Problem Set 1
Physics 386 / Spring 1997
Professor Klaus Schulten

Problem 1: Normalization and Expectation Values

Normalize the wave function

$$\phi(x) \;=\; \frac{c}{a^2 + x^2} \tag{1}$$

and find the expectation values of x and x^2 for this wave function. *The range of x for this wave function is $(-\infty, \infty)$.*

Problem 2: Particle in a Box

For the particle in the box, as treated in class, determine the probability that a particle in the n-th stationary state ($n = 1, 2, \ldots$) is found in the right side ($x \geq a/2$) of the box.

Problem 3: Interaction of an Electron in a Box with Light

An electron is moving in a one-dimensional box. Choose the size of the box such that the energy difference of the transition from stationary state with $n = 1$ to the stationary state with $n = 2$ matches the energy of red ($\lambda = 8000$ Å) light. Do the same for blue ($\lambda = 4000$ Å) light.

Problem 4: Wave Packet in One-Dimensional Box - Difficult

Describe the time-dependence of a particle moving in a one-dimensional box as described through the wave equation

$$i\hbar \partial_t \, \psi(x,t) \;=\; -\frac{\hbar^2}{2m} \partial_x^2 \, \psi(x,t) \, , \tag{2}$$

boundary conditions

$$\psi(x,t) \;=\; 0 \quad \text{for } x \;=\; 0, a \tag{3}$$

and initial condition

$$\psi(x,0) \; = \; \left[\frac{1}{2\pi\sigma^2}\right]^{\frac{1}{4}} \exp\left(-\frac{(x-a/2)^2}{2\sigma^2} \; + \; i\,k_0\,x\right) \; , \quad \sigma \; = \; \frac{a}{8}, \; k_0 \; = \; \frac{10}{a} \; . \tag{4}$$

Follow the computational procedure presented in class. In calculating the expansion coefficients $c_n(0)$ assume that the Gaussian above is very small outside the box such that one can assume

$$c_n(0) \; = \; \int_{-\infty}^{+\infty} dx' \, \underbrace{\psi(x',0)}_{=f(x')} \phi_n(x') \tag{5}$$

Determine the leading 10 coefficients and write down an expression for the wave function $\psi(x,t)$ in terms of these coefficients. Explain why we can use just the first ten coefficients to get a reasonable approximation to the wave function.

Optional: Computer simulation of the particle in a box. Determine the wave function at $t = nt_0$ for $t_0 = 0.02m\,a^2/\hbar$ for $n = 0,1,\ldots$ (choose the upper number as you wish). You can use software such as Mathematica or Maple to perform much of the algebra. Plot the result. What happens when you vary x_o? When you vary k_o?

This problem set needs to be handed in by Monday, February 17, 1997.