

Chem 333
September 19, 2006

Background

Use *Mathematica* wherever you can to simplify integrals and differentiate (*hint*: don't try to combine too many functions in a single input line; the larger the combination, the larger the chance for error)

Particle in a 1-D Box ($0 \leq x \leq a$) wave function:

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

Problems

1. Calculate the expectation value for the particle's energy, $\langle E \rangle$, when $\Psi = \psi_n$
2. Is $\langle E \rangle$ also an eigenvalue of \hat{H} ?
3. How does the *relative* energy separation of two states change as the quantum number becomes large?

$$\text{Relative energy separation} \equiv (E_{n+1} - E_n) / E_n$$

4. Calculate the expectation value for the particle's momentum, $\langle p \rangle$, when $\Psi = \psi_n$
5. Is ψ_n an eigenfunction of the momentum operator?
6. Under what conditions would you expect to measure $\langle p \rangle$? Under what conditions would you expect to measure an eigenvalue of the momentum operator?
 - a. Extra credit problem: How could you determine these eigenvalues? (*Hint*: the completeness theorem suggests another way of looking at ψ_n .)
7. Calculate the expectation value for the particle's position, $\langle x \rangle$, when $\Psi = \psi_n$
8. $\langle x \rangle$ and $P(x)dx$ provide different information about position. Explain.