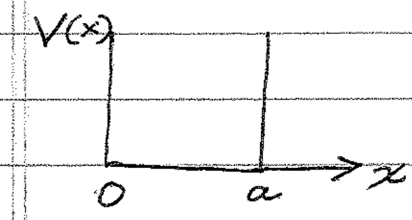
Infinite Square Well



$$V(x) = 0 \quad 0 \leq x \leq a$$
$$= \infty \quad \text{otherwise}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \rightarrow \frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi = -k^2\psi,$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$.

This second order equation has a solution of the form:

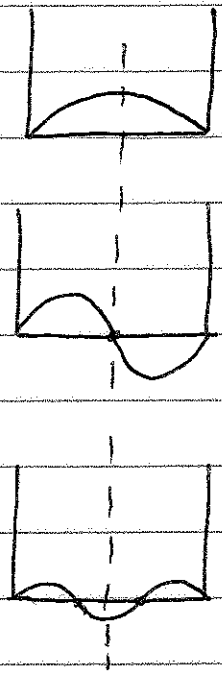
$$\psi(x) = A\sin kx + B\cos kx$$

with the boundary condition $\psi(0) = \psi(a) = 0$.

$$\psi(0) = 0 \rightarrow \psi(x) = A\sin kx \quad (B = 0)$$

$$\psi(a) = 0 \rightarrow \sin ka = 0 \rightarrow ka = n\pi$$
$$n = 1, 2, 3, \ldots$$
$$\rightarrow k_n = \frac{n\pi}{a}$$

$$k_n = \sqrt{\frac{2mE_n}{\hbar^2}} \rightarrow E_n = \frac{\hbar^2 k_n^2}{2m}$$



$n=1$ $\quad \sin\left(\frac{\pi x}{a}\right)$ 0 nodes even about $x = a/2$

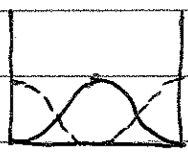
$n=2$ $\quad \sin\left(\frac{2\pi x}{a}\right)$ 1 node odd about $x = a/2$

$n=3$ $\quad \sin\left(\frac{3\pi x}{a}\right)$ 2 node even about $a/2$

Normalization:

$$\int_0^a |A|^2 \sin^2(kx)\,dx = \int_0^a |A|^2 \cos^2(kx)\,dx$$

$$= \frac{1}{2}\int_0^a |A|^2 \left(\sin^2(kx) + \cos^2(kx)\right) dx$$



$$= \frac{1}{2}\int_0^a |A|^2\,dx = \frac{|A|^2 a}{2}$$

$$\rightarrow A = \sqrt{\frac{2}{a}}$$

Summary: $\psi_n(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi}{a}x\right)$

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

Orthogonality:

$$\int_0^a \psi_m^*(x)\psi_n(x)\,dx = 0 \quad \text{if } m \neq n$$

$$\int_0^a \psi_m^*(x)\psi_m(x)\,dx = 1 \quad \text{... normalization}$$

$$\int_0^a \psi_m^*(x)\psi_n(x)\,dx = \frac{2}{a}\int_0^a \sin\left(\frac{\pi m}{a}x\right)\sin\left(\frac{\pi n}{a}x\right)$$

Because $\cos(A+B) = \cos(A)\cos(B) - \sin(A)\sin(B)$
$\cos(A-B) = \cos(A)\cos(B) + \sin(A)\sin(B)$

$\rightarrow \cos(A-B) - \cos(A+B) = 2\sin(A)\sin(B)$

$$= \frac{1}{a}\int_0^a \left[\cos\left(\frac{\pi}{a}(m-n)x\right) - \cos\left(\frac{\pi}{a}(m+n)x\right)\right]dx$$

$$= \frac{1}{a}\left[\frac{1}{\frac{\pi}{a}(m-n)}\sin\left(\frac{\pi}{a}(m-n)x\right)\Big|_0^a - \frac{1}{\frac{\pi}{a}(m+n)}\sin\left(\frac{\pi}{a}(m+n)x\right)\Big|_0^a\right]$$

$= 0$ because $\sin(\pi \times \text{integer}) = 0$

$$\boxed{\text{Summary: } \int_0^a \psi_m^*(x)\psi_n(x) = \delta_{mn} \qquad \delta_{mn} = 1 \text{ if } m=n \text{ \& } 0 \text{ otherwise}}$$

Completeness:

Any nice function on [0, a] can be written in terms of the $\psi_n(x)$.

$$\boxed{f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x).}$$

$$\rightarrow \int_0^a \psi_m^*(x) f(x)\, dx = \sum_{n=1}^{\infty} c_n \underbrace{\int_0^a \psi_m^*(x)\psi_n(x)\, dx}_{\delta_{mn}} = c_m$$

$$\boxed{c_m = \int_0^a \psi_m^*(x) f(x)\, dx}$$

$$\rightarrow f(x) = \sum_{n=1}^{\infty} \left(\int_0^a \psi_n^*(x') f(x')\, dx' \right) \psi_n(x)$$

$$= \sum_{n=1}^{\infty} \int_0^a \psi_n^*(x') \psi_n(x) f(x')\, dx'$$

$$= \int_0^a \underbrace{\left\{ \sum_{n=1}^{\infty} \psi_n^*(x')\psi_n(x) \right\}}_{\text{What is this?} \Longrightarrow} f(x')\, dx'$$

(extra)

$$\sum_{n=1}^{\infty} \psi_n^*(x')\psi_n(x) = \frac{2}{a}\sum_{n=1}^{\infty} \sin\left(\frac{\pi n x'}{a}\right)\sin\left(\frac{\pi n x}{a}\right)$$

$$= \frac{1}{a}\sum_{n=1}^{\infty} \cos\left(\frac{\pi n(x-x')}{a}\right) - \frac{1}{a}\sum_{n=1}^{\infty} \cos\left(\frac{\pi n(x+x')}{a}\right)$$

Now $\cos\theta = \frac{1}{2}(e^{i\theta}+e^{-i\theta})$ so the sum is:

$$= \frac{1}{2a}\left(\sum_{n=1}^{\infty} e^{i\pi n(x-x')/a} + e^{-i\pi n(x-x')/a}\right) + \frac{1}{2a}$$

cancel

$$- \frac{1}{2a}\left(\sum_{n=1}^{\infty} e^{i\pi n(x+x')/a} + e^{-i\pi n(x+x')/a}\right) - \frac{1}{2a}$$

The reason I have included $0 = \frac{1}{2a} - \frac{1}{2a}$ is that the sum can now be written as:

$$= \frac{1}{2a}\sum_{n=-\infty}^{+\infty} e^{i\pi n(x-x')/a} - \frac{1}{2a}\sum_{n=-\infty}^{+\infty} e^{i\pi n(x+x')/a}$$

$$= \lim_{N\to\infty} \frac{1}{2a}\sum_{n=-N}^{N} e^{i\pi n(x-x')/a} - \frac{1}{2a}\sum_{n=-N}^{N} e^{i\pi n(x+x')/a}$$

This sum is a geometric series:

$$\sum_{n=0}^{\infty} z^n = \frac{1}{1-z}$$

$$\left.\begin{aligned} \sum_{n=-N}^{\infty} z^n &= \frac{z^{-N}}{1-z} \\ \sum_{n=N+1}^{\infty} z^n &= \frac{z^{N+1}}{1-z} \end{aligned}\right\} \rightarrow \sum_{n=-N}^{N} z^n = \frac{z^{-N} - z^{N+1}}{1-z}$$

$$= (z^{N+1} - z^{-N})/(z-1)$$

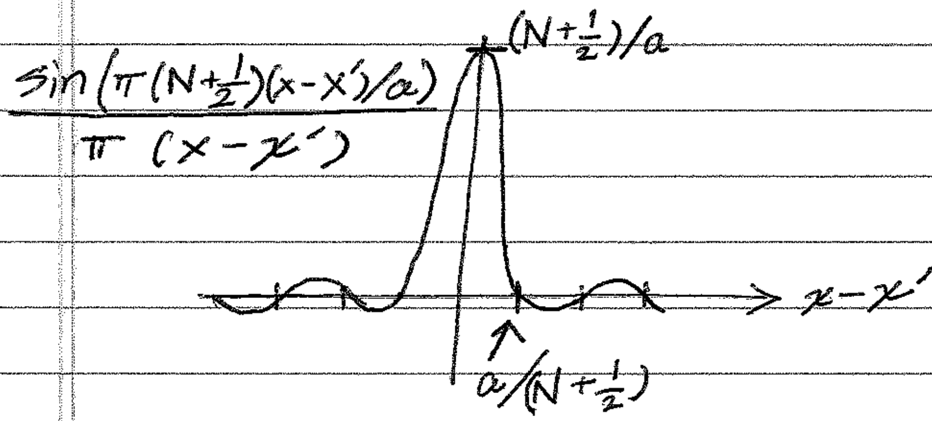
$$= \frac{z^{N+\frac{1}{2}} - z^{-(N+\frac{1}{2})}}{z^{1/2} - z^{-1/2}}$$

For our series $z = e^{i\pi(x-x')/a}$ or $e^{i\pi(x+x')/a}$.
Thus, our sum reduces to

$$= \lim_{N\to\infty} \frac{1}{2a}\,\frac{\sin\left(\pi(N+\frac{1}{2})(x-x')/a\right)}{\sin\left(\pi\frac{1}{2}(x-x')/a\right)} - \frac{1}{2a}\,\frac{\sin\left(\pi(N+\frac{1}{2})(x+x')/a\right)}{\sin\left(\pi\frac{1}{2}(x+x')/a\right)}$$

Both of these functions are strongly peaked when the denominator vanishes. Near $x = x'$,

$$\frac{1}{2a}\,\frac{\sin\left(\pi(N+\frac{1}{2})(x-x')/a\right)}{\sin\left(\pi\frac{1}{2}(x-x')/a\right)} \approx \frac{1}{\cancel{2}\cancel{a}}\,\frac{\sin\left(\pi(N+\frac{1}{2})(x-x')/a\right)}{\pi\frac{1}{\cancel{2}}(x-x')/\cancel{a}}$$



As $N\to\infty$ this becomes more strongly peaked and narrower; however, the area remains 1 because

$$\int_{-\infty}^{+\infty} dx\,\frac{\sin(\alpha x)}{\pi x} = 1.$$

(extra)

In physics we write a function that has no width (as $N \to \infty$), but area 1 as a delta function.

$$\delta(x) = \lim_{N\to\infty} \frac{1}{2a} \frac{\sin(\pi(N+\frac{1}{2})(x)/a)}{\pi x}$$

$$\int_{-\infty}^{+\infty} \delta(x)\,dx = \underline{1}$$

Our original sum is thus

$$\sum_{n=1}^{\infty} \psi_n^*(x')\psi_n(x) = \delta(x-x') - \delta(x+x'),$$

but on the interval $[0,a]$ $x+x' \neq 0$. Consequently the completeness condition is

$$\boxed{\sum_{n=1}^{\infty} \psi_n^*(x')\psi_n(x) = \delta(x-x').}$$