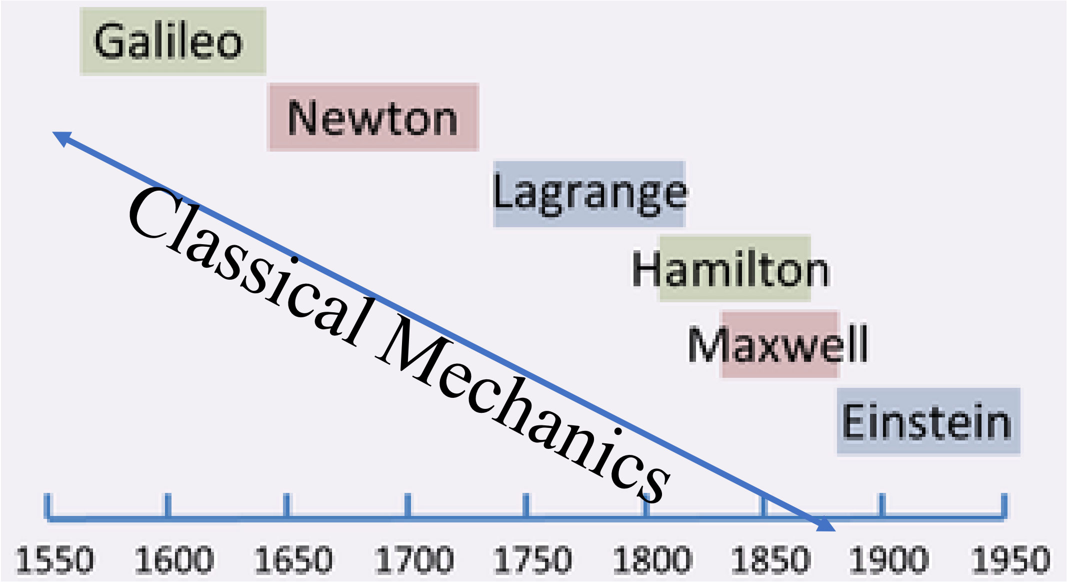
Evolution in Mechanics

@Citizendium



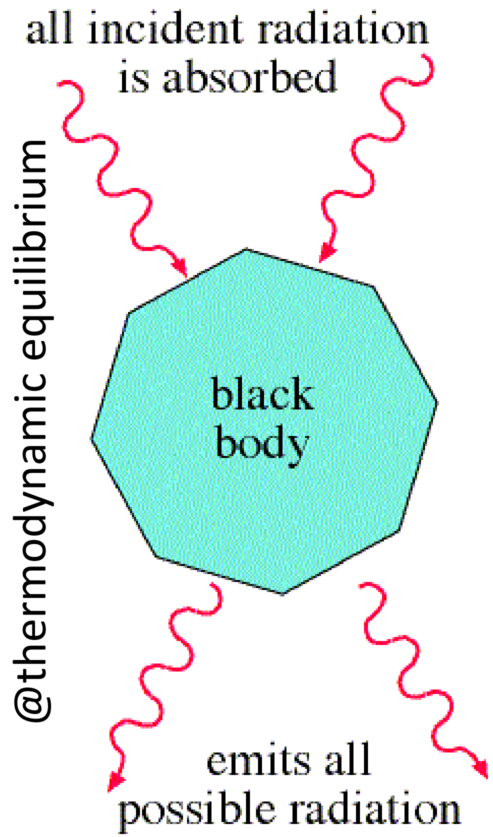
	Newtonian Mechanics	Lagrangian Mechanics	Hamiltonian Mechanics
Principle	Force = $m \times accln$	Principle of Least Action	Reformulation of Lagrangian Mechanics (in Phase space coordinates (x,p))
Driving Equation	$m\ddot{x} = F$	Lagrange's Eq. $\frac{d}{dt}\left\{\frac{\partial L}{\partial \dot{x}}\right\} = \frac{\partial L}{\partial x}$ $L = K.E - P.E.$	$\dot{p} = -\frac{\partial H}{\partial x}, \dot{x} = \frac{\partial H}{\partial p}$ $H = K.E. + P.E.$

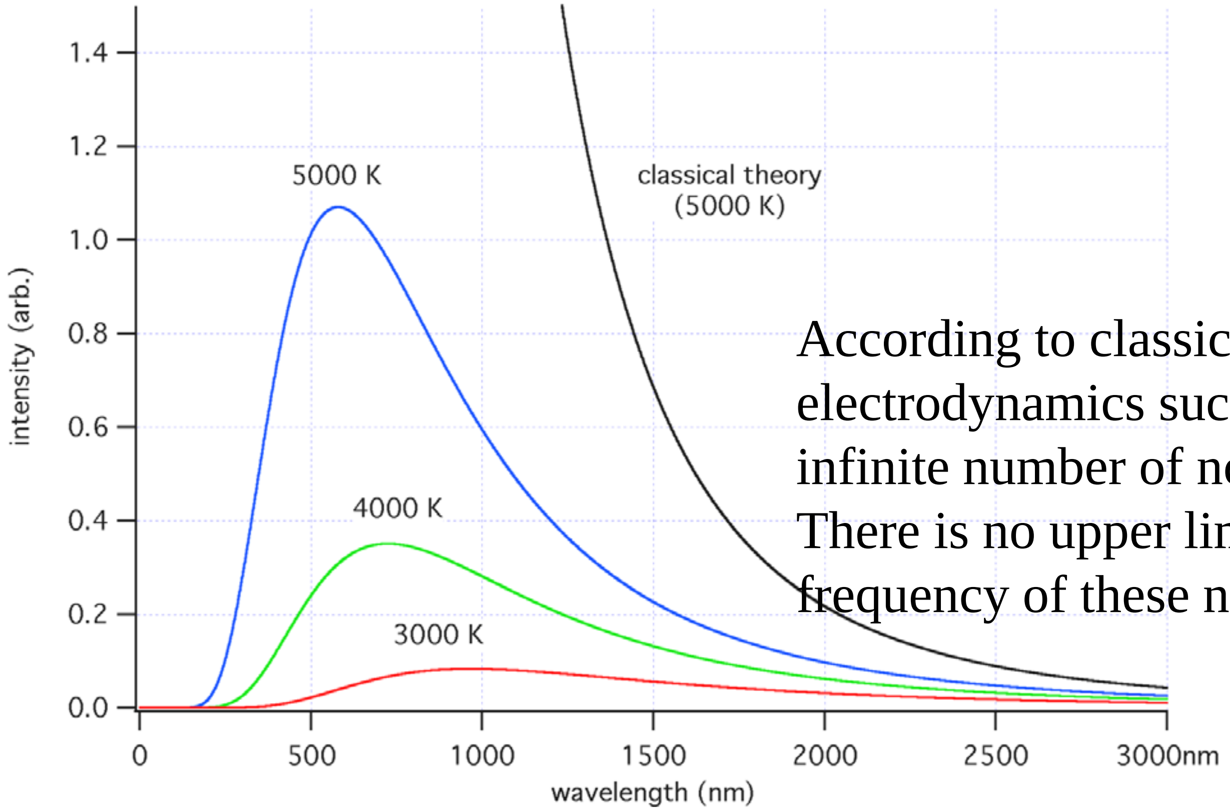
	Newtonian Mechanics	Lagrangian Mechanics	Hamiltonian Mechanics
Principle	Force = $m \times accln$	Principle of Least Action: minimum energy path	Reformulation of Lagrangian Mechanics (in Phase space coordinates (x,p))
Driving Equation	$m\ddot{x} = F$	Lagrange's Eq. $\frac{d}{dt}\left\{\frac{\partial L}{\partial \dot{x}}\right\} = \frac{\partial L}{\partial x}$ $L = K.E - P.E.$	$\dot{p} = -\frac{\partial H}{\partial x}, \dot{x} = \frac{\partial H}{\partial p}$ $H = K.E.+P.E.$
Co-ordinates	Cartesian Coordinates	Cartesian Coordinates	Canonical Coordinates
Require-ments & Basis	Cause = Effect; Vectorial in Nature; Does not have systematic method for deriving conservation law	Start from 1st Principle; Based on scalar function: Energy in terms of Lagrangian. Not ideal for Non-conservative system, Like friction	Converting 2nd order differential Lagrange's equation to 1st order Hamilton's Equations.

Classical → Quantum Mechanics

Despite the huge success of Classical Mechanics

- ➢ There are certain experimental results bothered physicists during end part of 19^{th} Century
- ➢ Most of the properties of light ←Explained with Classical Mech.
- ➢ Means light as wave following wave equation
- ➢ **Ultraviolet catastrophe of Black Body Radiation could not**



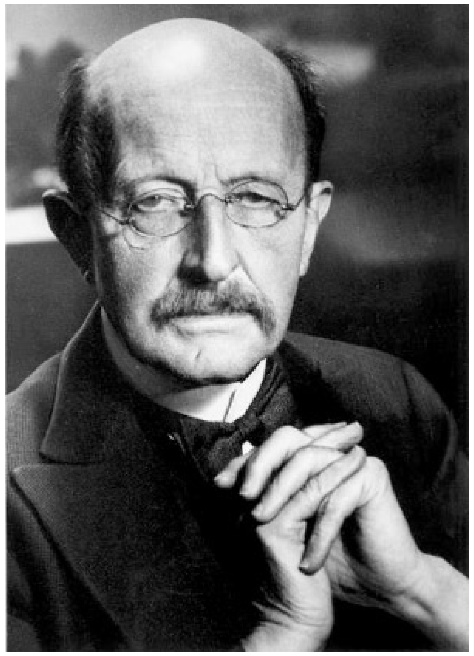


According to classical electrodynamics such a cavity has infinite number of normal modes. There is no upper limit to the frequency of these normal modes

Classical → Quantum Mechanics

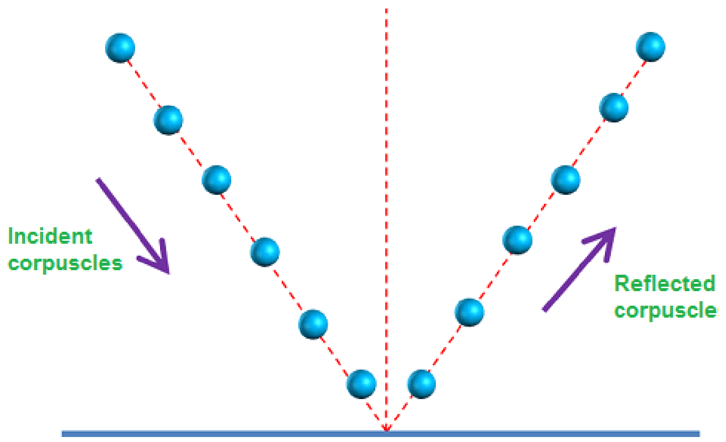
Despite the huge success of Classical Mechanics

- There are certain experimental results bothered physicists during end part of 19^{th} Century
- Most of the properties of light ←Explained with Classical Mech.
- Means: light as wave following wave equation
- Ultraviolet catastrophe of Black Body Radiation could not
- Eventually understood discrete quanta !!!
- Particle (Photon) picture of light wave



Max Karl Ernst Ludwig Planck
1858-1947

Many years back Newton proposed → Corposcular Theory



However,

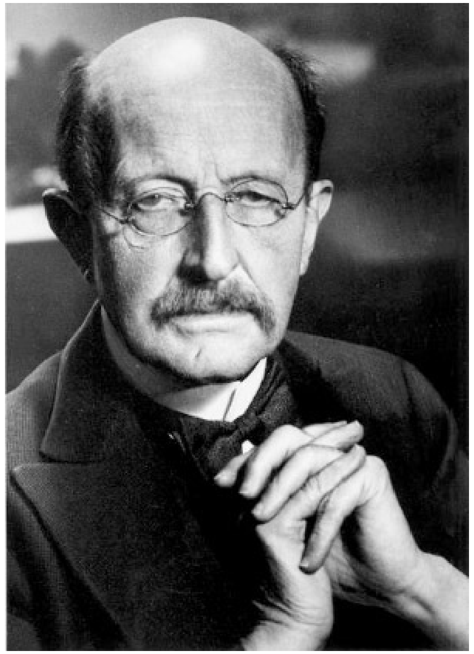
- Particle (Photon) picture of light wave
- Max Planck's hypothesis of light (@1900)
- laid foundation of particle-like behavior of light

Classical → Quantum Mechanics

The density of radiant energy in the cavity per unit wavelength interval, at the wavelength λ, and at the temperature T

$$E(\lambda,T)=\frac{8\pi hc}{\lambda^5}\times\frac{1}{e^{\frac{hc}{\lambda kT}}-1}$$

Planck's Radiation Law



Max Karl Ernst Ludwig Planck
1858-1947

**Energy of wave is related with frequency and quantized $E=nh\nu$

*The average energy in a normal mode is of the order of kT.

*The probability of emission of high energy photons with high frequency gets smaller for a given temperature when $h\nu >> kT$. There is not enough energy available for emitting these photons.

Other examples:
Waves behaving as particles

Experiments

1. Photoelectric effect (1902)
2. Compton effect (1922)
3. Pair Production (1932, Anderson)

*Theoretical proposal: Dirac (1928)

Wave-Particle duality

de Broglie postulate (PhD Thesis 1924)

$$\lambda = \frac{h}{p}$$

$$p\lambda = h$$

$$E = h\nu = \frac{h}{T}$$

$$ET = h$$

***Mass of an e- = 9.109383×10^{-28} gm;
Velocity is obtained from the given kinetic energy of 1000 eV

$$p = \sqrt{2m\,K.E.} = \sqrt{(1000\ eV)\left(\frac{1.6\times10^{-19}\text{J}}{1\ eV}\right)2(9.109383\times10^{-31}\ kg)}$$

$$= 1.7\ \times\ 10^{-23}\ \text{kg. m/s}$$

$$\lambda = \frac{h}{p}$$

$$= \frac{6.626069\times10^{-34}\ kg\cdot m^2/s}{1.7\times10^{-23} kg\cdot m/s}$$

$$= 3.87\times10^{-11}\ m$$

$$= 38.9\ pm$$

Wave-Particle duality

de Broglie postulate (PhD Thesis 1924)

$$\lambda = \frac{h}{p}$$

$$p\lambda = h$$

$$E = h\nu = \frac{h}{T}$$

$$ET = h$$

***Mass of a tennis ball = 0.11 kg;
Velocity = 44.7 m/s

$$\lambda = \frac{h}{mv} = \frac{6.626069 \times 10^{-34}\ kg \cdot m^2/s}{(0.11\ kg)(44.7\ m/s)} = 1.3 \times 10^{-34} m$$

Particles behaving as waves

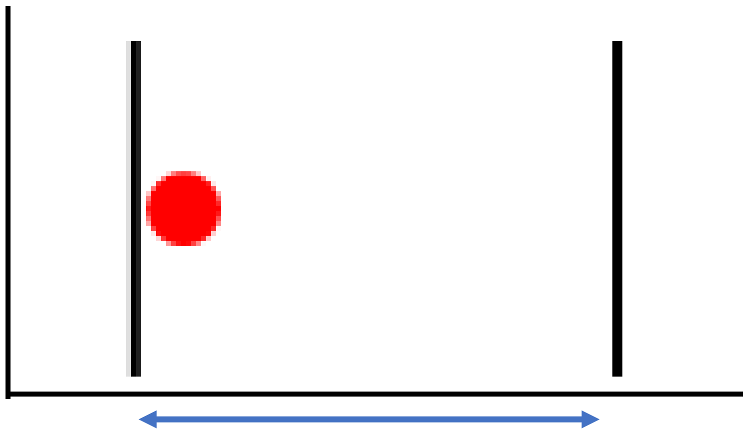
Experiments

Electron diffraction

Davisson –Germer (USA)
and Thompson (UK) (1927)

Electron microscope

Confining Particle in small box

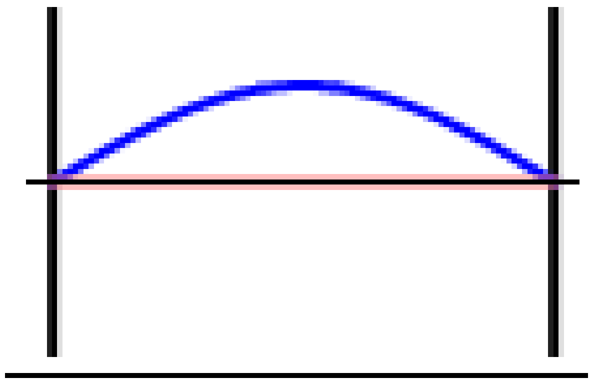


L~ $10\ \mu m\ or\ \ 100nm$

- If this particle has wave behavior
- The wave has to fit in the length
- Remember, if it is hard wall,
- Amplitude of the wave =0 @wall

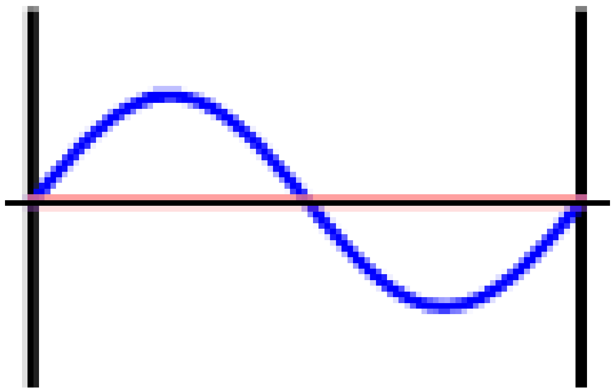
WF: Wavefunction

- Real part of WF
- Imaginary part of WF



Fundamental wave with $L = \frac{\lambda}{2}$

Ground State of the wave $E = \frac{h}{T}$



1^{st} excited wave with $L = \ \lambda$

Energy of 1^{st} excited state $E = \frac{2h}{T} = 2h\nu$

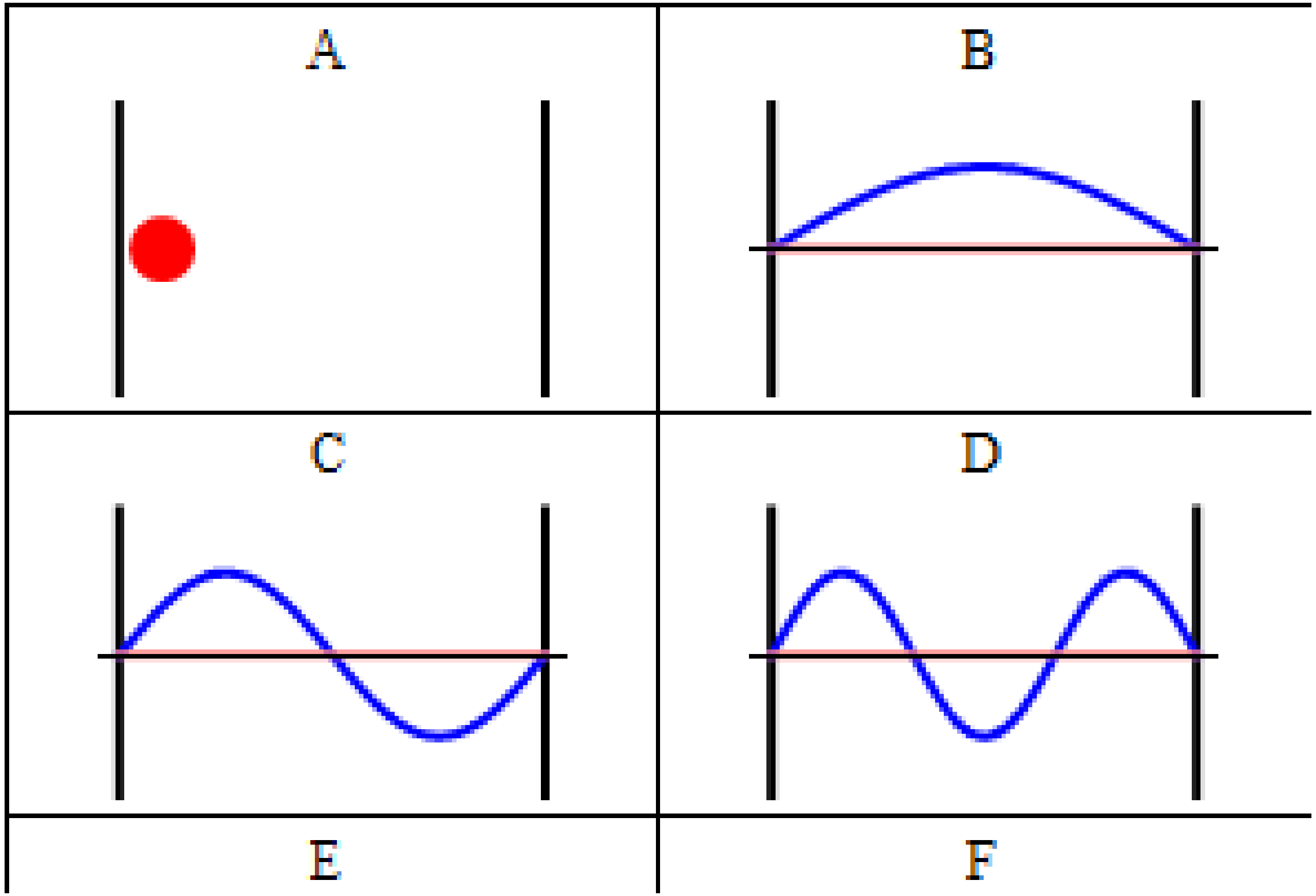
Confining Particle in small box

- Energy of the particle discretized
- Possible energy levels

$$\left.\begin{aligned} E_1 &= h\nu \\ E_2 &= 2h\nu \\ E_3 &= 3h\nu \\ &\vdots \\ E_n &= nh\nu \\ E_\infty &= \infty h\nu \end{aligned}\right\}$$

Question:
- Are the states are Equally probable??
- Is there any hierarchy?

- Nature says: most probable state →Ground State
- But, probability of other excited states is finite, but decreases with “n”.

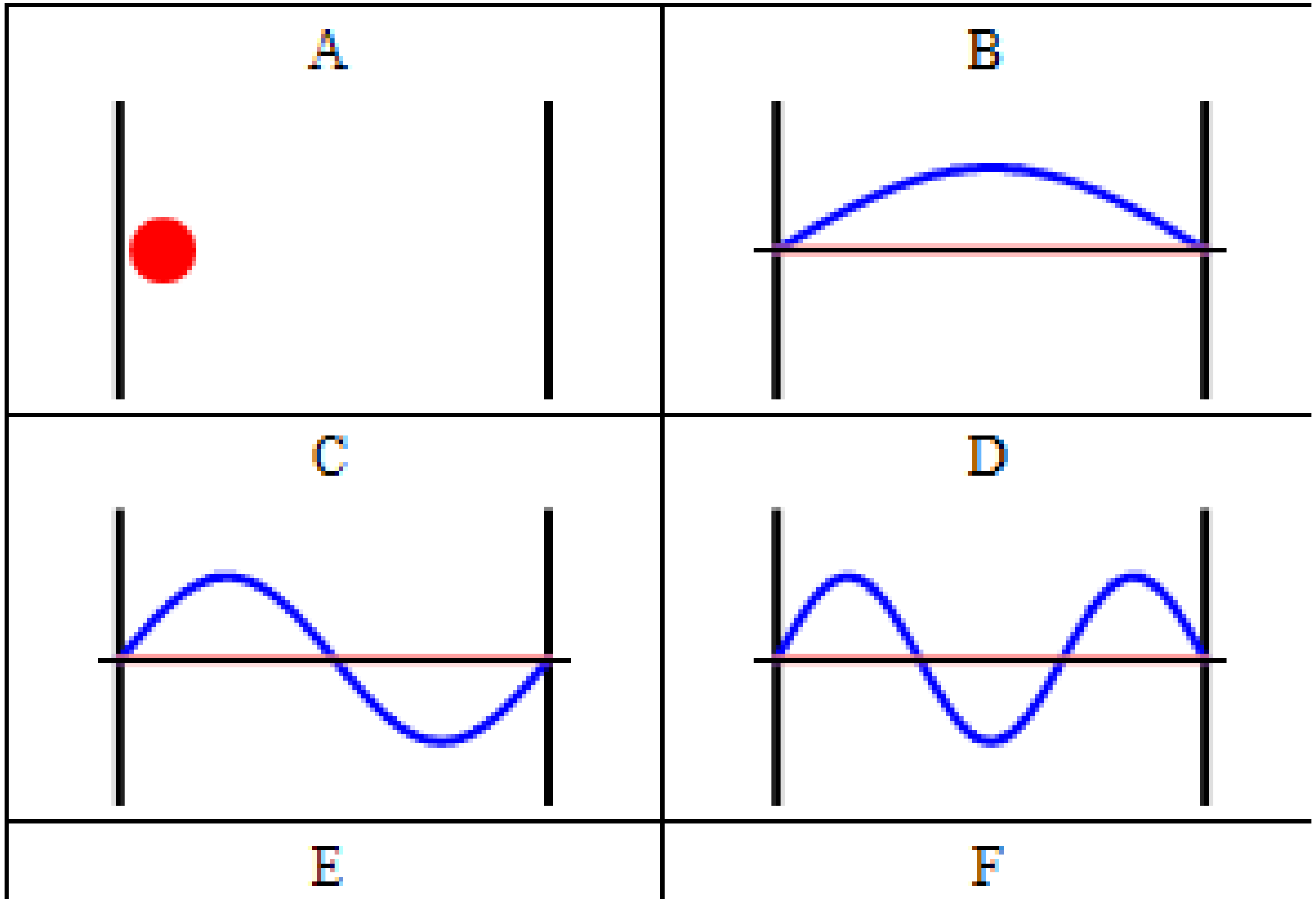


Confining Particle in small box

Look: Ground state wavefunction!

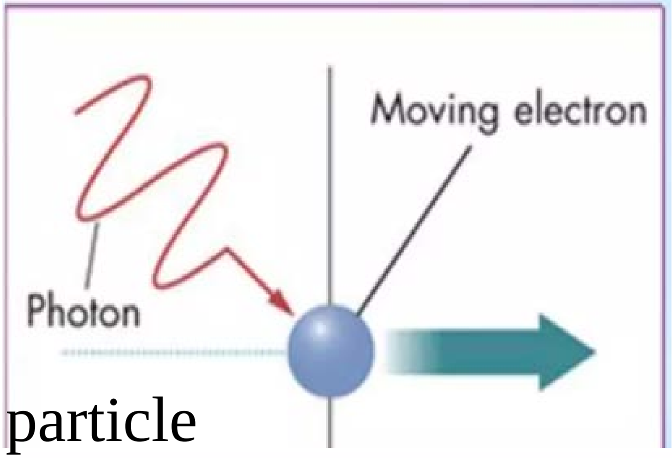
- Probability of finding the particle @box center is maximum
- As we go towards wall, prob. decreases and becomes 0 @wall
- Measurement of position will have uncertainty, but in the range between the wall
- Position uncertainty dictates its canonically conjugate variable → momentum uncertainty (through Hamilton equations)
- This understanding → uncertainty of canonically conjugate variables

➔ Uncertainty Relation



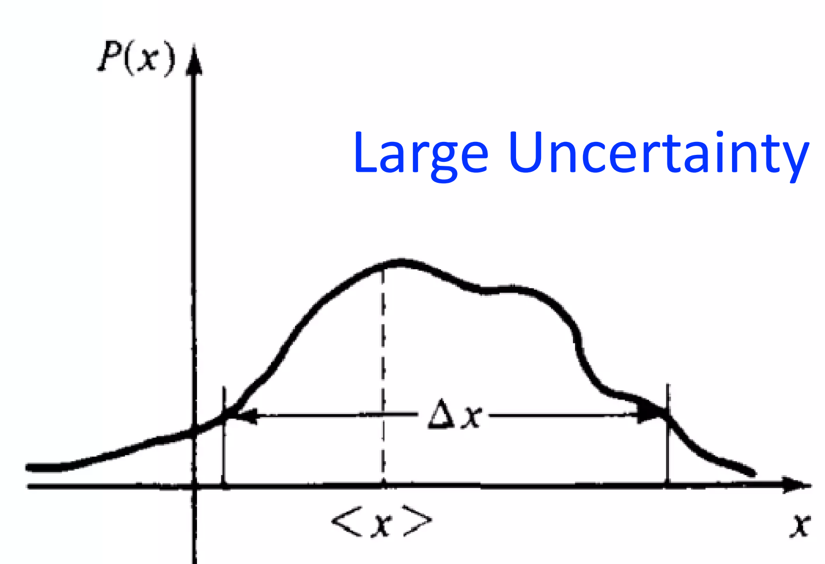
Understanding the Uncertainty

Why do we get uncertainty?

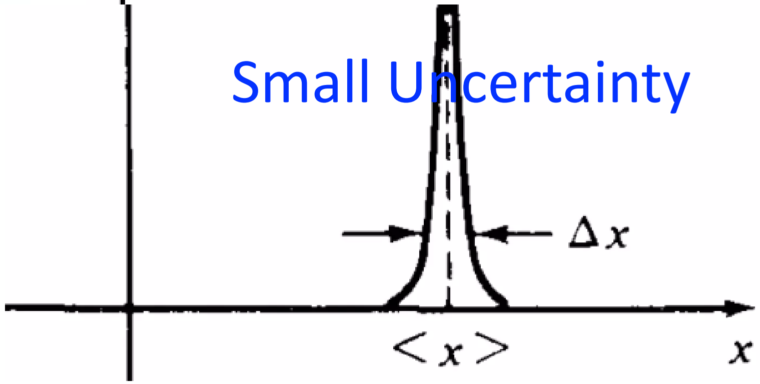


- Measurement requires interaction with probe?
- For very small particle: Interaction changes property of the small particle
- Accurate measurement of position
  ←→ requires shorter wavelength of light
  ←→ Shorter wavelength of light→ High energy photon
- Expect high energy or momentum will be transferred
  from photon to particle to get position accurately.

Uncertainty Definition: $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$

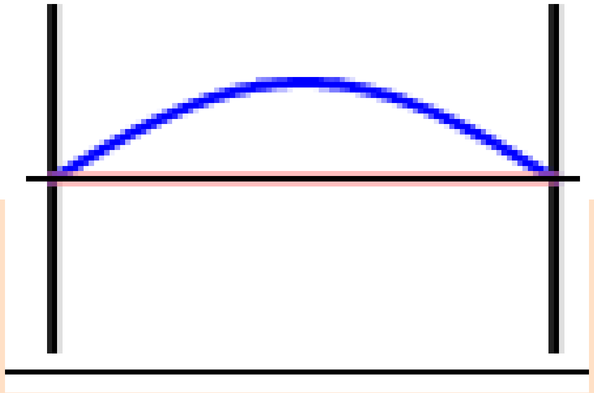


- This uncertainty measurement error or inaccuracy of the setup
- You can think about infinitely accurate experimental setup
- Still you can not avoid this quantum uncertainty
- This is fundamental and inherent in nature.



$$p = \frac{h}{\lambda} \Longrightarrow$$

Fixed momentum → Fixed wavelength



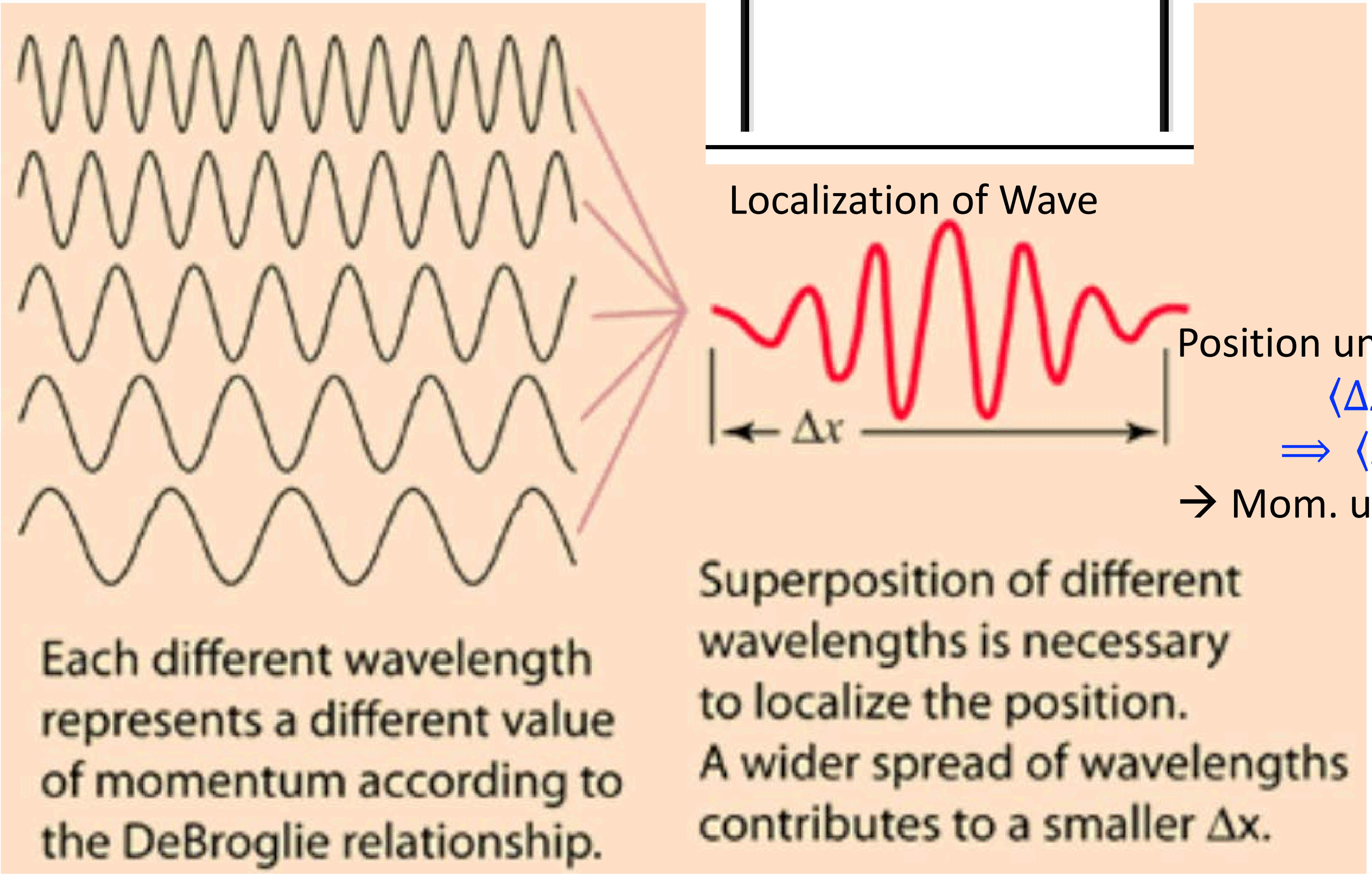
$\lambda_1 \rightarrow p_1 \Longrightarrow$

$\lambda_2 \rightarrow p_2 \Longrightarrow$

$\lambda_3 \rightarrow p_3 \Longrightarrow$

$\lambda_4 \rightarrow p_4 \Longrightarrow$

$\lambda_4 \rightarrow p_4 \Longrightarrow$



Localization of Wave

Position uncertainty

$\langle \Delta x \rangle$

$\Longrightarrow \langle \Delta p_x \rangle$

→ Mom. uncertainty

@hyperphysics

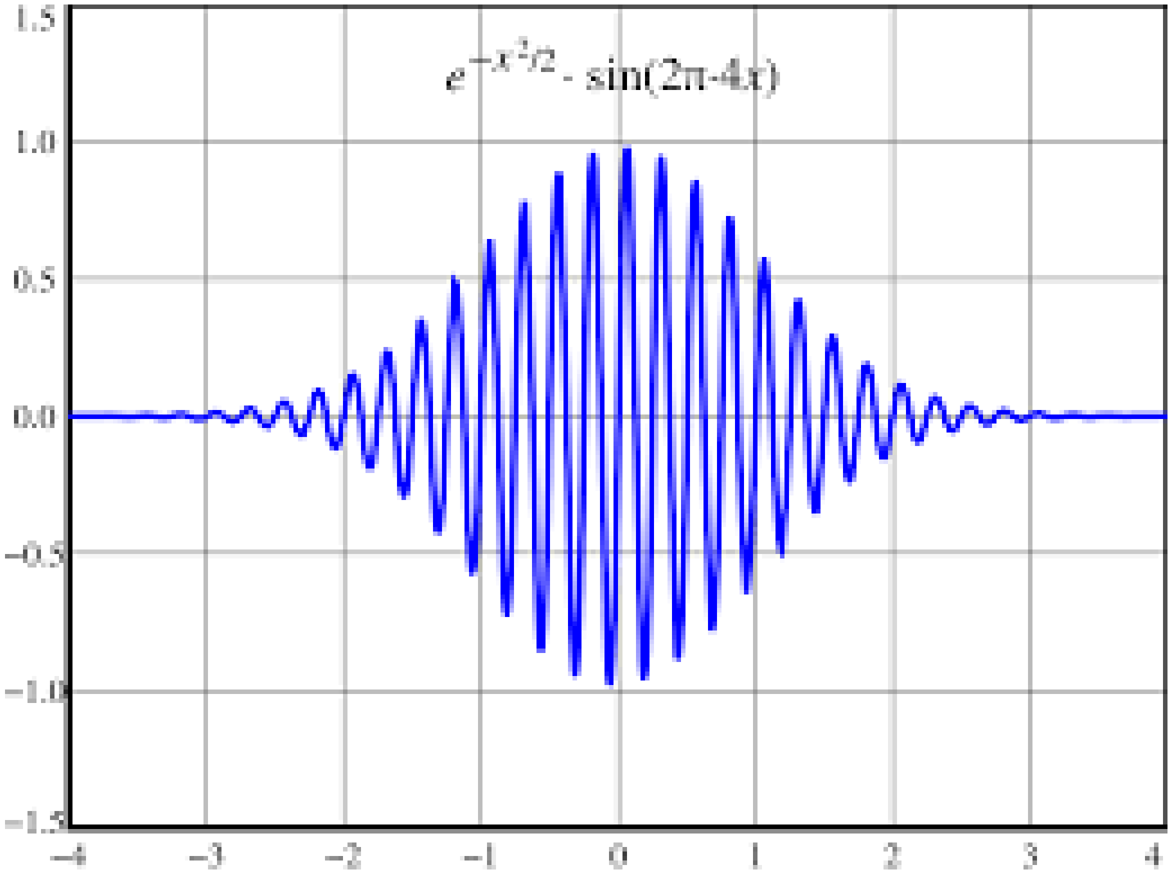
Heisenberg's Uncertainty Relations

Consider, Gaussian wave packets: $\langle A \rangle = \int_{-\infty}^{\infty} y^*(x) A(x) y(x) dx$

$$\langle \Delta x \rangle \langle \Delta p_x \rangle \geq \frac{\hbar}{2};$$

$$\langle \Delta z \rangle \langle \Delta p_z \rangle \geq \frac{\hbar}{2};$$

$$\langle \Delta y \rangle \langle \Delta p_y \rangle \geq \frac{\hbar}{2};$$



$$\langle \Delta x \rangle \langle \Delta p_x \rangle \sim \frac{\hbar}{2}; etc$$

Minimum Uncertainty

Single-slit diffraction: Δx in slit-width, changes Δp_x

This principle is of great importance in understanding many phenomena

Electrons confined in atoms

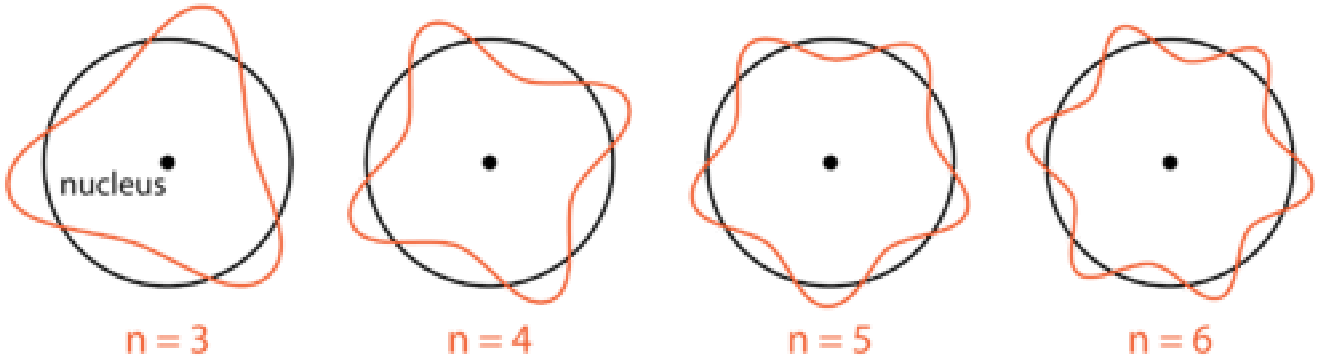
Max. movement span of electron: Diameter of atom

$$x \sim 10^{-10} m \qquad \Delta p \sim \hbar / \Delta x$$

$$x \sim \Delta x \qquad \Delta p \sim p$$

Electron Cloud inside atom

@https://mipt.ru/en/



Standing Wave of electron orbital

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Kinetic Energy of Electron in Atom

$$E = p^2/2m = \hbar^2/(2m(\Delta x)^2)$$

$$= (10^{-34})^2/(2 \times 10^{-30} \times (10^{-10})^2)$$

J eV

We know, Hydrogen atom ionisation potential : 13.6 eV

This is in combination with Nuclear attraction potential energy

This principle is of great importance in understanding many phenomena

Hydrogen atom: Ground state

$$E = \frac{\hbar^2}{2m(\Delta r)^2} - \frac{e^2}{4\pi\epsilon_0 \Delta r}$$

$$\frac{\partial E}{\partial \Delta r} = -\frac{\hbar^2}{m(\Delta r)^3} + \frac{e^2}{4\pi\epsilon_0 (\Delta r)^2} = 0$$

$$\Rightarrow \Delta r = \frac{4\pi\epsilon_0}{me^2}\,\hbar^2$$

$$\Delta r = \frac{(1.05 \times 10^{-34})^2}{9 \times 10^9 \times 9.1 \times 10^{-31} \times (1.6 \times 10^{-19})^2}$$

$$= 0.528 \times 10^{-10} \text{ m} = 0.528 \text{ A}^\circ$$ Bohr radius

Minimum energy

$$\boxed{\Delta r = \frac{4\pi\epsilon_0}{me^2}}$$

This principle is of great importance in understanding many phenomena

particles confined in nucleus

Size of the nucleus

$$E = p^2/2m = \hbar^2/(2m(\Delta x)^2)$$

$$= (10^{-34})^2/(2\times4\times1.67\times10^{-27}\times4\times(10^{-15})^2)$$

$$\boxed{= 2\times10^{-13}\ \mathrm{J} \sim 1\ \mathrm{MeV}}$$

This principle is of great importance in understanding many phenomena

Harmonic oscillator: Ground state

$$E = \frac{p_x^2}{2m} + \frac{1}{2}kx^2$$

$$x \sim \Delta x$$

$$\Delta p_x \sim p_x \sim \hbar / 2\Delta x$$

$$E = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}k(\Delta x)^2$$

$$\frac{\partial E}{\partial \Delta x} = -\frac{\hbar^2}{4m(\Delta x)^3} + k(\Delta x) = 0$$

$$\Rightarrow (\Delta x)^2 = \frac{\hbar}{2\sqrt{mk}}$$

Zero point energy

Consequences of Zero Point Energy

- We found consequence of Heisenberg uncertainty is the zero point energy
- We had earlier calculated radius of hydrogen atom using the uncertainty relation
- Other way to say, zero point energy decides the span of electron

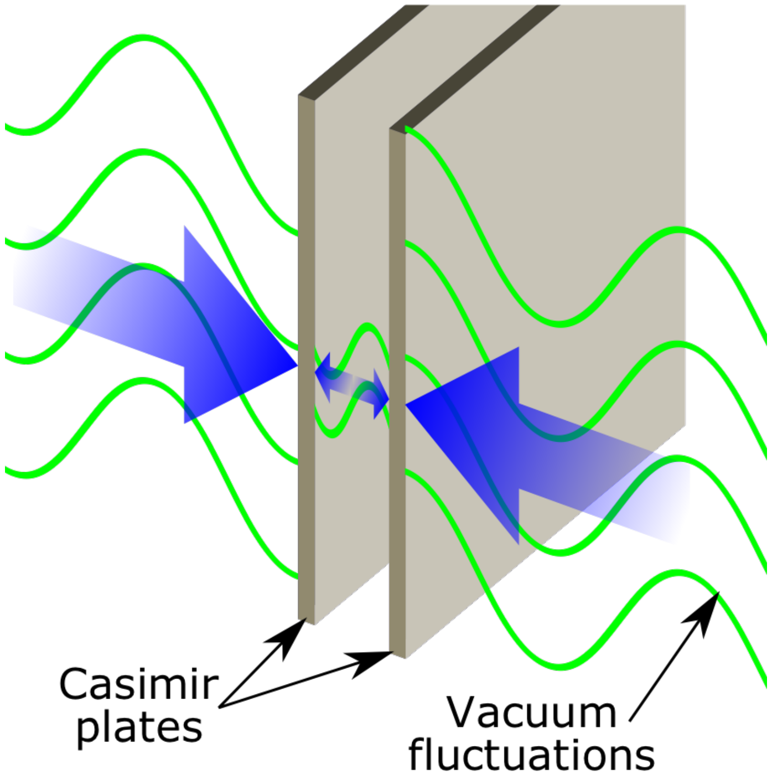
- In 1934 Paul Dirac and W. Heisenberg: Vacuum Fluctuation
  - Vacuum does not mean empty.
  - $(\Delta E)(\Delta t) \sim \hbar \implies$ Within Δt time, e^- & e^+ can be generated & destroyed in vacuum $\implies$ Sea of transient charges always present : Energy of Vacuum randomly changes temporaily

$\implies$ Consequence, we can not measure bare charge: e^+ cloud around test e^-

$\implies$ Experimentally verified theory: Physical charge of e^- matches with theoretically evaluated value up to 10 decimal places

Endless Creation Out of Nothing: https://www.scientificamerican.com/article/

- In 1948 Hendrik Casimir showed:
  one consequence of the zero-point field is an attractive force between two uncharged, perfectly conducting parallel plates, the so-called Casimir effect.



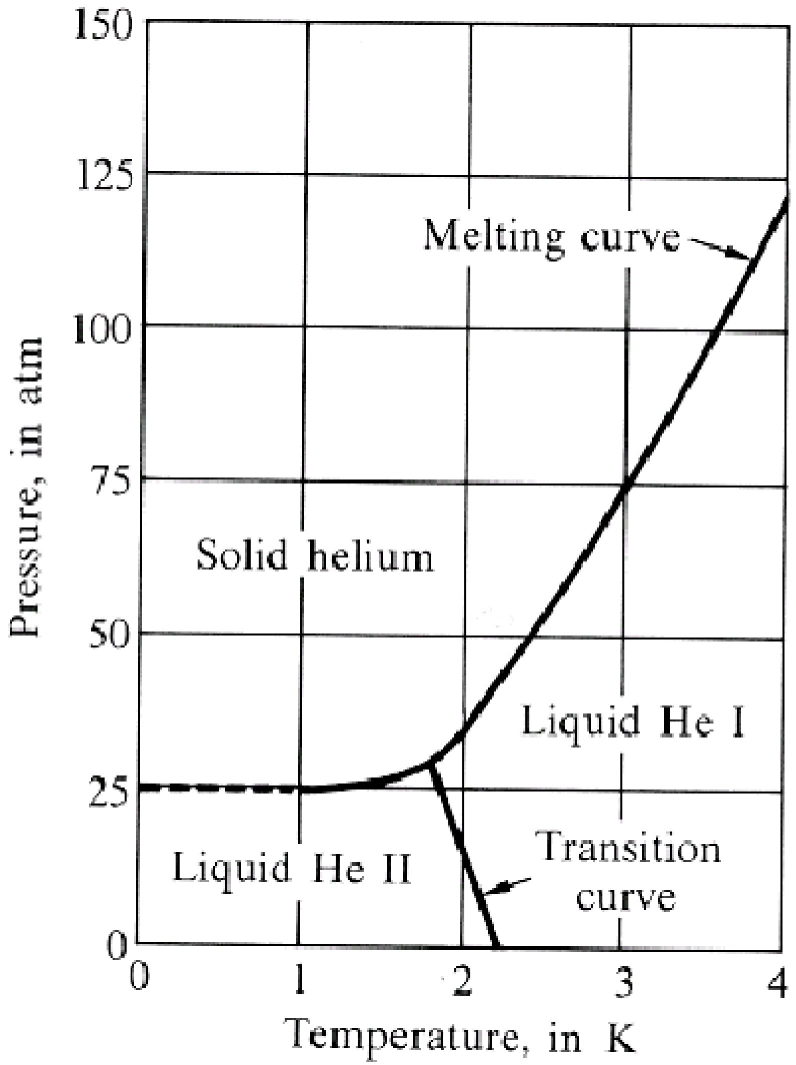
Consequences of Zero Point Energy

Helium atom:

- It remains liquid @absolute zero temperature.
- The large vibrational zero-point energy is responsible for this

For Fermion Gas:

- Degeneracy Pressure



Dynamics of Particle in Quantum Mechanics

Dynamics of Particle

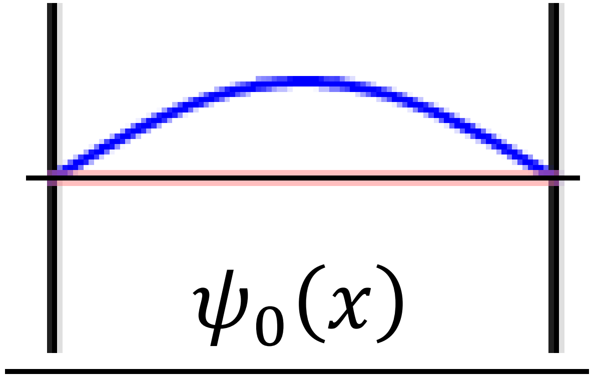
	Newtonian Mechanics	Lagrangian Mechanics	Hamiltonian Mechanics	Quantum Mechanics
Principle	Force = $m \times accl^n$	Principle of Least Action	Reformulation of Lagrangian Mechanics (in Phase space coordinates (x,p))	Hamilton's Equation of motion
Driving Equation	$m\ddot{x} = F$	Lagrange's Eq. $\frac{d}{dt}\left\{\frac{\partial L}{\partial \dot{x}}\right\} = \frac{\partial L}{\partial x}$ $L = K.E - P.E.$	$\dot{p} = -\frac{\partial H}{\partial x}, \dot{x} = \frac{\partial H}{\partial p}$ $H = K.E. + P.E.$	x *and* p *are not simple* dynamical variables. They are self-adjoint Canonical conjugate operators

$\hat{x}$ & $\hat{p}$: Operate on states representing the system

Example of states representing system: Energy states of particle in box

Position Operator

$\hat{x}$

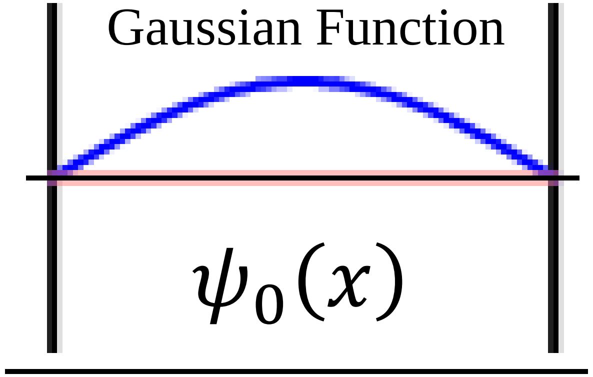


: $x\,\psi_0(x)$: Wavefunction

Measured value

Momentum Operator: Canonically conjugate operator (Fourier transform dual)

$\hat{p}$



: $p\,\psi_0(x)$

Consider Plane wave

$$\psi(x,t) = e^{\frac{i}{\hbar}(px - Et)}$$

$$\frac{\partial \psi(x,t)}{\partial x} = \frac{ip}{\hbar} e^{\frac{i}{\hbar}(px-Et)} = \frac{ip}{\hbar}\psi.$$

$$\boxed{\hat{p} = -i\hbar \frac{\partial}{\partial x}}$$

Time Evaluation of Quantum System

Momentum operator: $\hat{p}_x \equiv -i\hbar \dfrac{\partial}{\partial x}$

Total energy operator: $\hat{E} \equiv i\hbar \dfrac{\partial}{\partial t}$

Now the total energy of a particle is just the sum of the kinetic energy and the potential energy:

$$E = p^2/2m + V$$

In "operator" form this becomes:

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m}(-i\hbar)^2 \frac{\partial^2 \psi}{\partial x^2} + V\psi$$

Rearranging we get Schrödinger's equation: (one dimensional version)

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t}}$$

Schrödinger's equation

Things to note from Schrödinger's eqn.

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=i\hbar\frac{\partial\psi}{\partial t}}$$

(i) The equation is linear in ψ that is there are no terms like ψ^2 or $\left(\frac{\partial\psi}{\partial x}\right)^2$.

(ii) The equation is homogeneous, that is there are no terms independent of ψ

Taken together these features mean that if ψ is a solution to the equation, then so is $c\psi$ where c is any complex number.

This implies that any linear combination of solutions is also a solution

Differences between Schrödinger and classical wave equations

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=i\hbar\frac{\partial\psi}{\partial t}$$

K.E. + P.E. = Total Energy

$$\frac{\partial^2 y}{\partial x^2}=\frac{1}{\mathrm{v}^2}\frac{\partial^2 y}{\partial t^2}$$

Schrödinger Wave Equation	Classical Wave Equation
Eqn. derived for total energy	Eqn. derived from force
First order derivative w.r.t. time	Second order derivative w.r.t time
Complex Equation	Real Equation
➔ ψ must be complex	➔ y is a displacement : Real

Interpretation of the wavefunction

What does $\psi(x, t)$ tell us?

c.f. Young's slit experiment: high probability of detecting particle at bright fringes, low probability at dark fringes

• for light expect probability of detecting a photon to be proportional to the *intensity* of E.M. wave.

Phase of $\psi(x,t)$ is not observable.
The probability of finding a particle in the range x to $x+dx$ at time t is proportional to $|\psi(x,t)|^2\, dx$

Define: $P(x,t)\, dx. \propto |\psi(x,t)|^2\, dx$

Need to normalise probabilities: $$\int_{-\infty}^{\infty} P(x)\, dx = 1$$

(**one** particle!)

Normalisation of wavefunction

$$P(x,t)\,dx. \propto |\psi(x,t)|^2\,dx$$

To get rid of proportional sign we need a constant of proportionality: $P(x,t)\,dx. = A\,|\psi(x,t)|^2\,dx.$

Eliminate A by using the normalisation: $\int_{-\infty}^{\infty} P(x)\,dx = 1$

$$A\int_{-\infty}^{\infty} |\psi(x,t)|^2\,dx = 1$$

It follows that: $A = \dfrac{1}{\int_{-\infty}^{\infty} |\psi(x,t)|^2\,dx}$

If we normalise the wavefunction so that $\int_{-\infty}^{\infty} |\psi(x,t)|^2\,dx = 1$

we can define $\boxed{P(x,t) = |\psi\,(x,t)|^2}$

Time independent Schrödinger equation

Time-dependent, Schrödinger equation: $$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Suppose time-independent potential, then we expect the total energy to be a constant.

Example: $V(x,t)$ ~ Potential due to oscillating dipole → $V(x)$ ~ due to constant dipole

"Separation of variables": $\psi(x,t) = u(x)\,f(t)$

Insert into Schrödinger equation:

$$-\frac{\hbar^2}{2m}f(t)\frac{\partial^2 u(x)}{\partial x^2} + V(x)u(x)f(t) = i\hbar u(x)\frac{\partial f(t)}{\partial t}$$

Divide through by $u(x)\,f(t)$:

$$\underbrace{-\frac{\hbar^2}{2m}\frac{1}{u(x)}\frac{\partial^2 u(x)}{\partial x^2} + V(x)}_{\text{LHS}} = \underbrace{i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}}_{\text{RHS}}$$

Only depends on x

Only depends on t

Time independent Schrödinger equation $$-\frac{\hbar^2}{2m}\frac{1}{u(x)}\frac{\partial^2 u(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}$$

- The only way a function of x = a function of t, $\forall x,t$ $\Longrightarrow$ L.H.S.=R.H.S. constant.
- Call the constant E (we will show later this is the total energy).

RHS becomes: $$i\hbar\frac{\partial f(t)}{\partial t} = E\, f(t)$$

Integrating: $$\int\frac{\partial f}{f} = \frac{E}{i\hbar}\int\partial t \longrightarrow \boxed{f(t) = f(0)\exp(-i\,E\,t/\hbar)}$$

LHS becomes: $$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} + V(x)\,u(x) = E\,u(x)}$$

This is called the time-independent Schrödinger equation

ψ has a solution of the form: $$\psi(x,t) = u(x)\exp(-i\,E\,t/\hbar)$$

Probability density is independent of time: $$|\psi(x,t)|^2 = |u(x)|^2$$

'Solving' the Schrödinger equation:

What do we want? Usually, the <u>allowed energy levels</u>.

<u>First:</u> Assume a solution - e.g. $u(x) = A\sin(kx)$ (TISE)

<u>Second:</u> Substitute solution into Schrödinger equation.
That gives relationship between E (and V) and k

<u>Third:</u> Use boundary conditions (e.g., u and du/dx continuous)
to solve for allowed values of k (e.g. in terms of well size, a)

<u>Fourth:</u> Use earlier relationship between E (and V) and k to
obtain allowed values of E

Example of solution of T.I.S.E:
Particle in a box: infinite potential well

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

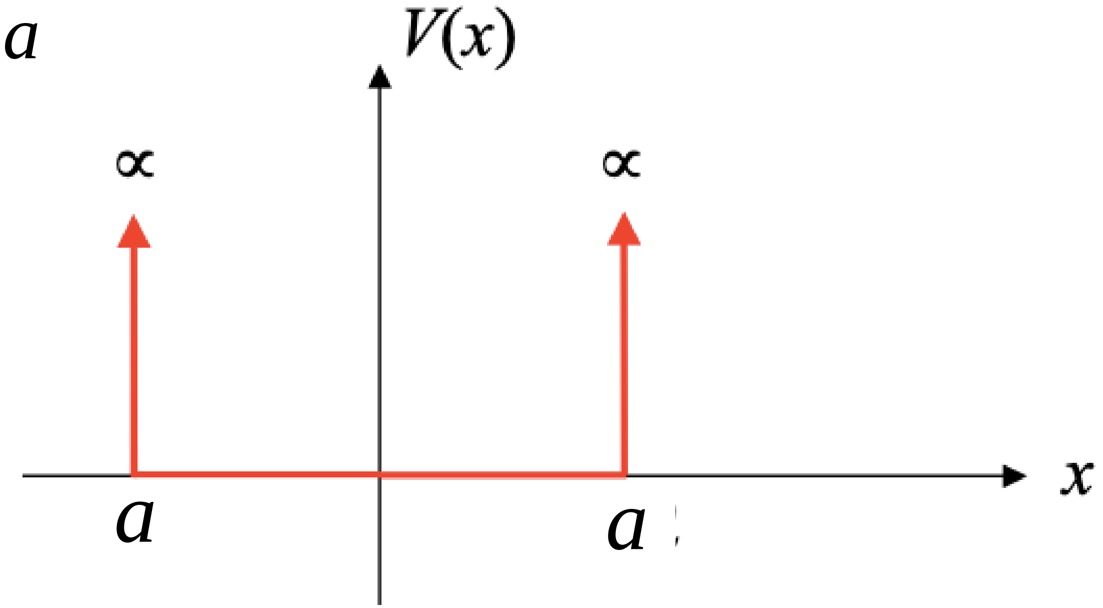
Box in one dimension with walls at $-a$ and $+a$

$$V(x) = 0 \quad \text{for } |x| \le a,$$

$$V(x) = \infty \quad \text{for } |x| > a$$

For $|x| \le a$, T.I.S.E becomes:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} = E\,u(x)$$



Boundary condition: $u(x)$ must vanish for $|x| > a$,

Types of solution (I)

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} = E\,u(x)$$

A possible solution is: $u(x)=A\,sin(kx)$

Check:

$$\frac{\partial u}{\partial x} = Ak\cos(kx)$$

$$\frac{\partial^2 u}{\partial x^2} = -Ak^2\sin(kx)$$

Insert into T.I.S.E.: $\frac{\hbar^2 k^2}{2m}A\sin(kx) = E\;A\sin(kx)$

Therefore it is a solution as long as: $E = \frac{\hbar^2 k^2}{2m}$

Boundary condition: $u(x) = 0$ for $|\,x\,| > a$

implies $sin(kx) = 0$ for $|\,x\,| = a$. True if $ka=m\pi$ (m integer)

Types of solution (II)

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} = E\,u(x)}$$

Another type of solution is: $u(x)=B\,cos(kx)$

Check:

$$\frac{\partial u}{\partial x} = -Bk\sin(kx)$$

$$\frac{\partial^2 u}{\partial x^2} = -Bk^2\cos(kx)$$

Insert into T.I.S.E.: $$\frac{\hbar^2 k^2}{2m}B\cos(kx) = E\ B\cos(kx)$$

Therefore it is a solution as long as: $$E = \frac{\hbar^2 k^2}{2m}$$

Boundary condition: $u(x) = 0$ for $|x| > a$ implies

$cos(kx) = 0$ for $|x| = a$. True if $ka=m\pi/2$ (m odd integer)

Summary of solutions:

$u(x)=A\sin(kx)$

$u(x)=B\cos(kx)$

$ka=m\pi$ (m integer)

$ka=n\pi/2$ (n odd integer)

Equivalently: $ka=n\pi/2$

(n even integer)

$n = 2, 4, 6, 8, \ldots..$

$$\boxed{k=\frac{n\pi}{2a}}$$

$n = 1, 3, 5, 7, \ldots..$

$$\boxed{E=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2\pi^2n^2}{8ma^2}}$$

Energy levels for a particle in a box

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{8ma^2} \qquad n = 1,2,3,4,5,6,7,8,\ldots\ldots.$$

Solutions for energy are called energy eigenvalues

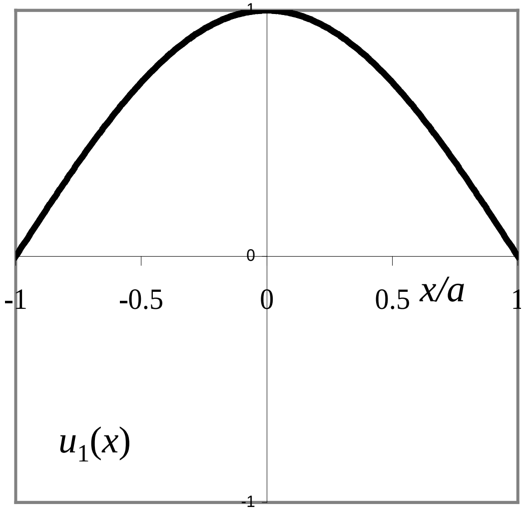
Wavefunctions for particle in a box

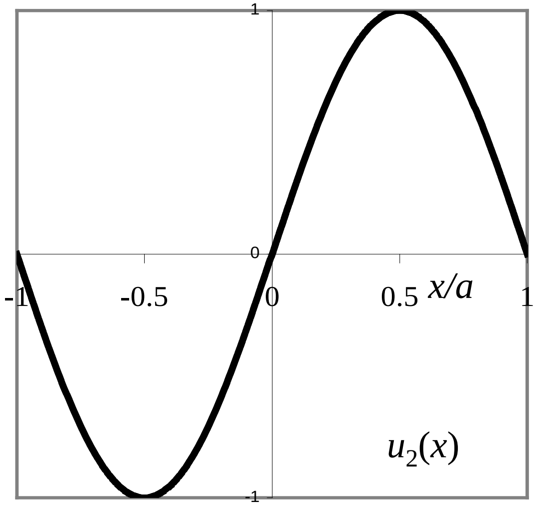
$u(x)=B\,cos(n\pi\, x/2a)$

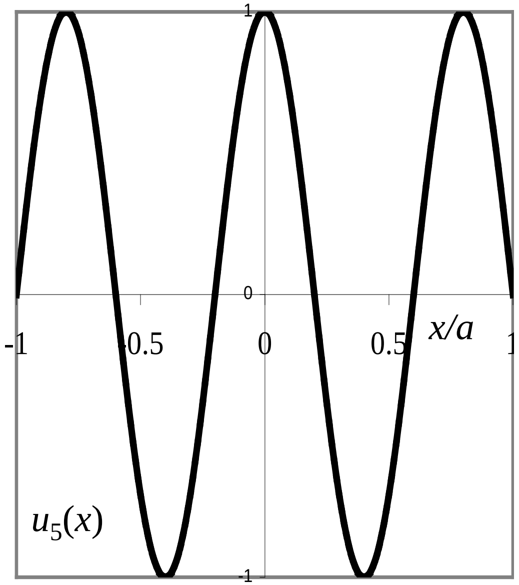
$n = 1, 3, 5, 7,\ldots..$

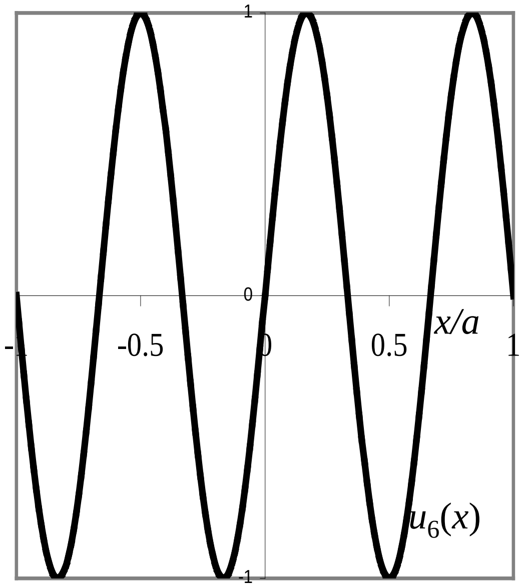
$u(x)=A\,sin(n\pi\, x/2a)$

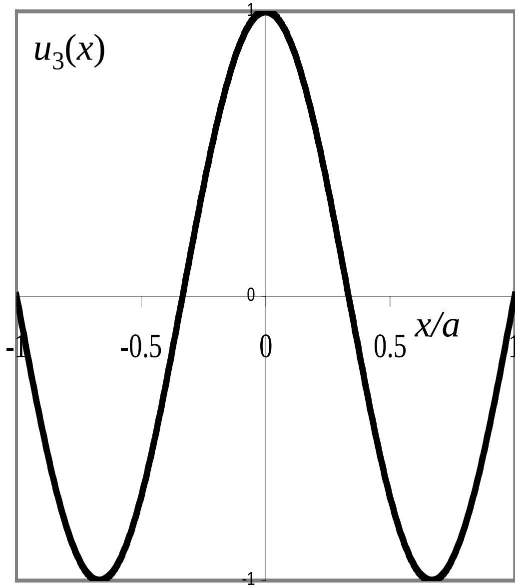
$n = 2, 4, 6, 8,\ldots..$

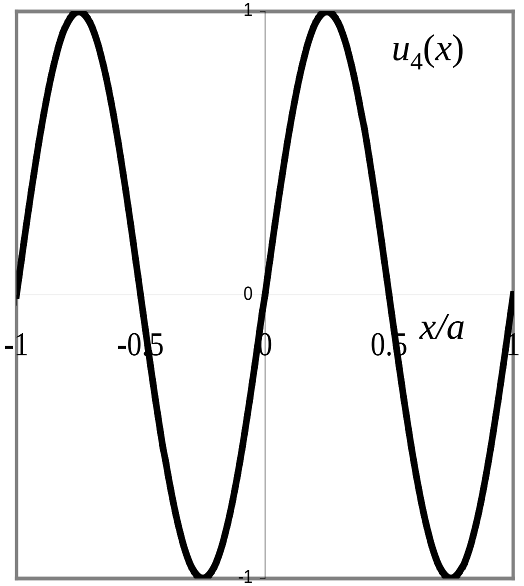












Solutions for wavefunctions are called eigenfunctions

Normalisation

$u(x) = A\ \sin(n\pi x/2a)$ or $B\ \cos(n\pi x/2a)$ Values of A, B ?

Normalisation condition: $\int_{-\infty}^{\infty} |\psi(x,t)|^2\, dx = 1$ ← As we know one particle is present @x ∈ $[-\infty, \infty]$

In the present case we only need to integrate between $-a$ and $+a$ since $u(x)$ vanishes outside this range:

$$\int_{-a}^{a} |\psi(x,t)|^2 dx = \int_{-a}^{a} A^2 \sin^2\left(\frac{n\pi x}{2a}\right) dx = \frac{A^2}{2}[x]_{-a}^{a} = A^2 a = 1$$

- It follows that: $A = \dfrac{1}{\sqrt{a}}$.
- Similarly it can be shown that $B = \dfrac{1}{\sqrt{a}}$

Takes care time evolution of wavefunction; making Sure # of particle is not changing over time

Normalised eigenfunctions:

$$\psi_n(x,t) = u_n(x)\exp(-i\,E_n\,t\,/\,\hbar) = \frac{1}{\sqrt{a}}\cos\left(\frac{n\pi x}{2a}\right)\exp\left(-\frac{iE_n t}{\hbar}\right)$$

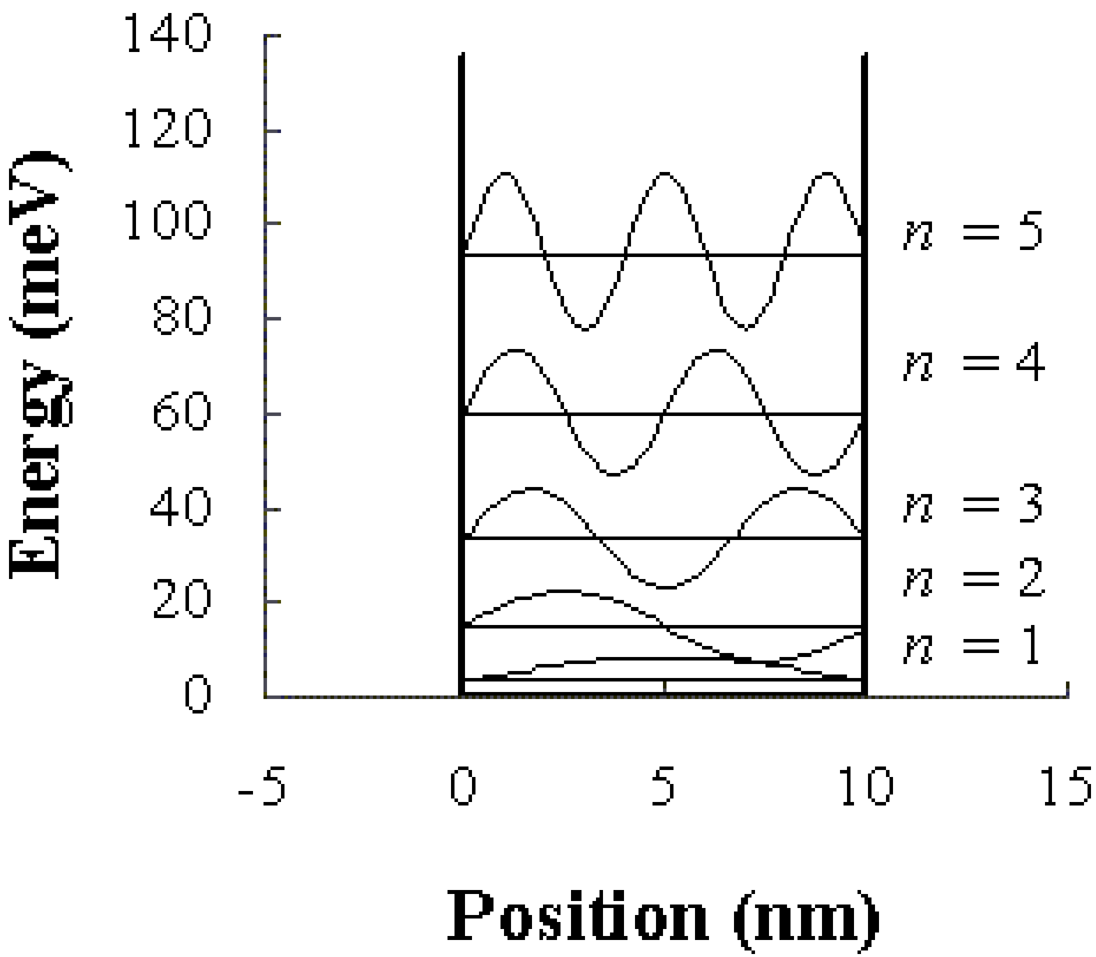
n =1, 3, 5,...

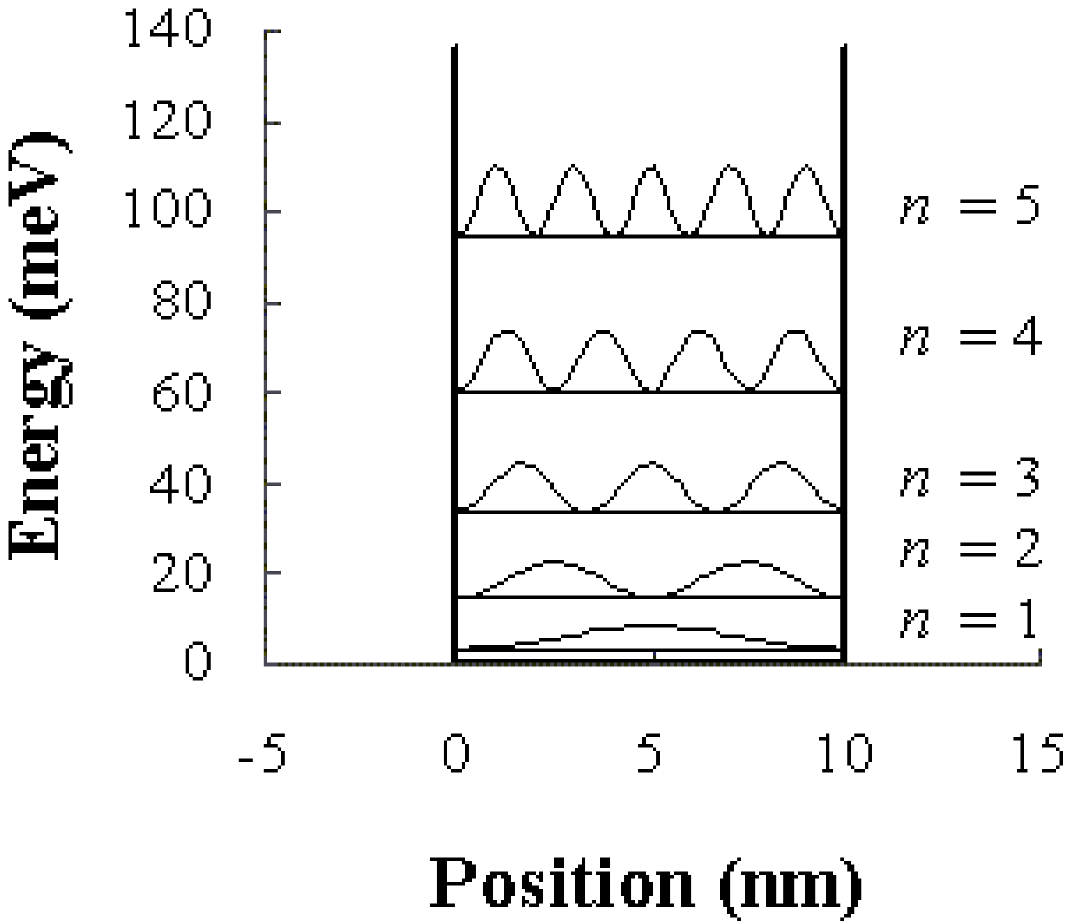
n =2, 4, 6.....

$$\psi_n(x,t) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi x}{2a}\right)\exp\left(-\frac{iE_n t}{\hbar}\right)$$

Probability density $P(x,t) = |\psi(x,t)|^2$

For first five eigenfunctions for particle in a box of width 10 nm





http://labman.phys.utk.edu/phys222core/modules/m10/wave_functions.html

Zero point energy

The lowest energy state for a particle in a box is $E_1 = \dfrac{\hbar^2 \pi^2}{8ma^2}$

Classically, Lowest possible energy should be zero.

- Why can't the energy be zero?

Heisenberg uncertainty relation $\Delta p \, \Delta x \approx \hbar$

Particle is confined in box, so $\Delta x \sim a$.

Must be an uncertainty in momentum $\Delta p \approx \dfrac{\hbar}{a}$

Since momentum cannot be zero (st~~a~~tic), minimum energy must be of order

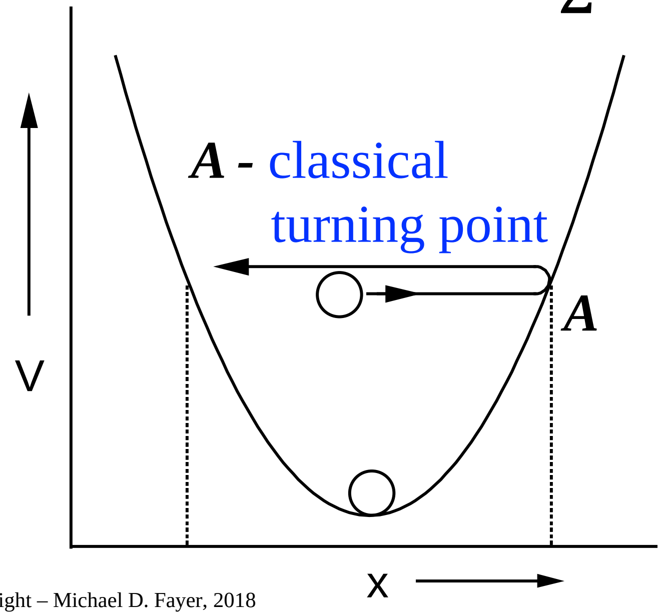
$$E_{\min} \approx \frac{(\Delta p)^2}{2m} \approx \frac{\hbar^2}{2ma^2}$$

(Qualitative Agreement with E_1!!)

Particle in Harmonic Oscillator: Quantum Mechanics point of View

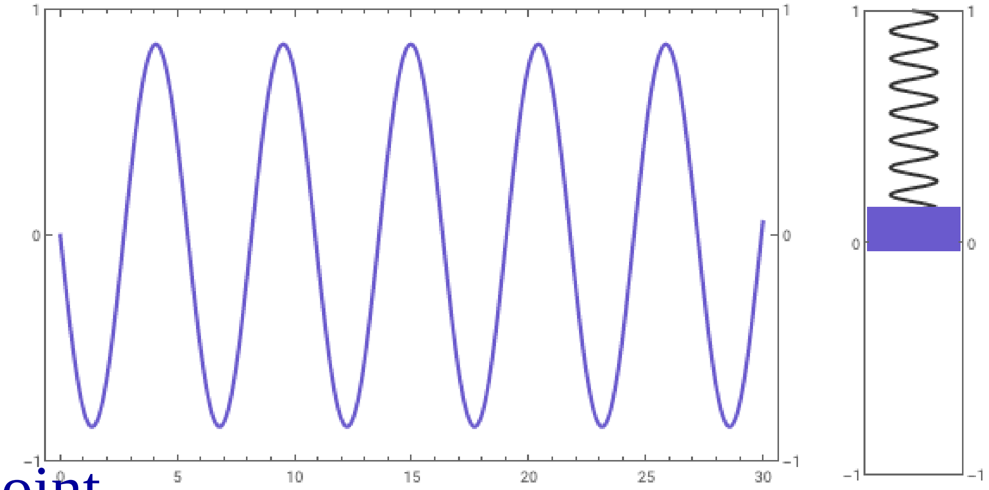
Potential : $V(x) = \frac{1}{2}kx^2$

Classical Mechanics: $m\ddot{x} = -kx$



Real Solution: $x(t) = A\cos kx$ with energy $E = \frac{1}{2}kA^2$

A can take on any value ➔ Energy is continuous.

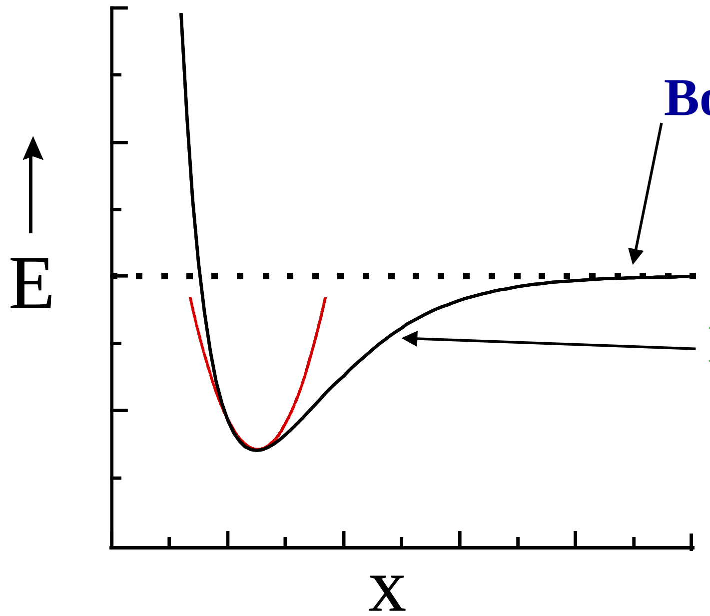


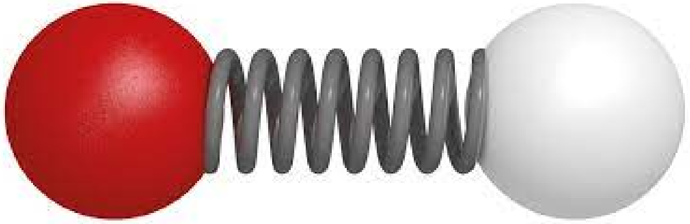
- Classical particle can never be past turning point.
- Turning point K.E. zero; potential energy max.
- Particle can be stationary at bottom of well, know position, $x = 0$; know momentum, $p = 0$.

$$\therefore \Delta x \Delta p = 0$$

Example: Quantum Harmonic Oscillator

Simplest model of molecular vibrations





- **Bonds between atoms act as "springs".**
- **Near bottom of molecular potential well,**
  molecular potential approximately parabolic

Harmonic Oscillator.

One Dimensional Quantum Harmonic Oscillator in the Schrödinger Representation

$H|\psi\rangle = E|\psi\rangle$ Where, $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$

- $\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - (2\pi^2 m\nu^2)x^2]\psi(x) = 0$

Define $\alpha = 2\pi m\nu/\hbar$

$\lambda = \frac{2mE}{\hbar^2}$

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \left(\lambda - \alpha^2 x^2\right)\psi(x) = 0}$$

Find $\psi(x)$!!

Must obey Born Conditions

- **finite everywhere**
- **single valued**
- **Continuous**
- **first derivative continuous**

Case: 1 $\alpha^2 x^2 \gg \lambda$ Therefore, λ can be dropped.

This is negligible compared to the 1st term as $x \to \infty$.

$$\frac{d^2\psi}{dx^2} = \alpha^2 x^2 \psi$$

$$\frac{d^2\psi}{dx^2} = \alpha^2 x^2 e^{\pm\frac{\alpha}{2}x^2} \pm \alpha e^{\pm\frac{\alpha}{2}x^2}$$

Two solutions

$$e^{-\frac{\alpha}{2}x^2}$$

This is O.K. at

$$x = \pm\infty$$

$$e^{+\frac{\alpha}{2}x^2}$$

*Remember $\alpha = \frac{2\pi m\nu}{\hbar} \geq 0$

This blows up at $x = \pm\infty$

Not finite everywhere.

Therefore, large x solution is

$$\psi(x) = e^{-\frac{\alpha}{2}x^2}$$

For all x

$$\psi(x) = e^{-\frac{\alpha}{2}x^2} f(x)$$

Must find this.

***How to derive $f(x)$?

$$\boxed{\frac{d^2\psi(x)}{dx^2}+\left(\lambda-\alpha^2x^2\right)\psi(x)=0} \Longrightarrow \psi(x)=e^{-\frac{\alpha}{2}x^2}f(x)$$

Need second derivative in Schrödinger equation

$$\frac{d^2\psi(x)}{dx^2}=e^{-\frac{\alpha}{2}x^2}(\alpha^2x^2f-\alpha f-2\alpha x f'+f'')$$

With $f'=\dfrac{df}{dx}$ **and** $f''=\dfrac{d^2f}{dx^2}$

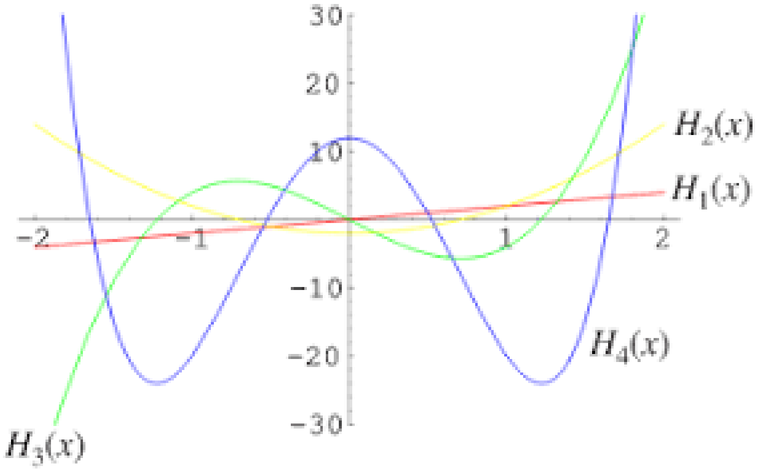
Substitute $\dfrac{d^2\psi(x)}{dx^2}$ **and** $\psi(x)$ **into the original equation**

and divide by $e^{-\frac{\alpha}{2}x^2}$ **gives**

$$f''-2\alpha x f'+(\lambda-\alpha)f=0$$

- **Equation only in *f*.**
- **Solve for *f* and have** $\psi(x)$

Solution will be Hermite polynomial



Quantization of Energy

If there are a finite number of terms in the series for $\underline{H}(\gamma)$, wavefunction does not blow up. Goes to zero at infinity.

$$e^{-\gamma^2/2}\gamma^n$$ The exponential goes to zero faster than γ^n blows up.

To make series finite, truncate by choice of λ → One can show $\lambda = (2n+1)\alpha, n = \text{integer}$

Therefore, $\lambda = \dfrac{2mE}{\hbar^2} = (2n+1)\,2\pi m\nu/\hbar$

definition of λ **definition of α**

$$E_n = \left(n + \frac{1}{2}\right)h\nu$$

n is the quantum number

$n = 0 \qquad E_0 = 1/2\,h\nu$

Lowest energy, not zero. Called zero point energy.

Energy levels equally spaced by $h\nu$.

Energy Levels

Correspond to each n: $$E_n = \left(n + \frac{1}{2}\right) h\nu$$

Wavefunctions

$$\psi_n(x) = N_n e^{-\frac{\gamma^2}{2}} H_n(\gamma)$$

$$\gamma = \sqrt{\alpha}\, x \qquad \alpha = 2\pi m\nu / \hbar$$

$$N_n = \left\{ \left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \frac{1}{2^n n!} \right\}^{\frac{1}{2}}$$

normalization constant

Ground state($n = 0$) $$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha}{2}x^2} = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\gamma^2}{2}}$$

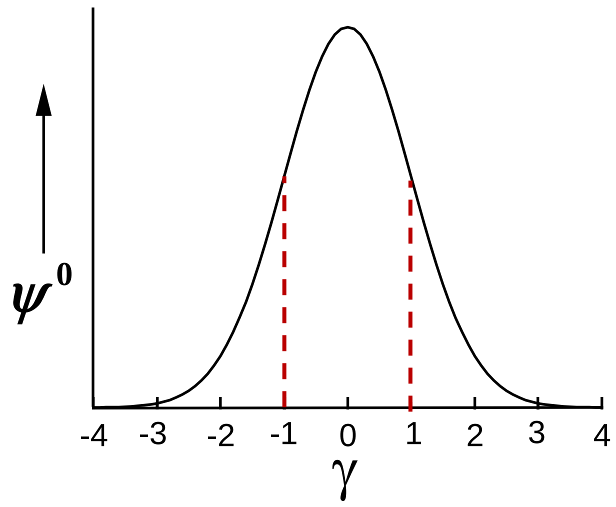
This is a Gaussian.
Minimum uncertainty.

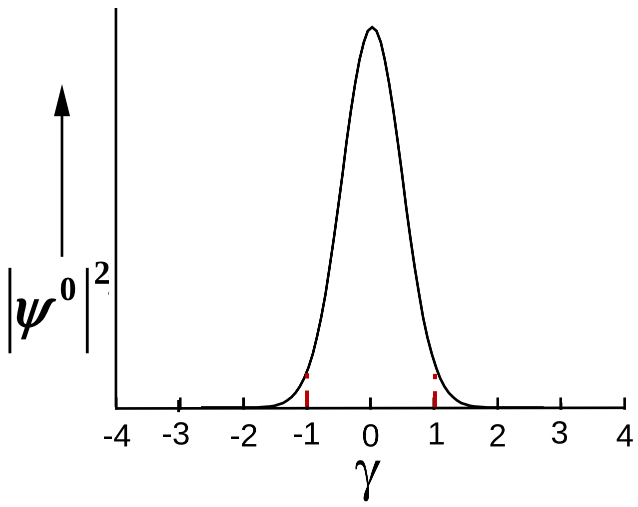
Hermite Polynomials

$$H_0(\gamma) = 1\gamma^0$$
$$H_1(\gamma) = 2\gamma$$
$$H_2(\gamma) = 4\gamma^2 - 2\gamma^0$$
$$H_3(\gamma) = 8\gamma^3 - 12\gamma$$
$$H_4(\gamma) = 16\gamma^4 - 48\gamma^2 + 12\gamma^0$$
$$H_5(\gamma) = 32\gamma^5 - 160\gamma^3 + 120\gamma$$
$$H_6(\gamma) = 64\gamma^6 - 480\gamma^4 + 720\gamma^2 - 120\gamma^0$$

** Given an oscillator $0 \le \alpha \to$ Large Number

Ground State of Quantum Harmonic Oscillator





Classical turning points

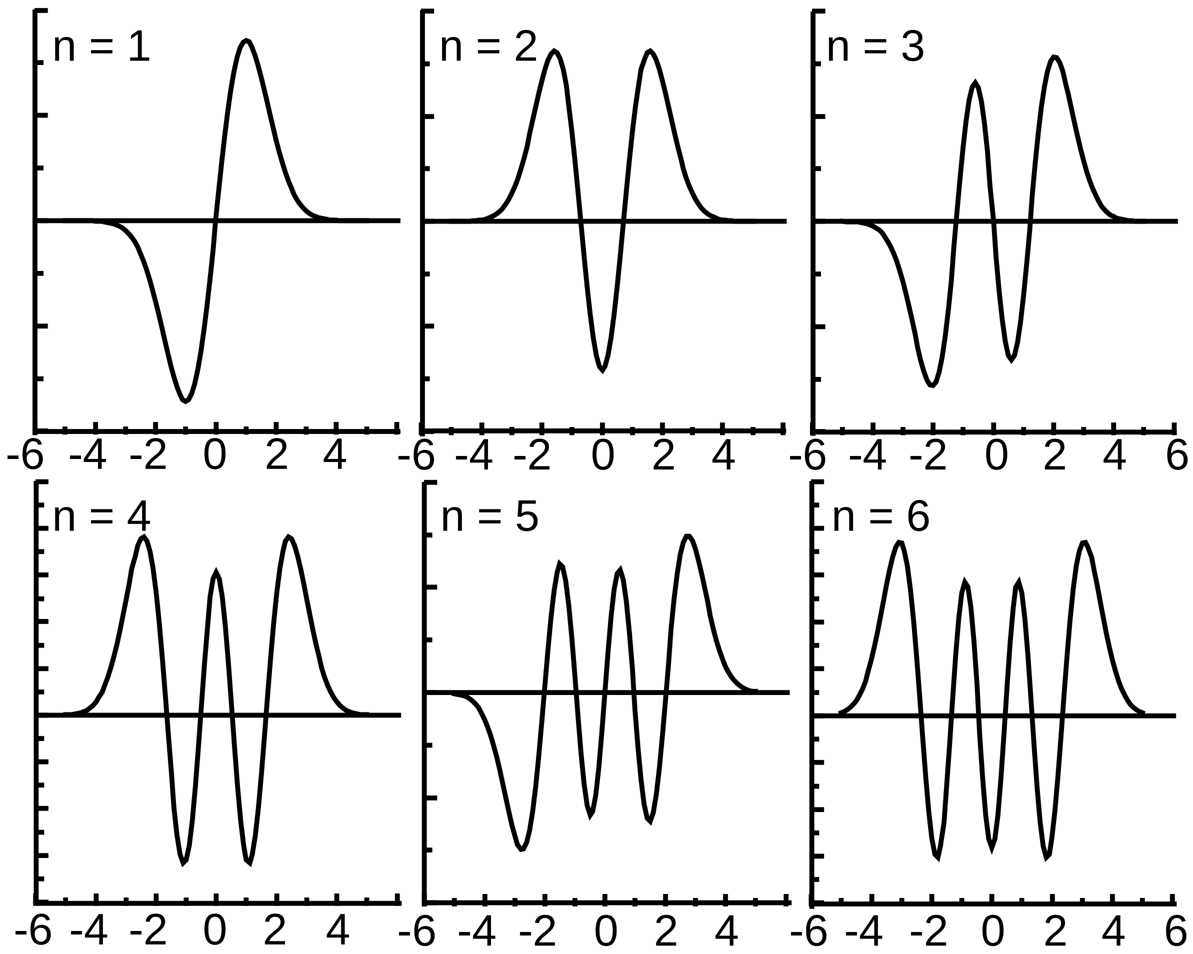
$$\underbrace{1/2\,kx^2}_{\text{potential energy}} = \underbrace{1/2\,h\nu}_{\text{total energy}}$$

$$\therefore \quad x^2 = \frac{h\nu}{k}$$

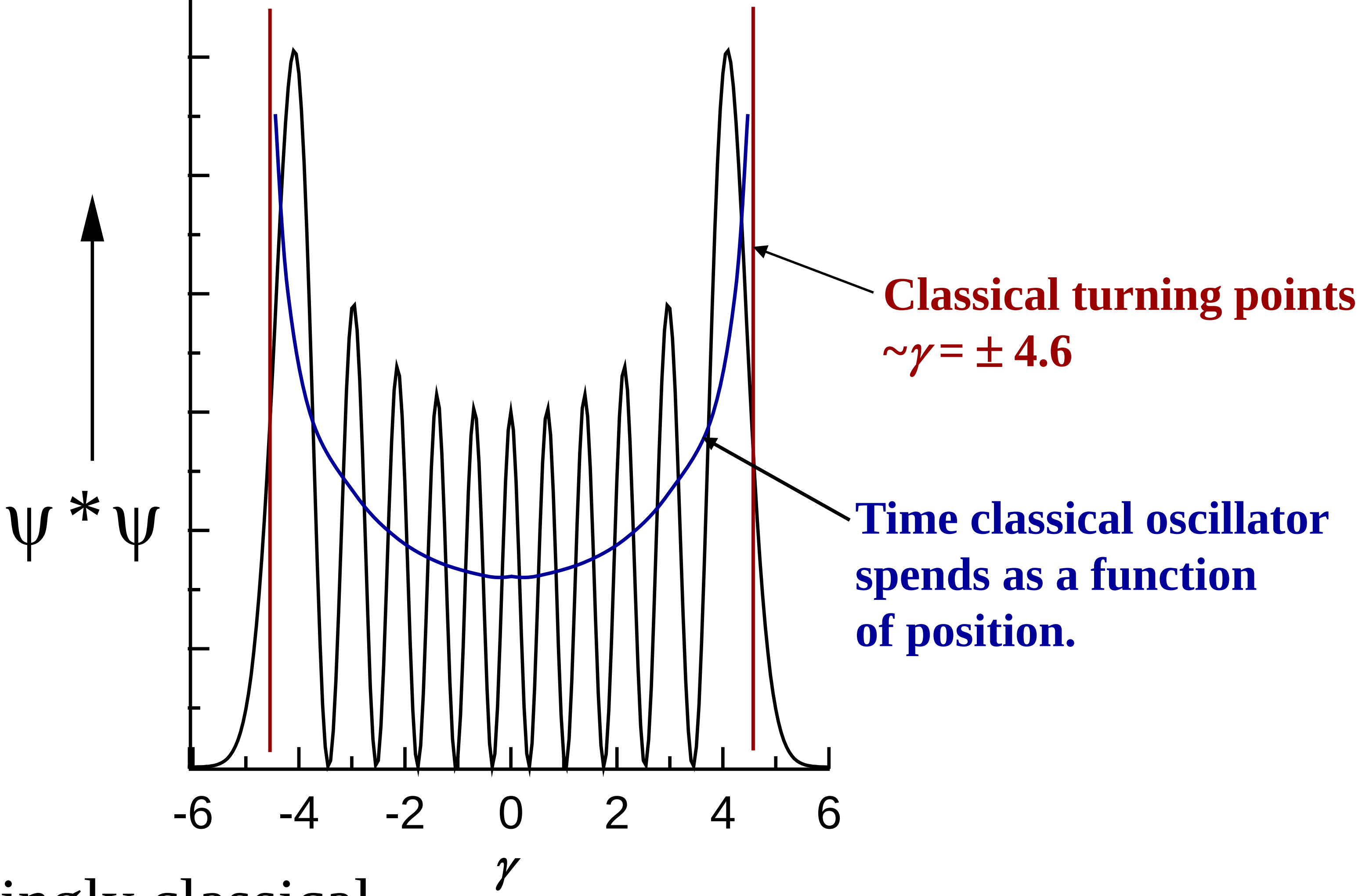
$$x = \pm\sqrt{h\nu / k} = \pm\gamma$$

classical turning points - wavefunction extends into classically forbidden region.

More wavefunctions - larger *n*, more nodes



Comparison of Quantum HO With Classical HO



Looks increasingly classical.
For large object, nodes so closely spaced because n very large that can't detect nodes.