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 for a particle moving in a potential V is

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

where ψ is the wavefunction and E is the energy. 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.

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

$$\psi(x) = e^{ikx} v(x), \qquad v(x + l) = v(x), \tag{2}$$

where k is a real number. Hence, "allowed solutions" to (1) are those which 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 $\psi(x)$ does not necessarily have this property.

2 Numerical Work

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,

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

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

> **Programming Task:** Given some $x_{\max}$, write a program which solves (1) for $0 < x < x_{\max}$. The solution depends on the value of E, and on the boundary values $\psi(0)$ and $\psi'(0)$.
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> 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 $x_{\max}$;
>
> Your program should be able to plot the solution ψ as a graph. When running the program, you will need to select a suitable step for your numerical integration.

Question 1 Consider the case

$$a = 2, \qquad \psi(0) = 1, \qquad \psi'(0) = 0, \qquad x_{\max} = 150$$

Run your program for some energies in the range $-2.0 < E < 1.5$ and report the results for ψ. You should choose the values of E to illustrate the different kinds of solution that you find. Your report should discuss the accuracy of the numerical methods which you use.

Note: In this question and throughout this project, you should provide graphs that illustrate clearly the behaviour that you observe. Note that very large numbers of graphs are *unlikely to be effective* in communicating this information.

Question 2 Remember, the physically-relevant energies E are those for which ψ remains finite as $|x| \to \infty$. These "allowed" values of the energy are grouped into bands.

For the parameters of question 1, 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. In order to determine which energy values are allowed, you may want to consider the effect of increasing $x_{\max}$, it should be adequate to consider $x_{\max} \leqslant 500$ but you may consider higher values if you wish.

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 $\psi(0) = 0$, $\psi'(0) = 1$?

Question 3 The allowed solutions can be expressed as linear combinations of Bloch functions, as defined in (2). 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.

Question 4 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?

