Tutorial 9 - Operators

Hilbert Space

Quantum theory is based on two constructs: *wave functions* and *operators*. Mathematically, wave functions satisfy the defining conditions for abstract *vectors*, and operators act on them as *linear transformations*. So the natural language of quantum mechanics is *linear algebra*. However, in quantum mechanics the “vectors” we encounter are (for the most part) *functions*, who live in *infinite*-dimensional spaces. For physical states we limit ourselves to

$$f(x) \quad \text{such that} \quad \int_a^b |f(x)|^2 \, dx < \infty,$$

also known as $L^2(a,b) = L^2(\Omega,\alpha)$ or *Hilbert space*.

Question 1:

1. For what range of ν is the function $f(x) = x^\nu$ in Hilbert space, on the interval $(0,1)$? Assume ν is real, but not necessarily positive.
2. For the specific case $\nu = 1/2$, is $f(x)$ in this Hilbert space? What about $xf(x)$? How about $\frac{d}{dx}f(x)$?

Solution:

1. Taking the inner product

$$\langle f(x) | f(x) \rangle = \int_0^1 f^* f dx = \int_0^1 x^{2\nu} dx = \frac{1 - 0^{2\nu+1}}{2\nu+1},$$

   the second term is 0 only if $2\nu + 1 > 0$, i.e. $\nu > -1/2$. For the case of $\nu = -1/2$ we have

$$\langle f(x) | f(x) \rangle = \int_0^1 x^{-1} dx = \ln(1) - \ln(0) = 0 + \infty,$$

   thus $f(x) = x^\nu$ is only in Hilbert space if $\boxed{\nu > -1/2}$.

2. From (1) we see that for $\nu = 1/2$ the function $f(x)$ is in Hilbert space.
   In a similar way $xf(x) = x^{3/2}$ is also in Hilbert space, but $df/dx = x^{-1/2}$ is not.

Hermitian Operators - Observables

Given a Hilbert space $L^2(\Omega,\alpha)$ with an inner product $\langle \cdot | \cdot \rangle$, and a continuous linear operator $\hat{Q}$, there exist an operator $\hat{Q}^\dagger$ which follows

$$\left\langle f | \hat{Q} g \right\rangle = \left\langle \hat{Q}^\dagger f | g \right\rangle,$$

where $\hat{Q}^\dagger$ is known as the *Hermitian conjugate* of $\hat{Q}$. If $\hat{Q} = \hat{Q}^\dagger$ then it is said that $\hat{Q}$ is a *Hermitian operator*. Since any measured physical quantity must be real, we require that all observables are represented via Hermitian operators.

Question 2:

Prove that the eigenvalues of an Hermitian operator are real.

Solution:

Considering a Hermitian operator $\hat{Q}$ with the eigenvalues equation

$$\hat{Q}\left|\psi_n\right\rangle = q_n\left|\psi_n\right\rangle .$$

Taking the inner product of this equation with $\langle\psi_n|$ we find

$$\left\langle\psi_n|\hat{Q}\psi_n\right\rangle = q_n\left\langle\psi_n|\psi_n\right\rangle \quad \text{and also} \quad \left\langle\psi_n|\hat{Q}\psi_n\right\rangle = \left\langle\hat{Q}\psi_n|\psi_n\right\rangle = q_n^*\left\langle\psi_n|\psi_n\right\rangle ,$$

where we used the fact that $\hat{Q}^\dagger = \hat{Q}$. Thus, since $\langle\psi_n|\psi_n\rangle \neq 0$ we find that $\boxed{q_n = q_n^*}$, i.e. the eigenvalue of any Hermitian operator is real.

Question 3:

Show that the momentum operator $\hat{p}$ is Hermitian, and find the Hermitian conjugate of the derivative operator $\hat{D} \equiv \partial/\partial x$.

Solution:

Taking the product of $\hat{p}\left|g\right\rangle$ and $\langle f|$ we find

$$\langle f|\hat{p}g\rangle = \int_{-\infty}^{\infty} f^*\left(-i\hbar\right)\frac{dg}{dx}dx = \cancel{-i\hbar f^* g\Big|_{-\infty}^{\infty}} + \int_{-\infty}^{\infty}\left(-i\hbar\frac{df}{dx}\right)^* g dx = \langle\hat{p}f|g\rangle ,$$

thus $\boxed{\hat{p}^\dagger = \hat{p}}$. Using this property we can write

$$\left(-i\hbar\hat{D}\right)^\dagger = -i\hbar\hat{D} \quad \rightarrow \quad \boxed{\hat{D}^\dagger = -\hat{D}}.$$

Question 4:

Given the two Hermitian operators $\hat{A}$ and $\hat{B}$. Show that if $\hat{A}\hat{B} = \hat{B}\hat{A}$ then $\hat{A}$ and $\hat{B}$ can be simultaneously diagonalized (e.g. diagonalized in the same basis) and vice versa.

Solution:

If $\hat{A}$ and $\hat{B}$ share the same eigenbasis, i.e.

$$\hat{A}\left|\psi\right\rangle = a\left|\psi\right\rangle \quad \text{and} \quad \hat{B}\left|\psi\right\rangle = b\left|\psi\right\rangle,$$

then taking the product

$$\left\langle\psi\right|\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)\psi\Big\rangle = \left\langle\psi\right|\left(\hat{A}b - \hat{B}a\right)\psi\Big\rangle = \left\langle\psi\right|(ba - ab)\,\psi\rangle = 0 \quad \rightarrow \quad \boxed{\hat{A}\hat{B} = \hat{B}\hat{A}}.$$

This can be also shown in terms of the unitary transformation U, such that

$$U^{-1}\hat{A}U = D_1 \quad \text{and} \quad U^{-1}\hat{B}U = D_2,$$

where D_1 and D_2 are diagonal matrices. Then,

$$U^{-1}\hat{A}\hat{B}U = U^{-1}\hat{A}UU^{-1}\hat{B}U = D_1D_2 = D_2D_1 = U^{-1}\hat{B}UU^{-1}\hat{A}U = U^{-1}\hat{B}\hat{A}U \quad \rightarrow \quad \boxed{\hat{A}\hat{B} = \hat{B}\hat{A}}.$$

Now, going the other way, if $\hat{A}\hat{B} = \hat{B}\hat{A}$ then, let us consider $\left|\psi\right\rangle$, the eigenstate of $\hat{A}$, then we have

$$\left\langle\psi\right|\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)\psi\Big\rangle = a\left\langle\psi\right|\left(\hat{B} - \hat{B}\right)\psi\Big\rangle = 0,$$

where we used the hermiticity of $\hat{A}$. But this only holds if $\left|\psi\right\rangle$ is also an eigenstate of $\hat{B}$, namely $\hat{B}\left|\psi\right\rangle = b\left|\psi\right\rangle$.

Commutation Relation

Two operators which follow $\hat{A}\hat{B} = \hat{B}\hat{A}$ are said to be commutable operators. The commutation relation of two operators plays an important role in quantum physics, and it is useful to define the *commutator* of $\hat{A}$ and $\hat{B}$ as

$$\left[\hat{A}, \hat{B}\right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}.$$

Some important properties of the commutator are:

- $\left[\hat{A}, \hat{B}\right] = -\left[\hat{B}, \hat{A}\right]$.
- $\left[\hat{A}, \hat{A}\right] = 0$.
- $\left[\hat{A}, \left[\hat{B}, \hat{C}\right]\right] + \left[\hat{B}, \left[\hat{C}, \hat{A}\right]\right] + \left[\hat{C}, \left[\hat{A}, \hat{B}\right]\right] = 0$.
- $\left[\hat{A}, \hat{B}\hat{C}\right] = \left[\hat{A}, \hat{B}\right]\hat{C} + \hat{B}\left[\hat{A}, \hat{C}\right]$.
- If $\left[\hat{A}, \hat{C}\right] = \left[\hat{B}, \hat{C}\right] = 0$, where $\hat{C} = \left[\hat{A}, \hat{B}\right]$, then

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

  therefore, if $F\left(\hat{B}\right)$ is an analytic function of $\hat{B}$, then

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

Question 5:

Calculate the following commutation relations:

- $[\hat{x},\hat{p}]$.
- $\left[\hat{x},\hat{p}^2\right]$.
- $[\hat{x}^n,\hat{p}]$.

Solution:

Using a test wave function ψ, we have

$$[\hat{x},\hat{p}]\,\psi = -i\hbar\left(x\frac{d\psi}{dx} - \frac{d}{dx}(x\psi)\right) = -i\hbar\left(\cancel{x\frac{d\psi}{dx}} - \psi - \cancel{x\frac{d\psi}{dx}}\right) = i\hbar\psi \quad \rightarrow \quad \boxed{[\hat{x},\hat{p}] = i\hbar}.$$

Now, using the commutator properties we can write

$$\left[\hat{x},\hat{p}^2\right] = [\hat{x},\hat{p}]\,\hat{p} + \hat{p}\,[\hat{x},\hat{p}] = 2i\hbar\hat{p} \quad \rightarrow \quad \boxed{\left[\hat{x},\hat{p}^2\right] = 2i\hbar\hat{p}},$$

and

$$[\hat{x},[\hat{x},\hat{p}]] = [\hat{x},i\hbar] = 0 \quad \rightarrow \quad [\hat{x}^n,\hat{p}] = n\hat{x}^{n-1}\,[\hat{x},\hat{p}] = i\hbar n\hat{x}^{n-1} \quad \rightarrow \quad \boxed{[\hat{x}^n,\hat{p}] = i\hbar n\hat{x}^{n-1}}.$$

Generalized Ehrenfest Theorem

Consider how fast changes some observable $Q(x,p,t)$,

$$\begin{aligned}
\frac{d}{dt}\langle Q\rangle &= \frac{d}{dt}\left\langle \Psi|\hat{Q}\Psi\right\rangle \\
&= \left\langle \frac{\partial\Psi}{\partial t}|\hat{Q}\Psi\right\rangle + \left\langle \Psi|\frac{\partial\hat{Q}}{\partial t}\Psi\right\rangle + \left\langle \Psi|\hat{Q}\frac{\partial\Psi}{\partial t}\right\rangle \\
&= \left\langle \frac{1}{i\hbar}\hat{H}\Psi|\hat{Q}\Psi\right\rangle + \left\langle \frac{\partial\hat{Q}}{\partial t}\right\rangle + \left\langle \Psi|\hat{Q}\frac{1}{i\hbar}\hat{H}\Psi\right\rangle \\
&= \frac{i}{\hbar}\left\langle \Psi|\left(\hat{H}\hat{Q} - \hat{Q}\hat{H}\right)\Psi\right\rangle + \left\langle \frac{\partial\hat{Q}}{\partial t}\right\rangle,
\end{aligned}$$

where we used the Schrödinger equation $i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$. Therefore we find

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

also known as the *generalized Ehrenfest theorem*.

Question 6:

1. Consider a particle moving under the influence of the potential $V(x) = kx^n$. Calculate the time derivative of $\langle \hat{x} \rangle$ and $\langle \hat{p} \rangle$.

2. The results from (1) resemble Newton's equations for classical motion. Show that in fact, this is only true for $n \leq 2$ i.e. for a free particle, a constant force and a harmonic potential.

Solution:

1. The Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + k\hat{x}^n.$$

Using the generalized Ehrenfest theorem, considering the fact that the operators do not depend explicitly on t, we have

$$\frac{d}{dt}\langle \hat{p} \rangle = \frac{i}{\hbar}\left\langle \left[\hat{H}, \hat{p}\right] \right\rangle + \cancel{\left\langle \frac{\partial \hat{p}}{\partial t} \right\rangle} = \frac{i}{\hbar}\left\langle \frac{1}{2m}\cancel{\left[\hat{p}^2, \hat{p}\right]} + k\left[\hat{x}^n, \hat{p}\right] \right\rangle = -\left\langle kn\hat{x}^{n-1} \right\rangle = -\left\langle \nabla V \right\rangle \quad \rightarrow \quad \boxed{\frac{d}{dt}\langle \hat{p} \rangle = -\langle \nabla V \rangle},$$

and

$$\frac{d}{dt}\langle \hat{x} \rangle = \frac{i}{\hbar}\left\langle \left[\hat{H}, \hat{x}\right] \right\rangle + \cancel{\left\langle \frac{\partial \hat{x}}{\partial t} \right\rangle} = \frac{i}{\hbar}\left\langle \frac{1}{2m}\left[\hat{p}^2, \hat{x}\right] + k\cancel{\left[\hat{x}^n, \hat{x}\right]} \right\rangle = \frac{i}{\hbar}\left\langle \frac{1}{2m}\left(\hat{p}\left[\hat{p}, \hat{x}\right] + \left[\hat{p}, \hat{x}\right]\hat{p}\right) \right\rangle = \frac{\langle \hat{p} \rangle}{m} \quad \rightarrow \quad \boxed{\frac{d}{dt}\langle \hat{x} \rangle = \frac{\langle \hat{p} \rangle}{m}}.$$

2. Newton's classical laws of motion state that

$$m\frac{d^2}{dt^2}\langle x \rangle = \frac{d}{dt}\langle p \rangle = -\nabla V\left(\langle x \rangle\right),$$

thus we need to check whether $\langle \nabla V(x) \rangle \stackrel{?}{=} \nabla V(\langle x \rangle)$, where

$$\langle \nabla V(x) \rangle = \int \psi^* \nabla V(x)\, \psi dx \quad \text{and} \quad \nabla V(\langle x \rangle) = \nabla V\left(\int \psi^* x \psi dx\right).$$

Thus

$$n = 0: \quad \nabla V = 0 \quad \rightarrow \begin{cases} \langle \nabla V(x) \rangle = \int \psi^*(0)\, \psi dx = 0 \\ \nabla V(\langle x \rangle) = 0 \end{cases} \quad \rightarrow \quad \langle \nabla V(x) \rangle = \nabla V(\langle x \rangle),$$

$$n = 1: \quad \nabla V = k \quad \rightarrow \begin{cases} \langle \nabla V(x) \rangle = \int \psi^* k \psi dx = k \\ \nabla V(\langle x \rangle) = k \end{cases} \quad \rightarrow \quad \langle \nabla V(x) \rangle = \nabla V(\langle x \rangle),$$

$$n = 2: \quad \nabla V = 2kx \quad \rightarrow \begin{cases} \langle \nabla V(x) \rangle = \int \psi^* 2kx \psi dx = 2k\langle x \rangle \\ \nabla V(\langle x \rangle) = 2k\langle x \rangle \end{cases} \quad \rightarrow \quad \langle \nabla V(x) \rangle = \nabla V(\langle x \rangle),$$

$$n > 2: \quad \nabla V = nkx^{n-1} \quad \rightarrow \begin{cases} \langle \nabla V(x) \rangle = \int \psi^* nk\psi x^{n-1} dx = nk\left\langle x^{n-1} \right\rangle \\ \nabla V(\langle x \rangle) = nk\langle x \rangle^{n-1} \end{cases} \quad \rightarrow \quad \langle \nabla V(x) \rangle \neq \nabla V(\langle x \rangle) \text{ if } \left\langle x^{n-1} \right\rangle \neq \langle x \rangle^{n-1}$$

Therefore, Ehrenfest theorem corresponds to the Newtonian case up to 2$^{\text{nd}}$ order.

Question 7:

1. Show that the function $e^{\hat{A}}\hat{B}e^{-\hat{A}}$, can be written in terms of a sum of commutators.
   Hint: use the function $F\left(\hat{A},\hat{B},\lambda\right) \equiv e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}$ to expand the exponents on powers of λ, then take $\lambda = 1$.

2. For the harmonic oscillator
$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2,$$
   calculate:
   (a) $e^{i\hat{H}t/\hbar}\hat{x}e^{-i\hat{H}t/\hbar}$.
   (b) $e^{i\hat{H}t/\hbar}\hat{p}e^{-i\hat{H}t/\hbar}$.

Solution:

1. Writing F as
$$F\left(\hat{A},\hat{B},\lambda\right) \equiv e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}, \quad \text{so that } F\left(\hat{A},\hat{B}\right) = F\left(\hat{A},\hat{B},\lambda\right)|_{\lambda=1}$$
   we can see that
$$\frac{\partial F}{\partial\lambda} = \hat{A}e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}} - e^{\lambda\hat{A}}\hat{B}e^{-\lambda\hat{A}}\hat{A} = \left[\hat{A},F\right],$$
$$\frac{\partial^2 F}{\partial\lambda^2} = \left[\hat{A},\frac{\partial F}{\partial\lambda}\right] = \left[\hat{A},\left[\hat{A},F\right]\right],$$
$$\frac{\partial^3 F}{\partial\lambda^3} = \left[\hat{A},\left[\hat{A},\left[\hat{A},F\right]\right]\right],$$
   and so forth. In addition we note that $F(\lambda = 0) = \hat{B}$, thus, Taylor expanding around $\lambda = 0$ we have
$$F = \sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\frac{\partial^n F}{\partial\lambda^n}\Big|_{\lambda=0} = \hat{B} + \lambda\left[\hat{A},\hat{B}\right] + \frac{\lambda^2}{2}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] + \frac{\lambda^3}{3}\left[\hat{A},\left[\hat{A},\left[\hat{A},\hat{B}\right]\right]\right] + \ldots$$
   Now, taking $\lambda = 1$ we get
$$\boxed{e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + \left[\hat{A},\hat{B}\right] + \frac{1}{2}\left[\hat{A},\left[\hat{A},\hat{B}\right]\right] + \ldots}$$

2. Using the result of (1) we can write
$$e^{i\hat{H}t/\hbar}\hat{Q}e^{-i\hat{H}t/\hbar} = \hat{x} + \left[\hat{H},\hat{Q}\right] + \frac{1}{2}\left[\hat{H},\left[\hat{H},\hat{Q}\right]\right] + \ldots$$
   (a) For $\hat{x}$,
$$\left[\hat{H},\hat{x}\right] = \left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2,\hat{x}\right] = \frac{1}{2m}\left[\hat{p}^2,\hat{x}\right] = -\frac{i\hbar}{m}\hat{p},$$
$$\left[\hat{H},\left[\hat{H},\hat{x}\right]\right] = \left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2,-\frac{i\hbar}{m}\hat{p}\right] = -\frac{i\omega^2\hbar}{2}\left[\hat{x}^2,\hat{p}\right] = \hbar^2\omega^2\hat{x},$$
$$\left[\hat{H},\left[\hat{H},\left[\hat{H},\hat{x}\right]\right]\right] = \left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2,\hbar^2\omega^2\hat{x}\right] = \frac{\omega^2\hbar^2}{2m}\left[\hat{p}^2,\hat{x}\right] = -\frac{i\hbar}{m}\hbar^2\omega^2\hat{p},$$
   and so forth, so that
$$\begin{aligned} e^{i\hat{H}t/\hbar}\hat{x}e^{-i\hat{H}t/\hbar} &= \hat{x} + \frac{1}{m\omega}\omega t\hat{p} - \frac{1}{2!}(\omega t)^2\hat{x} - \frac{1}{3!}\frac{1}{m\omega}(\omega t)^3\hat{p} + \ldots \\ &= \hat{x}\left(1 - \frac{1}{2!}(\omega t)^2 + \frac{1}{4!}(\omega t)^4 + \ldots\right) + \frac{1}{m\omega}\left(\omega t - \frac{1}{3!}(\omega t)^3 + \frac{1}{5!}(\omega t)^5 + \ldots\right)\hat{p} \\ &= \hat{x}\cos\omega t + \frac{1}{m\omega}\hat{p}\sin\omega t. \end{aligned}$$
$$\boxed{e^{i\hat{H}t/\hbar}\hat{x}e^{-i\hat{H}t/\hbar} = \hat{x}\cos\omega t + \frac{1}{m\omega}\hat{p}\sin\omega t}.$$

(b) In the same manner

$$\left[\hat{H},\hat{p}\right] = \left[\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2\hat{x}^2,\hat{p}\right] = \frac{1}{2}m\omega^2\left[\hat{x}^2,\hat{p}\right] = i\hbar m\omega^2\hat{x},$$
$$\left[\hat{H},\left[\hat{H},\hat{p}\right]\right] = \left[\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2\hat{x}^2, i\hbar m\omega^2\hat{x}\right] = i\frac{\hbar\omega^2}{2}\left[\hat{p}^2,\hat{x}\right] = \hbar^2\omega^2\hat{p},$$
$$\left[\hat{H},\left[\hat{H},\left[\hat{H},\hat{p}\right]\right]\right] = \left[\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2\hat{x}^2, \hbar^2\omega^2\hat{p}\right] = \frac{1}{2}m\omega^2\hbar^2\omega^2\left[\hat{x}^2,\hat{p}\right] = i\hbar m\omega^2\hbar^2\omega^2\hat{x},$$

and so forth, so that, counting the $(it/\hbar)$ factors for each $\hat{H}$ as well,

$$\begin{aligned}
e^{i\hat{H}t/\hbar}\hat{p}e^{-i\hat{H}t/\hbar} &= \hat{p} - m\omega\left(\omega t\right)\hat{x} - \frac{1}{2!}\left(\omega t\right)^2\hat{p} + \frac{1}{3!}m\omega\left(\omega t\right)^3\hat{x} + \frac{1}{4!}\left(\omega t\right)^4\hat{p} + \dots \\
&= \hat{p}\left(1 - \frac{1}{2!}\left(\omega t\right)^2 + \frac{1}{4!}\left(\omega t\right)^4 + \dots\right) + m\omega\left(-\omega t + \frac{1}{3!}\left(\omega t\right)^3 - \frac{1}{5!}\left(\omega t\right)^5 + \dots\right)\hat{x} \\
&= \hat{p}\cos\omega t - m\omega\hat{x}\sin\omega t.
\end{aligned}$$

$$\boxed{e^{i\hat{H}t/\hbar}\hat{p}e^{-i\hat{H}t/\hbar} = \hat{x}\cos\omega t + \frac{1}{m\omega}\hat{p}\sin\omega t}.$$

In the future, you will encounter another framework in which the operators are the ones we propagate in time instead of the states, so that

$$\left\langle\Psi\left(x,t\right)|\hat{Q}|\Psi\left(x,t\right)\right\rangle = \left\langle\psi\left(x\right)|e^{i\hat{H}t/\hbar}\hat{Q}e^{-i\hat{H}t/\hbar}|\psi\left(x\right)\right\rangle \equiv \left\langle\psi\left(x\right)|\hat{Q}\left(t\right)|\psi\left(x\right)\right\rangle,$$

this is called the Heisenberg picture, in contrast to the Schrödinger picture we've been working with so far. So what we've just calculated are the *time dependent* position and momentum operators $\hat{x}\left(t\right)$ and $\hat{p}\left(t\right)$, for the harmonic oscillator.