Course: Engineering Physics
PHY 1701

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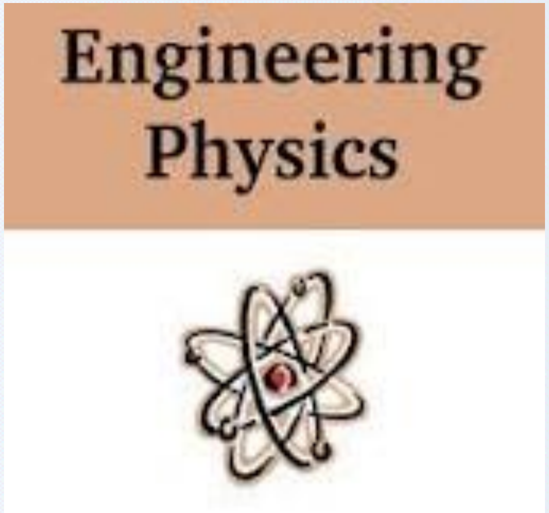
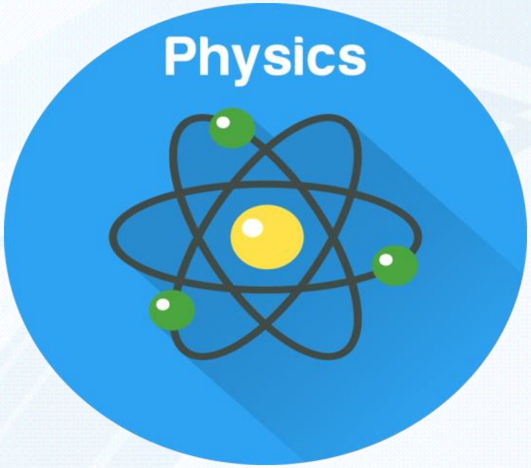
Outline

- ➢ **Eigen Values**
- ➢ **Eigen Functions**
- ➢ **Particle in a 1D Box**



Resources:

Concepts of Modern Physics (Arthur Beiser)
Pages: 198 – 202



Schrodinger Equation

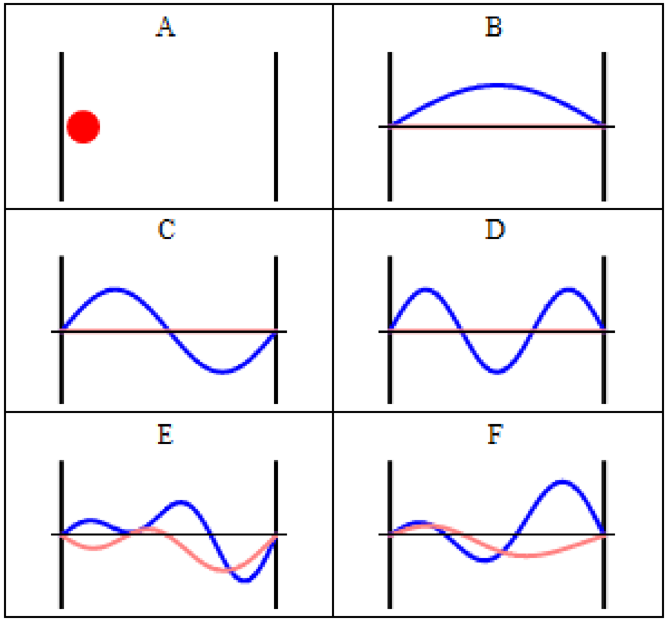
Steady-state Schrodinger equation in one dimension:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

Steady-state Schrodinger equation in three dimension:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2}E\psi = 0$$

Standing Waves in Stretched String



$$\lambda = \frac{1}{3}L$$

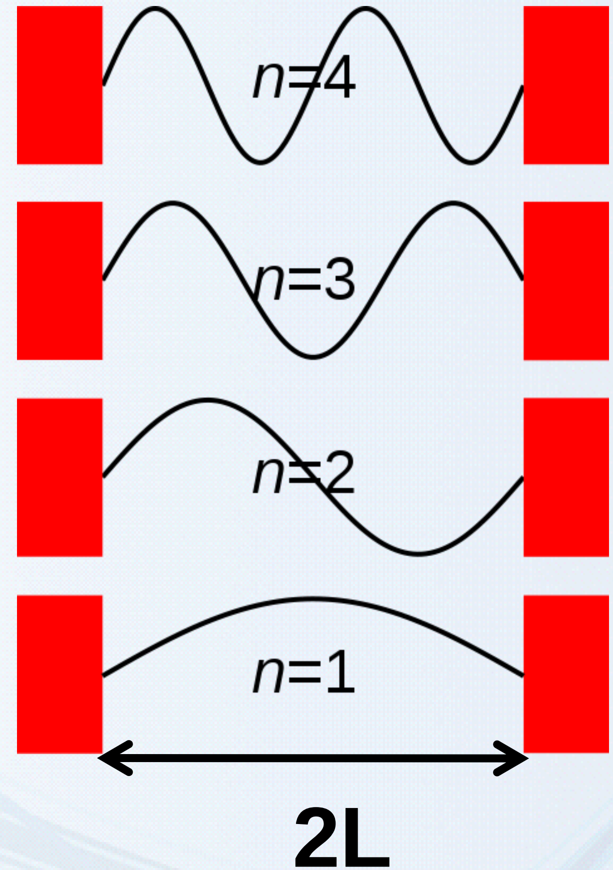
$$\lambda = \frac{2}{5}L$$

$$\lambda = \frac{1}{2}L$$

$$\lambda = \frac{2}{3}L$$

$$\lambda = L$$

$$\lambda = 2L$$



$$\lambda_n = \frac{2L}{n+1} \qquad n = 0,1,2,3 \ldots ..$$

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Eigenvalues & eigenfunctions

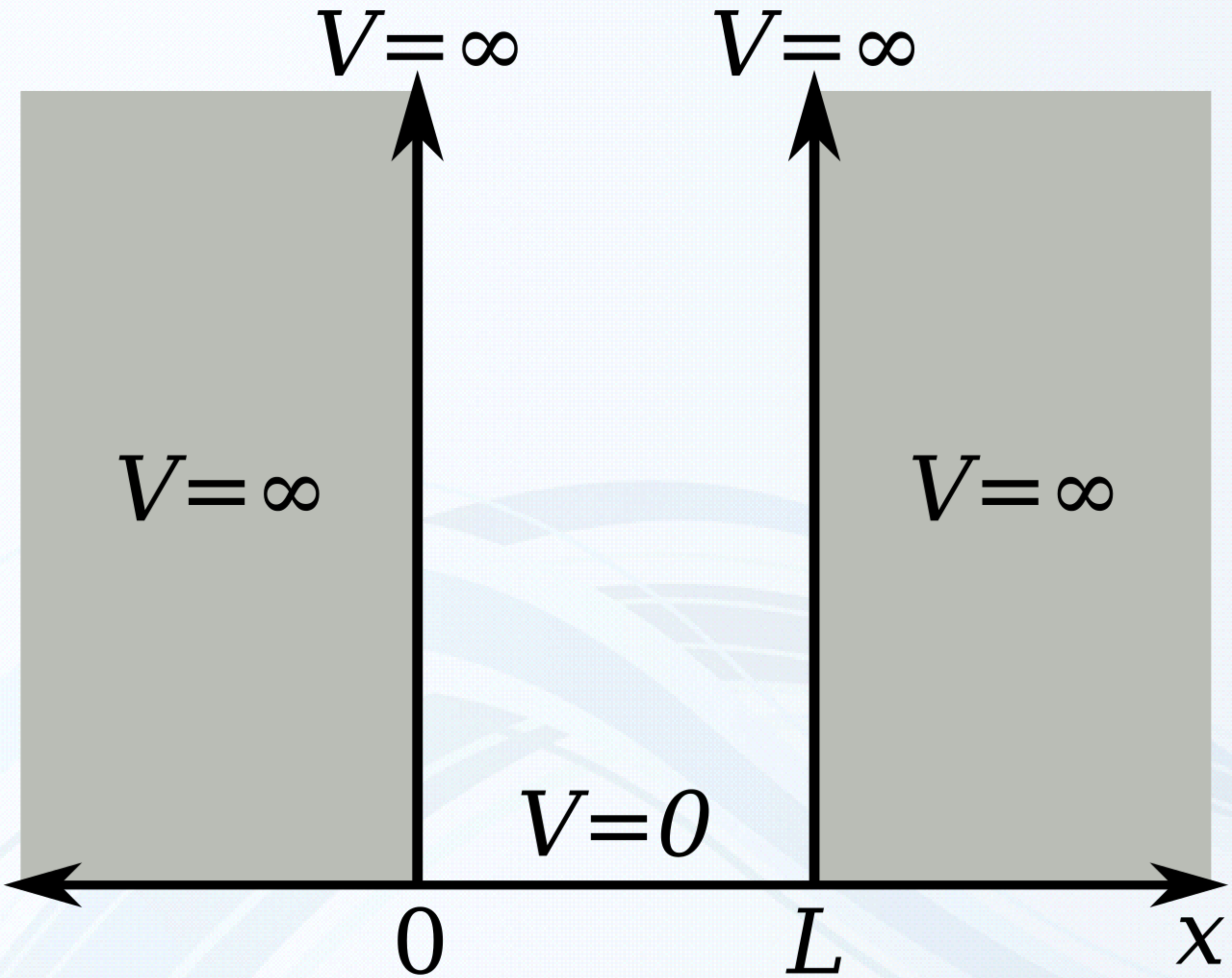
The values of energy E_n for which Schrodinger's steady-state equation can be solved are called eigen values

And the corresponding wave function ψ_n are called eigen functions.

The term "eigen" come from German "eigenwert" meaning **"proper or characteristic value"**

Eigen funktion → **"proper or characteristic function"**

Particle in a 1D Box



Particle motion:

X=0
X=L
Infinite hard walls

Particle does not lose energy
→total energy is constant

Wave function ψ is 0 for x ≤ 0 and x ≥ L

Particle in a 1D Box

Within the box the Schrodinger equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

Here, since U=0 (potential energy)

The total derivative $d^2\psi/dx^2$ is the same as the partial derivative $\partial^2\psi/\partial x^2$ because ψ is a function of only with x in this problem

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Particle in a 1D Box

Therefore,

$$\psi = A\sin\frac{\sqrt{2mE}}{\hbar}x + B\cos\frac{\sqrt{2mE}}{\hbar}x$$

Now, applying the boundary condition, the wave function $\psi(x) = 0$ for $x \leq 0$ and $x \geq L$

$\psi = 0$ for $x = 0$ and $x = L$

Since Cos0=1 → the second term cannot describe the particle because it does not vanish at x=0

Particle in a 1D Box

Since sin0 = 0, we have only first term

That is

$$\frac{\sqrt{2mE}}{\hbar} L = n\pi \qquad n = 1,2,3,\ldots$$

The sines of the angles π, 2 π, 3 π, …. are all zero

The particle in a box is $E_n = \dfrac{n^2\pi^2\hbar^2}{2mL^2}$ $\qquad n = 1,2,3,\ldots..$

Particle in a 1D Box

of $|\psi_n|^2$ over all space is finite, as we can see by integrating $|\psi_n|^2\,dx$ from $x = 0$ to $x = L$ (since the particle is confined within these limits). With the help of the trigonometric identity $\sin^2\theta = \frac{1}{2}(1 - \cos 2\theta)$ we find that

$$\begin{aligned}
\int_{-\infty}^{\infty} |\psi_n|^2\,dx &= \int_0^L |\psi_n|^2\,dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \\
&= \frac{A^2}{2}\left[\int_0^L dx - \int_0^L \cos\left(\frac{2n\pi x}{L}\right) dx\right] \\
&= \frac{A^2}{2}\left[x - \left(\frac{L}{2n\pi}\right)\sin\frac{2n\pi x}{L}\right]_0^L = A^2\left(\frac{L}{2}\right) \qquad (5.43)
\end{aligned}$$

To normalize ψ we must assign a value to A such that $|\psi_n|^2\,dx$ is *equal* to the probability $P\,dx$ of finding the particle between x and $x + dx$, rather than merely proportional to $P\,dx$. If $|\psi_n|^2\,dx$ is to equal $P\,dx$, then it must be true that

$$\int_{-\infty}^{\infty} |\psi_n|^2\,dx = 1 \qquad (5.44)$$

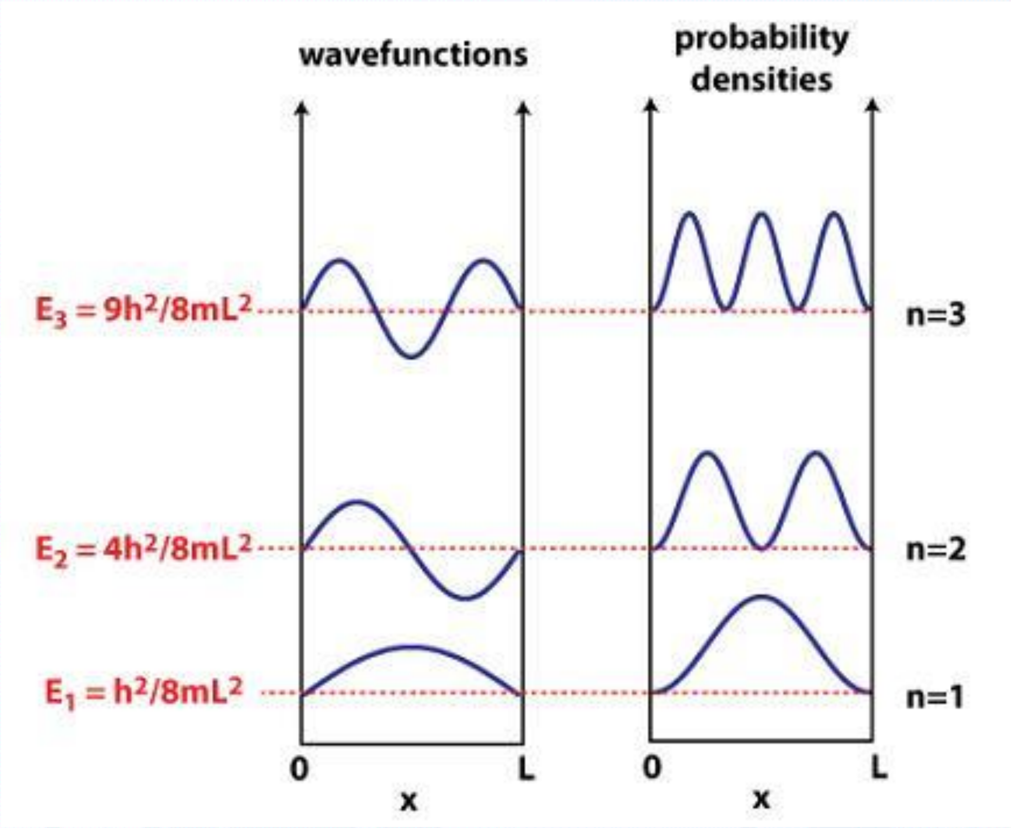
Comparing Eqs. (5.43) and (5.44), we see that the wave functions of a particle in a box are normalized if

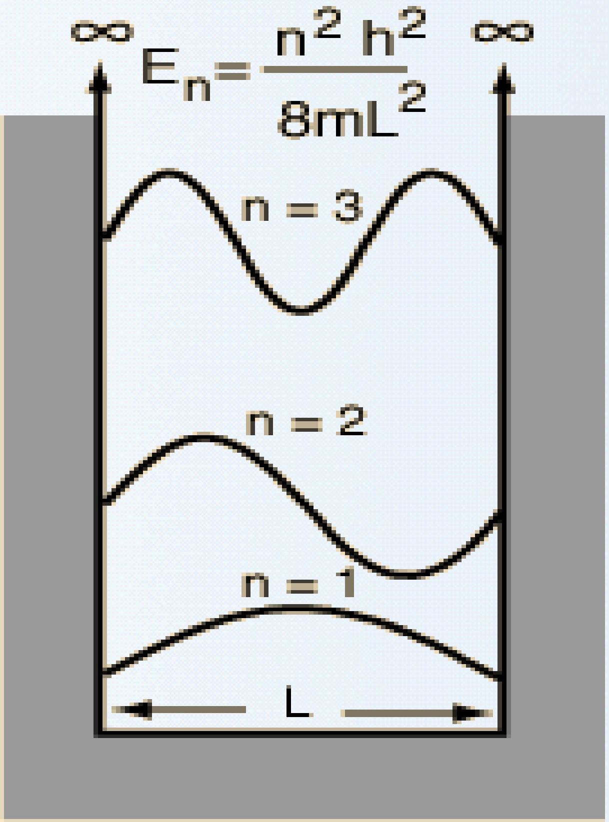
$$A = \sqrt{\frac{2}{L}} \qquad (5.45)$$

The normalized wave functions of the particle are therefore

Particle in a box $$\psi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \qquad n = 1, 2, 3, \ldots \qquad (5.46)$$

Particle in a 1D Box





Discrete energy levels and eigen functions of a particle in a box

Numerical

Example 3.4

An electron is in a box 0.10 nm across, which is the order of magnitude of atomic dimensions. Find its permitted energies.

Solution

Here $m = 9.1 \times 10^{-31}$ kg and $L = 0.10$ nm $= 1.0 \times 10^{-10}$ m, so that the permitted electron energies are

$$E_n = \frac{(n^2)(6.63 \times 10^{-34}\ \text{J}\cdot\text{s})^2}{(8)(9.1 \times 10^{-31}\ \text{kg})(1.0 \times 10^{-10}\ \text{m})^2} = 6.0 \times 10^{-18} n^2\ \text{J}$$
$$= 38 n^2\ \text{eV}$$

The minimum energy the electron can have is 38 eV, corresponding to $n = 1$. The sequence of energy levels continues with $E_2 = 152$ eV, $E_3 = 342$ eV, $E_4 = 608$ eV, and so on (Fig. 3.11). If such a box existed, the quantization of a trapped electron's energy would be a prominent feature of the system. (And indeed energy quantization is prominent in the case of an atomic electron.)

Numerical

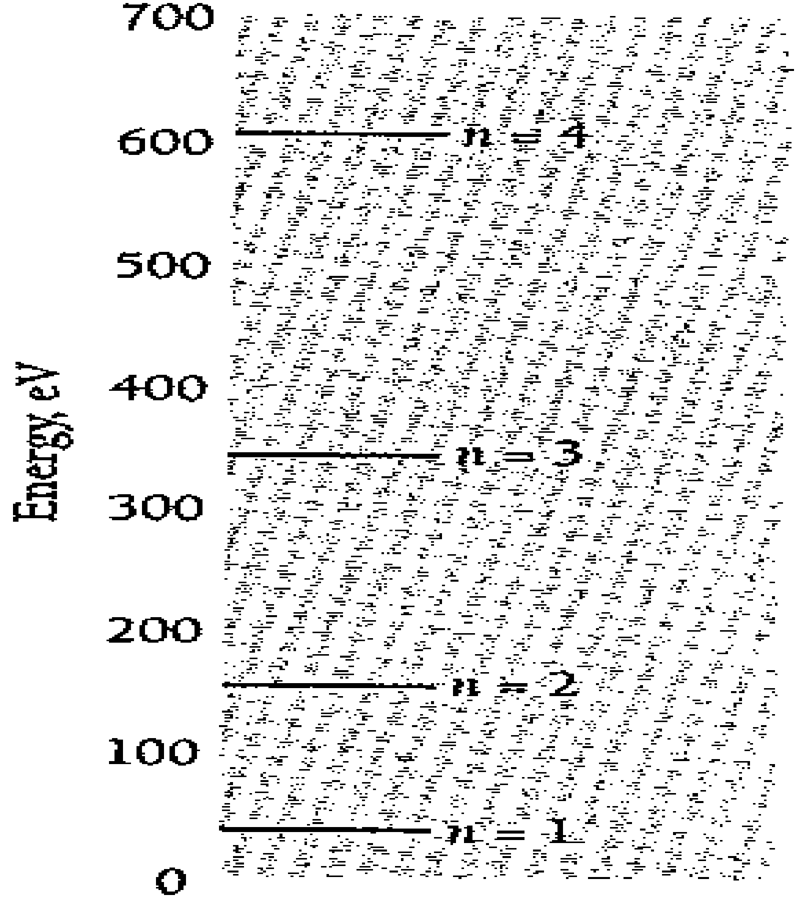


Figure 3.11 Energy levels of an electron confined to a box 0.1 nm wide.

Numerical

A 10-g marble is in a box 10 cm across. Find its permitted energies.

Solution

With $m = 10\text{ g} = 1.0 \times 10^{-2}\text{ kg}$ and $L = 10\text{ cm} = 1.0 \times 10^{-1}\text{ m}$,

$$E_n = \frac{(n^2)(6.63 \times 10^{-34}\text{ J}\cdot\text{s})^2}{(8)(1.0 \times 10^{-2}\text{ kg})(1.0 \times 10^{-1}\text{ m})^2}$$

$$= 5.5 \times 10^{-64} n^2\text{ J}$$

Numerical

The minimum energy the marble can have is 5.5×10^{-64} J, corresponding to $n = 1$. A marble with this kinetic energy has a speed of only 3.3×10^{-31} m/s and therefore cannot be experimentally distinguished from a stationary marble. A reasonable speed a marble might have is, say, $\frac{1}{3}$ m/s—which corresponds to the energy level of quantum number $n = 10^{30}$! The permissible energy levels are so very close together, then, that there is no way to determine whether the marble can take on only those energies predicted by Eq. (3.18) or any energy whatever. Hence in the domain of everyday experience, quantum effects are imperceptible, which accounts for the success of Newtonian mechanics in this domain.