Chem 3322 homework #6, due March 8, 2024

<u>Problem 1</u> – angular momentum

Angular momentum in classical mechanics measures the 'amount of rotation'. It is analogous to linear momentum, which measures the 'amount of motion'. In classical mechanics, angular momentum is conserved. The definition of angular momentum for a point particle is given by

$$\underline{L} = \underline{r} \times \underline{p} \tag{1}$$

namely by the cross product of the position vector with the (linear) momentum vector.

a) From this definition, show that, in quantum mechanics, the z-component of the angular momentum operator is given by

$$\hat{L}_z = -i\hbar \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right) \tag{2}$$

b) Let us assume that our particle motion is restricted to the x-y plane. In this case, we can transform to plane polar coordinates. The transformations and reverse transformations are

$$\begin{aligned} x &= r\cos\theta & \qquad r &= \sqrt{x^2+y^2} \\ y &= r\sin\theta & \qquad \theta &= \arctan(y/x) \end{aligned} \tag{3}$$

Show that, in plane polar coordinates,

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\theta} \tag{4}$$

Hint: you must use the chain rule

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} \quad \text{and} \quad \frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta} \tag{5}$$

and you will need the derivative of arctan:

$$\frac{\partial \arctan(x)}{\partial x} = \frac{1}{1+x^2} \tag{6}$$

c) For the doubly degenerate excited states of the particle-on-a-ring model, we can write the stationary states in real form (as we did in class) as $\psi_{\text{sin}} = A\sin(n\theta)$ and $\psi_{\text{cos}} = A\cos(n\theta)$ or in complex form as $\psi_+ = Ae^{in\theta}$ and $\psi_- = Ae^{-in\theta}$.

Using ψ_+ determine the value of the normalization constant A. (It is the same value for all 4 wavefunctions.)

d) If we think of the ring as lying in the x-y plane, our transformations from part (b) can be used. Using the transformed $\hat{L}_z$ operator, find the expectation value of the angular momentum for each of the 4 wavefunctions ψ_{sin}, ψ_{cos}, ψ_+, and ψ_-

e) Find the standard deviation of the angular momentum for each of the 4 wavefunctions.

f) Which of the 4 wavefunctions are eigenfunctions of the $\hat{L}_z$ operator? For those that are, give the corresponding eigenvalue. In light of this result, comment on your answers from parts (d) and (e).

g) Explain the results (give a physical interpretation) of parts (d), (e), and (f). Remember that the real forms (ψ_{sin}, ψ_{cos}) and the complex forms (ψ_+, ψ_-) are linear combinations of each other through the Euler relation $e^{i\xi} = \cos\xi + i\sin\xi$.

Problem 2 – **expectation values**

For a particle in a 1d box, use the normalized wavefunctions derived in class to compute

$$a)\ \langle x \rangle \qquad b)\ \langle x^2 \rangle \qquad c)\ \langle p_x \rangle \qquad d)\ \langle p_x^2 \rangle \tag{7}$$

for the ground state. Interpret the results of parts a) and c) physically.

Problem 3 – **uncertainty**

a) Using the results of Problem 2), determine the standard deviations Δx and Δp_x.

b) Find the value of the product $\Delta x\ \Delta p_x$. This kind of product of standard deviations is called an uncertainty product. It can be proved that, for any normalized ψ,

$$\Delta x\ \Delta p_x \geq \frac{\hbar}{2} \tag{8}$$

known as the Heisenberg Uncertainty Principle. Your result should, of course, be consistent with this inequality. Verify this.

<u>Problem 4</u> – particle in a box energies

For the particle in a one dimensional box with quantum number n, work out a) the expected value of the potential energy, b) the expected value of the kinetic energy, and c) compare the sum of these two expected values to the energy value E_n which we calculated in class.

<u>Problem 5</u> – harmonic oscillator energies

Recall the harmonic oscillator model has potential energy $V(x) = m\omega^2 x^2/2$. For the ground state,

$$\psi_0(x) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2} \tag{9}$$

where $\alpha = m\omega/2\hbar$. First, prove (by integrating) that $\psi_0(x)$ is normalized. Next, work out a) the expected value of the potential energy, b) the expected value of the kinetic energy, and c) compare the sum of these two expected values to the energy E_0 which we calculated in class. For the integrals in this question you will need to use integral tables or online resources to help you, for example https://www.wolframalpha.com/