5 Quantum Mechanics

5.1 Band Structure

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 Schrödinger equation is

\[ \frac{d^2 \psi}{dx^2} + (E - V(x))\psi = 0. \]  

(1)

The object of this exercise is to verify by numerical methods that ‘allowed’ energy eigenvalues of (1) may have a band structure when \( V(x) \) is periodic. An ‘allowed’ value of \( E \) is such that the corresponding solution of (1) remains finite as \( |x| \to \infty \).

For \( V(x) \), consider an infinite series of nearly parabolic sections, each of width \( 2a \), viz, for positive \( x \),

\[ V(x) = - (x - c_j)^2 \left[ 1 + \frac{1}{20} (x - c_j)^2 \right] \]

where the positions of the maxima are given by \( c_j = (2j + 1)a \) with \( j = \text{floor}(x/2a) \), i.e. the greatest integer less than or equal to \( (x/2a) \). This may be considered to be a model for an electron in a crystal lattice.

2 Numerical Work

Write a program which will:

(i) input values for \( E \) and suitable initial conditions for \( \psi \);

(ii) integrate (1) for positive \( x \) up to \( x_{\text{max}} \), where \( x_{\text{max}} = 150 \) is sufficient to look for the lowest energy band, but may need to be increased looking for higher energy bands;

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

Take \( a = 2.0 \) and \( \psi(0) = 1, \psi'(0) = 0 \).

You may use any ordinary differential equation (ODE) solver you wish, such as MATLAB’s ode45. Whichever solver you use, you will be expected to comment on its accuracy and any tests you did to choose input values such as tolerances.

In order to be fairly certain that \( \psi(x) \) remains bounded in bands for which \( E > 0 \), you may have to increase \( x_{\text{max}} \). It should be adequate for the purposes of this project to take \( x_{\text{max}} \leq 500 \), but you may take it higher if you wish.

**Question 1** What ODE solver or algorithm are you using? What parameters, such as tolerances, does it require as input, and how can you be sure the ones you have chosen are sensible?
**Question 2**  Find 5 band boundaries in the range $-2.5 < E < 1.5$ to two decimal places, by “trial and error.” Tabulate or otherwise present the values of $E$ corresponding to these boundaries.

**Question 3**  Present plots of $\psi(x)$ near to all band boundaries investigated and in the middle of any two bands. Comment on how the plots demonstrate you have correctly located band boundaries.

**Question 4**  For any periodic $V(x)$ with period $\ell$, the solutions are Bloch functions of the form

$$\psi = e^{ikx}v(x) \quad v(x + \ell) = v(x),$$

where $v(x)$ is a periodic function with the same period $\ell$ and $k$ can be complex. Derive a formula which will allow you to extract $k$ from your numerical results. [You should not have to use fast Fourier transform (FFT) methods.]

**Question 5**  Plot the dispersion relation $E(k)$. Can you find a relationship?

**Question 6**  Plot the Bloch function for some value of $E$ choosing a suitable function $v(x)$ and compare it with the numerical solution.

**Question 7**  Compare your numerical results with those expected from the ‘nearly free’ and ‘tightly bound’ models. Which is the most appropriate model for the different energy bands?