Physics 486 Discussion 7 – Hermitian Operators and Commutators

On the back page are the 4 postulates of Quantum Mechanics as tabulated by R. Shankar in his QM textbook, Ch. 4. Jain has an expanded version in §10.5, where he enumerates 7 postulates that amount to the same thing. Shankar’s version has the advantage of conciseness, plus a helpful Classical Mechanics column for comparison; Jain’s version has the advantage of being more explicit and less jargon-heavy.

POSTULATE 1 says that all available information about the state of a quantum system at time \( t \) is encoded in the system’s wavefunction \(|\Psi(t)\rangle\), which is a member of the Hilbert Space \( \cong \text{Inner Product Space} \) of square-integrable complex-valued functions with inner product

\[
\langle f | g \rangle \equiv \int_{-\infty}^{+\infty} f^*(x) \, g(x) \, dx .
\]

POSTULATE 2 says that every measurable property \( Q \) of a system is associated with a Hermitian operator \( \hat{Q} \). This is the new concept we will explore today. For a single particle in one spatial dimension, the phase-space observables \( x \) and \( p \) are represented by these Hermitian operators:

\[
\hat{x} = x \quad \hat{p} = -i\hbar \frac{\partial}{\partial x}
\]

All other dynamical properties \( Q \) of the particle can be computed from these as \( \hat{Q}(\hat{x}, \hat{p}) \).

Problem 1 : What Are Hermitian Operators?  

Hermitian operators are those associated with measurable quantities in QM. What properties must they possess? Measurements are real, so the expectation values of a Hermitian operator \( \hat{Q} \) must be real numbers, i.e. \( \langle \hat{Q} \rangle^\ast = \langle \hat{Q} \rangle \). We can take this as the definition of a Hermitian operator.

Since \( \langle \hat{Q} \rangle = \int_{-\infty}^{+\infty} \psi^\ast(x) \, \hat{Q} \, \psi(x) \, dx \), which is \( \langle \psi | \hat{Q} \psi \rangle \) in our new bra-ket notation,

and \( \langle \hat{Q} \rangle^\ast = \int_{-\infty}^{+\infty} \psi^\ast(x) \, \hat{Q}^\ast \, \psi^\ast(x) \, dx = \int_{-\infty}^{+\infty} (\hat{Q} \, \psi(x))^\ast \, \psi(x) \, dx \), which is \( \langle \hat{Q} \psi | \psi \rangle \).

Thus \( \langle \psi | \hat{Q} \psi \rangle = \langle \hat{Q}^\ast \psi | \psi \rangle \) is an equivalent definition to \( \langle \hat{Q} \rangle^\ast = \langle \hat{Q} \rangle \).

One more equivalence: as you will show on your homework, the above definitions are also equivalent to this:

\[
\langle g | \hat{Q} \, h \rangle = \langle \hat{Q} \, g | h \rangle
\]

for any two functions \( g(x) \) and \( h(x) \). This is the standard definition of a Hermitian operator \( \hat{Q} \), e.g. the one you will find in Wikipedia. Now, on to the properties of these operators!

(a) Prove that all eigenvalues of a Hermitian operator are REAL. Recall the definition of eigen-things: if

1 Q1 (b) evaluate \( \langle Q \rangle \) and \( \langle Q^2 \rangle \) for the eigenstate \( \psi_q \) with eigenvalue \( q \) … it is really easy to show that \( \langle Q^n \rangle = q^n \) in an eigenstate!  
(c) What do you want to show? Write it down. … You want to show \( \langle f_1 | f_2 \rangle = 0 \) … Use the eigen-property of \( f_1 \) to replace it with something involving \( \hat{Q} \) … \( f_i = \hat{Q} \, f_i / q_i \) … use the Hermitian property of \( \hat{Q} \) to move it to the other side … use \( q_1 \neq q_2 \) …  
(d) \( A_p = 1 / \sqrt{2\pi\hbar} \) (e) not normalizable … \( B_0 = 1 \) (f) hint: integrate by parts … hermiticity condition: \( C = \) imaginary  
(g) hermiticity condition: \( A = \) real  
(h) yes!!! (i) yes  
(j) hint: evaluate \( \{\hat{x}, \hat{p}\} \psi(x) \) i.e. give the operators some function \( \psi(x) \) to work on, that will make your calculation much more clear … answer: \( \{\hat{x}, \hat{p}\} = i\hbar \)  
(k) hermiticity condition: \( \{\hat{A}, \hat{B}\} = 0 \).

2 About eigen-things: “Eigen” is German for “one’s own”. Eigenart means “characteristic feature” or “distinctiveness” … Eigeninitiative means “his/her own idea” … Eigenleistung means “personal contribution” … In this vein, an eigenfunction of an operator \( Q \) is a function that is special to that operator in that the operator doesn’t change the shape of the eigenfunction at all, it just multiplies it by a scalar, which is the associated eigenvalue. The eigen-things of an operator \( Q \) are very personal to \( Q \).
\[ \hat{Q}f_q = qf_q \]

for some function \( f_q \) and some scalar \( q \), then \( f_q \) is an eigenfunction of \( \hat{Q} \) with eigenvalue \( q \). For your proof, evaluate the Hermitian condition \( \langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle \) for an eigenfunction \( f_q \) and see what condition that imposes on the eigenvalue \( q \).

(b) It is really important that those eigenvalues are real because they represent measurable values! We need to be very clear on something: an eigenfunction \( \psi_q \) of \( \hat{Q} \) with eigenvalue \( q \) is a state of definite \( Q \) i.e. the only possible value that the quantity \( Q \) can take if it is measured is the eigenvalue \( q \). To prove this, show that the variance \( \sigma_Q^2 = \langle Q^2 \rangle - \langle Q \rangle^2 \) is zero when the system is in an eigenstate of \( Q \), and so the only possible value you can measure is the average value \( \langle Q \rangle \) … which is what?

(c) Prove that two different eigenfunctions \( f_1 \) and \( f_2 \) of a Hermitian operator with different eigenvalues \( q_1 \) and \( q_2 \) are ORTHOGONAL. Hints are in the checkpoint.

(d) What are the eigenfunctions of the momentum operator? Show that \( \psi_p(x) = A_p e^{i(p/\hbar)x} \) works, with eigenvalue \( p \). Then, figure out what normalization constant \( A_p \) you need to make these un-normalizable plane-wave eigenfunctions obey Dirac orthonormality, i.e. 
\[ \langle \psi_{p_1} | \psi_{p_2} \rangle = \delta(p_2 - p_1) \]

You will need to use this fabulously useful representation of the Dirac \( \delta \) function that you found last week:
\[ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} \, dx = \delta(K) \]

(e) What are the eigenfunctions of the position operator? Show that \( \psi_{x_0}(x) = B_0 \delta(x - x_0) \) works, with eigenvalue \( x_0 \). Now to find the normalization constant \( B_0 \)! Are these eigenfunctions normalizable? If not, find the value of \( B_0 \) that makes the eigenfunctions obey Dirac orthonormality, i.e. 
\[ \langle \psi_{x_1} | \psi_{x_2} \rangle = \delta(x_2 - x_1) \]

(f) The momentum operator \( \hat{p}_x = -i\hbar \partial/\partial x \) represents one broad class of operators: derivatives \( \partial/\partial x, \partial/\partial y, \partial/\partial z, \partial/\partial t \). The energy operator \( \hat{E} = i\hbar \partial/\partial t \) is in this class. Consider a general first-derivative operator \( \hat{A} \) with a constant factor \( C \) out in front: \( \hat{A} = C(\partial/\partial x) \). In general, \( C \) can be complex. Is this \( \hat{A} \) operator Hermitian? You will find that it is, but only if you impose a condition on \( C \); what is that condition?

(g) The position operator \( \hat{x} = x \) represents the other class of operators: multiplicative functions \( A(x,y,z,t) \). The potential-energy operator \( \hat{V} = V(x,t) \) is in this class. Consider a general multiplicative-function operator \( \hat{A} = A(x,t) \) . In general, the function \( A(x,t) \) can be complex. Is this \( \hat{A} \) operator Hermitian? You will find that it is, but only if you impose a condition on \( A \); what is that condition?

(h) Do \( \hat{p} \) and \( \hat{x} \) obey the constraints you found in (f) & (g), i.e. are they Hermitian operators?

(i) Additional operators can be formed by adding and/or multiplying the two classes of operators you just investigated. First consider addition: let \( \hat{A} \) and \( \hat{B} \) be Hermitian operators. Is \( \hat{A} \pm \hat{B} \) Hermitian?

(j) Before we tackle multiplication, you must realize that the product of two operators is not necessarily commutative! We define the commutator of two operators as follows: \( [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \). Calculate the extremely important commutator \( [\hat{x}, \hat{p}] \). It is not zero! It will appear in a famous relation very soon.

(k) And now multiplication of operators: if \( \hat{A} \) and \( \hat{B} \) are Hermitian operators, is the product \( \hat{A}\hat{B} \) Hermitian? You will find that the answer is yes only if a certain condition is met. What is that condition?
Appendix: Postulates of QM from R. Shankar, "Principles of Quantum Mechanics"

Classical Mechanics

I. The state of a particle at any given time is specified by the two variables \( x(t) \) and \( p(t) \), i.e., as a point in a two-dimensional phase space.

II. Every dynamical variable \( \omega \) is a function of \( x \) and \( p \): \( \omega = \omega(x, p) \).

Quantum Mechanics

I. The state of the particle is represented by a vector \( |\psi(t)\rangle \) in a Hilbert space.

II. The independent variables \( x \) and \( p \) of classical mechanics are represented by Hermitian operators \( X \) and \( P \) with the following matrix elements in the eigenbasis of \( X^\dagger \):

\[
\langle x'|X|x\rangle = x\delta(x - x')
\]

\[
\langle x'|P|x\rangle = -i\hbar\delta'(x - x')
\]

The operators corresponding to dependent variables \( \omega(x, p) \) are given Hermitian operators

\[
\Omega(X, P) = \omega(x \rightarrow X, p \rightarrow P)
\]

III. If the particle is in a state given by \( x \) and \( p \), the measurement\(\parallel\) of the variable \( \omega \) will yield a value \( \omega(x, p) \).

The state will remain unaffected.

IV. The state variables change with time according to Hamilton's equations:

\[
\dot{x} = \frac{\partial \mathcal{H}}{\partial p}
\]

\[
\dot{p} = -\frac{\partial \mathcal{H}}{\partial x}
\]

IV. The state vector \( |\psi(t)\rangle \) obeys the Schrödinger equation

\[
i\hbar \frac{d}{dt} |\psi(t)\rangle = \mathcal{H} |\psi(t)\rangle
\]

where \( H(X, P) = \mathcal{H}(x \rightarrow X, p \rightarrow P) \) is the quantum Hamiltonian operator and \( \mathcal{H} \) is the Hamiltonian for the corresponding classical problem.