Quantum Theory for Mathematicians

Erik Herrera

February 4, 2025

Problem 1. Suppose that $\phi(t)$ and $\psi(t)$ are differentiable functions with values in a Hilbert space $\mathbf{H}$, meaning that the limit

$$\frac{d\phi}{dt} := \lim_{h\to 0} \frac{\phi(t+h)-\phi(t)}{h}$$

exists in the norm topology of $\mathbf{H}$ for each t, and similarly for $\psi(t)$. Show that

$$\frac{d}{dt}\langle \phi(t), \psi(t)\rangle = \left\langle \frac{d\phi}{dt}, \psi(t)\right\rangle + \left\langle \phi(t), \frac{d\psi}{dt}\right\rangle.$$

Proof. By direct computation,

$$\begin{aligned}
\frac{d}{dt}\langle \phi(t), \psi(t)\rangle &= \lim_{h\to 0} \frac{\langle \phi(t+h), \psi(t+h)\rangle - \langle \phi(t), \psi(t)\rangle}{h} \\
&= \lim_{h\to 0} \frac{\langle \phi(t+h), \psi(t+h)\rangle - \langle \phi(t), \psi(t+h)\rangle + \langle \phi(t), \psi(t+h)\rangle - \langle \phi(t), \psi(t)\rangle}{h} \\
&= \lim_{h\to 0} \left\langle \frac{\phi(t+h)-\phi(t)}{h}, \psi(t+h)\right\rangle + \lim_{h\to 0} \left\langle \phi(t), \frac{\psi(t+h)-\psi(t)}{h}\right\rangle
\end{aligned}$$

By the Cauchy-Schwarz inequality,

$$\lim_{h\to 0} \left| \left\langle \phi(t), \frac{\psi(t+h)-\psi(t)}{h} - \frac{d\psi}{dt}(t)\right\rangle \right| \leq \lim_{h\to 0} \|\phi(t)\| \left\| \frac{\psi(t+h)-\psi(t)}{h} - \frac{d\psi}{dt}(t)\right\| = 0$$

Hence,

$$\lim_{h\to 0} \left\langle \phi(t), \frac{\psi(t+h)-\psi(t)}{h}\right\rangle = \left\langle \phi(t), \frac{d\psi}{dt}(t)\right\rangle$$

Similarly,

$$\lim_{h\to 0} \left\langle \frac{\phi(t+h)-\phi(t)}{h}, \psi(t)\right\rangle = \left\langle \frac{d\phi}{dt}(t), \psi(t)\right\rangle$$

Thus,

$$\begin{aligned}
\lim_{h\to 0} \left\langle \frac{\phi(t+h)-\phi(t)}{h}, \psi(t+h)\right\rangle &= \lim_{h\to 0} \left\langle \frac{\phi(t+h)-\phi(t)}{h}, \psi(t+h)-\psi(t)+\psi(t)\right\rangle \\
&= \lim_{h\to 0} \left\langle \frac{\phi(t+h)-\phi(t)}{h}, \psi(t+h)-\psi(t)\right\rangle + \left\langle \frac{d\phi}{dt}(t), \psi(t)\right\rangle \\
&= \left\langle \frac{d\phi}{dt}(t), \psi(t)\right\rangle
\end{aligned}$$

since the Cauchy-Schwarz inequality implies that

$$\begin{aligned}
\lim_{h\to 0}\left|\left\langle \frac{\phi(t+h)-\phi(t)}{h}, \psi(t+h)-\psi(t)\right\rangle\right| &\leq \lim_{h\to 0}\left\|\frac{\phi(t+h)-\phi(t)}{h}\right\|\|\psi(t+h)-\psi(t)\| \\
&= \lim_{h\to 0} h\left\|\frac{\phi(t+h)-\phi(t)}{h}\right\|\left\|\frac{\psi(t+h)-\psi(t)}{h}\right\| \\
&= 0\left\|\frac{d\phi}{dt}(t)\right\|\left\|\frac{d\psi}{dt}(t)\right\| \\
&= 0
\end{aligned}$$

Therefore, we have the desired result:

$$\frac{d}{dt}\langle\phi(t),\psi(t)\rangle = \left\langle \frac{d\phi}{dt}(t), \psi(t)\right\rangle + \left\langle \phi(t), \frac{d\psi}{dt}(t)\right\rangle$$

■

Problem 2. Suppose A and B are operators on a finite-dimensional Hilbert space and suppose that $AB - BA = cI$ for some constant c. Show that $c = 0$. Note: This shows that the commutation relations in (3.8) are a purely infinite-dimensional phenomenon.

Proof. Taking the trace of the commutator, we find

$$\mathrm{Tr}(AB - BA) = \mathrm{Tr}(AB) - \mathrm{Tr}(BA) = \mathrm{Tr}(AB) - \mathrm{Tr}(AB) = 0$$

because the trace is additive and cyclic. This means that $c = 0$ if $AB - BA = cI$.

■

Problem 3. If A is a bounded operator on a Hilbert space $\mathbf{H}$, then there exists a unique bounded operator A^* on H satisfying $\langle\phi, A\psi\rangle = \langle A^*\phi, \psi\rangle$ for all ϕ and ψ in H. (Appendix A.4.3.) The operator A^* is called the adjoint of A, and A is called self-adjoint if $A^* = A$.

1. Show that for any bounded operator A and constant $c \in \mathbb{C}$, we have $(cA)^* = \bar{c}A^*$, where $\bar{c}$ is the complex conjugate of c.

   Proof. This follows from the sesquilinearity of the inner product:

   $$\langle\phi, cA\psi\rangle = c\langle\phi, A\psi\rangle = c\langle A^*\phi, \psi\rangle = \langle\bar{c}A^*, \psi\rangle$$

   ■

2. Show that if A and B are self-adjoint, then the operator

   $$\frac{1}{i\hbar}[A, B]$$

   is also self-adjoint.

Proof. It is clear that the adjoint is additive:

$$\langle \phi, (A+B)\psi \rangle = \langle \phi, A\psi \rangle + \langle \phi, B\psi \rangle = \langle A^*\phi, \psi \rangle + \langle B^*\phi, \psi \rangle = \langle (A^* + B^*)\phi, \psi \rangle$$

We can also see that $(AB)^* = B^*A^*$:

$$\langle \phi, AB\psi \rangle = \langle A^*\phi, B\psi \rangle = \langle B^*A^*\phi, \psi \rangle$$

Using the previous part of the problem, we then see that

$$\left(\frac{1}{i\hbar}(AB - BA)\right)^* = \frac{-1}{i\hbar}(B^*A^* - A^*B^*) = \frac{-1}{i\hbar}(BA - AB) = \frac{1}{i\hbar}(AB - BA)$$

■

Problem 4. Verify Proposition 3.19 using Proposition 3.14. Note that the operator $V'(X)$ means simply the operator of multiplication by the function $V'(x)$.

Proof. From Proposition 3.14, we know that

$$\frac{d}{dt}\langle X \rangle = \left\langle \frac{1}{i\hbar}[X, H] \right\rangle = \frac{1}{2i\hbar m}\langle [X, P^2] \rangle \tag{1}$$

and

$$\frac{d}{dt}\langle P \rangle = \left\langle \frac{1}{i\hbar}[P, H] \right\rangle = \frac{1}{i\hbar}\langle [P, V(X)] \rangle \tag{2}$$

As a lemma, we show that $[A, B^n] = nB^{n-1}[A, B]$ if $[[A, B], B] = 0$. This is clearly true for the case of $n = 1$. By Proposition 3.15,

$$[A, B^n] = [A, B^{n-1}B] = [A, B]B^{n-1} + B[A, B^{n-1}]$$

Using induction, we see that

$$[A, B^n] = [A, B]B^{n-1} + (n-1)BB^{n-2}[A, B] = [A, B]B^{n-1} + (n-1)B^{n-1}[A, B]$$

Because $[A, B]$ and B commute, this gives $[A, B^n] = nB^{n-1}[A, B]$ as desired. Applying this to (1) and (2) gives

$$\frac{d}{dt}\langle X \rangle = \frac{1}{i\hbar m}\langle P[X, P] \rangle = \frac{1}{m}\langle P \rangle$$

and

$$\frac{d}{dt}\langle P \rangle = \frac{1}{i\hbar}\langle V'(X)[P, X] \rangle = -\langle V'(X) \rangle$$

■

Problem 5. Suppose that ψ is a unit vector in $L^2(\mathbb{R})$ such that the functions $x\psi(x)$ and $x^2\psi(x)$ also belong to $L^2(\mathbb{R})$. Show that

$$\left\langle X^2 \right\rangle_\psi > (\langle X \rangle_\psi)^2$$

Hint: Consider the integral

$$\int_{-\infty}^{\infty} (x-a)^2 |\psi(x)|^2 dx$$

where $a = \langle X \rangle_\psi$.

Proof. We begin by computing the variance of X:

$$\begin{aligned}
\left\langle (X - \langle X \rangle)^2 \right\rangle &= \int (x - \langle X \rangle)^2 |\psi(x)|^2 dx \\
&= \int x^2 |\psi(x)|^2 dx - 2\langle X \rangle \int x |\psi(x)|^2 dx + \langle X \rangle^2 \int |\psi(x)|^2 dx \\
&= \langle X^2 \rangle - 2\langle X \rangle^2 + \langle X \rangle^2 \\
&= \langle X^2 \rangle - \langle X \rangle^2
\end{aligned}$$

Because the left side is positive, we conclude that $\langle X \rangle^2 < \langle X^2 \rangle$.

■

Problem 6. Consider the Hamiltonian $\hat{H}$ for a quantum harmonic oscillator, given by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{k}{2}x^2$$

where k is the spring constant of the oscillator. Show that the function

$$\psi_0(x) = \exp\left\{ -\frac{\sqrt{km}}{2\hbar} x^2 \right\}$$

is an eigenvector for $\hat{H}$ with eigenvalue $\hbar\omega/2$, where $\omega := \sqrt{k/m}$ is the classical frequency of the oscillator. Note: We will explore the eigenvectors and eigenvalues of $\hat{H}$ in detail in Chap. 11.

Proof. By direction calculation, we see that

$$\begin{aligned}
\frac{d^2}{dx^2}\psi_0(x) &= \frac{d^2}{dx^2} \exp\left\{ -\frac{\sqrt{km}}{2\hbar} x^2 \right\} \\
&= \frac{d}{dx}\left(-\frac{\sqrt{km}}{\hbar} x \exp\left\{ -\frac{\sqrt{km}}{2\hbar} x^2 \right\} \right) \\
&= -\frac{\sqrt{km}}{\hbar} \exp\left\{ -\frac{\sqrt{km}}{2\hbar} x^2 \right\} + \frac{km}{\hbar^2} x^2 \exp\left\{ -\frac{\sqrt{km}}{2\hbar} x^2 \right\}
\end{aligned}$$

Therefore,

$$\begin{aligned}
\hat{H}\psi_0(x) &= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{k}{2}x^2\right)\psi_0(x) \\
&= \frac{\hbar}{2}\sqrt{\frac{k}{m}}\exp\left\{-\frac{\sqrt{km}}{2\hbar}x^2\right\} - \frac{kx^2}{2}\exp\left\{-\frac{\sqrt{km}}{2\hbar}x^2\right\} + \frac{kx^2}{2}\exp\left\{-\frac{\sqrt{km}}{2\hbar}x^2\right\} \\
&= \frac{\hbar\omega}{2}\psi_0(x)
\end{aligned}$$

■

Problem 7. Prove Proposition 3.23.

Hint: Show that $[P(t), \hat{H}] = ([P, \hat{H}])(t)$ and $[X(t), \hat{H}] = ([X, \hat{H}])(t)$.

Proof. We begin by showing the hint:

$$[P(t), H] = P(t)H - HP(t) = e^{itH/\hbar}Pe^{-itH/\hbar}H - He^{itH/\hbar}Pe^{-itH/\hbar} = e^{itH/\hbar}[P, H]e^{-itH/\hbar}$$

since H commutes with itself. Likewise, $[X(t), H] = [X, H](t)$ Using the computation from problem 4, we find

$$\frac{dX(t)}{dt} = \frac{1}{i\hbar}[X(t), H] = \frac{1}{i\hbar}[X, H](t) = \frac{1}{m}P(t)$$

and

$$\frac{dP(t)}{dt} = \frac{1}{i\hbar}[P(t), H] = \frac{1}{i\hbar}[P, H](t) = -(V'(X))(t) = -V'(X(t))$$

■

Problem 8. 1. Find the general solution to (3.43), where E is a negative real number. Show that the only such solution that satisfies the boundary conditions (3.44) is identically zero.

Proof. Solutions to 3.43 with negative E have the form

$$\psi(x) = Ae^{\omega x} + Be^{-\omega x}, \text{ where } \omega = \frac{\sqrt{-2mE}}{\hbar}$$

The boundary conditions $\psi(0) = 0$ implies that $B = -A$. Adding the further condition $\psi(L) = 0$ requires

$$Ae^{\omega L} - Ae^{-\omega L} = A(e^{\omega L} - e^{-\omega L}) = 0$$

which means that $A = 0$.

■

2. Establish the same result as in Part (1) for $E = 0$.

Proof. Solutions to 3.43 with $E = 0$ have the form

$$\psi(x) = Ax + B$$

boundary conditions $\psi(0) = \psi(L) = 0$ imply that $A = B = 0$.

∎

Problem 9. 1. Suppose ϕ and ψ are smooth functions on $[0, L]$ satisfying the boundary conditions (3.44). Using integration by parts, show that

$$\langle \phi, \hat{H}\psi \rangle = \langle \hat{H}\phi, \psi \rangle$$

where $\hat{H} = -\left(\hbar^2/2m\right) d^2/dx^2$ and where

$$\langle \phi, \psi \rangle = \int_0^L \overline{\phi(x)}\psi(x)dx$$

Proof. By direct computation,

$$\langle \phi, H\psi \rangle = \int_0^L \overline{\phi(x)} \left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi(x)dx$$

Using integration by parts twice, this is equal to

$$\langle \phi, H\psi \rangle = \int_0^L \left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \right) \overline{\phi(x)}\psi(x)dx = \int_0^L \overline{\left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \right) \phi(x)}\psi(x)dx = \langle H\phi, \psi \rangle$$

since we have vanishing boundary conditions.

∎

2. Show that the result of Part (a) fails if ϕ and ψ are arbitrary smooth functions (not satisfying the boundary conditions).

Proof. Let $\psi(x) = 1$ and $\phi(x) = Ax^2$, where A is the appropriate normalization constant. Notice that $H\psi(x) = 0$ and $H\phi(x) = -A\frac{\hbar^2}{2m}$. Therefore,

$$\langle \phi, H\psi \rangle = \int_0^L Ax^2 \cdot 0dx = 0$$

and

$$\langle H\phi, \psi \rangle = \int_0^L -A\frac{\hbar^2}{2m} \cdot 1dx = -\frac{AL\hbar^2}{2m}$$

This shows that $\langle \phi, H\psi \rangle$ and $\langle H\phi, \psi \rangle$ do not agree for arbitrary smooth ϕ, ψ.

∎

Problem 10. Let $\hat{J}_1, \hat{J}_2$, and $\hat{J}_3$ be the angular momentum operators for a particle moving in $\mathbb{R}^3$. Using the canonical commutation relations (Proposition 3.25), show that these operators satisfy the commutation relations

$$\frac{1}{i\hbar}\left[\hat{J}_1, \hat{J}_2\right] = \hat{J}_3; \quad \frac{1}{i\hbar}\left[\hat{J}_2, \hat{J}_3\right] = \hat{J}_1; \quad \frac{1}{i\hbar}\left[\hat{J}_3, \hat{J}_1\right] = \hat{J}_2.$$

This is the quantum mechanical counterpart to Exercise 19 in the previous chapter.

Proof. By direct computation, we see that $[J_1, J_2] =$

$$[X_2P_3 - X_3P_2, X_3P_1 - X_1P_3] = [X_2P_3, X_3P_1] - [X_3P_2, X_3P_1] - [X_2P_3, X_1P_3] + [X_3P_2, X_1P_3]$$

The second and third terms vanish while

$$[X_2P_3, X_3P_1] = X_2P_1[P_3, X_3] = -i\hbar X_2P_1$$

and

$$[X_3P_2, X_1P_3] = X_1P_2[X_3, P_3] = i\hbar X_1P_2$$

Thus,

$$\frac{1}{i\hbar}[J_1, J_2] = X_1P_2 - X_2P_1 = J_3$$

By symmetry,

$$\frac{1}{i\hbar}[J_2, J_3] = J_1 \quad \text{and} \quad \frac{1}{i\hbar}[J_3, J_1] = J_2.$$

■