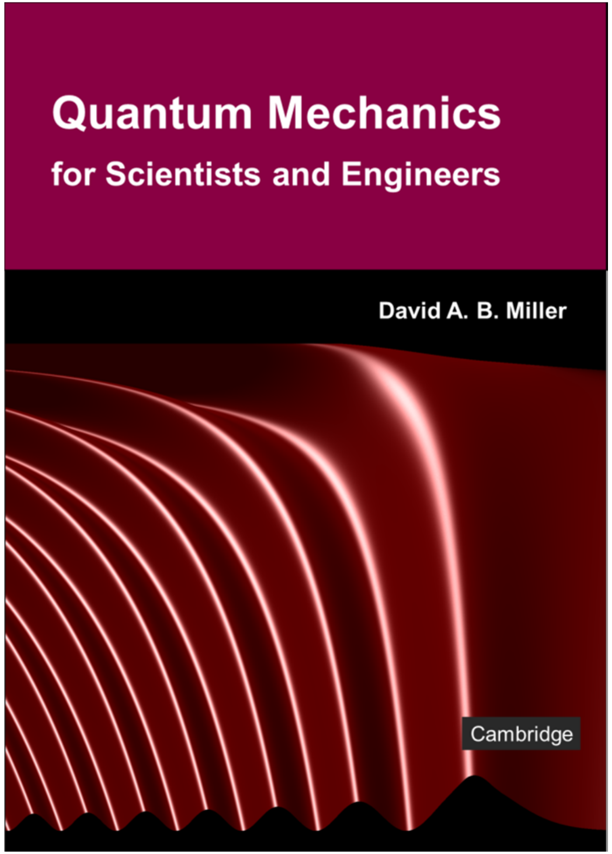
2.3 Particle in a box

Slides: Video 2.3.4 Solving for the particle in a box

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.6 (first part)



The particle in a box

Solving for the particle in a box

Quantum mechanics for scientists and engineers

David Miller

Particle in a box

We consider a particle of mass m

with a spatially-varying potential $V(z)$ in the z direction

so we have a Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2}+V(z)\psi(z)=E\psi(z)$$

where E is the energy of the particle

and $\psi(z)$ is the wavefunction

Particle in a box

Suppose the potential energy is a simple "rectangular" potential well

thickness L_z

Potential energy is constant inside

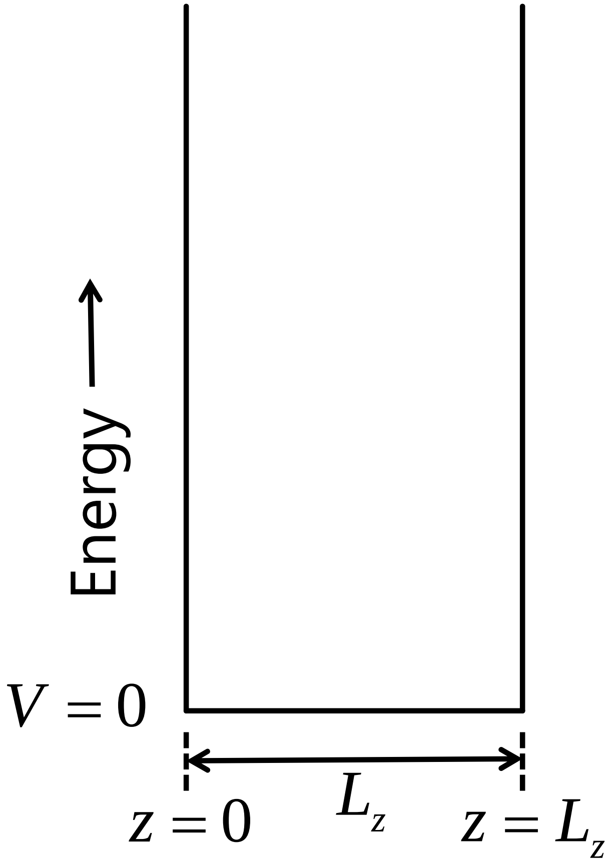
we choose $V = 0$ there

rising to infinity at the walls

i.e., at $z = 0$ and $z = L_z$

We will sometimes call this

an infinite or infinitely deep (potential) well



Particle in a box

Because these potentials at $z = 0$ and at $z = L_z$ are infinitely high

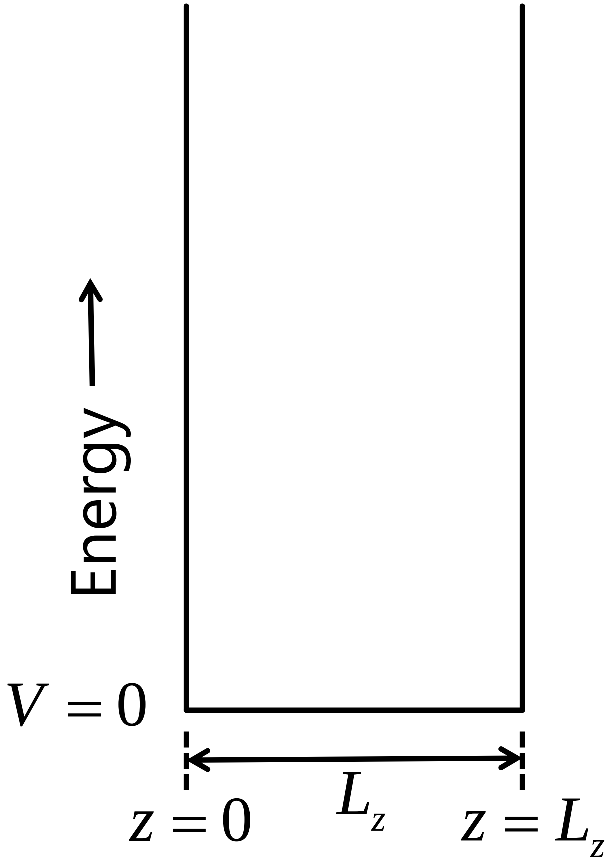
but the particle's energy E is presumably finite

we presume there is no possibility of finding the particle outside

i.e., for $z < 0$ or $z > L_z$

so the wavefunction ψ is 0 there

so ψ should be 0 at the walls



Particle in a box

With these choices

inside the well

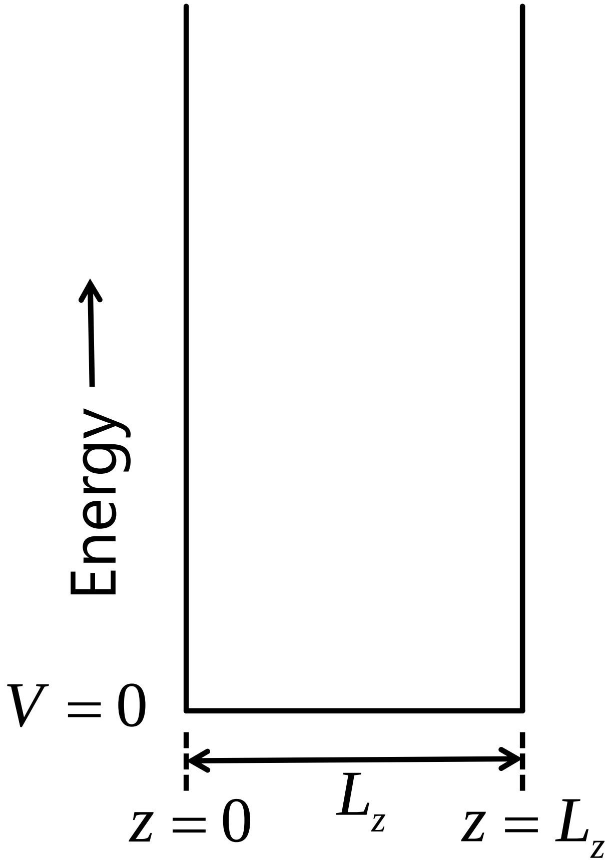
the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2}+V(z)\psi(z)=E\psi(z)$$

becomes $$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2}=E\psi(z)$$

with the boundary conditions

$\psi(0)=0$ and $\psi(L_z)=0$



Particle in a box

The general solution to the equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(z)}{dz^2} = E\psi(z)$$

is of the form

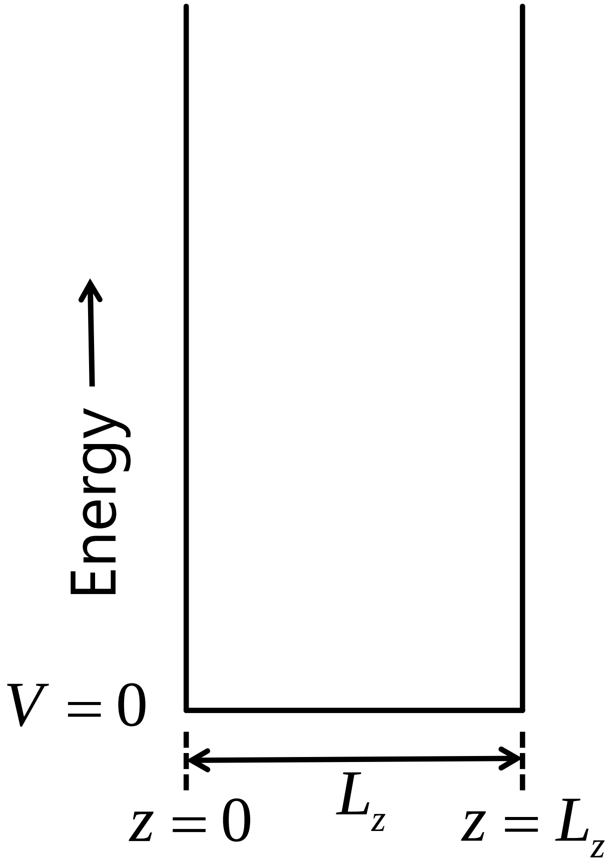
$$\psi(z) = A\sin(kz) + B\cos(kz)$$

where A and B are constants

and $k = \sqrt{2mE/\hbar^2}$

The boundary condition $\psi(0) = 0$

means $B = 0$ because $\cos(0) = 1$



Particle in a box

With now $\psi(z) = A\sin(kz)$

and the condition $\psi(L_z) = 0$

kz must be a multiple of π, i.e.,

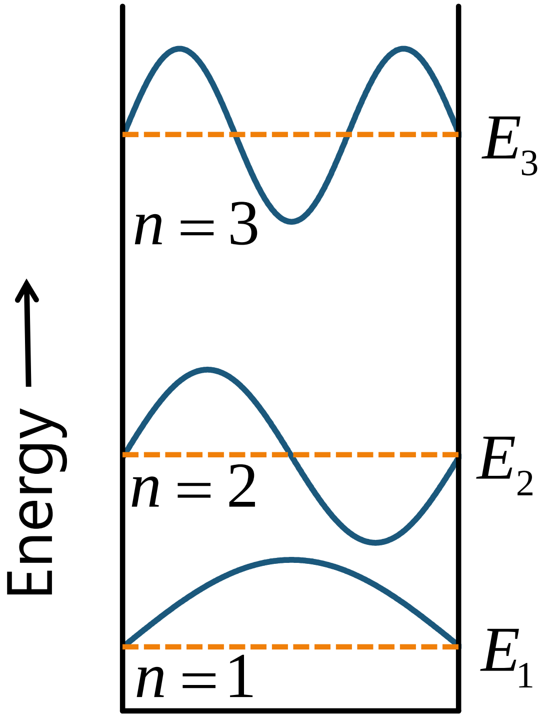
$$k = \sqrt{2mE/\hbar^2} = n\pi / L_z$$

where n is an integer

Since, therefore, $E = \dfrac{\hbar^2 k^2}{2m}$

the solutions are

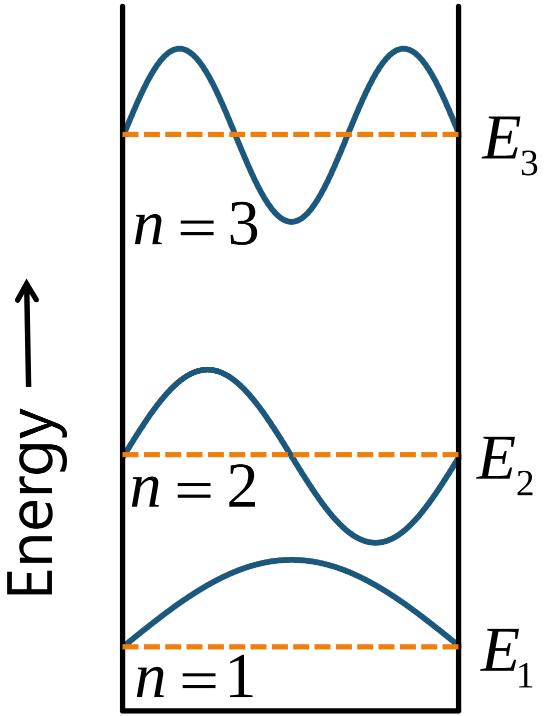
$$\psi_n(z) = A_n \sin\left(\frac{n\pi z}{L_z}\right) \text{ with } E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_z}\right)^2$$



Particle in a box

We restrict n to positive integers $n = 1, 2, \ldots$ for the following reasons

- Since $\sin(-a) = -\sin(a)$ for any real number a
  - the wavefunctions with negative n are the same as those with positive n
    - within an arbitrary factor, here -1
  - the wavefunction for $n = 0$ is trivial
    - the wavefunction is 0 everywhere



$$\psi_n(z) = A_n \sin\left(\frac{n\pi z}{L_z}\right)$$

Particle in a box

We can normalize the wavefunctions

$$\int_0^{L_z} |A_n|^2 \sin^2\left(\frac{n\pi z}{L_z}\right) dz = |A_n|^2 \frac{L_z}{2}$$

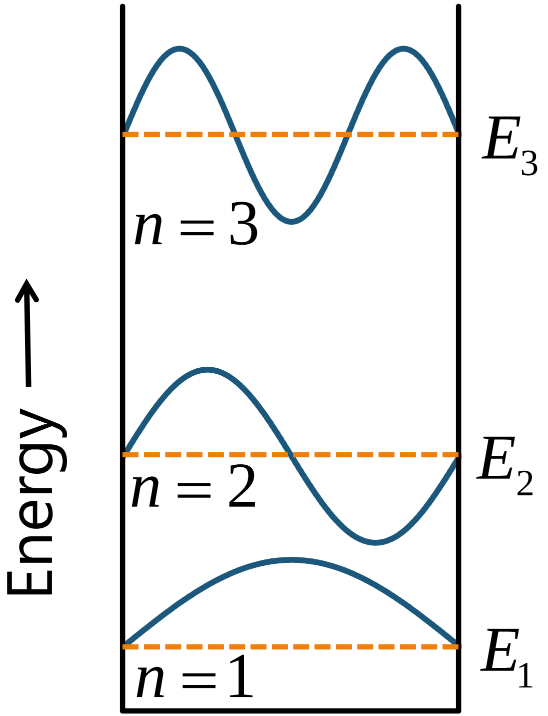
To have this integral equal 1

choose $|A_n| = \sqrt{2 / L_z}$

Note A_n can be complex

All such solutions are arbitrary within a unit complex factor

Conventionally, we choose A_n real for simplicity in writing



Particle in a box

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_z}\right)^2$$

$$\psi_n(z) = \sqrt{\frac{2}{L_z}}\sin\left(\frac{n\pi z}{L_z}\right)$$

$$n = 1,\ 2,\ \ldots$$