CHEM 361B - Lecture 6 Activity

The Particle in a Box

1. The Schrödinger equation for a particle of mass m constrained to move on a circle of radius a is

$$-\frac{\hbar^2}{2I}\frac{d^2\psi}{d\theta^2} = E\psi(\theta)$$

where $I = ma^2$ is the moment of inertia and θ is the angle that describes the position of the particle around the ring.

   (a) The solution to this differential equation takes the form

$$\psi(\theta) = Ae^{in\theta}$$

   Show that $n = \pm\sqrt{2IE}/\hbar$

   (b) Argue that the appropriate boundary condition is $\psi(\theta) = \psi(\theta + 2\pi)$ and use this condition to show that $n = 0, \pm 1, \pm 2, \ldots$

   (c) Show that the energy of the particle on a ring is

$$E = \frac{n^2\hbar^2}{2I} \quad n = 0, \pm 1, \pm 2, \ldots$$

   (d) What is the physical significance of the sign of the integers n?

   (e) Show that the normalisation constant A is $\sqrt{1/2\pi}$.

   (f) Show that the probability of finding a particle in the $n = 2$ energy level between $\pi/2 \leq \theta \leq 3\pi/4$ is 1/8.

   (g) This solution to the Schrödinger Equation can be used to describe some spectroscopic data for benzene. Benzene has a radius of 1.39 Å. Show that the wavelength of the lowest energy photon required to excite the ground state of benzene is 210 nm. For reference, the experimental absorption is 268 nm.

2. We can draw a comparison between classical and quantum particles trapped in boxes

	Classical	Quantum
$\langle x \rangle$	$a/2$	$a/2$
$\langle x^2 \rangle$	$a^2/3$	$\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}$
σ_x	$a/\sqrt{12}$	$\frac{a}{2\pi n}\sqrt{\frac{\pi^2 n^2}{3} - 2}$

Show that $\langle x^2 \rangle$ and σ_x for the quantum particle matches the classical particle when $n \to \infty$. What conclusion can you draw from this result? To support your conclusion, draw the probability density for a classical particle in a box and the highly excited quantum particle in a box.