

Problem 1: Finite quantum well

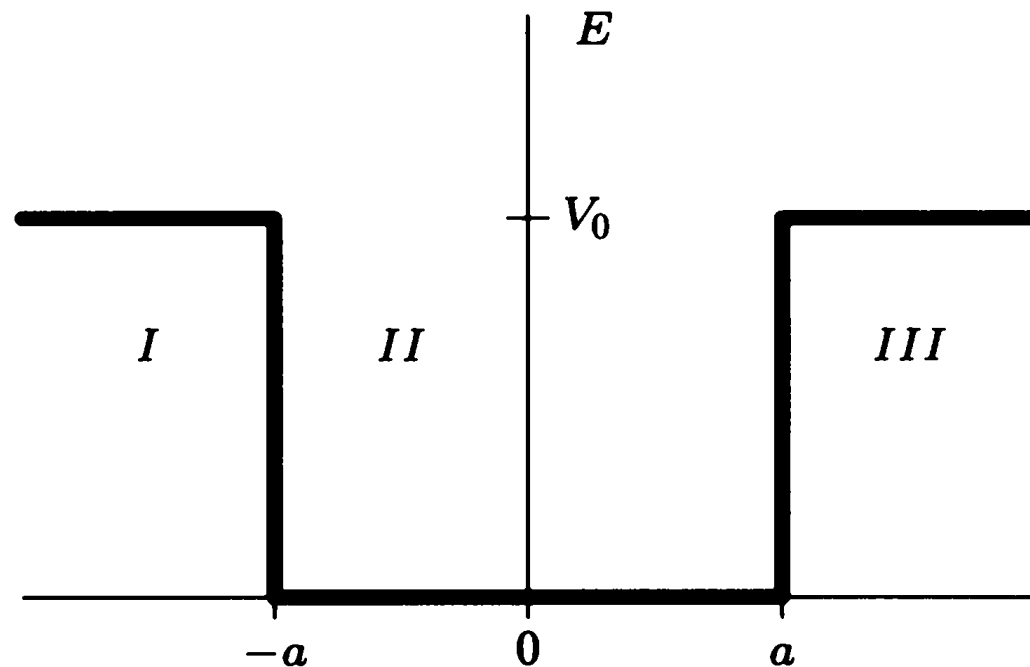


FIGURE 2.8 The finite square well.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(V_0 - E)\psi = 0, \text{ Schroedinger Equation}$$

Analytical solution of the wave function

In region II the general solution is

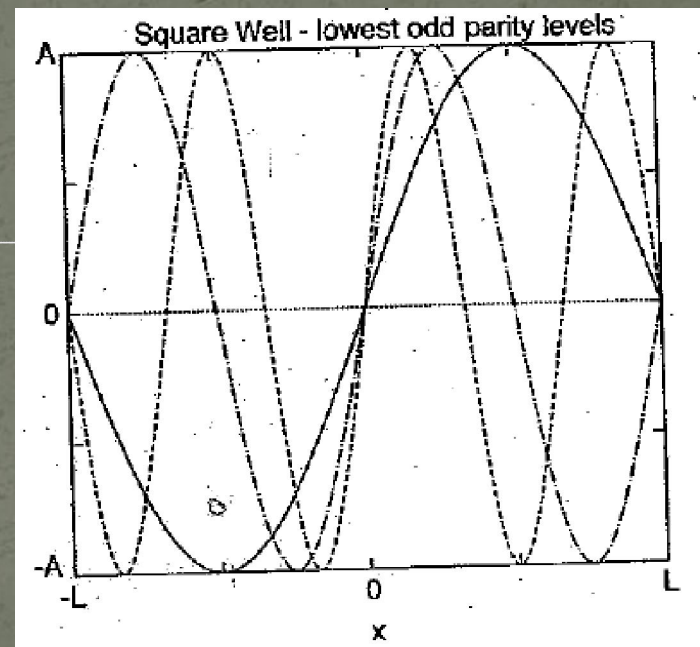
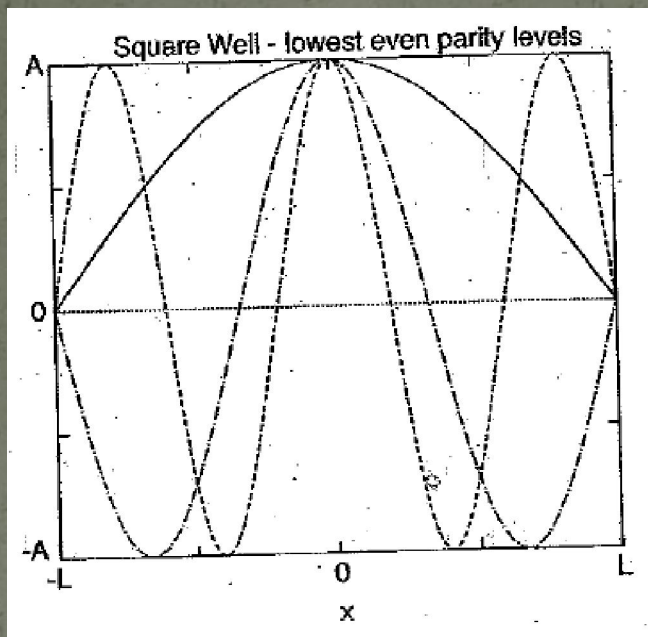
$$\psi_{II} = A \sin \alpha x + B \cos \alpha x, \quad \alpha = \sqrt{\frac{2mE}{\hbar^2}},$$

while in region III it must be

$$\psi_{III} = F e^{-\beta x}$$

How about ψ_I ?

Old and Even solutions



Continuity at $x = -a$

$$-A \sin \alpha a + B \cos \alpha a = C e^{-\beta a}$$

$$\alpha A \cos \alpha a + \alpha B \sin \alpha a = \beta C e^{-\beta a},$$

Discontinuity at $x = a$

$$A \sin \alpha a + B \cos \alpha a = F e^{-\beta a}$$

$$\alpha A \cos \alpha a - \alpha B \sin \alpha a = -\beta F e^{-\beta a}.$$

Even States: $A = 0, \quad B \neq 0, \quad C = F, \quad \beta \cos \alpha a = \alpha \sin \alpha a.$

Odd States: $A \neq 0, \quad B = 0, \quad C = -F, \quad \alpha \cos \alpha a = -\beta \sin \alpha a.$

where $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$ and $\beta = \sqrt{2m(V_0 - E)/\hbar^2}.$

Problems:

Plot the function

$$f(E) = \beta \cos \alpha a - \alpha \sin \alpha a$$

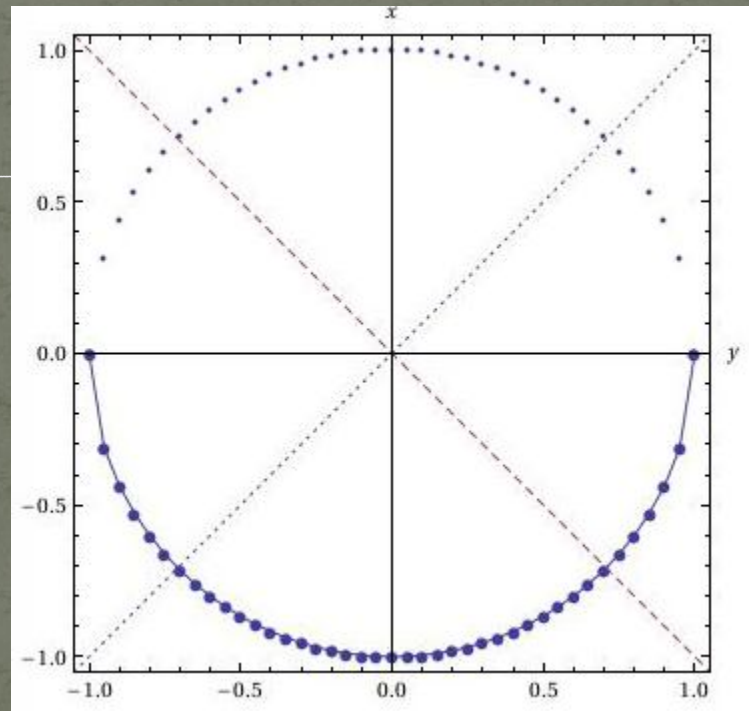
as a function of energy.

Given $V_0 = 10 \text{ eV}$, $a = 3 \text{ \AA}$, and $m = 1 m_e$

Find the lowest even and lowest odd solutions to the square well problem, with $a = 3 \text{ \AA}$, $m = 1 m_e$, and $V_0 = 10 \text{ eV}$. Plot the potential and the wavefunctions associated with these eigenvalues. (The convention is to align the zero baseline of the wavefunction with the energy eigenvalue.)

Problem 2

- The graph as shown is produced using Show[], Plot and ListPlot. The equation for a circle with unit radius is $x^2 + y^2 = 1$. Produce the graph.



Problem 3: Use (i) stochastic method, (ii) Simpson rule, (iii) trapezoid rule, (ii) Mathematica method to evaluate the area of a gaussian with $\mu = 0$, $\sigma = 1$, for x in $[-0.5, 0.5]$.

Problem 4: Find the root of $e^x = -x + 2$ using the (i) bisection method, (ii) Newton-Raphson method, (iii) Mathematica method.

Problem 5: There are three roots in $x \sin x = -1.5x + 3$. Write a programme to find all of them (use whatever method suit to your taste)