Homework 9 - Operators

Question 1:

We define the commutator of two operators $\hat{A}$ and $\hat{B}^{\wedge}$ by $\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$. Prove the following identities:

1. $\left[\hat{A},\hat{B}\right]=-\left[\hat{B},\hat{A}\right]$.
2. $\left[\hat{A},\hat{A}\right]=0$.
3. $\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]=0$.
4. $\left[\hat{A},\hat{B}\hat{C}\right]=\hat{B}\left[\hat{A},\hat{C}\right]+\left[\hat{A},\hat{B}\right]\hat{C}$.
5. $\left[\hat{A}\hat{B},\hat{C}\right]=\hat{A}\left[\hat{B},\hat{C}\right]+\left[\hat{A},\hat{C}\right]\hat{B}$.
6. If $\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]=\left[\hat{B},\left[\hat{A},\hat{B}\right]\right]=0$, then

$$\left[\hat{A}^{n},\hat{B}\right]=n\hat{A}^{n-1}\left[\hat{A},\hat{B}\right]\qquad\text{and}\qquad\left[\hat{A},\hat{B}^{n}\right]=n\hat{B}^{n-1}\left[\hat{A},\hat{B}\right],$$

and therefore if $F\left(\hat{B}\right)$ is an analytical function of $\hat{B}$ we get:

$$\left[\hat{A},F\left(\hat{B}\right)\right]=\frac{dF\left(\hat{B}\right)}{d\hat{B}}\left[\hat{A},\hat{B}\right].$$

Solution:

1. $\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}=-\left(\hat{B}\hat{A}-\hat{A}\hat{B}\right)=-\left[\hat{B},\hat{A}\right]$.
2. $\left[\hat{A},\hat{A}\right]=\hat{A}\hat{A}-\hat{A}\hat{A}=0$.
3. Opening the commutators

$$\begin{aligned}\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]&=\left[\hat{A},\hat{B}\hat{C}\right]-\left[\hat{A},\hat{C}B\right]+\left[\hat{C},\hat{A}\hat{B}\right]-\left[\hat{C},B\hat{A}\right]+\left[\hat{B},\hat{C}\hat{A}\right]-\left[B,\hat{A}\hat{C}\right]\\&=\underline{\hat{A}\hat{B}\hat{C}}-\underline{\underline{\hat{B}\hat{C}\hat{A}}}-\underline{\underline{\underline{\hat{A}\hat{C}\hat{B}}}}+\overline{\hat{C}\hat{B}\hat{A}}+\overline{\overline{\hat{C}\hat{A}\hat{B}}}-\underline{\hat{A}\hat{B}\hat{C}}\\&\quad-\overline{\hat{C}\hat{B}\hat{A}}+\overline{\overline{\overline{\hat{B}\hat{A}\hat{C}}}}+\underline{\underline{\hat{B}\hat{C}\hat{A}}}-\overline{\overline{\hat{C}\hat{A}\hat{B}}}-\overline{\overline{\overline{\hat{B}\hat{A}\hat{C}}}}+\underline{\underline{\underline{\hat{A}\hat{C}\hat{B}}}}\\&=0.\end{aligned}$$

4. $\left[\hat{A},\hat{B}\hat{C}\right]=\hat{A}\hat{B}\hat{C}-\hat{B}\hat{C}\hat{A}=\hat{A}\hat{B}\hat{C}-\hat{B}\hat{A}\hat{C}+\hat{B}\hat{A}\hat{C}-\hat{B}\hat{C}\hat{A}=\left(\hat{A}\hat{B}-\hat{B}\hat{A}\right)\hat{C}+\hat{B}\left(\hat{A}\hat{C}-\hat{C}\hat{A}\right)=\left[\hat{A},\hat{B}\right]\hat{C}+\hat{B}\left[\hat{A},\hat{C}\right]$.

5. $\left[\hat{A}\hat{B},\hat{C}\right] = \hat{A}\hat{B}\hat{C} - \hat{C}\hat{A}\hat{B} = \hat{A}\hat{B}\hat{C} - \hat{A}\hat{C}\hat{B} + \hat{A}\hat{C}\hat{B} - \hat{C}\hat{A}\hat{B} = \hat{A}\left(\hat{B}\hat{C} - \hat{C}\hat{B}\right) + \left(\hat{A}\hat{C} - \hat{C}\hat{A}\right)\hat{B} = \hat{A}\left[\hat{B},\hat{C}\right] + \left[\hat{A},\hat{C}\right]\hat{B}$.

6. Checking for $n = 1$ is trivial, then assuming this holds for $n-1$ we have

$$\begin{aligned}
\left[\hat{A}^n,\hat{B}\right] &= \hat{A}^{n-1}\left[\hat{A},\hat{B}\right] + \left[\hat{A}^{n-1},\hat{B}\right]\hat{A} \\
&= \hat{A}^{n-1}\left[\hat{A},\hat{B}\right] + (n-1)\,\hat{A}^{n-2}\left[\hat{A},\hat{B}\right]\hat{A} \\
&= \hat{A}^{n-1}\left[\hat{A},\hat{B}\right] + (n-1)\,\hat{A}^{n-2}\left(\hat{A}\left[\hat{A},\hat{B}\right] - \cancel{\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]}\right) \\
&= n\hat{A}^{n-1}\left[\hat{A},\hat{B}\right],
\end{aligned}$$

where we used $\hat{C}\hat{A} = \hat{A}\hat{C} - \left[\hat{A},\hat{C}\right]$, with $\hat{C} = \left[\hat{A},\hat{B}\right]$. Similarly,

$$\begin{aligned}
\left[\hat{A},\hat{B}^n\right] &= \hat{B}^{n-1}\left[\hat{A},\hat{B}\right] + \left[\hat{A},\hat{B}^{n-1}\right]\hat{B} \\
&= \hat{B}^{n-1}\left[\hat{A},\hat{B}\right] + (n-1)\,\hat{B}^{n-2}\left[\hat{A},\hat{B}\right]\hat{B} \\
&= n\hat{B}^{n-1}\left[\hat{A},\hat{B}\right].
\end{aligned}$$

Question 2:

Given an operator $\hat{A}$, we define it's hermitian conjugate,$\hat{A}^\dagger$ such that $\left\langle \psi_1|\hat{A}\psi_2\right\rangle = \left\langle \hat{A}^\dagger\psi_1|\psi_2\right\rangle$.

1. Show that if $\hat{A} = a$ (just multiplication by a scalar) then $\hat{A}^\dagger = a^*$.
2. Find the Hermitian conjugate of the derivative operator $\hat{D} \equiv \frac{\partial}{\partial x}$.

   An Hermitian operator is an operator that satisfies $\hat{A}^\dagger = \hat{A}$.

3. Let $\hat{A}$ and $\hat{B}$ be two Hermitian operators. We define the operator $\hat{C} \equiv \hat{A} + i\hat{B}$. Is this operator Hermitian? If not, find its Hermitian conjugate $\hat{C}^\dagger$.
4. Given two commuting operators $\hat{A}$ and $\hat{B}$, and let φ be an eigenstate of $\hat{B}$ with eigenvalue b. Show that $\hat{A}\varphi$ is also an eigenstate of $\hat{B}$, with the same eigenvalue b.
5. From (4), deduce that if b is non-degenerate (there is only one eigenstate associated with it), then φ is also an eigenstate of $\hat{A}$.

Solution:

1. Since $\left\langle \psi|\hat{A}\psi\right\rangle = a\left\langle \psi|\psi\right\rangle$, then $\left\langle \psi|\hat{A}\psi\right\rangle = \left\langle \hat{A}^\dagger\psi|\psi\right\rangle = a^*\left\langle \psi|\psi\right\rangle$. Thus $\boxed{\hat{A}^\dagger = a^*}$.
2. Using the fact that $\hat{p} = -i\hbar\hat{D}$ is Hermitian,

$$\hat{p}^\dagger = \hat{p} \quad \rightarrow \quad i\hbar\hat{D}^\dagger = -i\hbar\hat{D} \quad \rightarrow \quad \boxed{\hat{D}^\dagger = -\hat{D}}.$$

3. Taking the Hermitian conjugate

$$\hat{C}^\dagger = \hat{A}^\dagger - i\hat{B}^\dagger = \hat{A} - i\hat{B} \neq \hat{C},$$

   we see that $\hat{C}$ is not Hermitian.

4. Taking the inner product

$$\left[\hat{A},\hat{B}\right]|\varphi\rangle = \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)|\varphi\rangle = 0 \quad \rightarrow \quad \hat{B}\hat{A}\,|\varphi\rangle = b\hat{A}\,|\varphi\rangle\,,$$

   thus $\hat{A}\,|\varphi\rangle$ is also an eigenvector of $\hat{B}$ with an eigenvalue b.

5. If b has only one eigenstate, then
$$b\hat{A}\left|\varphi\right\rangle \neq b\left|\varphi\right\rangle,$$
which means that $\left|\varphi\right\rangle$ must be an eigenstate of $\hat{A}$ with some eigenvalue a such that
$$b\hat{A}\left|\varphi\right\rangle = ab\left|\varphi\right\rangle \neq b\left|\varphi\right\rangle.$$

Question 3:

Consider a three-dimensional vector space spanned by an orthonormal basis $\left|1\right\rangle, \left|2\right\rangle, \left|3\right\rangle$. Kets $\left|\alpha\right\rangle$ and $\left|\beta\right\rangle$ are given by
$$\left|\alpha\right\rangle = i\left|1\right\rangle - 2\left|2\right\rangle - i\left|3\right\rangle \quad \text{and} \quad \left|\beta\right\rangle = i\left|1\right\rangle + 2\left|3\right\rangle.$$

1. Construct $\left\langle\alpha\right|$ and $\left\langle\beta\right|$ in terms of the dual basis $\left\langle 1\right|, \left\langle 2\right|, \left\langle 3\right|$.
2. Find $\langle\alpha|\beta\rangle$ and $\langle\beta|\alpha\rangle$, and confirm that $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$.
3. Find all nine matrix elements of the operator $\hat{A} \equiv \left|\alpha\right\rangle\left\langle\beta\right|$, in this basis, and construct the matrix A. Is it Hermitian?

Solution:

1. Using the fact that $\langle\alpha|\alpha\rangle = 1$, hence $\left\langle\alpha\right| = \left|\alpha\right\rangle^\dagger$, taking the Hermitian conjugate we find
$$\boxed{\left\langle\alpha\right| = -i\left\langle 1\right| - 2\left\langle 2\right| + i\left\langle 3\right| \quad \text{and} \quad \left\langle\beta\right| = -i\left\langle 1\right| + 2\left\langle 3\right|}.$$

2. Taking the inner products we find
$$\boxed{\langle\alpha|\beta\rangle = 1 + 2i \quad \text{and} \quad \langle\beta|\alpha\rangle = 1 - 2i = \langle\alpha|\beta\rangle^*}.$$

3. Representing the operator $\hat{A}$ as a matrix that acts on the vector space states,
$$\hat{A}\left|\psi\right\rangle = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} \left|1\right\rangle \\ \left|2\right\rangle \\ \left|3\right\rangle \end{pmatrix},$$
we can find the elements by taking the inner products $\left\langle i|\hat{A}|i\right\rangle$:
$$A_{11} = \langle 1|\alpha\rangle\langle\beta|1\rangle = (i)(-i) = 1; \quad A_{21} = \langle 1|\alpha\rangle\langle\beta|1\rangle = (i)(0) = 0; \quad A_{31} = \langle 1|\alpha\rangle\langle\beta|1\rangle = (i)(2) = 2i;$$
$$A_{12} = \langle 1|\alpha\rangle\langle\beta|2\rangle = (-2)(-i) = 2i; \quad A_{22} = \langle 1|\alpha\rangle\langle\beta|1\rangle = (-2)(0) = 0; \quad A_{32} = \langle 1|\alpha\rangle\langle\beta|1\rangle = (-2)(2) = -4;$$
$$A_{13} = \langle 1|\alpha\rangle\langle\beta|3\rangle = (-i)(-i) = -1; \quad A_{23} = \langle 1|\alpha\rangle\langle\beta|1\rangle = (-i)(0) = 0; \quad A_{33} = \langle 1|\alpha\rangle\langle\beta|1\rangle = (-i)(2) = -2i.$$
thus
$$A = \begin{pmatrix} 1 & 0 & 2i \\ 2i & 0 & -4 \\ -1 & 0 & -2i \end{pmatrix},$$
which is singular and therefore is not Hermitian.

Question 4:

Prove the uncertainty principle, relating the uncertainty in position to the uncertainty in energy:
$$\sigma_x\sigma_H \geq \frac{\hbar}{2m}\left|\langle p\rangle\right|.$$
For stationary states this does not tell you much—why not?

Solution:

Using the generalized uncertainty principle

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \left\langle \left[\hat{A}, \hat{B} \right] \right\rangle \right)^2,$$

calculating the commutator

$$\left[\hat{x}, \frac{\hat{p}^2}{2m} + V(\hat{x}) \right] = \frac{1}{2m} \left[\hat{x}, \hat{p}^2 \right] + \cancel{\left[\hat{x}, V(\hat{x}) \right]} = \frac{1}{2m} \left(\left[\hat{x}, \hat{p} \right] \hat{p} + \hat{p} \left[\hat{x}, \hat{p} \right] \right) = \frac{i\hbar \hat{p}}{m},$$

we find

$$\boxed{\sigma_x \sigma_H \geq \frac{\hbar}{2m} \left| \langle p \rangle \right|}.$$

For stationary states $\sigma_H = 0$ and $\langle p \rangle = 0$, then we get the trivial relation $0 \geq 0$.

Question 5:

1. Use the generalized Ehrenfest theorem

$$\frac{d}{dt} \langle Q \rangle = \frac{i}{\hbar} \left\langle \left[\hat{H}, \hat{Q} \right] \right\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle,$$

   to show that

$$\frac{d}{dt} \langle xp \rangle = 2 \langle T \rangle - \left\langle x \frac{\partial V}{\partial x} \right\rangle,$$

   where T is the kinetic energy.

2. In a stationary state the left side is zero (why?) so

$$2 \langle T \rangle = \left\langle x \frac{\partial V}{\partial x} \right\rangle.$$

   This is called the *virial theorem*. Use it to prove that $\langle T \rangle = \langle V \rangle$ for stationary states of the harmonic oscillator.

Solution:

1. Replacing Q with xp we have

$$\begin{aligned} \frac{d}{dt} \langle xp \rangle &= \frac{i}{\hbar} \left\langle \left[\hat{H}, \hat{x}\hat{p} \right] \right\rangle + \cancel{\left\langle \frac{\partial (\hat{x}\hat{p})}{\partial t} \right\rangle} \\ &= \frac{i}{\hbar} \left\langle \left[\frac{\hat{p}^2}{2m} + V(\hat{x}), \hat{x}\hat{p} \right] \right\rangle \\ &= \frac{i}{\hbar} \left(\left\langle \frac{1}{2m} \left[\hat{p}^2, \hat{x}\hat{p} \right] \right\rangle + \langle [V(\hat{x}), \hat{x}\hat{p}] \rangle \right). \end{aligned}$$

   Now,

$$\begin{aligned} \left[\hat{p}^2, \hat{x}\hat{p} \right] &= \hat{x} \cancel{\left[\hat{p}^2, \hat{p} \right]} + \left[\hat{p}^2, \hat{x} \right] \hat{p} = -2i\hbar \hat{p}^2, \\ [V(\hat{x}), \hat{x}\hat{p}] &= \hat{x} [V(\hat{x}), \hat{p}] + \cancel{[V(\hat{x}), \hat{x}]} \hat{p} = i\hbar \hat{x} \frac{\partial V}{\partial x}, \end{aligned}$$

   where we used the property $[f, \hat{p}] = i\hbar \partial f / \partial x$. Thus

$$\frac{d}{dt} \langle xp \rangle = \frac{i}{\hbar} \left(\left\langle -\frac{1}{2m} 2i\hbar p^2 \right\rangle + \left\langle i\hbar x \frac{\partial V}{\partial x} \right\rangle \right) = 2 \langle T \rangle - \left\langle x \frac{\partial V}{\partial x} \right\rangle,$$

   where $\hat{T} \equiv \hat{p}^2 / 2m$.

2. For stationary states all expectation values are time-independent, thus

$$2\langle T\rangle = \left\langle x\frac{\partial V}{\partial x}\right\rangle,$$

calculating the right-hand-side, for harmonic oscillator we find

$$\left\langle x\frac{\partial V}{\partial x}\right\rangle = \left\langle 2m\omega^2 x^2\right\rangle = 2\langle V\rangle \quad \rightarrow \quad \boxed{\langle T\rangle = \langle V\rangle}.$$