Lesson 6: Solutions of the Schrödinger equation

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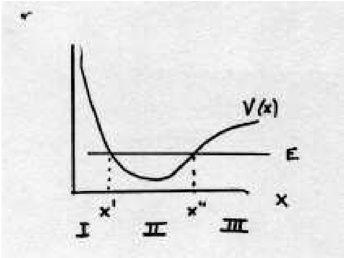
- $\phi(x)$ and $\phi'(x)$ finite, single-valued and continuous
  $\phi'(x)$ may be discontinuous if there are discontinuities in the potential



x' y x'' classical turning points

- **Bound** state $\longrightarrow$ the classically allowed range is finite $\longrightarrow$ it is not allowed any value of energy $\longrightarrow$ quantized values (**"unbound states"** are called **"scattering states"**)

  Bound state $\longrightarrow$ $E < V(-\infty)$ and $V(+\infty)$

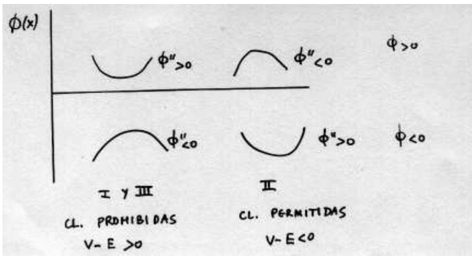
  Scattering states $\longrightarrow$ $E > V(-\infty)$ or/and $V(+\infty)$
- Bound states eigenfunctions of the Hamiltonian are nondegenerate in one dimension
- Bound states eigenfunctions of the Hamiltonian can always be chosen real in one dimension

- **Bound-state** eigenfunctions of Hamiltonians corresponding to even potentials $V(x) = V(-x)$ have good parity (are odd or even)
- For bound states the minimum eigenvalue of $\hat{H}$ is larger than the bottom of the potential (**Zero-Point Energy**)

From the time-independent Schrodinger equation

$$\frac{d^2\phi(x)}{dx^2} \;=\; \frac{2m}{\hbar^2}\,[V(x) - E]\,\phi(x)$$

- classically forbidden regions sign$(\frac{d^2\phi}{dx^2}) \;=\;$ sign ϕ
- classically allowed regions sign$(\frac{d^2\phi}{dx^2}) \;=\; -$sign ϕ



- the wave function has no zeros in forbidden regions containing $\pm\infty$
- for $x = \pm\infty$ $\phi(x) \rightarrow 0$ (if ϕ is normalizable $\leftrightarrow$ bound state)
- in classically allowed regions $|V - E|$ larger $\rightarrow$ larger T kinetic energy $\rightarrow$ larger p (momentum) $\rightarrow$ smaller λ (semiclassical reasoning)
- in classically allowed regions if $E_1 < E_2$ (eigenvalues of $\hat{H}$) $\rightarrow$ $T_1 < T_2$ (in every point) $\rightarrow$ $\lambda_1 > \lambda_2$ $\rightarrow$ ϕ_2 oscillates more than ϕ_1 (semiclassical reasoning)
- for bound states, at a given energy, in the classically allowed region larger $E - V$ implies larger T $\rightarrow$ larger v $\rightarrow$ less probability $\rightarrow$ lower amplitude (semiclassical reasoning)

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- if two eigenfunctions of the Hamiltonian cross in a classically allowed region $\rightarrow$ the one with larger $|\frac{d^2\phi}{dx^2}|$ is of higher energy

$$\phi_1(x) = \phi_2(x) \text{ and } |\frac{d^2\phi_1}{dx^2}| > |\frac{d^2\phi_2}{dx^2}| \rightarrow E_1 > E_2$$

- **the ground state** (the eigenstate of $\hat{H}$ lower in energy) has no zeros in the classically allowed region. The next (first excited state) has one, and so on
- exceptions can be found for our semiclassical reasonings

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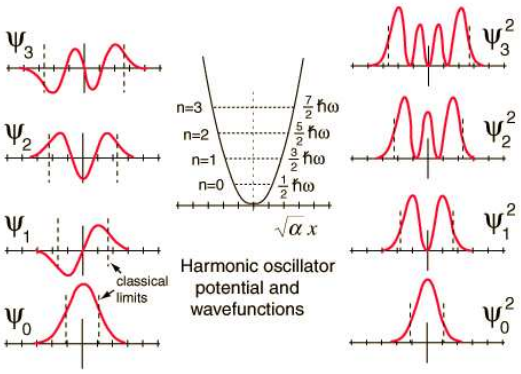
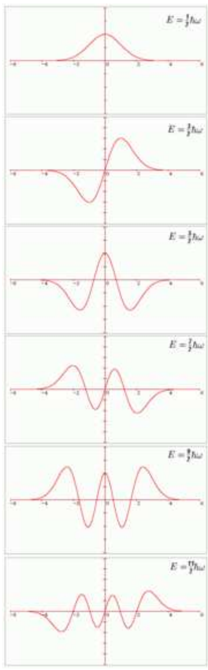

Ψ_3
Ψ_2
Ψ_1
Ψ_0
n=3
n=2
n=1
n=0
$\frac{7}{2}\hbar\omega$
$\frac{5}{2}\hbar\omega$
$\frac{3}{2}\hbar\omega$
$\frac{1}{2}\hbar\omega$
$\sqrt{\alpha}\,x$
classical limits
Harmonic oscillator
potential and
wavefunctions
Ψ_3^2
Ψ_2^2
Ψ_1^2
Ψ_0^2



Constant potential: free particle

$V(x) \; = \; 0$ the particle is not bound to any region of space $\rightarrow$ any value of energy is allowed, there is no quantization of it (the energy is quantized when the classical range of motion of the particle is finite)

$\hat{H} \; \neq \; \hat{H}(t) \; \rightarrow \; < \hat{H} >$ is conserved

$\frac{\partial V}{\partial x} \; = \; 0 \; \rightarrow \; < \hat{p}_x >$ is conserved

$\hat{H}$ and $\hat{p}_x$ are constants of motion

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} \; = \; E\phi$$

$$\frac{d^2\phi}{dx^2} \; + \; \frac{2mE}{\hbar^2}\phi \; = \; 0$$

$$\frac{d^2\phi}{dx^2} \; + \; k^2\phi \; = \; 0$$

$$\phi(x) \; = \; e^{\pm\, ikx} \quad ; \quad k \; = \; \frac{\sqrt{2mE}}{\hbar} \quad ; \quad E \; = \; \frac{\hbar^2 k^2}{2m}$$

General solution $\phi(x) \; = \; A\, e^{ikx} \; + \; B\, e^{-ikx}$

$$\Psi(x,t) \; = \; \left(A\, e^{ikx} \; + \; B\, e^{-ikx}\right) e^{-\frac{iEt}{\hbar}}$$

$$\hat{p}_x\, e^{\pm\, ikx} \; = \; -\, i\hbar\frac{\partial}{\partial x}e^{\pm\, ikx} \; = \; \pm\, \hbar k e^{\pm\, ikx} \; = \; \pm\, \sqrt{2mE}\, e^{\pm\, ikx}$$

$e^{\pm\, ikx}$ are eigenfunctions of $\hat{p}_x$ with eigenvalues $\pm\, \hbar k$

e^{ikx} plane wave traveling towards increasing values of x

e^{-ikx} plane wave traveling towards decreasing values of x

for e^{ikx} (or e^{-ikx}) $\Delta\hat{p}_x \; = \; 0 \quad \rightarrow \quad \Delta\hat{x} \; = \; \infty$

We could have used a potential $V(x) = V_0 \quad \forall x$

The solution obtained is valid if we make the change $E \to E - V_0$

Normalization of the wave function

$$\int_{-\infty}^{\infty} dx\, e^{-ikx}\, e^{ik'x} = 2\pi\delta(k-k')$$

If $k = k'$ non-normalized

If $k \neq k' \to$ orthogonal functions (eigenfunctions of $\hat{p}_x$ associated with different eigenvalues)

The wave function represents a **beam of particles**, not a particle (for particles the wave function must be square integrable). Possible constants in the wave function are related to the flux of particles (unbound states)

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Square well of infinite depth

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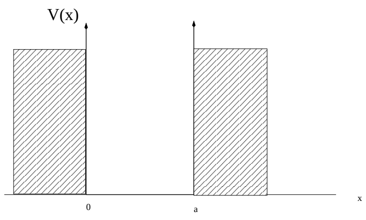
$$V(x) = \begin{cases} \infty & \begin{cases} x \leq 0 \\ x \geq a \end{cases} \\ \\ 0 & 0 \leq x \leq a \end{cases}$$

$$\phi(x) = 0 \begin{cases} x \leq 0 \\ x \geq a \end{cases}$$

particle confined in a one-dimensional box



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Boundary conditions $\phi(0) = 0 \;\; ; \;\; \phi(a) = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} = E\phi \qquad 0 \le x \le a$$

$$\frac{d^2\phi}{dx^2} + k^2\phi = 0 \; ; \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\phi(x) = A\,e^{ikx} + B\,e^{-ikx}$$

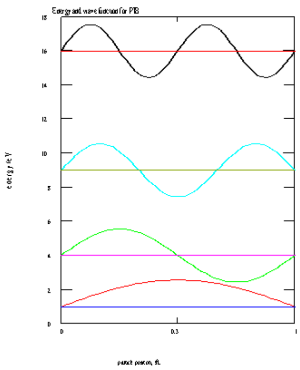
$$\phi(0) = 0 \quad \rightarrow \quad A + B = 0$$

$$\phi(a) = 0 \rightarrow Ae^{ika} + B\,e^{-ika} = A\left(e^{ika} - e^{-ika}\right) = 2iA\sin ka = 0$$

$$k_n = \frac{n\pi}{a} \quad ; \quad n = 1, 2, 3, \cdots$$

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

All eigenstates are bound ones (∞)



$$\phi_n(x) \;=\; 2A\;\sin\left(\frac{n\pi x}{a}\right)\;;\; n=1,2,3,\cdots (n=0\;\rightarrow\;\phi_0(x)=0)$$

- Overall factor i (modulus 1) can be taken out (a constant factor of modulus 1, the so-called **phase**, is undetermined in the wave function) since $\phi(x)$ and $e^{i\delta}\phi(x)$ with $\delta \in \mathcal{R}$ represent the same state)

Determination of A (normalization constant)

$$\begin{aligned} 1 \;&=\; \int_{-\infty}^{\infty} |\phi|^2\,dx \;=\; 4\,|A|^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right)\,dx \;= \\ &=\; 4\,|A|^2 \int_0^{n\pi} \frac{a}{n\pi} \sin^2 y\,dy \;=\; 2|A|^2\,a \end{aligned}$$

$$\left(\int \sin^2 y\,dy \;=\; \frac{1}{2}(y - \frac{1}{2}\sin 2y)\right)$$

$$|A| \;=\; \frac{1}{\sqrt{2a}} \quad\rightarrow\quad A \;=\; \frac{1}{\sqrt{2a}}\,e^{i\alpha}\;\;;\;\;\alpha\;\text{ real}$$

in $x \;=\; 0$ and $x \;=\; a$ the potential is discontinuous $\;\rightarrow\;$ in addition it becomes <u>infinite</u> $\;\rightarrow\;$ $\phi'(x)$ is <u>discontinuous</u> (if it was not infinite $\phi'(x)$ would be continuous)

Symmetric infinite well of length a

$$V(x') = \begin{cases} \infty & \begin{cases} x' \leq -\frac{a}{2} \\ x' \geq \frac{a}{2} \end{cases} \\ 0 & -\frac{a}{2} \leq x' \leq \frac{a}{2} \end{cases}$$

$x' \;=\; x - \frac{a}{2}\;\;;\qquad \Phi_n(x') \;=\; \phi_n(x) \;=\; \phi_n(x' + \frac{a}{2})$

$$\sin(A+B) \;=\; \sin A \cos B \;+\; \sin B \cos A$$

$$\Phi_n(x') = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x'}{a} + \frac{n\pi}{2}\right)$$
$$= \sqrt{\frac{2}{a}} \left[\cos\frac{n\pi x'}{a}\sin\frac{n\pi}{2} + \sin\frac{n\pi x'}{a}\cos\frac{n\pi}{2}\right]$$

n even $\rightarrow \sin\frac{n\pi}{2} = 0 \;;\; \cos\frac{n\pi}{2} = (-1)^{\frac{n}{2}}$

$$\Phi_n(x') = \sqrt{\tfrac{2}{a}}(-1)^{\frac{n}{2}}\sin\tfrac{n\pi x'}{a} \rightarrow \sqrt{\tfrac{2}{a}}\sin\tfrac{n\pi x'}{a}$$

n odd $\rightarrow \sin\frac{n\pi}{2} = (-1)^{\frac{n-1}{2}} \;;\; \cos\frac{n\pi}{2} = 0$

$$\Phi_n(x') = \sqrt{\tfrac{2}{a}}(-1)^{\frac{n-1}{2}}\cos\tfrac{n\pi x'}{a} \rightarrow \sqrt{\tfrac{2}{a}}\cos\tfrac{n\pi x'}{a}$$

Think of well of length $2L$!

Bibliography

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