L15-Infinite Square Well

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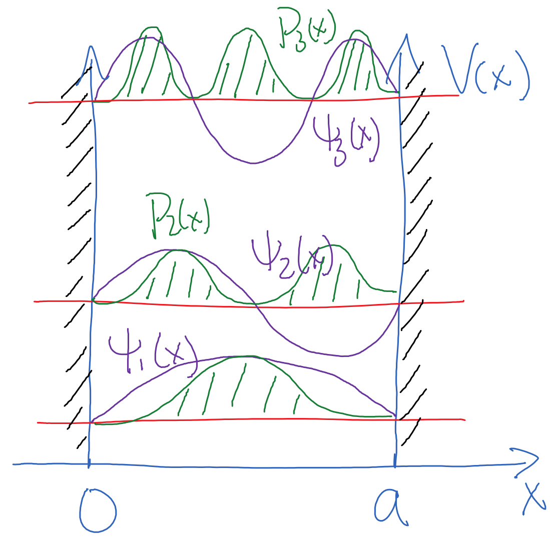

* Simplest case of TISE, but illustrates steps to any problem:

  a) solve 2nd order ODE in each smooth region of the potential
  $\Rightarrow A f_1(x;E) + B f_2(x;E)$

  b) combine solutions using Boundary Conditions:
  $\psi \to 0$ @ $\pm\infty$; ψ continuous, ψ' continuous if $V(x)$ finite
  determines all but one of $A_1, B_1, A_2, B_2, \ldots$
  plus a quantized spectrum of eigenfn's: $\hat{A}\psi_n = E_n \psi_n$

  c) normalized $\psi_n(x)$ form a complete set of orthogonal basis functions for $\psi(x)$
  $\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}$, use orthogonality to determine $c_n = \langle \psi_n | \Psi_0 \rangle$ from initial state $\Psi_0(x)$

* solution: $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + 0\psi = E\psi = \frac{\hbar^2 k^2}{2m}\psi$

$$\frac{d^2}{dx^2}\psi = -k^2\psi \quad \Rightarrow \quad \psi = A\sin(kx) + B\cos(kx)$$

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

$$\psi(0) = 0 = A\cancel{\sin(0)} + B\cos(0) \quad \Rightarrow \quad B = 0$$

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

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

* normalization: $\langle \psi_n | \psi_m \rangle = \int_0^a dx\, |A|^2 \sin(k_n x) \sin(k_m x)$

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

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

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

* Two properties guarenteed by Sturm-Liouville:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n x) \qquad E_n = \frac{\hbar^2 k_n}{2m} \qquad k_n = \frac{n\pi}{a} \qquad n = 1, 2, 3, \ldots$$

$\langle \psi_n | \psi_m \rangle = \delta_{nm}$ — orthogonality (independence)

$\sum_n |\psi_n\rangle \langle \psi_n| = I$ — closure (completeness) — Dirichlet's theorem

* amplitudes: $|\psi\rangle = \sum_n |\psi_n\rangle \underbrace{\langle \psi_n | \psi \rangle}_{c_n} = \sum_n |\psi_n\rangle \underbrace{c_n}$ complex constant

$$\langle \psi_n | f \rangle = \sum_m \underbrace{\langle \psi_n | \psi_m \rangle}_{\delta_{mn}} c_m = c_n = \int_0^a dx\, \psi_n^* \psi(x)$$

or $\quad |\psi\rangle = \int_0^a dx\, |x\rangle \langle x | \psi \rangle = \int_0^a dx\, |x\rangle\, \psi(x)$

$\psi(x)$, c_n are components of $|\psi\rangle$ in different bases.

note: $\langle \psi | \psi \rangle = \sum_n \langle \psi | \psi_n \rangle \langle \psi_n | \psi \rangle = \sum_n c_n^* c_n = \sum_n |c_n|^2 = 1$

just as $\langle \psi | \psi \rangle = \int_0^a dx \langle \psi | x \rangle \langle x | \psi \rangle = \int_0^a dx\, \psi^*(x)\, \psi(x) = \int_0^a dx\, |\psi(x)|^2 = 1$

$|x\rangle \to |\psi_n\rangle$ or $\psi(x) \to c_n$ is a unitary transformation

* symmetry: even/odd states, since $V(x)$ symmetric

* general solution: $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin(k_n x) e^{-iE_n t/\hbar}$

initial state: $\Psi(x,0) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin(k_n x) \cancel{e^{-iE_n 0/\hbar}}$ 1

$$c_n = \langle \psi_n | \Psi_0 \rangle = \int_0^a dx \sqrt{\frac{2}{a}} \sin(k_n x) \cdot \Psi(x,0)$$

* expected value of energy: $\langle H \rangle = \langle \Psi | H | \Psi \rangle$

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

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

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

* exercise 2.4

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

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

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

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

$$\langle p\rangle_n = \langle \psi_n | -i\hbar \frac{\partial}{\partial x} | \psi_n\rangle = 0$$ 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!