L14-Infinite Square Well

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* 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.

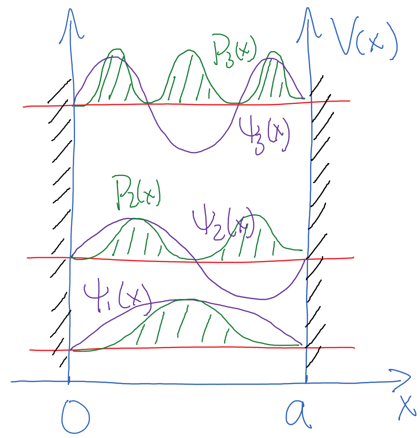
  - in Q.M., we solve for the "modes" (standing waves) with fixed ends.

* 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.
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.S.E. has the form

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

(The "completeness" of $\psi_n(x)$ is also gearanteed 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:

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

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

* Application of these steps to the infinite square well:

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

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

b) There is only one region!

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

$$\psi(0) = 0 = A\,\cancel{\sin(0)} + B\cos(0) \implies B = 0$$

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

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

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

c) $\langle \Psi_n | \Psi_m \rangle = \int_0^a dx\, |A|^2 \sin(k_n x)\sin(k_m x)$

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

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

$= 0$ if $n \neq m$ or $|A|^2 \frac{a}{2} \equiv 1$ 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) $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}}\sin(k_n x)e^{-iE_n t/\hbar}$ where $c_n = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\Psi(x,0)\,dx$

Note: $\langle \Psi|\Psi\rangle = \left\langle \sum_{m=1}^{\infty} c_m \Psi_m(x) \Big| \sum_{n=1}^{\infty} c_n \Psi_n(x) \right\rangle = \int_a^b \sum_{m,n} c_m^* c_n \Psi_m^*(x)\Psi_n(x)\,dx$

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

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

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

e) Example: expected value of energy:

$\langle H\rangle = \langle \Psi|H|\Psi\rangle = \sum_n \langle \Psi|\underbrace{H|\Psi_n\rangle}_{E_n|\Psi_n\rangle}\langle \Psi_n|\Psi\rangle = \sum_n E_n c_n c_n^* = \sum_n E_n |c_n|^2$

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!

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

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 $p_n^2 = \hbar^2 k_n^2$

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

use Mathematica!