Today in Physics 237: the infinite square well

Our first Schrödinger equation solution:

- A quantum confined to an infinite square well
- Orthonormality and completeness of sines and cosines
- Evaluation of Fourier coefficients *via* Fourier's Trick
- Use of the general solution to the Schrödinger equation for the infinite square well.

L-R: Mortimer Brewster (Cary Grant), Jonathan "Johnny" Brewster (Raymond Massey), and Dr. Herman Einstein (Peter Lorre), in *Arsenic and Old Lace* (1944).

Quantum confined to an infinite square well

- … is simple but instructive: $V(x)\begin{cases} =0, & 0<x<a \\ \\ \rightarrow\infty, & x\le 0,\ge a \end{cases}$.

- Without solving the Schrödinger equation we already know that Ψ = 0 where $V\rightarrow\infty$, because the quantum cannot get to those regions. Infinite force toward the well, $F=-dV/dx\rightarrow\pm\infty\left(x=\substack{0\\a}\right)$, is exerted on a particle encountering the walls; waves would encounter perfect reflectivity.
  - These facts provide the boundary conditions for our solution to the Schrödinger equation.

- Within the well a quantum is free. With $k^2\equiv 2mE/\hbar^2$, $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi \quad\Rightarrow\quad \frac{d^2\psi}{dx^2}+k^2\psi=0$.

- This is familiar to you as the harmonic-oscillator equation; a **particular** solution is

$$\psi(x)=A\sin kx+B\cos kx \quad , \quad \text{or equivalently} \quad \psi(x)=A'e^{ikx}+B'e^{-ikx} \quad ,$$

the equivalence dictated by Euler's formula $e^{iu}=\cos u+i\sin u.$ We will use sines and cosines in the following.

Quantum confined to an infinite square well (continued)

- We can evaluate *B*, and find the values of *k* for which solutions exist, by applying the boundary conditions $\psi(x)=0$ at *x* = 0 and *x* = *a*. Presuming a nontrivial solution – i.e. that $A \neq 0$ and $ka \neq 0$,

$$\psi(0)=B\cos 0=0 \quad \Rightarrow \quad B=0 \quad .$$

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

- Thus only a **discrete spectrum** of energies is permitted for each sinusoidal solution: $\boxed{E_n=\frac{n^2\pi^2\hbar^2}{2ma^2}}$.
- Ordinarily we could also use continuity of *dψ*/*dx* at the walls to determine the remaining unknown constant *A*. This isn't allowed here because *V* is infinite there (so formally *dψ*/*dx* is undefined), so instead we normalize:

$$1=\int_{-\infty}^{\infty}|\psi|^2 dx=|A|^2\int_0^a \sin^2\frac{n\pi x}{a}dx=|A|^2\frac{a}{n\pi}\int_0^{n\pi}\sin^2 u\,du=|A|^2\frac{a}{n\pi}\frac{n\pi}{2}$$

see Lecture 2, page 5

$$\Rightarrow \quad A=\sqrt{\frac{2}{a}} \quad , \quad \boxed{\psi_n(x)=\sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}} \quad .$$

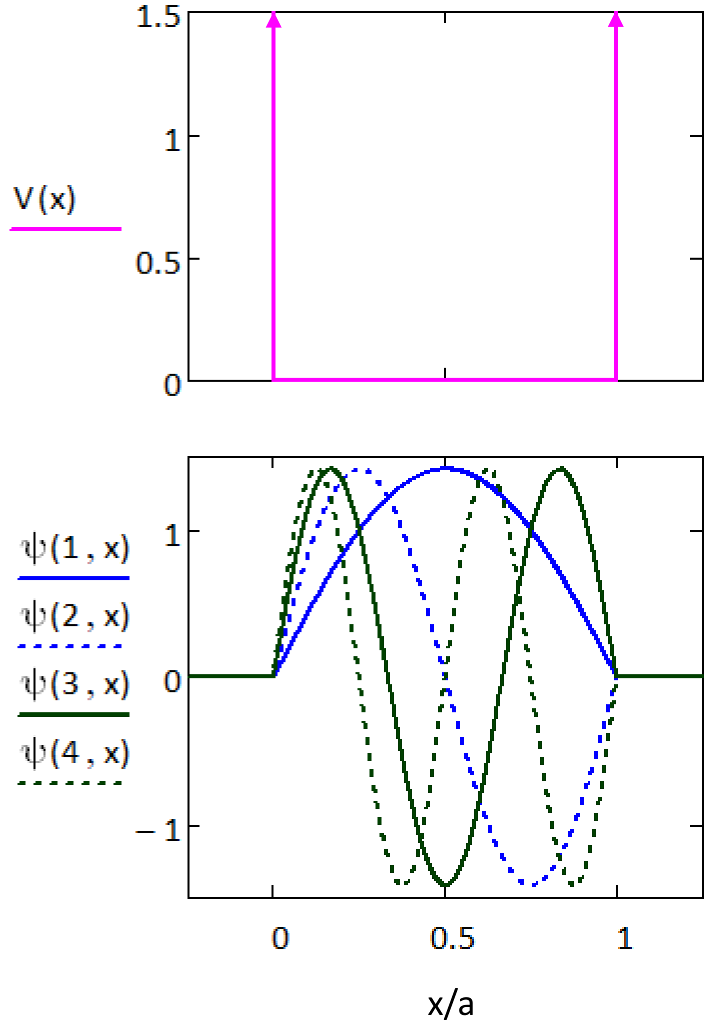
In quantum-ese we say that the $\psi_n(x)e^{-iE_n t/\hbar}$ are **eigenstates** of the Hamiltonian, with **eigenvalues** E_n.

Properties of the particular solutions

- Alternately even and odd, with respect to the center of the well: even if *n* is odd, and *vice versa*.
  - As *V* is an even function of *x*; viz. Problem 2.1c, Lecture 3.
- *n* + 1 zero-crossings (**nodes**).
- Sinusoidal solutions mean that important properties of sines and cosines are inherited:
  - wavefunctions for different *n* are **orthonormal**:

$$\int_0^a \psi^*{}_m(x)\psi_n(x)\,dx = \delta_{mn} = \begin{cases} 1 \text{ if } m = n \\ 0 \text{ otherwise} \end{cases}$$

  - this set of wavefunctions is **complete:** one can express any wavefunction for a quantum confined to an infinite square well as a linear combination of the $\psi_n(x)$.



Properties of the particular solutions (continued)

- That the $\psi_n(x)$ are orthonormal is demonstrated by Griffiths (p. 33); the missing step involves remembering a trig identity:

  $$\cos(u \pm v) = \cos u \cos v \mp \sin u \sin v \quad \text{, or in this case,} \quad \cos\left(\frac{m\pi x}{a} \pm \frac{n\pi x}{a}\right) = \cos\frac{m\pi x}{a}\cos\frac{n\pi x}{a} \mp \sin\frac{m\pi x}{a}\sin\frac{n\pi x}{a} \quad .$$

  Subtract the upper of these expressions (+/-) from the lower (-/+) and you get from the first to the second line of the proof.

- That the sines and cosines are complete – or equivalently e^{ikx} and e^{-ikx} – is a result called **Dirichlet's theorem** by some, and has been presented/will be presented to you in MATH 281.

- With our complete orthonormal set of $\psi_n(x)$ we can compose a **general** solution for the wavefunction $\Psi(x,t)$ in the infinite square well: it is a linear combination of all the $\psi_n(x)$, in the form of a **Fourier series** (once again see MATH 281):

  $$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{a}\right) e^{-in^2\pi^2\hbar t/2ma^2} \quad .}$$

The general solution

- Among the things one can do with the general solution is to specify a (valid) wavefunction at some specific time, say $t = 0$, and receive from the general solution the wavefunction at all other times.
  - Note that, although the particular solutions $\psi_n(x)e^{-iE_nt/\hbar}$ are stationary states – have time-independent expectation values for the observables – the general solution $\Psi(x,t)$ is not stationary.

- Once a valid initial ($t = 0$) wavefunction is specified, one then calculates the **Fourier coefficients**: the constants c_n which determine the initial mixture of particular solutions $\psi_n(x)$.

- And – as is familiar to recent victims of PHYS 217 – one does this by exploiting the orthonormality of the $\psi_n(x)$, with **Fourier's Trick:** with $\Psi(x,0)$ as the initial wave function, one extracts the c_n from the sum by multiplying through by $\psi_m^*(x)$ and integrating over x:

$$\int_0^a \psi_m^*\Psi(x,0)dx = \int_0^a \sum_n^\infty \psi_m^* c_n \psi_n dx = \sum_n^\infty c_n \int_0^a \psi_m^* \psi_n dx = \sum_n^\infty c_n \delta_{mn} = c_m \quad ; \quad \boxed{c_n = \int_0^a \psi_n^* \Psi(x,0)dx} \ .$$

How to use the general solution

I presume you will read Examples 2.1-2.3 carefully before doing this week's workshop problems. Here's an additional example of the use of the general solution $\Psi(x,t)$ for the infinite square well, including ancient pop culture content.

Problem 2.5. A quantum in the infinite square well has as its initial wavefunction $\Psi(x,0)=A\left[\psi_1(x)+\psi_2(x)\right]$.

a. Normalize $\Psi(x,0)$; that is, find *A*. Once normalized, it will stay normalized for all *t*.

b. Find $\Psi(x,t)$ and $\left|\Psi(x,t)\right|^2$. Express the latter as a sinusoidal function of time, as in Example 2.1. Let $\omega\equiv\pi^2\hbar/2ma^2$.

c. Compute $\langle x\rangle$. Notice that it oscillates in time. What is the angular frequency of the oscillation? What is the amplitude of the oscillation? (If your amplitude is greater than *a*/2, go directly to jail.)

d. Compute $\langle p\rangle$. (As Peter Lorre would say, "Do eet ze *kveek* vay, Johnny.")
The quote paraphrases a line by Lorre's character Dr. Einstein in Frank Capra's *Arsenic and Old Lace* (1944).

e. If you measured the energy of this quantum, what values might you get, and what is the probability of getting each of them? Find $\langle H\rangle$. How does it compare with E_1 and E_2?

Problem 2.5

orthogonal: integrate to zero

a. $$1=\int\left|\Psi(x,0)\right|^2dx=\left|A\right|^2\int_0^a\left(\psi_1^*+\psi_2^*\right)\left(\psi_1+\psi_2\right)dx=\left|A\right|^2\int_0^a\left(\psi_1^*\psi_1+\psi_2^*\psi_1+\psi_1^*\psi_2+\psi_2^*\psi_2\right)dx=2\left|A\right|^2\quad\Rightarrow\quad\boxed{A=\frac{1}{\sqrt{2}}}\ .$$

normalized

b. $$c_n=\int_0^a\psi_n^*\Psi(x,0)dx=A\int_0^a\psi_n^*\left(\psi_1+\psi_2\right)dx=A\left(\delta_{n1}+\delta_{n2}\right)\quad\Rightarrow\quad c_1=c_2=A=\frac{1}{\sqrt{2}},c_{>2}=0\quad .$$

$$\Psi(x,t)=\left(c_1\psi_1e^{-iE_1t/\hbar}+c_2\psi_2e^{-iE_2t/\hbar}\right)=\frac{1}{\sqrt{a}}\left[\sin\frac{\pi x}{a}e^{-i\pi^2\hbar t/2ma^2}+\sin\frac{2\pi x}{a}e^{-i4\pi^2\hbar t/2ma^2}\right]$$

$$\boxed{=\frac{e^{-i\omega t}}{\sqrt{a}}\left[\sin\frac{\pi x}{a}+\sin\frac{2\pi x}{a}e^{-3i\omega t}\right]}\ .$$

Use Euler's formula,

$\cos u=\left(e^{iu}+e^{-iu}\right)/2$:

$$\left|\Psi(x,t)\right|^2=\frac{1}{a}\left(\sin\frac{\pi x}{a}+\sin\frac{2\pi x}{a}e^{3i\omega t}\right)\left(\sin\frac{\pi x}{a}+\sin\frac{2\pi x}{a}e^{-3i\omega t}\right)=\frac{1}{a}\left[\sin^2\frac{\pi x}{a}+\sin^2\frac{2\pi x}{a}+\left(e^{3i\omega t}+e^{-3i\omega t}\right)\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\right]$$

$$\boxed{=\frac{1}{a}\left[\sin^2\frac{\pi x}{a}+\sin^2\frac{2\pi x}{a}+2\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\cos3\omega t\right]}\ .$$

Problem 2.5 (continued)

$$\text{c.}\langle x\rangle = \int \Psi^*(x,t)\,x\,\Psi(x,t)\,dx = \frac{1}{a}\int_0^a x\left[\sin^2\frac{\pi x}{a} + \sin^2\frac{2\pi x}{a} + 2\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\cos 3\omega t\right]dx \quad .$$

$$\frac{1}{a}\int_0^a x\sin^2\frac{\pi x}{a}\,dx = a\int_0^1 u\sin^2\pi u\,du = \frac{a}{4} = \frac{1}{a}\int_0^a x\sin^2\frac{2\pi x}{a}\,dx \quad .$$

$$\frac{2\cos 3\omega t}{a}\int_0^a x\,\underline{\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}}\,dx = \frac{\cos 3\omega t}{a}\int_0^a x\left(\underline{\cos\frac{\pi x}{a} - \cos\frac{3\pi x}{a}}\right)dx = -\frac{16a\cos 3\omega t}{9\pi^2} \quad .$$

Same trig identity as used on page 5

See page 11 below for details of the integrals.

$$\langle x\rangle = \frac{a}{4} + \frac{a}{4} - \frac{16a\cos 3\omega t}{9\pi^2} = \boxed{\frac{a}{2}\left(1 - \frac{32}{9\pi^2}\cos 3\omega t\right)} \left\{\begin{array}{l} \text{Amplitude } \boxed{\dfrac{32}{9\pi^2}\dfrac{a}{2}} < \dfrac{a}{2} \quad , \\ \text{angular frequency } 3\omega = \boxed{\dfrac{3\pi^2\hbar}{2ma^2}} \quad . \end{array}\right.$$

Problem 2.5 (continued)

d. By the quick way, G&S mean to return to the means of Lecture 2, page 9, rather than doing another expectation-value integral:

$$\langle p\rangle = m\frac{d}{dt}\langle x\rangle = \left(\frac{ma}{2}\right)\left(-\frac{32}{9\pi^2}\right)(-3\omega\sin 3\omega t) = \boxed{\frac{8\hbar}{3a}\sin 3\omega t} \quad .$$

e. From part a: $\int\left|\Psi(x,t)\right|^2 dx = \left|A\right|^2\int_0^a\left(\psi_1^*\psi_1 + \psi_2^*\psi_2\right)dx = \frac{1}{2}+\frac{1}{2}$. Only one of two energy eigenstates would be found by a measurement, either n = 1 or n = 2, with equal probability. And thus a measurement of H would return either $\boxed{E_1 = \frac{\pi^2\hbar^2}{2ma^2} \text{ or } E_2 = \frac{2\pi^2\hbar^2}{ma^2}}$. You could guess from this that the expectation value of H would be the average of these two values, and sure enough, using orthonormality and the fact that ψ_1 and ψ_2 are eigenstates of $\hat{H}$,

$$\langle H\rangle = \int\Psi^*(x,t)\hat{H}\Psi(x,t)dx = \frac{1}{2}\int_0^a\left(\psi_1^*\hat{H}\psi_1 + \psi_2^*\hat{H}\psi_2\right)dx = \boxed{\frac{1}{2}(E_1+E_2) = \frac{5}{4}\frac{\pi^2\hbar^2}{ma^2}} \quad .$$

The integrals in Problem 2.5c

- Use the trig identity $\sin^2\alpha = (1-\cos 2\alpha)/2$ – derived in the same way as the identity on page 5 – and do it for $\alpha = 2j\pi$ with integer *j*, so we get the first two integrals we need at once. Following the use of the identity is an integration by parts to get rid of the factor of *u*:

$$\int_0^1 u\sin^2 j\pi u\,du = \frac{1}{2}\int_0^1 u\left(1-\cos 2j\pi u\right)du = \left.\frac{u^2}{4}\right|_0^1 - \frac{1}{2}\int_0^1 u\cos 2j\pi u\,du \qquad \begin{cases} v = \dfrac{1}{2j\pi}\sin 2j\pi u \\ dv = \cos 2j\pi u\,du \end{cases}$$

$$= \frac{1}{4} - \frac{1}{2}\frac{u}{2j\pi}\left.\cancelto{0}{\sin 2j\pi u}\right|_0^1 + \frac{1}{2}\frac{1}{2j\pi}\int_0^1 \sin 2j\pi u\,du = \frac{1}{2} + \frac{1}{2}\left(\frac{1}{2j\pi}\right)^2 \int_0^{2j\pi} \sin w\,dw$$

$$= \frac{1}{4} + \frac{1}{2}\left(\frac{1}{2j\pi}\right)^2 \left[-\cos w\right]_0^{2j\pi} = \frac{1}{4} + \frac{1}{2}\left(\frac{1}{2j\pi}\right)^2 \left[\cancelto{0}{-1+1}\right] = \frac{1}{4}\ .$$

Same result for any value of integer *n.*

So $\boxed{\dfrac{1}{a}\displaystyle\int_0^a x\sin^2\frac{\pi x}{a}dx = \frac{a}{4} = \frac{1}{a}\int_0^a x\sin^2\frac{2\pi x}{a}dx}$.

Compare page 9

The integrals in Problem 2.5c (continued)

- The next integrals have integrands with products of *u* and cos *Au,* like the last ones, so again they involve integration by parts to get rid of the factor of *u.* The only difference is that here *A* is an odd multiple of π instead of an even one. Again we take *j* to be an integer, so our odd integer is 2*j* + 1 instead of our former even 2*j*, and the integration by parts goes like this:

$$\int_0^1 u\cos(2j+1)\pi u\,du \left\{\begin{array}{l} v=\dfrac{1}{(2j+1)\pi}\sin(2j+1)\pi u \\ \\ dv=\cos(2j+1)\pi u\,du \end{array}\right\} = \frac{u}{(2j+1)\pi}\overset{0}{\sin(2j+1)\pi u}\Big|_0^1 - \frac{1}{(2j+1)\pi}\int_0^1 \sin(2j+1)\pi u\,du$$

$$= -\left(\frac{1}{(2j+1)\pi}\right)^2 \int_0^{(2j+1)\pi} \sin w\,dw = +\left(\frac{1}{(2j+1)\pi}\right)^2 \cos w\Big|_0^{(2j+1)\pi}$$

$$= \left(\frac{1}{(2j+1)\pi}\right)^2(-1-1) = -2\left(\frac{1}{(2j+1)\pi}\right)^2 \quad .$$

The integrals in Problem 2.5c (continued)

- Our integrals have cosine factors with *j* = 0 and 1. Picking up from page 9, just as the identity on page 5 is used, we use our new result in the second line:

$$\frac{2\cos 3\omega t}{a}\int_0^a x\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}dx = \frac{\cos 3\omega t}{a}\int_0^a x\left(\cos\frac{\pi x}{a}-\cos\frac{3\pi x}{a}\right)dx = a\cos 3\omega t\int_0^1 u\left(\cos\pi u-\cos 3\pi u\right)du$$

$$=\left(a\cos 3\omega t\right)\left(-\frac{2}{\pi^2}+\frac{2}{9\pi^2}\right)\coloneqq-\frac{16a\cos 3\omega t}{9\pi^2}\quad .$$

Compare page 9