A. 15.5: Decaying waves

As we saw in this chapter, in one dimension, a periodic potential opens a band gap such that there are no plane-wave eigenstates between energies $\epsilon_0(G/2) - |V_G|$ and $\epsilon_0(G/2) + |V_G|$ with $G$ a reciprocal lattice vector. However, at these forbidden energies, decaying (evanescent) waves still exist. Assume the form

$$\psi(x) = e^{-\kappa x}[Ae^{ikx} + Be^{i(k-G)x}],$$

with $0 < \kappa \ll k$ and $\kappa$ real. Using first order degenerate perturbation theory (as in problem 15.1), find $\kappa$ as a function of energy for $k = G/2$. For what range of $V_G$ and $E$ is your result valid?

B. 15.6: Kronig-Penney Model

Consider electrons of mass $m$ in a so-called “delta-function comb” potential in one dimension

$$V(x) = aU \sum_n \delta(x - na).$$

(a) Argue using the Schrödinger equation that in-between delta functions, an eigenstate of energy $E$ is always of plane wave form $e^{ikx}$, with

$$|q_E| = \sqrt{2mE/\hbar}.$$

Using Bloch’s theorem, conclude that we can write an eigenstate with energy $E$ as

$$\psi(x) = e^{ikx}u_E(x),$$

where $u_E(x)$ is a periodic function defined as

$$u_E(x) = e^{-ikx}[A \sin(q_E x) + B \cos(q_E x)] \quad 0 < x < a,$$

and $u_E(x) = u_E(x + a)$ defines $u$ outside of this interval.

(b) Using continuity of the wave function at $x = 0$ derive

$$B = e^{-ika}[A \sin(q_E a) + B \cos(q_E a)],$$

and using the Schrödinger equation to fix the discontinuity in slope at $x = 0$ derive

$$q_E A - e^{-ika}q_E[A \cos(q_E a) - B \sin(q_E a)] = \frac{2maUa}{\hbar^2}.$$

Solve these two equations to obtain

$$\cos(ka) = \cos(q_E a) + \frac{maUa}{\hbar^2 q_E \sin(q_E a)}.$$

The left-hand side of this equations is always between $-1$ and $1$, but the right-hand side is not. Conclude that there must be values of $E$ for which there are no solutions of the Schrödinger equation – hence concluding that there are gaps in the spectrum.

(c) For small values of the potential $U$ show that this result agrees with the predictions of the nearly free electron model (i.e., determine the size of the gap at the zone boundary).