CHEM 312: Home assignment C

C1: In each case, show that $f(x)$ is the eigenfunction of $\hat{A}$.

(a) $\hat{A} = d^2/dx^2, \quad f(x) = \cos(\omega x)$

(b) $\hat{A} = 4d^2/dx^2 + 2d/dx + 7, \quad f(x) = e^{\alpha x}$

Answer

To check whether or not a function is an eigenfunction of an operator, we apply the operator on the function first and then we check whether or not the result is a constant times the original function.

(a)

$$\hat{A}f = \frac{d^2 \cos(\omega x)}{dx^2} = \frac{d}{dx}(-\omega \sin(\omega x)) = -\omega^2 \cos(\omega x) = -\omega^2 f$$

Since the result of $\hat{A}$ on f is a constant $-\omega^2$ times f, this function is an eigenfunction.

(b)

$$\begin{aligned}(4d^2/dx^2 + 2d/dx + 7)e^{\alpha x} &= (4\frac{d^2 e^{\alpha x}}{dx^2} + 2\frac{de^{\alpha x}}{dx} + 7e^{\alpha x}) \\ &= (4\alpha^2 e^{\alpha x} + 2\alpha e^{\alpha x} + 7e^{\alpha x}) = (4\alpha^2 + 2\alpha + 7)e^{\alpha x}\end{aligned}$$

By the same reasoning, $e^{\alpha x}$ is an eigenfunction of the above operator.

C2: (a) Write out the operator $\hat{A}^2$ for $\hat{A} = \frac{d}{dx} + x$.

(b) What is the value of the commutator $\left[x, \frac{d}{dx}\right]$?

[Hint: Make sure to use a test function to get the proper operators]

Answer

(a) We can expand the square of a sum of operators in the same way as we would expand the square of a sum of two numbers

$$(a + b)^2 = a^2 + b^2 + ab + ba$$

except that we cannot write $ab + ba$ as $2ab$, because in general ab is not equal to ba for operators.

$$A^2 = (\frac{d}{dx} + x)^2 = \frac{d^2}{dx^2} + x^2 + x\frac{d}{dx} + \frac{d}{dx}x$$

(b) To calculate a commutator $[\hat{A}, \hat{B}]$, first write out the commutator $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. Next, act with the resulting operator on a general (test) function f. At the end, omit the function f.

$$\left[x, \frac{d}{dx}\right] f = \left(x\frac{d}{dx} - \frac{d}{dx}x\right) f = \left(x\frac{df}{dx} - \frac{dxf}{dx}\right) = \left(x\frac{df}{dx} - x\frac{df}{dx} - f\right) = (-1)f$$

$$\left[x, \frac{d}{dx}\right] = -1$$

C3: A quantum object moving in one dimension, between $-\infty \leq x \leq \infty$, is in a state represented by the wave function:

$$\psi(x) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{ax^2}{2}},$$

where a is a constant. Evaluate the average value of the kinetic energy of the object in this state. See the inside of the back cover of the textbook for the required integrals.

Answer

The expectation value of the kinetic energy operator is

$$\left\langle \hat{T} \right\rangle = \int_{-\infty}^{\infty} \psi^* \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi dx$$

Insert $\psi(x)$ is this equation to get

$$\left\langle \hat{T} \right\rangle = \int_{-\infty}^{\infty} \left(\left(\frac{a}{\pi}\right)^{1/4} e^{-\frac{ax^2}{2}}\right) \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) \left(\left(\frac{a}{\pi}\right)^{1/4} e^{-\frac{ax^2}{2}}\right) dx$$

$$= -\frac{\hbar^2}{2m}\left(\frac{a}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\frac{ax^2}{2}} \frac{d^2}{dx^2} e^{-\frac{ax^2}{2}} dx$$

Notice that since the function $\psi(x)$ is a real function, $\psi(x)^* = \psi(x)$. It is always convenient to factor all the constants out, as done in the last step above.

Calculate the second derivative of the wavefunction in the integrand

$$\int_{-\infty}^{\infty} (e^{-\frac{ax^2}{2}})(\frac{d}{dx})(-axe^{-\frac{ax^2}{2}})dx = \int_{-\infty}^{\infty} (e^{-\frac{ax^2}{2}})(-ae^{-\frac{ax^2}{2}} + a^2x^2e^{-\frac{ax^2}{2}})dx$$

$$\int_{-\infty}^{\infty} (-ae^{-ax^2} + a^2x^2e^{-ax^2})dx = \left[-a\int_{-\infty}^{\infty} e^{-ax^2}dx + a^2\int_{-\infty}^{\infty} x^2e^{-ax^2}dx\right]$$

The two integrals on the right hand side can be found on the inside back cover of the textbook. Notice that the integrand e^{-ax^2} is an even function so the integral from $-\infty$ to zero has the same value as the integral from zero to ∞.

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = 2\int_0^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = 2\int_0^{\infty} e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}}$$

After inserting the values of the integrals and simplifying, the end result is

$$\left\langle \hat{T} \right\rangle = \frac{\hbar^2 a}{4m}$$

Note 1: The result has to be a positive number, because kinetic energy is a positive quantity. The wavefunction is defined on the domain $(-\infty, \infty)$. In order for e^{-ax^2} to vanish at infinity (requirement of a proper wavefunction) a has to be a positive number.

Note 2: Whenever we use special functions like exponential or sine functions, the argument of the function should be unit-less. For example, ax^2 in e^{-ax^2} is unit-less, which means a has the dimension of $1/\text{Length}^2$. Check the dimension of the expectation value of the kinetic energy above!

C4: Can the position and kinetic energy operators have simultaneous eigenfunctions? Justify your answer.

Answer

If two operators commute, it is possible to find a function that is the simultaneous eigenfunction of the two operators. The opposite is also true: if two operators do not commute, it is not possible at all to find such a function. So to answer this question we need to calculate the commutator of the position and kinetic energy operators.

$$\left[x, \hat{T}\right] f = \left[x, -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right] f = -\frac{\hbar^2}{2m}\left(x\frac{d^2 f}{dx^2} - \frac{d^2 x f}{dx^2}\right) = -\frac{\hbar^2}{2m}\left(x\frac{d^2 f}{dx^2} - x\frac{d^2 f}{dx^2} - 2\frac{df}{dx}\right) = \left(\frac{\hbar^2}{m}\frac{d}{dx}\right) f$$

$$\left[x, \hat{T}\right] = \frac{\hbar^2}{m}\frac{d}{dx}$$