Quantum Physics PY1T20/PYU11P20

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Quantum Physics Lecture 11

Applications of Steady state Schroedinger Equation

Box of more than one dimension

Harmonic oscillator

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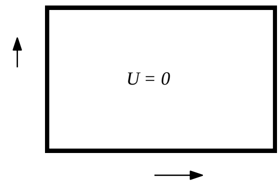
Waves/particles in a box of >1 dimension

Consider 2-D box
Potential $U = 0$ between $x = 0$ and $x = a$
And between $y = 0$ and $y = b$
U infinite elsewhere



Wavefunction Ψ expressed as $\Psi(x,y) = f(x)g(y)$ *- Separation of variables*

Steady state Schrödinger Equation inside box, where $U = 0$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi(x,y)}{\partial x^2} + \frac{\partial^2\Psi(x,y)}{\partial y^2}\right) = E\Psi(x,y) \qquad (\textit{Recall } H\Psi = E\Psi)$$

Put in $\Psi(x,y) = f(x)g(y)$ - noting partial differentials!

Waves/particles in a 2-D box (cont.)

$$-\frac{\hbar^2}{2m}\left(g(y)\frac{\partial^2 f(x)}{\partial x^2} + f(x)\frac{\partial^2 g(y)}{\partial y^2}\right) = Ef(x)g(y)$$

Thus
$$-\frac{\hbar^2}{2m}\left(\frac{1}{f(x)}\frac{\partial^2 f(x)}{\partial x^2} + \frac{1}{g(y)}\frac{\partial^2 g(y)}{\partial y^2}\right) = E$$

Only one term is x dependent, and it equals a constant

$$\frac{\dfrac{\partial^2 f(x)}{\partial x^2}}{f(x)} = -C$$

So $\dfrac{\partial^2 f(x)}{\partial x^2} = -Cf(x)$ Which we have seen before…

Solutions, using boundary conditions, are $f(x) = A\sin\dfrac{n\pi x}{a}$ with $C = \dfrac{n^2\pi^2}{a^2}$

Similarly, for y dependence $g(y) = B\sin\dfrac{m\pi y}{b}$

Hence the energy levels in the box are $E_{n,m} = \dfrac{\hbar^2}{2m}\left(\dfrac{n^2\pi^2}{a^2} + \dfrac{m^2\pi^2}{b^2}\right)$

With **TWO** quantum numbers n,m needed to specify the state

Waves/particles in a 2-D box (cont.)

Ψ is specified by the quantum numbers *n & m*

There are as many states as there are possible *n,m* combinations *(N.B. n & m are positive)*

Two distinct wave functions are ***DEGENERATE*** if they have the same energy.

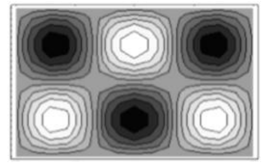
*e.g. the states 1,3 and 3,1 are **degenerate** if a = b*

If a/b is irrational there are no degeneracies

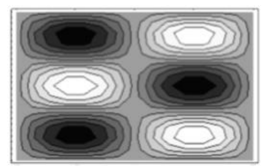
Readily extended to 3-D….

Useful, especially when filling box with more than one particle.

C.f. black body cavity



Examples:
2,3 and 3,2
wavefunctions



Harmonic Oscillator

Examples: mass on spring, diatomic molecule…

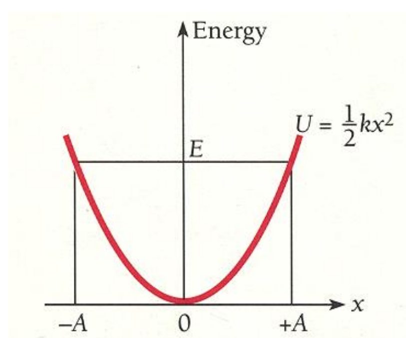
Hooke's Law: "restoring force" $F = -kx$

$$-kx = m\frac{d^2x}{dt^2}$$

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0$$

$$x = A\cos\omega t$$

Where $\omega = \sqrt{\frac{k}{m}}$



Potential energy $U = (1/2)kx^2$ (potential well, parabolic)

Expect (1) quantised energy,

(2) $E_{min} \neq 0$

(3) particle outside the classical limits A

Apply SSSE to Harmonic Oscillator

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \tfrac{1}{2}kx^2\right)\psi = 0$$

$$\text{or} \quad \frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{km}{\hbar^2}x^2\right)\psi = 0$$

$$\text{write} \quad y = \left(\frac{\sqrt{km}}{\hbar}\right)^{1/2} x \quad \text{and} \quad dy^2 = \left(\frac{\sqrt{km}}{\hbar}\right) dx^2$$

$$\boxed{\frac{d^2\psi}{dy^2} + \left(\alpha - y^2\right)\psi = 0} \quad \alpha = \frac{2mE}{\hbar^2} \Big/ \frac{\sqrt{km}}{\hbar} = \frac{2E}{\hbar}\sqrt{\frac{m}{k}} = \frac{2E}{\hbar\omega}$$

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Results for Harmonic Oscillator

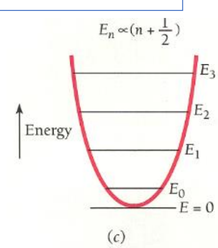
Solution requires:

$$\boxed{\frac{d^2\psi}{dy^2} + \left(\alpha - y^2\right)\psi = 0}$$

$$\alpha = 2n + 1 \quad \text{for} \quad n = 0, 1, 2, 3 \ldots$$

$$E_n = \frac{\hbar\omega}{2}\alpha = \frac{\hbar\omega}{2}(2n+1) = \left(n + \tfrac{1}{2}\right)\hbar\omega$$

$E_0 = \frac{\hbar\omega}{2}$ ***a.k.a. "zero point energy***



Recall Planck's assumption & blackbody formula *(Lecture 8):*
Oscillator energies assumed $E_n = \hbar\omega n$

Later, found additional detail & statistics, C_v etc. but…
Right ideas on quantisation: *"fortunate guesswork!"*

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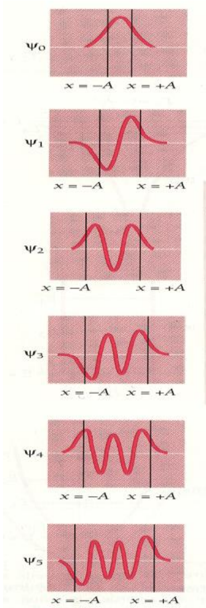
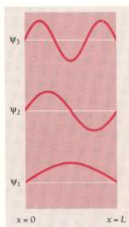
Wavefunctions of Harmonic Oscillator



Comparing with infinite square well case,
ψ has <u>approximately</u> same shape
<u>except</u>:



(1) width of well is changing

(2) ψ extends beyond classical limit

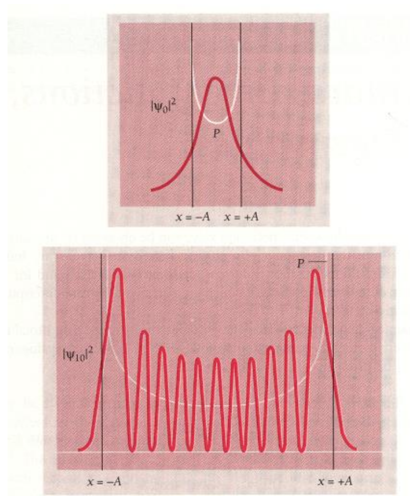
(3) amplitude increases at well edge

Look at (2) and (3) via the probability density…..

Probability Density of Harmonic Oscillator

(1) Finite probability of particle outside the classical limits

(2) the quantum picture only approaches the classical picture at large n values
(classical - probability maximum at extremities of oscillation - slower)
- Correspondence Principle



Footnote: compare square well [$E_n \propto n^2$] and harmonic oscillator [$E_n \propto (n + 1/2)$] and Bohr H atom [$E_n \propto -1/n^2$] for energies.
Differing shapes of the potential wells.