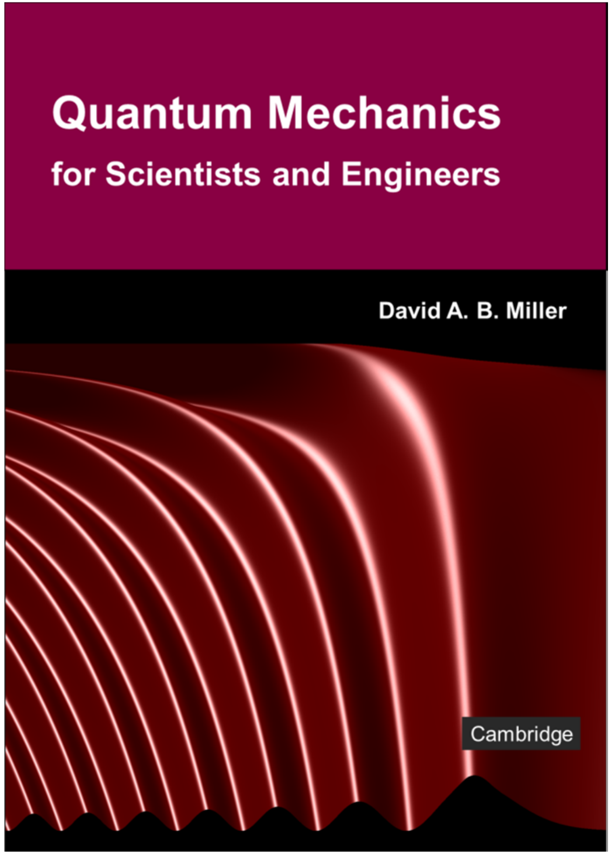
2.3 Particle in a box

Slides: Video 2.3.6 Nature of the particle-in-a-box solutions

Text reference: Quantum Mechanics for Scientists and Engineers

Section 2.6 (second part)



The particle in a box

Nature of particle-in-a-box solutions

Quantum mechanics for scientists and engineers

David Miller

Eigenvalues and eigenfunctions

Solutions

- with a specific set of allowed values of a parameter (here energy)
  - eigenvalues
- and with a particular function associated with each such value
  - eigenfunctions

can be called eigensolutions

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

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

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

Eigenvalues and eigenfunctions

Here

since the parameter is an energy

we can call the eigenvalues

eigenenergies

and we can refer to the eigenfunctions as the

energy eigenfunctions

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

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

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

Degeneracy

Note in some problems

- it can be possible to have more than one eigenfunction with a given eigenvalue
  - a phenomenon known as
    - "degeneracy"

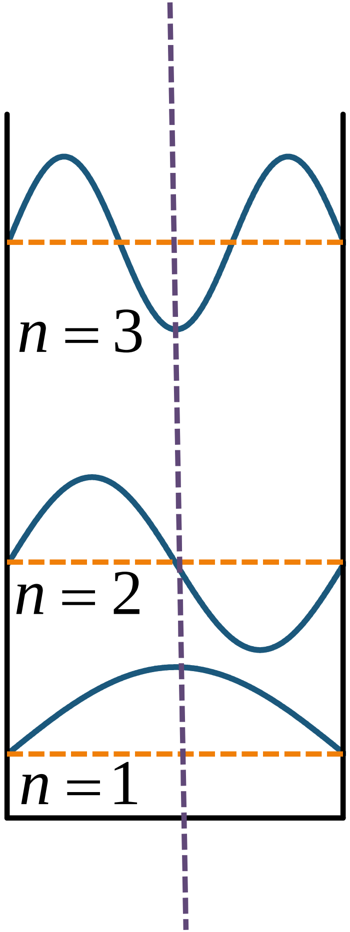
The number of such states with the same eigenvalue is called

- "the degeneracy"
  - of that state

Parity of wavefunctions

Note these eigenfunctions have definite symmetry

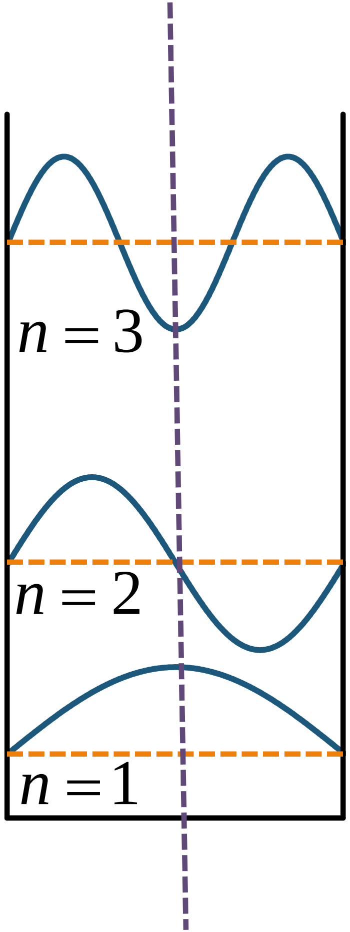
- the $n = 1$ function is the mirror image on the left of what it is on the right
  - such a function has "even parity" or is said to be an "even function"
- The $n = 3$ eigenfunction is also even



Parity of wavefunctions

The $n = 2$ eigenfunction is an inverted image

- the value at any point on the right of the center
  - is exactly minus the value at the "mirror image" point on the left of the center
- Such a function
  - has "odd parity"
  - or is said to be an "odd function"



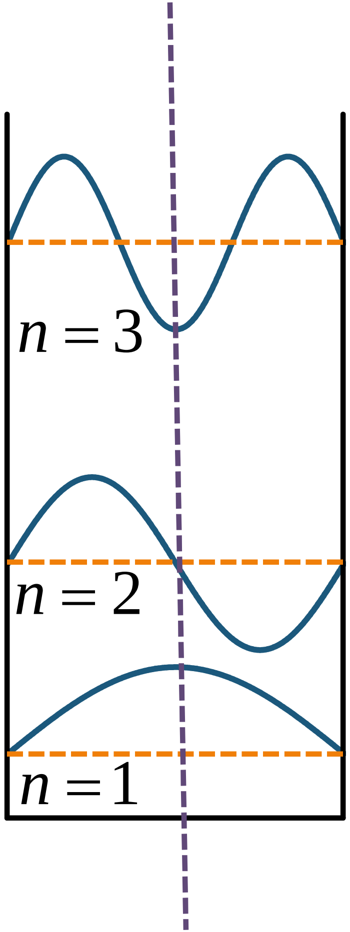
Parity of wavefunctions

For this symmetric well problem

- the functions alternate between being even and odd
  - and all the solutions are either even or odd
    - i.e., all the solutions have a "definite parity"

Such definite parity is common in symmetric problems

- it is mathematically very helpful



Quantum confinement

This particle-in-a-box behavior is very different from the classical case

1 – there is only a discrete set of possible values for the energy

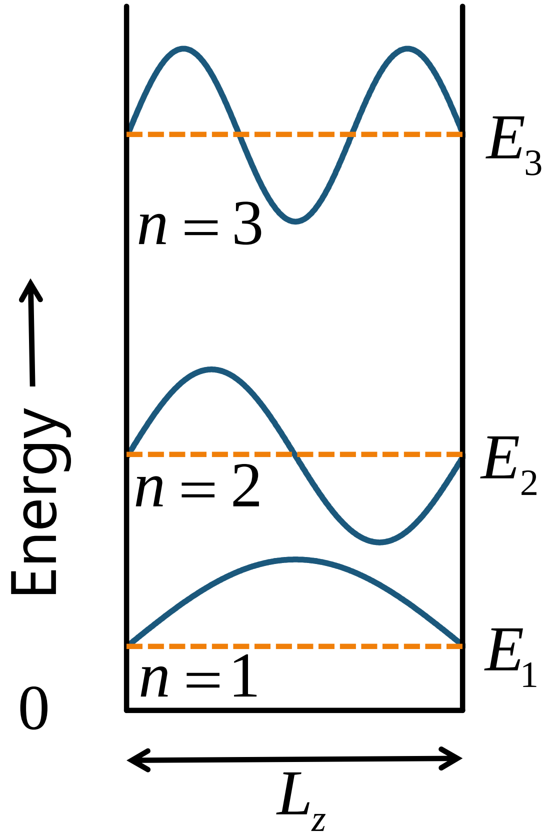
2 – there is a minimum possible energy for the particle

corresponding to $n=1$

here $E_1 = \left(\hbar^2 / 2m\right)\left(\pi / L_z\right)^2$

sometimes called a

"zero-point energy"



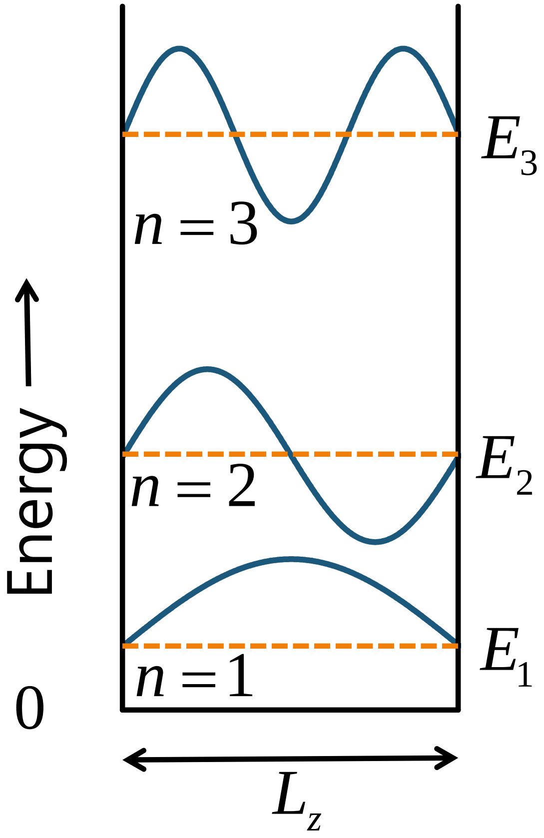
Quantum confinement

3 - the particle is not uniformly distributed over the box, and

its distribution is different for different energies

It is almost never found very near to the walls of the box

the probability obeys a standing wave pattern



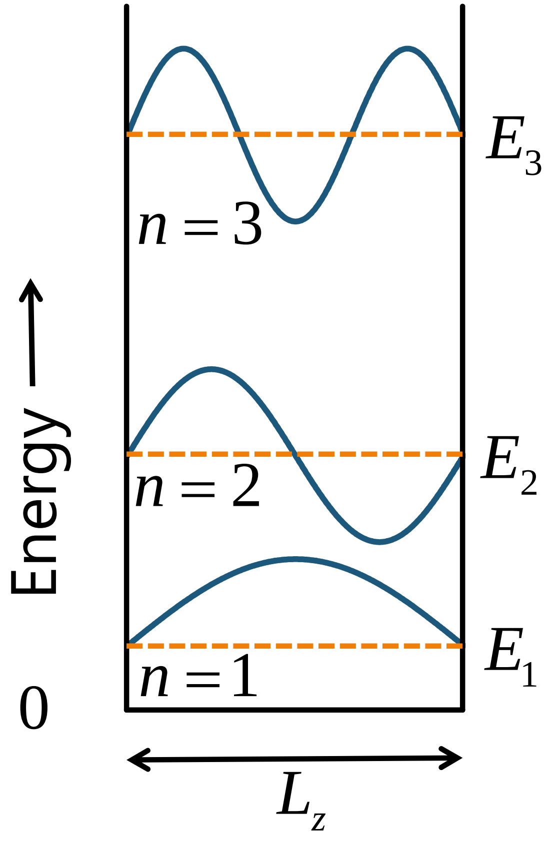
Quantum confinement

In the lowest state ($n = 1$),

- it is most likely to be found near the center of the box

In higher states,

- there are points inside the box where the particle will never be found

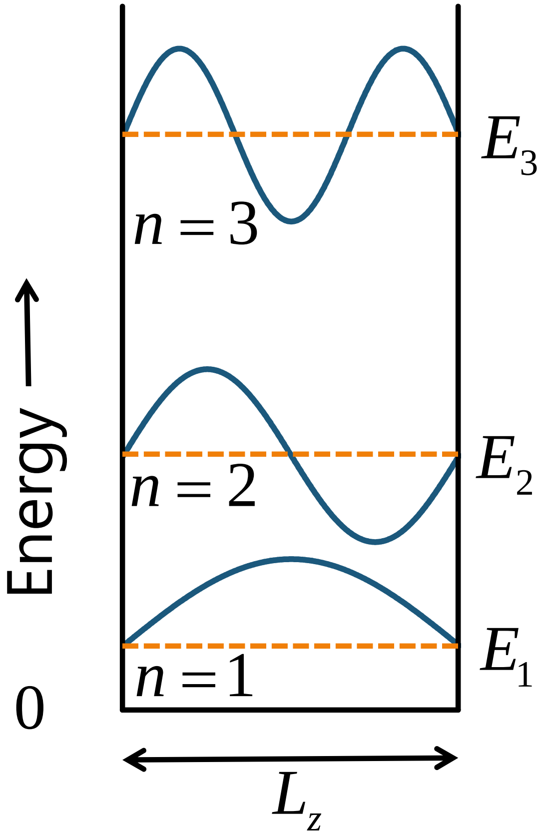


Quantum confinement

Note that

- each successively higher energy state
  - has one more "zero" in the eigenfunction

This is very common behavior in quantum mechanics



Energies in quantum mechanics

In quantum mechanical calculations

we can always use Joules as units of energy

but these are rather large

A very convenient energy unit

which also has a simple physical significance

is the electron-volt (eV) $\simeq 1.602 \times 10^{-19}$ J

the energy change of an electron in moving through an electrostatic potential change of 1V

Energy in eV = energy in Joules/e

e – electronic charge $= 1.602176565 \times 10^{-19}$ C (Coulombs)

Orders of magnitude

E.g., confine an electron in a 5 Å (0.5 nm) thick box

The first allowed level for the electron is

$$E_1 = \left(\hbar^2 / 2m_o\right)\left(\pi / 5\times10^{-10}\right)^2 \cong 2.4\times10^{-19}\,\text{J} \cong 1.5\ \text{eV}$$

The separation between the first and second allowed energies ($E_2 - E_1 \simeq 3E_1$)

is $\simeq 4.5\,\text{eV}$

which is a characteristic size of major energy separations between levels in an atom