Solutions of the Schrödinger equation

Quantum Mechanics Foundation Course: Problem Sheet 2

1 Time-independent Schrödinger equation

For 1-dimensional systems, the time-dependent Schrödinger equation is,

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right]\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t).$$

(i) Using separation of variables (Hint: $\Psi(x,t)=\psi(x)f(t)$), derive the time-independent Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x).$$

(ii) A uniform potential $V(x)=V_0$ acts on a particle. Show that its solution for the corresponding time-independent Schrödinger equation can be expressed as a superposition of plane waves,

$$\psi(x)=Ae^{ikx}+Be^{-ikx},$$

for $k=\sqrt{\frac{2m(E-V_0)}{\hbar^2}}$, where A and B are constants.

(iii) What form does the wavefunction adopt when $V_0>E$?

2 Infinite square well

A particle is constrained to a region in 1-dimensional space by a potential. The region begins at the origin and has a length a. The potential acting on the particle is defined as,

$$V(x)=\begin{cases}0, & \text{for} \quad 0\le x\le a\\ \infty, & \text{for} \quad x<0 \text{ and } x>a.\end{cases}$$

This is referred to as the 'particle in a box' model.

(i) Sketch the potential described above.

(ii) Using the time-independent Schrödinger equation, what is the value of the wavefunction outside the box?

(iii) What are the boundary conditions on the wavefunction?

(iv) Solving the Schrödinger equation subject to the above boundary conditions, find the allowed values of k?

(v) Show that the allowed forms of the wavefunction inside the box are:

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \quad .$$

(vi) Hence, show that the energy spectrum is given by:

$$E_n=\frac{n^2\pi^2\hbar^2}{2ma^2}$$

(vii) Using the formula in part (iv), sketch the first three wavefunctions. In a seperate plot, draw the first five energy levels (eigenvalues).

(viii) Estimate the ground state energy of an electron confined to a box of size $a=1$ Å. Is this result physically reasonable and why?

3 Finite square well

The same particle in a box model described above may be evaluated with a finite potential:

$$V(x) = \begin{cases} 0, & \text{for} \quad 0 \le x \le a \\ V, & \text{for} \quad x < 0 \text{ and } x > a. \end{cases}$$

(i) Sketch the form of the potential well.

(ii) Solve the time-independent Schrödinger equation seperately for each of the following regions:
$a)\, x < 0$ $\qquad b)\, 0 < x < a$ $\qquad c)\, x > 0$
Sketch the three solutions.

(iii) What are the boundary conditions satisfied by the wavefunction and its first derivative at $x = 0$ and $x = a$?

(iv) Graphically match the solutions found in part (ii) to provide a full wavefunction. Compared to the system in question 2 ($V = \infty$), is the particle confined to the box?

Section 2.5 of Alistair Rae's Quantum Mechanics provides the details to analytically match the solutions from each of the described regions to give the full wavefunction.

4 Harmonic oscillator

The potential describing a harmonic oscillator is given by $V(x) = \frac{1}{2}m\omega^2x^2$.

(i) Write down the corresponding time-independent Schrödinger equation.

(ii) Show that the wavefunction

$$\psi_g(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar}$$

is an eigenstate of the time-independent Schrödinger equation and find its energy.

(iii) Show that the wavefunction

$$\psi_e(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \sqrt{\frac{2m\omega}{\hbar}}\, x e^{-m\omega x^2/2\hbar}$$

is also an eigenstate of the time-independent Schrödinger equation and find its energy.

(iv) The energy spectrum for the harmonic oscillator is given by,

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad .$$

What energy levels do each of the above wavefunctions correspond to?

(v) What is the energy value for $n = 0$? Suggest a physical interpretation for this value. How does this compare to a classicial harmonic oscillator?

5 Recommended reading

- Quantum Mechanics - Alistair Rae - Chapters 1 & 2