11.4: Problems

Problem 11.4.1

Consider the operator $\hat{A}$ defined in Equation 11.1.1 as $\hat{A} = \hat{x} + \frac{d}{dx}$. Is it linear or non-linear? Justify.

Problem 11.4.2

Which of these functions are eigenfunctions of the operator $-\frac{d^2}{dx^2}$? Give the corresponding eigenvalue when appropriate. In each case k can be regarded as a constant.

$$f_1(x) = e^{ikx}$$

$$f_2(x) = \cos(kx)$$

$$f_3(x) = e^{-kx^2}$$

$$f_4(x) = e^{ikx} - cos(kx)$$

Problem 11.4.3

In quantum mechanics, the x, y and z components of the angular momentum are represented by the following operators:

$$\hat{L}_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_z = -i\hbar\left(\frac{\partial}{\partial\phi}\right)$$

The operator for the square of the magnitude of the orbital angular momentum, $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ is:

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

a) Show that the three 2p orbitals of the H atom are eigenfunctions of both $\hat{L}^2$ and $\hat{L}_z$, and determine the corresponding eigenvalues.

$$\psi_{2p0} = \frac{1}{\sqrt{32\pi a_0^3}} r e^{-r/2a_0}\cos\theta$$

$$\psi_{2p+1} = \frac{1}{\sqrt{64\pi a_0^3}} r e^{-r/2a_0}\sin\theta e^{i\phi}$$

$$\psi_{2p-1} = \frac{1}{\sqrt{64\pi a_0^3}} r e^{-r/2a_0}\sin\theta e^{-i\phi}$$

b) Calculate $\hat{L}_x\psi_{2p0}$. Is ψ_{2p0} and eigenfunction of $\hat{L}_x$?

c) Calculate $\hat{L}_y\psi_{2p0}$. Is ψ_{2p0} and eigenfunction of $\hat{L}_y$?

Problem 11.4.4

Prove that

$$\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$

Problem 11.4.5

For a system moving in one dimension, the momentum operator can be written as

$$\hat{p} = i\hbar\frac{d}{dx}$$

Find the commutator $[\hat{x}, \hat{p}]$

Note: $\hbar$ is defined as $h/2\pi$, where h is Plank's constant. It has been defined because the ratio $h/2\pi$ appears often in quantum mechanics.

Problem 11.4.6

We demonstrated that $\psi_1 s$ is not an eigenfunction of $\hat{T}$. Yet, we can calculate the average kinetic energy of a 1s electron, $\langle T\rangle$. Use Equation $11.3.1$ to calculate an expression for $\langle T\rangle$.

Problem 11.4.7

Use the Hamiltonian of Equation $11.3.5$ to calculate the energy of the electron in the 1s orbital of the hydrogen atom. The normalized wave function of the 1s orbital is:

$$\psi = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

Problem 11.4.8

The expression of Equation $11.3.1$ can be used to obtain the expectation (or average) value of the observable represented by the operator $\hat{A}$.

The state of a particle confined in a one-dimensional box of length a is described by the following wavefunction:

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) & \text{if } 0 \le x \le a \\ 0 & \text{otherwise} \end{cases}$$

The momentum operator for a one-dimensional system was introduced in Problem $11.4.5$.

a) Obtain an expression for $\hat{p}^2$ and determine if ψ is an eigenfunction of $\hat{p}$ and $\hat{p}^2$. If possible, obtain the corresponding eigenvalues.

Hint: $\hat{p}^2$ is the product $\hat{p}\hat{p}$.

b) Determine if ψ is an eigenfuction of $\hat{x}$. If possible, obtain the corresponding eigenvalues.

c) Calculate the following expectation values: $\langle x\rangle$, $\langle p^2\rangle$, and $\langle p\rangle$. Compare with the eigenvalues calculated in the previous questions.