Kronig-Penney model

We study a simple model for a one-dimensional crystal lattice, which was introduced by Kronig and Penney in 1931. The atomic potentials are taken to be rectangular, where the minima correspond to the atomic cores. The model is simplified even more by replacing the rectangular potentials by Dirac delta functions,

$$V(x) = V_0 \sum_{n=-\infty}^{\infty} \delta(x - an). \tag{1}$$

This is the so-called Kronig-Penney potential which is shown in Fig. 1A.

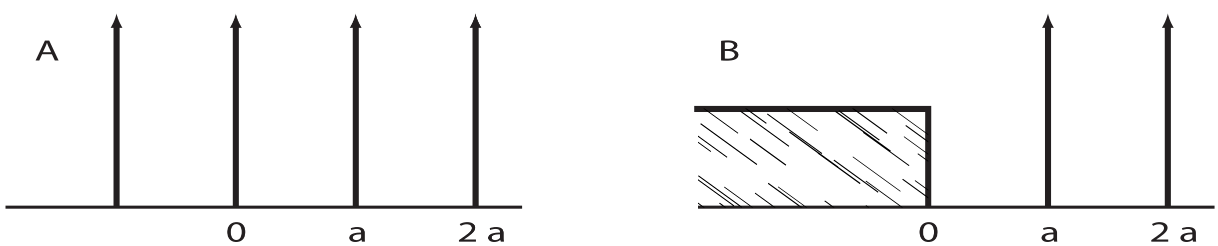

Figure 1: **A** Kronig-Penney potential $V(x)$. **B** Interface between a constant potential $U(x)$ and a Kronig-Penney potential.

Exercise 1.1 Energy bands

Using Bloch's Ansatz for the wave function in a periodic potential

$$\Psi(x + a) = \Psi(x)e^{ika}, \tag{2}$$

show that the energy in the Kronig-Penney potential for a given k obeys the equation

$$\cos\lambda = \frac{v}{2\beta}\sin\beta + \cos\beta, \tag{3}$$

where $\lambda = ka$, $\beta = a\sqrt{2mE/\hbar^2}$ and $v = 2mV_0a/\hbar^2$. In general, this equation can only be solved graphically or numerically. Show that the resulting band structure has band gaps (i.e., intervals where there exists no solution to Eq. (3)). Discuss the special cases where $v \to 0$ and $v \to \infty$.
Hint: Find the solution to the Schrödinger equation in the finite interval $(na, na + a)$ first. Then make use of the fact that the wave function has to be continuous everywhere. The integration of the Schödinger equation over the interval $(na - \eta, na + \eta)$ in the limit of $\eta \to 0$ yields another boundary condition for the derivative of the wave function.

Exercise 1.2 Density of states

Calculate the density of states of the Kronig-Penney model. What is the behavior of the density of states at the band boundaries?
Hint: The number of states per unit cell in the interval $(E, E + dE)$ is given by $\rho(E)dE$. Consider first a finite Kronig-Penney potential of length Na with periodic boundary conditions (N is the number of unit cells) such that the states can be indexed by discrete k-values. Convince yourself that

$$\rho(E) = \frac{a}{\pi}\left|\frac{dk}{dE}\right|. \tag{4}$$

The derivative dk/dE can be calculated using Eq. (3).

Exercise 1.3 Surface states

Consider now the potential

$$U(x) = \begin{cases} U_0 & x \leq 0, \\ V_0 \sum_{n=1}^{\infty} \delta(x - na) & x > 0, \end{cases} \tag{5}$$

which is shown in Fig. 1B.
Show that for $E < U_0 < \infty$ there is one additional state in every band gap which decays exponentially on both sides of $x = 0$. Show that the energy of this state is the solution of

$$\beta \cot \beta = \frac{u}{v} - \sqrt{u - \beta^2} \tag{6}$$

with $u = 2mU_0a^2/\hbar^2$.
Hint: The solution for $x > 0$ is given as in Ex. 1.1, but exponentially decaying. Thus, the energy eigenvalues should solve Eq. (3) within the band gaps. We set

$$\lambda = \begin{cases} i\mu & s = 1, \\ i\mu + \pi & s = -1, \end{cases} \tag{7}$$

where s is the sign of the right hand side of Eq. (3) where the Bloch ansatz implies that $\mu > 0$ for the wave function not to grow exponentially.
For $x < 0$ we use the ansatz

$$\Psi(x) = Ce^{\kappa x/a} \tag{8}$$

with $\kappa = \sqrt{u - \beta^2}$. Use the continuity of the wave function and its first derivative at $x = 0$ to find the energy.