For those who are not familiar with the δ-Dirac function: the potential can be considered as a square potential with width a and height V in the limit $a \to 0$, $V_0 \to \infty$ such that $aV_0 \to S$. The wave function is of the form $\psi(x) = a_- e^{ikx} + b_- e^{-ikx}$ for $x < 0$ and $\psi(x) = a_+ e^{ikx} + b_+ e^{-ikx}$ for $x > 0$ with $k = \sqrt{2Em}/\hbar$. The boundary condition at $x = 0$ imposes that the wave coefficients from the two sides are connected by the so-called *transfer matrix*,

$$\begin{pmatrix} a_+ \\ b_+ \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} a_- \\ b_- \end{pmatrix}. \quad (1)$$

Show that the transfer matrix T for the δ-Dirac potential is given by

$$T = \begin{pmatrix} 1 - iZ & -iZ \\ iZ & 1 + iZ \end{pmatrix}, \quad (2)$$

with $Z = \frac{\kappa}{k}$, $\kappa = mS/\hbar^2$.

Hint: Recall that the wave function is continuous while its derivative makes a jump across a δ-Dirac function.

(b) (∗) Compute the transmission and reflection coefficient. Show that $\det(T) = 1$.

(c) (10pts) Now we consider a periodic lattice of δ-Dirac potential with spatial period d, $V(x) = \sum_{n=-\infty}^{+\infty} S\delta(x - nd)$. The wave function is of the form $\psi(x) = a_n e^{ikx} + b_n e^{-ikx}$ for $nd < x < (n+1)d$ with $k = \sqrt{2Em}/\hbar$. The wave coefficients in adjacent cells are again related by the transfer matrix T determined above. Show that Bloch's theorem implies

$$\begin{pmatrix} a_{n+1} \\ b_{n+1} \end{pmatrix} = e^{iqd} \begin{pmatrix} e^{-ikd} & 0 \\ 0 & e^{+ikd} \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix}. \quad (3)$$

(d) (10pts) Using the results above to determine the spectral equation (or band-gap structure) of the electron in the potential, namely, the relation between E and q. You should obtain:

$$\cos(qd) = \cos(kd) + \frac{\kappa q}{kd} \sin(kd). \quad (4)$$

(e) (10pts) Sketch E as a function of q in the first Brillouin zone.