5 Quantum Mechanics

5.1 Band Structure (8 units)

This project relies on a knowledge of material covered in the Part II(D) course Applications of Quantum Mechanics.

1 Introduction

In suitable units, the Schrodinger equation is

$$\frac{d^2\psi}{dx^2} + \big(E - V(x)\big)\psi = 0. \tag{1}$$

In this exercise, we suppose that V is periodic, in which case the Schrodinger equation may be considered to be a model for an electron in a crystal lattice. You will seek solutions to the Schrodinger equation such that ψ remains finite as $|x| \to \infty$: these will be called "allowed solutions". You will verify that the energy values E for these solutions form a band structure.

Consider a specific choice for $V(x)$, which is an even function $[V(x) = V(-x)]$, formed from an infinite series of nearly parabolic sections, each of width $2a$. For positive x,

$$V(x) = \frac{3}{2}\left[1 - \cosh\left(x - (2r+1)a\right)\right] \tag{2}$$

where $r = \text{floor}(x/2a)$, i.e. the greatest integer less than or equal to $(x/2a)$.

2 Numerical Work

Given some x_{max}, you will write a program which solves (1) for $0 < x < x_{\text{max}}$. The solution depends on the value of E, and on the boundary values $\psi(0)$ and $\psi'(0)$.

Your program should

(i) input the values for E and x_{max}, and suitable boundary conditions for ψ;

(ii) solve the Schrodinger equation for x between 0 and x_{max};

(iii) display a graph of ψ against x for this range of x.

Take $a = 2$. Suggested values for other parameters are $\psi(0) = 1$, $\psi'(0) = 0$, $x_{\text{max}} = 150$, and $-2.0 < E < 1.5$. You will need to select a suitable step for your numerical integration.

Remember, you are seeking solutions for which ψ remains finite as $|x| \to \infty$. If such solutions exist then E is an "allowed" value of the energy. These allowed energy values are grouped into bands. In order to be fairly certain that an energy value is allowed, you may want to consider the effect of increasing x_{max}, it should be adequate to consider $x_{\text{max}} \leqslant 500$ but you may consider higher values if you wish. You should comment on the accuracy of the numerical methods which you use.

(i) Use trial and error to find five band boundaries in the range $-2.0 < E < 1.5$. Evaluate the energies of the band boundaries to two decimal places.

(ii) Make graphs showing representative solutions for ψ. You should show examples for energies that are near to all band boundaries, and examples taken from near the middle of two different bands. Comment on your results. Are the band boundaries affected by choosing different initial conditions for ψ, for example $\psi(0) = 0$, $\psi'(0) = 1$?

(iii) If $V(x)$ is periodic with period l, the solutions to (1) where ψ remains finite as $|x| \to \infty$ can always be written as linear combinations of Bloch functions. These are functions such that

$$\psi(x) = e^{ikx} v(x), \qquad v(x + l) = v(x),$$

where k is a real number. (Recalling the introduction, we can now make the precise statement that "allowed solutions" to (1) are those that can be expressed as linear combinations of Bloch functions.) One sees that $v(x)$ is a periodic function with the same period as V, but $\psi(x)$ has a different period in general.
Given a solution for ψ, show how you can extract k from your numerical results. How does the energy E depend on k? (It may be useful to make a sketch.) Make a graph in which you compare one of your numerical solutions with a suitably chosen linear combination of Bloch functions.

(iv) Compare your numerical results with those expected from the 'nearly free' and 'tightly bound' models of electrons in solids. Which is the most appropriate model for the different energy bands that you have found?

