Solution of Time-Independent Schrödinger Equation for a Finite One-Dimensional Square-Well Potential

A particle of mass m is confined inside a finite one-dimensional potential well of width a, with $V = 0$ inside the well ($-a/2 < x < a/2$) and $V = V_0 =$ constant outside the well ($|x| \geq a/2$). The potential V_0 is finite, but the energy of the particle $E < V_0$ so that it is bound.

The method of solution of the Time-Independent Schrödinger Equation follows the same steps as the other examples covered in the lectures, but the algebra is a little longer.

First write the general solution in each of the three regions.

$$\begin{array}{rrclrcl} x \leq -a/2: & V(x) & = & V_0, & \psi_1(x) & = & Ae^{Kx} + Be^{-Kx}, \\ -a/2 < x < a/2: & V(x) & = & 0, & \psi_2(x) & = & C\sin(kx) + D\cos(kx), \\ x \geq a/2: & V(x) & = & V_0, & \psi_3(x) & = & Fe^{-Kx} + Ge^{Kx}, \end{array}$$

where $k = \sqrt{2mE}/\hbar$ and $K = \sqrt{2m(V_0 - E)}/\hbar$.

The choice of the trigonometric form of the solution inside the well is because a bound standing-wave solution is expected. Outside the well exponentially decaying solutions are expected. These choices are for convenience, to keep the algebra as straightforward as possible.

Now apply conditions to determine the coefficients.

The wavefunction must remain finite everywhere.
As $x \to -\infty$, $e^{-Kx} \to \infty$, and so $B = 0$ to keep ψ_1 finite.
As $x \to +\infty$, $e^{Kx} \to \infty$, and so $G = 0$ to keep ψ_3 finite.

At the two well boundaries, $x = \pm a/2$, the wavefunction must be continuous.

$$\begin{array}{lrcll} \text{At } x = -a/2: & \psi_1(-a/2) & = & \psi_2(-a/2) & \\ \therefore & Ae^{-Ka/2} & = & C\sin(-ka/2) + D\cos(-ka/2) & \\ \therefore & -C\sin(ka/2) + D\cos(ka/2) & = & Ae^{-Ka/2}. & (1) \\ \text{At } x = +a/2: & \psi_2(a/2) & = & \psi_3(a/2) & \\ \therefore & C\sin(ka/2) + D\cos(ka/2) & = & Fe^{-Ka/2}. & (2) \end{array}$$

At the two well boundaries the first derivative of the wavefunction, $\psi' = d\psi/dx$, must be continuous.

$$\begin{array}{lrcll} \text{At } x = -a/2: & \psi_1'(-a/2) & = & \psi_2'(-a/2) & \\ \therefore & KAe^{-Ka/2} & = & kC\cos(-ka/2) - kD\sin(-ka/2) & \\ \therefore & C\cos(ka/2) + D\sin(ka/2) & = & (K/k)Ae^{-Ka/2}. & (3) \\ \text{At } x = +a/2: & \psi_2'(a/2) & = & \psi_3'(a/2) & \\ \therefore & kC\cos(ka/2) - kD\sin(ka/2) & = & -KFe^{-Ka/2} & \\ \therefore & C\cos(ka/2) - D\sin(ka/2) & = & -(K/k)Fe^{-Ka/2}. & (4) \end{array}$$

Equations (1)-(4) must be satisfied simultaneously.
Combine them in pairs to form four alternative equations.

$$\begin{array}{lrcll} (2) - (1) \to & 2C\sin(ka/2) & = & (F - A)\,e^{-Ka/2} & (5) \\ (3) + (4) \to & 2C\cos(ka/2) & = & -(K/k)(F - A)\,e^{-Ka/2} & (6) \\ (2) + (1) \to & 2D\cos(ka/2) & = & (F + A)\,e^{-Ka/2} & (7) \\ (3) - (4) \to & 2D\sin(ka/2) & = & (K/k)(F + A)\,e^{-Ka/2} & (8) \end{array}$$

Equations (5)-(8) must be satisfied simultaneously.

For equations (5) and (6) **both** to be true requires

$$\begin{array}{rccccr} \textbf{EITHER}: & C=0 & \textbf{and} & A=F & & \text{(9a)} \\ \textbf{OR}: & \cot(ka/2) & = & -K/k & & \text{(9b)} \end{array}$$

Condition (9b) comes from dividing equation (6) by equation (5).

For equations (7) and (8) **both** to be true requires

$$\begin{array}{rccccr} \textbf{EITHER}: & D=0 & \textbf{and} & A=-F & & \text{(10a)} \\ \textbf{OR}: & \tan(ka/2) & = & K/k & & \text{(10b)} \end{array}$$

Condition (10b) comes from dividing equation (8) by equation (7).

Therefore, to satisfy the boundary conditions, one of the conditions (9a) or (9b) must be true, **and** simultaneously one of the conditions (10a) or (10b) must be true.

If both (9a) and (10a) are true, then $C = D = 0$ and so $\psi_2 = 0$, which means that there is no particle inside the well. This is not an acceptable solution.

If both (9b) and (10b) are true, then

$$\begin{array}{rrcl} & \tan(ka/2) & = & -\cot(ka/2) \\ \therefore & \tan^2(ka/2) & = & -1, \end{array}$$

which is impossible, because both k and a are real numbers.
So conditions (9b) and (10b) **cannot** be simultaneously true.

Therefore there are two possibilities. **Either** conditions (9a) **and** (10b) are both true, **or** conditions (9b) **and** (10a) are both true. These generate two different sets of solutions for the finite square-well potential.

In the **first** set of solutions, $C = 0$ and $A = F$, so $\psi_2(x) = D\cos(kx)$ and $\psi_1(x) = \psi_3(-x)$.
These solutions are symmetric about the centre of the well ($x = 0$) and so have **even** parity.
The energy eigenvalues for these solutions can be found using equation (10b).

In the **second** set of solutions, $D = 0$ and $A = -F$, so $\psi_2(x) = C\sin(kx)$ and $\psi_1(x) = -\psi_3(-x)$.
These solutions are antisymmetric about the centre of the well ($x = 0$) and so have **odd** parity.
The energy eigenvalues for these solutions can be found using equation (9b).

Methods for solving equations (9b) and (10b), and the properties of the resulting wavefunctions, will be discussed further in the lectures.