L13-Infinite Square Well

Friday, October 16, 2015 07:16

* This is the simplest problem to solve in Quantum Mechanics: a one-dimensonal free particle except for an infinite repulsive force at $x=0$ (to the right) and at $x=a$ (to the left).

  - classically, it bounces back and forth between the 2 walls.

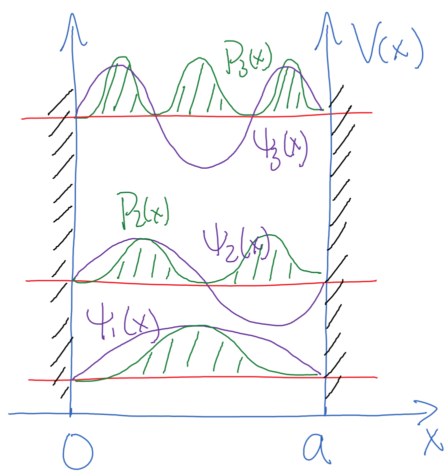
  - in Q.M., we solve for the "modes" (standing waves) with fixed ends.

* this problem will be used to illustrate the steps of QM. solutions:

  a) solve the 2nd order TISE (ODE) in each smooth region of the potential to get a general solution

  $$\psi(x) = A\, f_1(x; E) + B\, f_2(x; E)$$

  There are 2 unknown constants in each region, in addition to the constant E, which is the same in each region



  b) "Sew" the solutions together using:

  i) internal boundary conditions between neighbouring regions.
  $\Delta\psi = 0$ and $\Delta\psi' = 0$ (from integrating the TISE accross the boundary)

  ii) external boundary conditions (at the outer edges)
  $\psi \to 0$ at $x \to \infty$ and $x \to -\infty$

These boundary conditions can be solved for all but one of the unknown coeficients: A, B, C, D, ... ; E.
The final unknown is NOT E, but is the overall normalization.

In fact, this procedure will yield a whole "spectrum" of values of E_n with wavefunctions $\psi_n(x)$, where the index "n" indicates the number of [anti]nodes.

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where the index "n" indicates the number of [anti]nodes.
These are the standing waves of the T.I.S.E.

c) Normalize the wave functions: $\langle\psi_n|\psi_n\rangle \equiv \int \psi_n^*(x)\,\psi_n(x) = 1$
to determine the remaining constant. These functions $\psi_n(x)$ or $|\psi_n\rangle$ now form an "orthonormal basis" of the space of all possible wave functions using the "inner product"

$$\langle\psi_m|\psi_n\rangle \equiv \int \psi_m^*(x)\ \psi_n(x) = \delta_{mn} = \begin{cases} 1 \text{ if } m=n \\ 0 \text{ if } m\neq n \end{cases}$$

(This is guaranteed by the "Sturm-Liouville theorem")

d) The general solution to the T.D.SE. has the form

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\,\psi_n(x)\,e^{-iE_nt/\hbar}$$

(The "completeness" of $\psi_n(x)$ is also guaranteed by Sturm Liouville)

Use orthogonality of $|\psi_n\rangle$ to determine c_n from the initial state $\Psi_0(x)$.

$$\langle\psi_m|\Psi(x,0)\rangle = \langle\psi_m|\sum_{n=1}^{\infty} c_n\,\psi_n(x)\,\cancel{e^{-iE_n\cdot 0/\hbar}}\rangle = \sum_{n=1}^{\infty} c_n \underbrace{\langle\psi_m|\psi_n\rangle}_{\delta_{mn}} = c_m$$

e) Thus, the general solution to the TDSE, satisfying initial conditions $\Psi(x,0)$ and boundary conditions $\psi(\pm\infty)=0$ is:

$$\Psi(x,t) = \sum_{n=1}^{\infty} \int \psi_n^*(x)\,\Psi(x,0)\,dx \cdot \psi_n(x)\cdot e^{-iE_nt/\hbar} \equiv \underbrace{\sum_{n=1}^{\infty} |\psi_n\rangle e^{-iE_nt/\hbar}\langle\psi_n|}_{U(t)\ \text{time evolution op.}}\ |\Psi(x,0)\rangle$$

f) Calculate the probability of measuring an observable using $\Psi(x,t)$ and operators.

* Application of these steps to the infinite square well:

a) $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi + 0\psi = E\psi = \frac{\hbar^2k^2}{2m}\psi$ where $E = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}$

$\frac{d^2}{dx^2}\psi = -k^2\psi \implies \psi = A\sin(kx) + B\cos(kx)$ [general solution]

b) There is only one region!

if $x<0$ or $x>a$, $\psi(x)=e^{\pm\infty x}\to 0$.

$$\psi(0)=0=A\sin(0)+B\cos(0)\Rightarrow B=0$$

$$\psi(a)=0\Rightarrow A\sin(ka)=0\Rightarrow ka=n\pi \quad n=1,2,3,\ldots$$

thus $\psi(x)=A\sin(k_n x)$ on $0<x<a$

where $k_n=\frac{n\pi}{a}$ so $\boxed{E_n=\frac{\hbar^2k_n^2}{2m}=\frac{h^2n^2}{8ma^3}}$

c) $\langle\psi_n|\psi_m\rangle=\int_0^a dx\,|A|^2\sin(k_nx)\sin(k_mx)$

$$=|A|^2\int_0^a dx\,\tfrac{1}{2}\left[\cos(k_n-k_m)x-\cos(k_n+k_m)x\right]$$

$$=\tfrac{1}{2}|A|^2\left(\frac{\sin(k_n-k_m)x}{\underbrace{k_n-k_m}_{\text{if } n\neq m}}-\frac{\sin(k_n+k_m)x}{k_n+k_m}\right)\Bigg|_0^a \quad \text{but } k_na=n\pi$$

$$=0 \text{ if } n\neq m \quad \text{or} \quad |A|^2\frac{a}{2}\equiv 1 \text{ if } n=m\Rightarrow A=\sqrt{\frac{2}{a}}$$

thus $\boxed{\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)}$

Note: the symmetry of even ($n=1,3,\ldots$), odd ($n=2,4,6\ldots$) states.

d) $\Psi(x,t)=\sum_{n=1}^{\infty}c_n\sqrt{\frac{2}{a}}\sin(k_nx)e^{-iE_nt/\hbar}$ where $c_n=\int_0^a\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\Psi(x,0)\,dx$

Note: $\langle\psi|\psi\rangle=\left\langle\sum_{m=1}^{\infty}c_m\psi_m(x)\middle|\sum_{n=1}^{\infty}c_n\psi_n(x)\right\rangle=\int_a^b\sum_{m,n}c_m^*c_n\,\psi_m^*(x)\,\psi_n(x)\,dx$

$$=\sum_{m,n}c_m^*c_n\langle\psi_m|\psi_n\rangle=\sum_{m,n}c_m^*c_n\,\delta_{mn}=\sum_n c_n^*c_n=\sum_n|c_n|^2=1$$

This looks very similar to the normalization $\int|\psi(x)|^2dx=1$

because $\psi(x)$ and c_n are both components of $|\psi\rangle$ in different bases!

e) Example: expected value of energy:

$$\langle H\rangle=\langle\psi|H|\psi\rangle=\sum_n\langle\psi|\underbrace{H|\psi_n\rangle}_{E_n|\psi_n\rangle}\langle\psi_n|\psi\rangle=\sum_n E_nc_nc_n^*=\sum_n E_n|c_n|^2$$

$\overbrace{}^{E_n|\psi_n\rangle}$

is independent of time, since $\psi_n(x)$ stationary states: conservation of energy.

* Example: let $\Psi_0(x) = \frac{1}{\sqrt{a}}$ (uniform probability)

$$c_n = \langle \psi_n | \Psi_0 \rangle = \frac{\sqrt{2}}{a}\int_0^a dx \sin(k_n x)\cdot 1$$

note symmetry!

$$= \frac{\sqrt{2}}{a}\left(-\frac{\cos(k_n x)}{k_n}\Big|_0^a\right) = \frac{\sqrt{2}}{a}\,\frac{-(-1)^n+1}{n\pi/a} = \frac{\sqrt{8}}{n\pi}\,\delta_{n\,odd}$$

Mathematica: $\sum_{k=0}^{\infty}\frac{1}{(2k+1)^2} = \frac{\pi^2}{8} \Rightarrow \sum_{n=0}^{\infty}|c_n|^2 = 1$

$$\langle E \rangle = \sum_{n\,odd}|c_n|^2 E_n = \sum_{n\,odd}\left(\frac{\sqrt{8}}{n\pi}\right)^2\frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 \to \infty\,!$$

* exercise 2.4

$$\langle x \rangle_n = \langle \psi_n | x | \psi_n \rangle = \int_0^a dx\, |\psi_n|^2 x = \int_0^a dx\, \frac{2}{a}\sin^2 k_n x \cdot x$$

$$= \frac{2}{a}\left[-\frac{\cos(\cancel{2}k_n x)}{\cancel{8}k_n^2} - \frac{x\sin(\cancel{2}k_n x)}{\cancel{4}k_n} + \frac{x^2}{4}\right]_0^a = \frac{a}{2}$$

$$\langle x^2 \rangle_n = \langle \psi_n | x^2 | \psi_n \rangle = \frac{a^2}{6}\left(2 - \frac{3}{\pi^2 n^2}\right)$$

$$\sigma_{x,n}^2 = \langle x^2 \rangle_n - \langle x \rangle_n^2 = a^2\left(\frac{1}{12} - \frac{1}{2\pi^2 n^2}\right)$$

$$\langle p \rangle_n = \langle \psi_n | -i\hbar\frac{\partial}{\partial x} | \psi_n \rangle = 0$$ note: $d(uv) = u\,dv + v\,du$

$$\langle p^2 \rangle_n = \langle \psi_n | -\hbar^2\frac{\partial^2}{\partial x^2} | \psi_n \rangle = \hbar^2\frac{\pi^2 n^2}{a^2} = \hbar^2 k^2$$ so that $E_n = \frac{p_n^2}{2m}$

note: $[\hat{p}^2, H] = 0$ thus $|\psi_n\rangle$ has definite $p_n^2 = \hbar^2 k_n^2$

$$(\sigma_x \cdot \sigma_p)_n \geq \sqrt{a^2\left(\frac{1}{12} - \frac{1}{2\pi^2}\right)}\cdot\frac{\hbar\pi}{a} = \hbar\pi\sqrt{\frac{1}{12} - \frac{1}{2\pi^2}} = 0.5678\,\hbar \geq \frac{\hbar}{2}$$

use Mathematica!