Problem Set 0 CHEM 20100

- 9/13: **2.8** The details of several steps in the particle-in-a-box model in this chapter have been omitted. Work out the details of the following steps:
  - a. Show that if  $\Psi = A \sin rx + B \cos sx$  (A, B, r, and s are constants) is a solution to the wave equation for the one-dimensional box, then

$$r = s = \sqrt{2mE} \left(\frac{2\pi}{h}\right)$$

Solution.

$$\frac{-h^2}{8\pi^2 m} \cdot \frac{\partial^2 \Psi(x)}{\partial x^2} = E\Psi(x)$$

$$\frac{-h^2}{8\pi^2 m} \cdot \frac{\partial^2}{\partial x^2} \left( A \sin rx + B \cos sx \right) = E(A \sin rx + B \cos sx)$$

$$\frac{-h^2}{8\pi^2 m} \cdot \frac{\partial}{\partial x} \left( Ar \cos rx - Bs \sin sx \right) = E(A \sin rx + B \cos sx)$$

$$\frac{-h^2}{8\pi^2 m} \cdot \left( -Ar^2 \sin rx - Bs^2 \cos sx \right) = E(A \sin rx + B \cos sx)$$

$$\frac{Ar^2 h^2}{8\pi^2 m} \sin rx + \frac{Bs^2 h^2}{8\pi^2 m} \cos sx = AE \sin rx + BE \cos sx$$

$$0 = \left( \frac{Ar^2 h^2}{8\pi^2 m} - AE \right) \sin rx + \left( \frac{Bs^2 h^2}{8\pi^2 m} - BE \right) \cos sx$$

Choose x = 0.

$$= \frac{Bs^2h^2}{8\pi^2m} - BE$$

$$E = \frac{s^2h^2}{8\pi^2m}$$

$$\frac{8\pi^2mE}{h^2} = s^2$$

$$s = \sqrt{\frac{8\pi^2mE}{h^2}}$$

$$s = \sqrt{2mE} \frac{2\pi}{h}$$

With this result ...

$$0 = \left(\frac{Ar^2h^2}{8\pi^2m} - AE\right)\sin rx + \left(\frac{Bs^2h^2}{8\pi^2m} - BE\right)\cos sx$$

$$= \left(\frac{Ar^2h^2}{8\pi^2m} - AE\right)\sin rx + \left(B\left(\frac{s^2h^2}{8\pi^2m}\right) - BE\right)\cos sx$$

$$= \left(\frac{Ar^2h^2}{8\pi^2m} - AE\right)\sin rx + (BE - BE)\cos sx$$

$$= \left(\frac{Ar^2h^2}{8\pi^2m} - AE\right)\sin rx$$

Choose  $x = \frac{\pi}{2r}$ .

$$=\frac{Ar^2h^2}{8\pi^2m}-AE$$
 
$$r=\sqrt{2mE}\frac{2\pi}{h}$$

Problem Set 0 CHEM 20100

**d.** Show that substituting the value of r given in part c into  $\Psi = A \sin rx$  and applying the normalizing requirement gives  $A = \sqrt{2/a}$ .

Solution.

$$1 = \int_{\text{all space}} \Psi \Psi^* \, d\tau$$
$$= \int_0^a \left( A \sin \frac{n\pi x}{a} \right) \left( A \sin \frac{n\pi x}{a} \right) dx$$
$$= \int_0^a A^2 \sin^2 \frac{n\pi x}{a} \, dx$$

Use  $\sin^2 u = \frac{1-\cos 2u}{2}$ .

$$= A^{2} \int_{0}^{a} \frac{1 - \cos\frac{2n\pi x}{a}}{2} dx$$

$$= \frac{A^{2}}{2} \left( \int_{0}^{a} dx - \int_{0}^{a} \cos\frac{2n\pi x}{a} dx \right)$$

$$= \frac{A^{2}}{2} \left( [x]_{0}^{a} - \left[ \frac{a}{2n\pi} \sin\frac{2n\pi x}{a} \right]_{0}^{a} \right)$$

$$= \frac{A^{2}}{2} \left( (a - 0) - \left( \frac{a}{2n\pi} \sin 2n\pi - \frac{a}{2n\pi} \sin 0 \right) \right)$$

$$= \frac{A^{2}}{2} \left( a - \left( \frac{a}{2n\pi} \sin 2n\pi \right) \right)$$

Since n is an integer,  $\sin 2n\pi = 0$ .

$$= \frac{aA^2}{2}$$
$$\frac{2}{a} = A^2$$
$$A = \sqrt{\frac{2}{a}}$$