CEM 991 **Fall 2021**

Assignment No. 4 (25 pts.) **Due Date: November 5, 2021 (Friday)**

1. (8 pts.) The x, y, and z components of the angular momentum operator $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}} = -i\hbar(\hat{\mathbf{r}} \times \boldsymbol{\nabla})$ satisfy the following commutation relationships:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \tag{1}$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \tag{2}$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y. \tag{3}$$

Use the formulas

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \tag{4}$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \tag{5}$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \tag{6}$$

and the values of the elementary commutators involving the coordinate and momentum operators ($[\hat{x}, \hat{p}_x] = \imath\hbar\mathbf{1}$, $[\hat{x}, \hat{p}_y] = 0$, etc.) to prove Eq. (1). Then, use Eqs. (1)–(3) and algebraic properties of the commutator to show that $[\hat{L}^2, \hat{L}_z] = 0$, where $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$.
Hint: Use the following properties of the commutator: $[\hat{F}_1\hat{F}_2, \hat{G}] = \hat{F}_1[\hat{F}_2, \hat{G}] + [\hat{F}_1, \hat{G}]\hat{F}_2$ and $[\hat{F}_1\hat{F}_2, \hat{G}_1\hat{G}_2] = \hat{F}_1\hat{G}_1[\hat{F}_2, \hat{G}_2] + \hat{F}_1[\hat{F}_2, \hat{G}_1]\hat{G}_2 + \hat{G}_1[\hat{F}_1, \hat{G}_2]\hat{F}_2 + [\hat{F}_1, \hat{G}_1]\hat{G}_2\hat{F}_2$.

2. (6 pts.) Consider an operator

$$\hat{A} = \alpha\frac{\partial}{\partial x}, \tag{7}$$

where α is a complex number.

   (a) Find $\hat{A}^\dagger$ (the adjoint of $\hat{A}$).

   (b) Find values of α for which $\hat{A}$ becomes a Hermitian operator. Compare the result with an operator representing the x-component of the momentum $\mathbf{p}$. Please comment (briefly).

3. (6 pts.) Let A be the bounded linear operator whose domain is the entire Hilbert space $\mathscr{H}$ (so that you do not have to worry about the importance of domain in your calculations).

   (a) Show that $A^{\dagger\dagger} = A$ [$A^{\dagger\dagger}$ is defined as $(A^\dagger)^\dagger$].

   (b) Assume that operator A is unitary, so that $(Af, Ag) = (f, g)$ for every f, $g \in \mathscr{H}$. Show that each eigenvalue of the unitary operator A has an absolute value equal 1 (one).

4. (5 pts.) Use the equation

$$[\hat{x}, \hat{H}] = \frac{i\hbar}{m}\,\hat{p}_x \tag{8}$$

(cf. Problem 4 of Assignment No. 3) to prove that the expectation value of the momentum operator $\hat{p}_x$ in the state $u = u(x)$, which is an eigenstate of the Hamiltonian $\hat{H} = \frac{\hat{p}_x^2}{2m} + \hat{V}(x)$, where $V(x)$ is an arbitrary potential function, is zero.

SOLUTIONS

1. $$[\hat{L}_x, \hat{L}_y] = [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z]$$

$$= [\hat{y}\hat{p}_z, \hat{z}\hat{p}_x] - [\hat{y}\hat{p}_z, \hat{x}\hat{p}_z]$$

$$- [\hat{z}\hat{p}_y, \hat{z}\hat{p}_x] + [\hat{z}\hat{p}_y, \hat{x}\hat{p}_z]$$

Using the properties in the Hint, we obtain

$$[\overset{F_1}{\hat{y}}\,\overset{F_2}{\hat{p}_z}, \overset{G_1}{\hat{z}}\,\overset{G_2}{\hat{p}_x}] = \hat{y}\hat{z}\cancelto{0}{[\hat{p}_z, \hat{p}_x]} + \hat{y}[\hat{p}_z, \hat{z}]\hat{p}_x$$

$$+ \hat{z}\cancelto{0}{[\hat{y}, \hat{p}_x]}\hat{p}_z + \cancelto{0}{[\hat{y}, \hat{z}]}\hat{p}_x\hat{p}_z$$

$$= -\hat{y}\underbrace{[\hat{z}, \hat{p}_z]}_{i\hbar}\hat{p}_x = -i\hbar\,\hat{y}\hat{p}_x$$

$$[\underset{F_1}{\hat{y}}\,\underset{F_2}{\hat{p}_z},\ \underset{G_1}{\hat{x}}\,\underset{G_2}{\hat{p}_z}] = \hat{y}\hat{x}\cancelto{0}{[\hat{p}_z, \hat{p}_z]}$$

$$+\ \hat{y}\cancelto{0}{[\hat{p}_z, \hat{x}]}\hat{p}_z + \hat{x}\cancelto{0}{[\hat{y}, \hat{p}_z]}\hat{p}_z$$

$$+\ \cancelto{0}{[\hat{y}, \hat{x}]}\hat{p}_z^{\,2} = 0$$

$$[\underset{F_1}{\hat{z}}\,\underset{F_2}{\hat{p}_y},\ \underset{G_1}{\hat{z}}\,\underset{G_2}{\hat{p}_x}] = \hat{z}^2\cancelto{0}{[\hat{p}_y, \hat{p}_x]} + \hat{z}\cancelto{0}{[\hat{p}_y, \hat{z}]}\hat{p}_x$$

$$+\ \hat{z}\cancelto{0}{[\hat{z}, \hat{p}_x]}\hat{p}_y + \cancelto{0}{[\hat{z}, \hat{z}]}\hat{p}_x\hat{p}_y = 0$$

$$[\underset{F_1}{\hat{z}}\,\underset{F_2}{\hat{p}_y},\ \underset{G_1}{\hat{x}}\,\underset{G_2}{\hat{p}_z}] = \hat{z}\hat{x}\cancelto{0}{[\hat{p}_y, \hat{p}_z]} + \hat{z}\cancelto{0}{[\hat{p}_y, \hat{x}]}\hat{p}_z$$

$$+\ \hat{x}[\hat{z}, \hat{p}_z]\hat{p}_y + \cancelto{0}{[\hat{z}, \hat{x}]}\hat{p}_z\hat{p}_y$$

$$= \hat{x}\underbrace{[\hat{z}, \hat{p}_z]}_{i\hbar}\hat{p}_y = i\hbar\,\hat{x}\hat{p}_y\ .$$

Thus,

$$[\hat{L}_x, \hat{L}_y] = -i\hbar\,\hat{y}\hat{p}_x + i\hbar\,\hat{x}\hat{p}_y$$

$$= i\hbar\left(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right) = i\hbar\,\hat{L}_z .$$

We now calculate $[\hat{L}^2, \hat{L}_z]$. Using the properties of the commutator mentioned in the Hint, we obtain,

$$[\hat{L}^2, \hat{L}_z] = [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_z]$$

$$= [\overset{F_1F_2}{\hat{L}_x^2}, \overset{G}{\hat{L}_z}] + [\overset{F_1F_2}{\hat{L}_y^2}, \overset{G}{\hat{L}_z}]$$

$$+ \cancelto{0}{[\hat{L}_z^2, \hat{L}_z]} = \hat{L}_x[\hat{L}_x, \hat{L}_z]$$

$$+ [\hat{L}_x, \hat{L}_z]\,\hat{L}_x + \hat{L}_y[\hat{L}_y, \hat{L}_z]$$

$$+ \ [\hat{L}_y, \hat{L}_z]\hat{L}_y.$$

Using Eqs. (2) and (3), we obtain,

$$[\hat{L}^2, \hat{L}_z] = -\hat{L}_x[\hat{L}_z, \hat{L}_x] - [\hat{L}_z, \hat{L}_x]\hat{L}_x$$

$$+ \ \hat{L}_y[\hat{L}_y, \hat{L}_z] + [\hat{L}_y, \hat{L}_z]\hat{L}_y$$

$$= -\cancel{i\hbar\hat{L}_x\hat{L}_y} - \cancel{i\hbar\hat{L}_y\hat{L}_x}$$

$$+ \ \cancel{i\hbar\hat{L}_y\hat{L}_x} + \cancel{i\hbar\hat{L}_x\hat{L}_y}$$

$$= 0.$$

Thus,

$$[\hat{L}^2, \hat{L}_z] = 0,$$

which is what we had to show.

2. (a) We know that

$$\hat{A}^{\dagger} = \left(\alpha \frac{\partial}{\partial x}\right)^{\dagger} = \alpha^{*}\left(\frac{\partial}{\partial x}\right)^{\dagger}.$$

Let us find out what is $\left(\frac{\partial}{\partial x}\right)^{\dagger}$.

In general, the operator $\hat{F}^{\dagger}$ is defined by the condition

$$\int_{\Gamma} \varphi^{*}(\hat{F}\psi)\,d\tau = \int_{\Gamma} (\hat{F}^{\dagger}\varphi)^{*}\psi\,d\tau.$$

In our case, $\hat{F} = \frac{\partial}{\partial x}$, so that

$$\int_{\mathbb{R}^3} \varphi^{*}\left(\frac{\partial}{\partial x}\psi\right) dx\,dy\,dz =$$

$$= \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dx\,\varphi^{*}\frac{\partial\psi}{\partial x} \quad \underline{\underline{\text{integrating by parts}}}$$

$$= \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \left\{ \underbrace{\varphi^{*}\psi\Big|_{x=-\infty}^{x=\infty}}_{=0} - \int_{-\infty}^{\infty}\left(\frac{\partial\varphi}{\partial x}\right)^{*}\psi\,dx \right.$$

$$= -\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dx \left(\frac{\partial \varphi}{\partial x}\right)^* \psi$$

$$= \int_{\mathbb{R}^3} \left(-\frac{\partial}{\partial x}\varphi\right)^* \psi \, d\tau = \int_{\mathbb{R}^3} \left[\left(\frac{\partial}{\partial x}\right)^{\dagger} \varphi\right]^* \psi \, d\tau.$$

Thus, $$\left(\frac{\partial}{\partial x}\right)^{\dagger} = -\frac{\partial}{\partial x},$$

which means that

$$\hat{A}^{\dagger} = -\alpha^* \frac{\partial}{\partial x}.$$

$\therefore$

(b) From the condition $\hat{A}^{\dagger} = A$,

we obtain

$$\alpha \frac{\partial}{\partial x} = -\alpha^* \frac{\partial}{\partial x},$$

so that $\hat{A}$ is Hermitian if and only if (iff)

$$\alpha = -\alpha^*.$$

If $\alpha = a + bi$ $(a = \mathrm{Re}\,\alpha,\ b = \mathrm{Im}\,\alpha)$,
then

$$a + bi = -(a - bi) = -a + bi,$$

which implies that $a = 0$. Thus, $\hat{A}$ is Hermitian iff

$$\alpha = bi, \text{ where } b \text{ is a real}$$

number.

You know that

$$\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x} = -i\hbar\frac{\partial}{\partial x}.$$

Clearly, $\hat{p}_x$ is Hermitian, since in this case we can write,

$$\hat{p}_x = \alpha\frac{\partial}{\partial x}, \quad \alpha = -\hbar i$$

($\hbar$ is real).

Moreover, if we are interested in finding operators that might represent

$\hat{p}_x$ and that have the form

$$\alpha \frac{\partial}{\partial x},$$

we can ~~immediately~~ narrow our search to operators of the form

$$ib\frac{\partial}{\partial x}, \quad b\text{ - real},$$

since otherwise we would have to deal with operators that are not Hermitian.
(from this point of view, $b = -\hbar$ is a constant that guarantees the Hermiticity of $\hat{p}_x$).

3. (a) Consider

$$(A^{\dagger\dagger}f, g) = ((A^{\dagger})^{\dagger}f, g) \quad \text{turn-over-rule}$$

$$= (f, A^{\dagger}g) = (A^{\dagger}g, f)^{*} \quad \text{turn-over-rule}$$

$$= (g, Af)^{*} = (Af, g).$$

Thus,

$$(A^{\dagger\dagger}f, g) = (Af, g) \quad \forall_{f,g \in \mathcal{H}}$$

and, in consequence,

$$A^{\dagger\dagger}f = Af \quad \forall_{f \in \mathcal{H}}$$

$$\underline{\underline{A^{\dagger\dagger} = A}}.$$

(b) Consider

$$(Af, Af) = \|Af\|^2 .$$ For a unitary A,

$$(Af, Af) = (f, f) = \|f\|^2 .$$

Thus,

$$\|Af\| = \|f\| . \qquad (\star)$$

Assume that f is an eigenvector of A,

$$Af = \lambda f \quad , \quad \lambda \text{ - eigenvalue.}$$

We obtain,

$$\|Af\| = \|\lambda f\| = |\lambda| \, \|f\| \overset{\text{Eq.}}{\underset{(\star)}{=}} \|f\| .$$

Thus,

$$|\lambda| \, \|f\| = \|f\| .$$ Since $f \neq \Theta$ (f is an eigenvector, cannot be Θ), $\underline{|\lambda| = 1}$.

4. We have to calculate,

$$\langle \hat{p}_x \rangle \equiv \int_{-\infty}^{\infty} u^*(x)\, \hat{p}_x\, u(x)\, dx = (u, \hat{p}_x u),$$

where

$$\hat{H} u = E u .$$

According to the results of Problem 4 of Assignment No. 3, we can write,

$$[\hat{x}, \hat{H}] = \frac{i\hbar}{m} \hat{p}_x , \quad \text{or}$$

$$\hat{p}_x = \frac{m}{i\hbar} [\hat{x}, \hat{H}] .$$

Thus,

$$\langle \hat{p}_x \rangle = (u, \hat{p}_x u) =$$

$$= \frac{m}{i\hbar} (u, [\hat{x}, \hat{H}] u) =$$

$$= \frac{m}{i\hbar} (u, (\hat{x}\hat{H} - \hat{H}\hat{x}) u) =$$

$$= \frac{m}{i\hbar} \{ (u, \hat{x}\hat{H} u) - (u, \hat{H}\hat{x} u) \}$$

$$\xlongequal[\hat{H}\text{-hermitian}]{\hat{H}u=Eu} \frac{m}{i\hbar}\left\{(u, E\hat{x}u) - (\hat{H}u, \hat{x}u)\right\}$$

$$\xlongequal[E\text{-real}]{\hat{H}u=Eu} \frac{m}{i\hbar}\left\{E(u,\hat{x}u) - E(u,\hat{x}u)\right\}$$

$$= 0,$$

where we used the fact that $\hat{H}$ is hermitian (turn-over rule) and the fact that E is a real number.

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