Compiled

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1 Bound Energy states for particle in a semi-infinite potential wall

1.0.1 Let a particle of mass m_e in a box with potential ∞ for $x < 0$ and finite potential V_o for $x > a$ and we need to find the allowed bound energy states for the particle

Now since potential at $x < 0$ is ∞, $\Psi = 0$ in this region.In the region $0 \leq x \leq a$ can be solved as follows:-

$$-\frac{\hbar}{2m_e}\frac{d^2}{dx^2}\Psi(x) + V(x)\Psi(x) = E\Psi(x) \tag{1}$$

$$-\frac{\hbar}{2m_e}\frac{d^2}{dx^2}\Psi(x) + (0)\Psi(x) = E\Psi(x) \tag{2}$$

$$-\frac{\hbar}{2m_e}\frac{d}{dx^2}\Psi(x) = E\Psi(x) \tag{3}$$

$$\frac{d^2}{dx^2}\Psi(x) = -\frac{2m_eE}{\hbar^2}\Psi(x) \tag{4}$$

The general solution of this equation is of the form

$$\Psi(x) = A\cos kx + B\sin kx \text{ with } k = \sqrt{\frac{2m_eE}{\hbar^2}} \tag{5}$$

$$\tag{6}$$

Now $\Psi(x)$ must be 0 at \$ x = 0 \$ for function to be continuous. Therefore we have $A = 0$.Hence Ψ can be written as :-

$$\Psi(x) = B\sin(kx) \tag{7}$$

In the region $x > a$ we have :-

$$-\frac{\hbar}{2m_e}\frac{d^2}{dx^2}\Psi(x) + V(x)\Psi(x) = E\Psi(x) \tag{8}$$

$$-\frac{\hbar}{2m_e}\frac{d^2}{dx^2}\Psi(x) + V_o\Psi(x) = E\Psi(x) \tag{9}$$

$$\frac{d^2}{dx^2}\Psi(x) = \frac{2m_e(V_o - E)}{\hbar^2}\Psi(x) \tag{10}$$

$$\tag{11}$$

The general solution is :-

$$Ce^{Lx} + De^{-Lx} \text{ with } L = \sqrt{\frac{2m_e(V_o - E)}{\hbar^2}} \tag{12}$$

Now C must be zero as $\lim_{x\to\infty} Ce^{Lx} = \infty$.Hence Ψ can be written as :-

$$\Psi(x) = De^{-Lx} \tag{13}$$
$$\tag{14}$$

Now wavefunction must be continuous and differentiable a $x = a$, therefore

$$B\sin(Ka) = De^{-La} \text{ and } B * K\cos Ka = -D * Le^{-La} \tag{15}$$
$$1/K\tan Ka = -1/L \tag{16}$$
$$\sqrt{\frac{\hbar^2}{2m_eE}}\tan\sqrt{\frac{2m_eE}{\hbar^2}}a = -\sqrt{\frac{\hbar^2}{2m_e(V_o - E)}} \tag{17}$$
$$\tan\sqrt{\frac{2m_eE}{\hbar^2}}a = -\sqrt{\frac{E}{V_o - E}} \text{ this is our condition for finding energy in bound states} \tag{18}$$

Plotting the two sides of the equality witn energy of X axis and by assuming $a = 10^{-15}$ and $V_o = 0.000015$ we can se that the two curves intersect at discrete points which give us out bound state energy.
Next step is finding out normalization constants for the two wavefunctions. Now

$$\text{since } B\sin Ka = De^{-La} \tag{19}$$
$$D = B\sin Ka * e^{La} \tag{20}$$
$$\text{Condition for normalization :} \tag{21}$$
$$\int_{-\infty}^{\infty}\Psi^*(x)\Psi(x)\mathrm{d}x = 1 \tag{22}$$
$$|B|^2\int_0^a \sin^2 Kx\mathrm{d}x + |B|^2\sin^2 Ka * e^{2La}\int_a^{infty} e^{-2La} = 1 \tag{23}$$
$$B = \left[a/2 - \frac{1}{4K}\sin 2Ka + \frac{1}{2L}\sin^2 Ka\right]^{\frac{-1}{2}} \tag{24}$$

Plotting the wavefuntions by calculation B for each wavefunction separately for the four different energy levels, we get graphs as follows :-

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