

1. Physics 13: Schrödinger Equation Interpretation

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$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)+U(x)\Psi(x,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

- $\Psi(x,t)$ is complex and *i* appears on right
- 2nd order linear differential equation in 2(4) variables
- *U(x)* is potential function (e.g. mgx, $-k_{EM}e^2/x$, $(1/2)kx^2$)
- Simple example: free particle plane wave

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2. Plane wave in Schrödinger Equation

Plane wave in Schrödinger Equation

$$\Psi(x,t)=Ae^{i(kx-\omega t)}$$

let A be real

$$\mathrm{Re}(\Psi(x,t))=A\cos(kx-\omega t)$$

$$\mathrm{Im}(\Psi(x,t))=A\sin(kx-\omega t)$$

$$i\hbar\frac{\partial}{\partial t}\left[e^{i(kx-\omega t)}\right]=\hbar\omega\left[e^{i(kx-\omega t)}\right]$$

$$\frac{\partial}{\partial x}\left[e^{i(kx-\omega t)}\right]=ik\left[e^{i(kx-\omega t)}\right]$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[e^{i(kx-\omega t)}\right]=\frac{\hbar^2k^2}{2m}\left[e^{i(kx-\omega t)}\right]$$

Works as it should

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3. Stationary solutions

Stationary solutions

When U(x,t) is independent of time (U(x,t)=U(x)):

stationary states: $\Psi(x,t) = \psi(x)e^{-i\omega}$ with $E = \hbar\omega$

$$\rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\psi(x) \text{ ordinary diff.eq.}$$

Boundary conditions for physical solution:

$\psi(x)$ is continuous and $\frac{d\psi(x)}{dx}$ is also for $U(x)$ finite.

Note that the time dependent exponential was factored out leaving space variable dependence.

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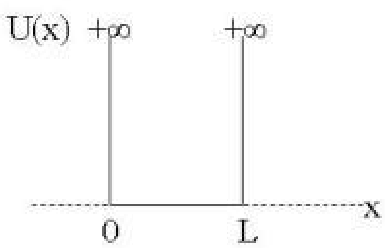
4. Particle in 1-dimensional box or square well

Particle in 1-dimensional box or Square Well



$U(x)=0 \quad 0<x<L$

$\quad = +\infty \quad x<0 \text{ or } x>L$

Can not have particle outside box, so $\psi(x)=0$ for $x<0$ or $x>L$

Continuity requires $\psi(0)=0$, $\psi(L)=0$

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

Mathematically equivalent to equation for standing waves on string of fixed ω - a mode

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5. Square well solutions

Square well solutions

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

Solutions of form $e^{\pm ikx}$ with $-k^2 = \frac{-2mE}{\hbar^2}$

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

General solution of form $\psi(x) = A\sin(kx) + B\cos(kx)$

Boundary conditions require $\psi(x) = A\sin(kx)$ with

$\psi(L) = 0 = A\sin(kL)$ So $kL = n\pi$ for any integer n

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6. Square well solutions cont'd

Square well solutions - 2

Then $\psi_n(x) = A_n \sin(k_n x) = A_n \sin(\frac{n\pi x}{L})$

$k_n = \frac{2\pi}{\lambda_n} = \frac{n\pi}{L} \rightarrow \lambda_n = \frac{2L}{n}$ just like string fixed at both ends

$E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2} = n^2\frac{h^2}{8mL^2} = n^2 E_1$ quantized energy

with $E_1 = \frac{h^2}{8mL^2}$ the minimum energy as allowed by Heisenberg

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7. Probability - normalization

Probability - normalization

$$\int_{-\infty}^{+\infty} dx\left|\psi_n(x)\right|^2 = \int_0^L dx A_n{}^2 \sin^2\left(\frac{n\pi x}{L}\right) = 1 \quad \text{normalization}$$

$$= A_n{}^2\left(\frac{L}{n\pi}\right)\int_0^{n\pi} d\vartheta \sin^2\vartheta = A_n{}^2\left(\frac{L}{n\pi}\right)\frac{n\pi}{2}$$

$$= A_n{}^2\frac{L}{2} \rightarrow A_n{}^{\lambda} = \sqrt{\frac{2}{L}}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \qquad \text{modes of the well (string)}$$

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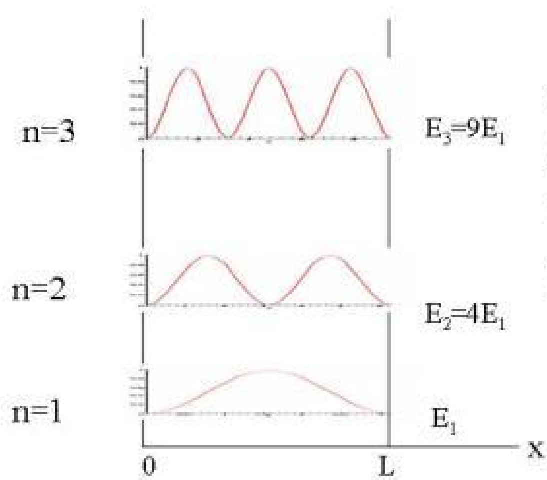
8. Particle states in the square well

Particle states in the square well



For probability in finite interval (x_1, x_2)

$$\int_{x_1}^{x_2} dx\left|\psi_n(x)\right|^2$$

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9. Where is the particle?

Where is the particle?

$$|\psi_n(x)|^2\,dx = \left(\frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right)\right)dx \quad \text{or} \quad \frac{1-\cos\left(\frac{2n\pi x}{L}\right)}{L}\,dx$$

Greatest probability to be where density is maximum:
center or x=L/2 for n=1; at x=L/4 and 3L/4 for n=2;
at x=L/6, L/2,5L/6 for n=3; etc.
But also places with 0 probability for each n.
Probability "clouds" within box.

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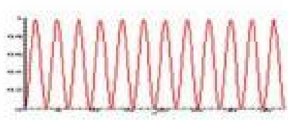
10. Implications of square well solutions

Implications of square well solutions

- Particle is not anywhere in particular - it is distributed - cloud
- Large n approaches uniform distribution



e.g. n=12

Bohr's Correspondence principle
QM ---> Classical as n --> ∞

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11. Average position in square well

Average position in square well

Always have $\langle x \rangle_n = \frac{L}{2}$ but $\langle x^2 \rangle_n$ will depend on n

and r.m.s. deviation $\sqrt{\left|\langle x^2 \rangle_n - \langle x \rangle_n{}^2\right|}$ varies with n.

$$\langle x^2 \rangle_n = \int_0^L dx \left(x^2 \frac{2}{L} \sin^2(n\pi x/L) \right)$$

Expectation value of x^2 or average over...

$$= \frac{2}{L} \left(\frac{L}{n\pi} \right)^3 \int_0^{n\pi} d\vartheta (\vartheta \sin \vartheta)^2 = L^2 \left(\frac{1}{3} - \frac{1}{2n^2\pi^2} \right)$$

$$\text{so} \quad \Delta x_{rms} = L\sqrt{\frac{1}{3} - \frac{1}{2n^2\pi^2} - \frac{1}{4}} = L\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}$$

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12. Average momentum in well

Average momentum in well

By symmetry $p_{ave} = \langle p \rangle = 0$ for all n.

So rms value is $\Delta p_{rms} = \sqrt{\langle p^2{}_n \rangle}$ but $p_n{}^2 = 2mE_n$

$$\Delta p_{rms} = \sqrt{2m \bullet n^2 \frac{h^2}{8mL^2}} = \frac{nh}{2L}$$

Joint uncertainty $\Delta p_n \Delta x_n = \frac{nh}{2}\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}} > \frac{\hbar}{2} (= 0.0796 h)$

for $n = 1$, get $\Delta p_1 \Delta x_1 = 0.0904\, h$

and $n >> 1$ gives $\frac{nh}{4\sqrt{3}}$ which grows with n

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13. 2-dimensional well LxL

2-dimensional well LxL

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y)+U(x,y)\psi(x,y)=E\psi(x,y)$$

For square box with $U=\infty$ for $x<0$ and $x>L$

and $y<0$ and $y>L$

and $U=0$ for $0<x<L$ and $0<y<L$

can factorize $\psi(x,y)=f(x)g(y)$

so $\psi(x,y)=A'\sin(n_x\pi x/L)\sin(n_y\pi y/L)$ with $A'=2/L$

Hence $E_{nx,ny}=\frac{h^2}{8mL^2}\left(n_x^{\ 2}+n_y^{\ 2}\right)$

2 quantum numbers note degeneracy, e.g. $E_{1,2}=E_{2,1}$

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14. Square wells - some conclusions

Square wells - some conclusions

- 3-dim --> 3 q.nos and more degeneracies
- E is not continuous for these “bound” systems
- Single particle “interferes” with itself to get stationary modes
- Real particle “traps” and quantum computers
- Charged particle transitions from E_{n1} to E_{n2} will be accompanied by $h\nu= E_{n1}- E_{n2}$
- Exemplar of bound particles

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15. Other potentials: Simple Harmonic Oscillator (SHO)

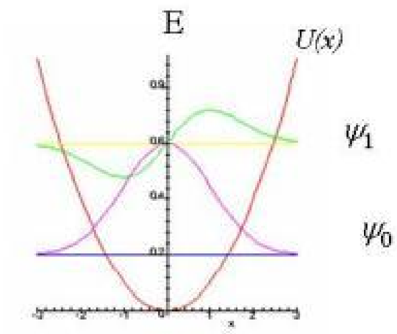
Other potentials: Simple Harmonic Oscillator (SHO)

SHO 1 dim. Force $= -kx$ and Potential $U(x) = \frac{1}{2}kx^2$

Lowest energy state $\psi_0(x) = Ae^{-\alpha x^2}$ (Gaussian form)

Check: $\frac{d}{dx}\psi_0(x) = -2ax\psi_0(x)$

$$\frac{d^2}{dx^2}\psi_0(x) = -2a\psi_0(x) + 4a^2x^2\psi_0(x)$$



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16. SHO (continued)

SHO (continued)

Substitute back into the stationary Schrödinger equation:

$$\frac{\hbar^2 a}{m}\psi_0(x) - \frac{2a^2\hbar^2}{m}x^2\psi_0(x) + \frac{1}{2}kx^2\psi_0(x) = E_0\psi_0(x)$$

x^2 terms must cancel so $a = \frac{\sqrt{km}}{2\hbar}$

Then $E_0 = \frac{\hbar^2}{m}\frac{\sqrt{km}}{2\hbar} = \frac{1}{2}\hbar\omega_0$ where ω_0 is the classical frequency!

In general the solutions occur for $E_n = (n + \frac{1}{2})\hbar\omega_0$

These are equally spaced energies.
Note that $|\psi_n(x)|^2$ is non-zero beyond classical turning points (where $U(x) \geq E_n$ and classical particle can not exist)

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17. Steps and barriers