The enigmatic wavefunction

Google Doodle, December 11, 2017

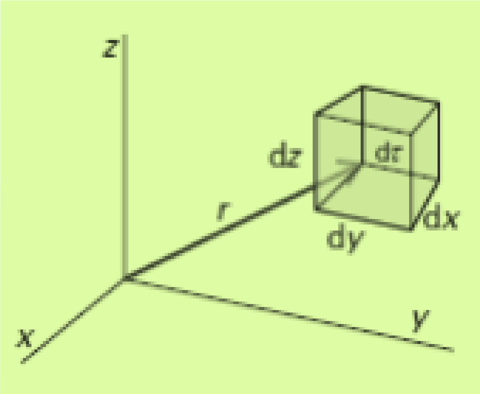
Born Interpretation

Classical wave equation:

$\boldsymbol{\Psi(x,t)}$ = Amplitude and $|\boldsymbol{\Psi(x,t)}|^2$ = Intensity

Quantum mechanical system:

- The state is completely specified by a wavefunction $\boldsymbol{\Psi(x,t)}$,which can be complex
- All possible information can be derived from $\boldsymbol{\Psi(x,t)}$
- Intensity is equivalent to Probability.
- $|\boldsymbol{\Psi(x,t)}|^2 = \boldsymbol{\rho(x)}$, probability density.
- $|\boldsymbol{\Psi(x,t)}|^2 \mathbf{dx} = \boldsymbol{P(x)}$, probability for finding the particle between $\boldsymbol{x}$ and $\boldsymbol{x} + \boldsymbol{dx}$
- In 3 dimensions, $\boldsymbol{P(x, y, z)} = |\boldsymbol{\Psi(x,y,z,t)}|^2 \mathbf{d\tau}$



Laws of Quantum Mechanics

The average value of the observable corresponding to operator Â is

$$\langle a \rangle = \int \Psi^* \hat{A} \Psi d\upsilon$$

Classical correspondence: Average values for a distribution function ***P(x)*** :

$$\langle x \rangle = \int_{-\infty}^{\infty} x P(x) \cdot dx \text{ and } \langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 P(x) \cdot dx$$

Quantum mechanical analogue:

$$\langle a \rangle = \int_{-\infty}^{+\infty} \widehat{A}.P(x)\,dx = \int_{-\infty}^{+\infty} \widehat{A}.|\Psi|^2\,dx \approx \int_{all\ space} \Psi^* \hat{A} \Psi\,dx = \langle \Psi | \widehat{A} | \Psi \rangle$$

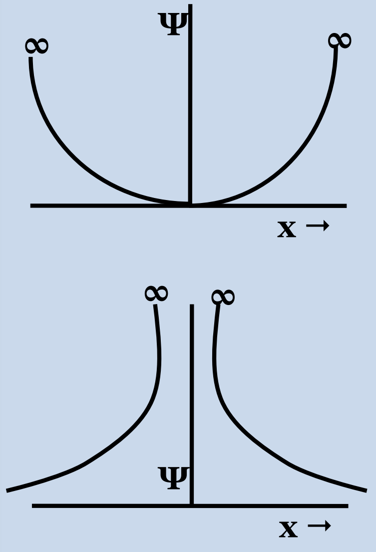
Normalization of Wavefunction

Since $\Psi^*\Psi d\tau$ is the probability, the total probability of finding the particle somewhere in space has to be unity

$$\iiint_{all\ space} \Psi^*(x,y,z).\Psi(x,y,z)dxdydz$$

$$= \int_{all\ space} \Psi^*\Psi d\tau = \langle \Psi | \Psi \rangle = 1$$

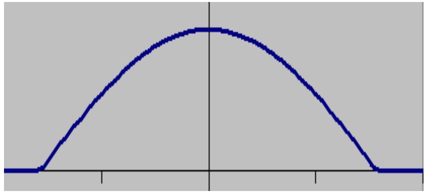
Divergent functions i.e. → ∞: Ψ can not be normalized, and therefore is NOT an acceptable wave function. However, a constant value C ≠ 1 is perfectly acceptable.

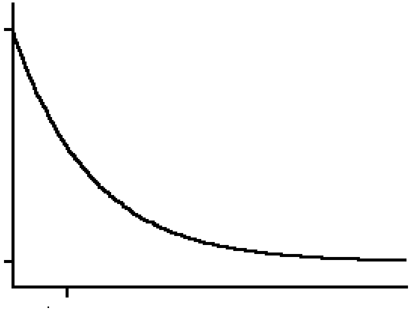


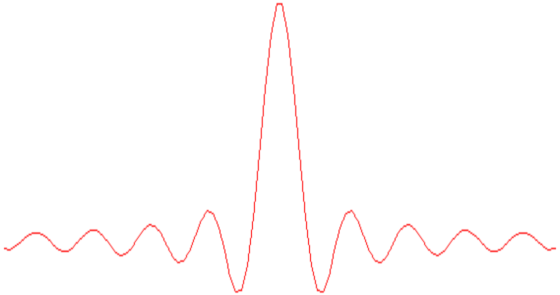
Unacceptable wavefunction

$\boldsymbol{\Psi}$ must vanish at ±∞, or more appropriately at the boundaries and $\boldsymbol{\Psi}$ must be finite

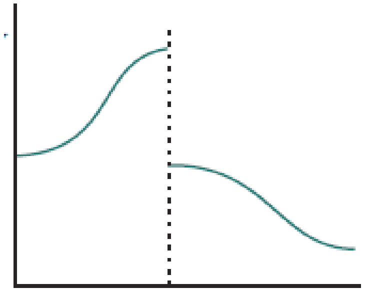
Acceptable wavefunctions



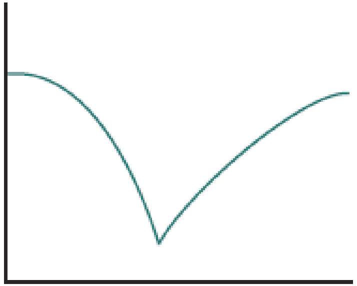




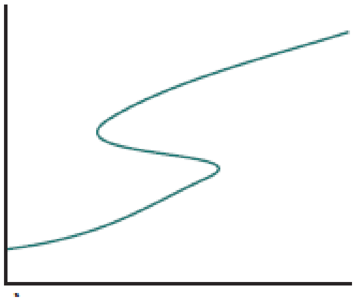
Restrictions on wavefunction



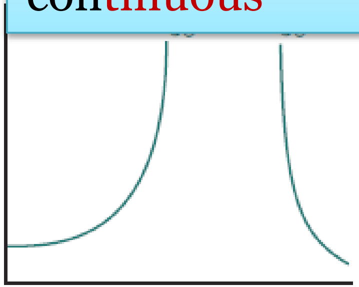
Unacceptable because $\boldsymbol{\psi}$ is not



Unacceptable because $d\boldsymbol{\psi}/dq$ is not continuous



Unacceptable because $\boldsymbol{\psi}$ is not single-valued



Unacceptable because $\boldsymbol{\psi}$ goes to infinity

Restrictions on wavefunction

ψ must be a solution of the Schrodinger equation

ψ must be normalizable: ψ must be finite and $\rightarrow$0 at boundaries/ $\pm\infty$

Ψ must be a continuous function of x,y,z

dΨ/dq must be must be continuous in q

Ψ must be single-valued

Ψ must be quadratically-intergrable
(square of the wavefunction should be integrable)

Origin of quantization

Quantum Mechanics

Examples of Exactly Solvable Systems

1. Free Particle
2. Particle in a Square-Well Potential
3. Hydrogen Atom

Free Particle

Time-independent Schrodinger equation

$$\hat{H}\psi = E\psi$$

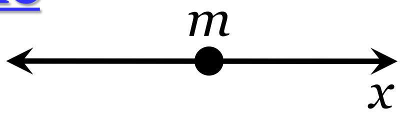
$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\cdot\psi(x)$$

For a free particle *V(x)*=0

There are no external forces acting

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

Free Particle



$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E \cdot \psi(x)$$

Second-order linear differential equation

Let us assume

$$\psi(x) = A\sin kx + B\cos kx$$

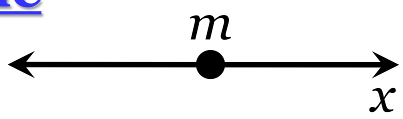
Trial Solution

$$y(x) = A\sin kx + B\cos kx$$

$$\frac{d}{dx}y(x) = \frac{d}{dx}\left(A\sin kx + B\cos kx\right) = k\left(A\cos kx - B\sin kx\right)$$

$$\frac{d^2}{dx^2}y(x) = -k^2\left(A\sin kx + B\cos kx\right) = -k^2 y(x)$$

Free Particle



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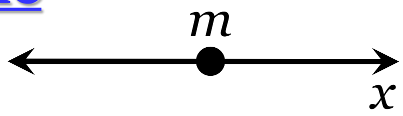
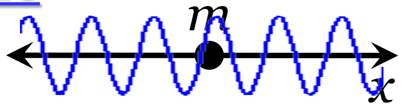


$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\cdot\psi(x)$$

$$\frac{\hbar^2}{2m}k^2\psi(x) = E\cdot\psi(x) \quad \Rightarrow \quad E = \frac{\hbar^2 k^2}{2m} \quad \Rightarrow \quad k = \pm\frac{\sqrt{2mE}}{\hbar}$$

Free Particle



de Broglie wave

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$$E = \frac{\hbar^2 k^2}{2m}$$

There are no restrictions on k

E can have any value

Energies of free particles are continuous

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

No Quantization **All energies are allowed**

Particle in 1-D Square-Well Potential