Department of Physics
University of California San Diego

Modern Physics (2D)
Prof. V. Sharma
Quiz # 7 (Feb 28 2003)

Some Relevant Formulae, Constants and Identities

$\lambda = \frac{h}{p}$; $\Delta x . \Delta p \geq \frac{h}{4\pi}$; $\Delta E . \Delta t \geq \frac{h}{4\pi}$

Time Dep. S. Eq: $-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$

Time Indep. S. Eq: $-\frac{\hbar^2}{2\text{m}}\frac{\partial^2 \psi(x)}{\partial x^2} + U(x)\psi(x) = E\ \psi(x)$

Particle of mass m in a rigid box of length L: $\text{E}_\text{n} = \frac{\text{n}^2\pi^2\hbar^2}{2mL^2}$

$\sin x = \frac{e^{ix} - e^{-ix}}{2i}$; $\cos x = \frac{e^{ix} + e^{-ix}}{2}$

$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + ...$

$\sin\alpha \sin\beta = \frac{1}{2}\left(\cos(\alpha - \beta) - \cos(\alpha + \beta)\right)$

$\int x^2 \sin^2 x\, dx = \frac{x^3}{6} - \left(\frac{x^2}{4} - \frac{1}{8}\right)\sin 2x - \frac{x\cos 2x}{4}$

$\int x \sin^2 x\, dx = \frac{\text{x}^2}{4} - \frac{x \sin 2x}{4} - \frac{\cos 2x}{8}$

$\int \sin^2 x\, dx = = -\frac{1}{2}\cos x \sin x + \frac{1}{2}\text{x} = \frac{1}{2}x - \frac{1}{4}\sin 2x$

Pl. write you answer in the Blue Book in indelible ink. Make sure your code number is prominently displayed on each page.

If you have trouble understanding the question, pl. ask the proctor

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Problem 1 : A Picket Fence Potential [12 pts] :
A one dimensional infinite potential well (or box with rigid walls) extends from **x = -L** to **x = L** and is divided into three sections by rigid interior walls (of infinite potential) at $x = -x_0$ and $x = x_0$, where $x_0 < L$. Each section contains one particle each of mass m in its ground state (a) draw a schematic of the configuration of potential "walls" and draw the wave function of the ground state for each particle cleanly (b) Write an expression for the total energy of this system in terms of x_0. (c) Use a well known rule of calculus to determine the value of x for which the total energy $E(x_0)$ is the minimum (d) what is the value of this total energy E?

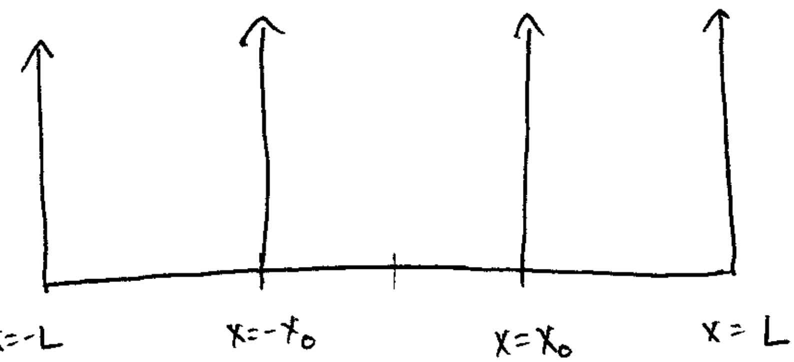
Problem 2: **Designer Wavefunctions [8 pts]:** Since the Schrodinger Equation is linear; we can add two solutions to find another. (a) find the normalization constant B for the combination

$$\psi(x) = B\left(\sin\frac{\pi}{L}x + \sin\frac{2\pi}{L}x\right)$$

of the wave functions for n=1 & n=2 states of a particle in a 1-dimensional rigid box of length L. This idea is needed for making Hydrogen bonds in chemistry or Quantum computers of tomorrow. (b) What is the expected value <x> for a particle in this state? Support your answer with a calculation.
(Note: The box goes from x=0 to x=L).

Phys 2D Quiz 7

a]



This is just a combo of 3 infinite wells, so the ground state is

(these bumps can be flipped over as well, in any combination).

b] E_1 for a well of length L is $\frac{\pi^2\hbar^2}{2mL^2}$

Here, we have 3 wells: The left one has length $L-x_0$
The middle has length $2x_0$
The right one has length $L-x_0$

So $$\boxed{E = \frac{\pi^2\hbar^2}{2m}\left[\frac{2}{(L-x_0)^2} + \frac{1}{(2x_0)^2}\right]}$$ (just add the energies!)

c] Find $\frac{\partial E}{\partial x_0} = \frac{\pi^2 \hbar^2}{2m}\left[\frac{-4}{(L-x_0)^3}\cdot(-1) - \frac{2}{(2x_0)^3}\cdot 2\right]$

$$= \frac{\pi^2 \hbar^2}{2m}\left[\frac{4}{(L-x_0)^3} - \frac{1}{2x_0^3}\right] = 0$$

So $\frac{(L-x_0)^3}{4} = 2x_0^3 \Rightarrow (L-x_0)^3 = 8x_0^3$

Thus $L - x_0 = 2x_0 \Rightarrow \boxed{x_0 = \frac{L}{3}}$

d] Plug in to part b to get

$$E = \frac{\pi^2 \hbar^2}{2m}\left[\frac{2}{\left(\frac{2L}{3}\right)^2} + \frac{1}{\left(\frac{2L}{3}\right)^2}\right] = \frac{\pi^2 \hbar^2}{2m}\cdot 3\left(\frac{3}{2L}\right)^2$$

$$\Rightarrow \boxed{E = \frac{27\pi^2 \hbar^2}{8mL^2}}$$

2a] $\psi(x) = B\left(\sin\left(\frac{\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right)\right)$

Normalize: $\int_0^L |\psi|^2 dx = 1$

$$\int_0^L |\psi|^2 dx = B^2 \int_0^L \left[\sin^2\left(\frac{\pi x}{L}\right) + 2\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) + \sin^2\left(\frac{2\pi x}{L}\right)\right] dx$$

We know from our study of the usual square well that $\int_0^L \sin^2\left(\frac{\pi x}{L}\right) dx = \frac{L}{2}$

and $\int_0^L \sin^2\left(\frac{2\pi x}{L}\right) dx = \frac{L}{2}$ (or can just do these).

$$\int_0^L \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{3\pi x}{L}\right) = \frac{1}{2}\int_0^L \left[\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right] dx = \frac{1}{2}\left[\frac{L}{\pi}\sin\left(\frac{\pi x}{L}\right)\Big|_0^L - \frac{L}{3\pi}\sin\left(\frac{3\pi x}{L}\right)\Big|_0^L\right]$$

$$= 0$$

So $B^2 \cdot \left[\frac{L}{2} + 0 + \frac{L}{2}\right] = B^2 L = 1 \Rightarrow \boxed{B = \frac{1}{\sqrt{L}}}$

b] $$\langle x \rangle = \int_0^L x|\psi|^2 dx = \int_0^L x \cdot \frac{1}{L}\left[\sin^2\left(\frac{\pi x}{L}\right) + 2\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) + \sin^2\left(\frac{2\pi x}{L}\right)\right] dx$$

Now, $$\int_0^L x\sin^2\left(\frac{\pi x}{L}\right) dx = \left(\frac{L}{\pi}\right)^2 \int_0^\pi x\sin^2 x \, dx = \frac{L^2}{\pi^2}\left[\frac{x^2}{4} - \frac{x\sin 2x}{4} - \frac{\cos 2x}{8}\right]_0^\pi$$

did a change of variables

$$= \frac{L^2}{\pi^2}\left[\frac{\pi^2}{4} - \frac{1}{8} + \frac{1}{8}\right] = \frac{L^2}{4}.$$

Similarly, $\int_0^L x\sin^2\left(\frac{2\pi x}{L}\right) = \left(\frac{L}{2\pi}\right)^2 \int_0^{2\pi} x\sin^2 x\,dx = \left(\frac{L}{2\pi}\right)^2 \left[\frac{x^2}{4} - \frac{x\sin 2x}{4} - \frac{\cos 2x}{8}\right|_0^{2\pi}$

$$= \frac{L^2}{4}.$$

Finally, $\int_0^L x\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) = \frac{1}{2}\int_0^L x\left[\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right]dx$

Int. by parts: $\int_0^L x\cos\left(\frac{\pi x}{L}\right)dx = \frac{L}{\pi}x\sin\left(\frac{\pi x}{L}\right)\Big|_0^L - \frac{L}{\pi}\int_0^L \sin\left(\frac{\pi x}{L}\right)dx$

$$= 0 + \left(\frac{L}{\pi}\right)^2\cos\left(\frac{\pi x}{L}\right)\Big|_0^L = -\frac{2L^2}{\pi^2}$$

and $\int_0^L x\cos\left(\frac{3\pi x}{L}\right)dx = \frac{L}{3\pi}x\sin\left(\frac{3\pi x}{L}\right)\Big|_0^L - \frac{L}{3\pi}\int_0^L \sin\left(\frac{3\pi x}{L}\right)dx$

$$= 0 + \left(\frac{L}{3\pi}\right)^2\cos\left(\frac{3\pi x}{L}\right)\Big|_0^L = \frac{L^2}{9\pi^2}(-2)$$

$\Rightarrow \int_0^L x\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) = \frac{1}{2}\left[-\frac{2L^2}{\pi^2} + \frac{2L^2}{9\pi^2}\right] = \frac{L^2}{\pi^2}\left(-\frac{8}{9}\right)$

So $\langle x\rangle = \frac{1}{L}\left[\frac{L^2}{4} + \frac{L^2}{4} - 2\frac{L^2}{\pi^2}\frac{8}{9}\right] = \boxed{L\left(\frac{1}{2} - \frac{16}{9\pi^2}\right)}$