Physics 486 Discussion 9 – Hermitian Operators

Problem 1 : The Final Word on Hermitian Operators *Hints & Checkpoints* [1]

We defined **Hermitian operators** in homework in a mathematical way: they are linear **self-adjoint** operators. As a reminder, every linear operator $\hat{Q}$ in a Hilbert space has an adjoint $\hat{Q}^\dagger$ that is defined as follows :

$$\boxed{\left\langle \hat{Q}^\dagger f \middle| g \right\rangle \equiv \left\langle f \middle| \hat{Q} g \right\rangle}$$

Hermitian operators are those that are equal to their own adjoints: $\boxed{\hat{Q}^\dagger = \hat{Q}}$.

Now for the physics properties of these operators. **Hermitian operators** are those associated with **observables** in quantum mechanics, i.e. with measurable quantities. What properties must they possess to fulfill this role? Measurements are **real**, so the **expectation values** of a Hermitian operator $\hat{Q}$ must be real numbers:

$$\boxed{\left\langle \hat{Q} \right\rangle^* = \left\langle \hat{Q} \right\rangle}.$$

We can take this as the physics definition of a Hermitian operator. Is it equivalent to the math definition? Let's use the familiar wavefunction representation for our proof :

Since $\left\langle \hat{Q} \right\rangle = \int_{-\infty}^{+\infty} \psi^*(x)\, \hat{Q}\, \psi(x)\, dx = \left\langle \psi \middle| \hat{Q}\, \psi \right\rangle$ in Dirac notation,

and $\left\langle \hat{Q} \right\rangle^* = \int_{-\infty}^{+\infty} \psi(x)\, \hat{Q}^*\, \psi^*(x)\, dx = \int_{-\infty}^{+\infty} \left(\hat{Q}\, \psi(x) \right)^* \psi(x)\, dx = \left\langle \hat{Q}\, \psi \middle| \psi \right\rangle$,

then $\left\langle \psi \middle| \hat{Q} \psi \right\rangle = \left\langle \hat{Q} \psi \middle| \psi \right\rangle$ is equivalent to $\left\langle \hat{Q} \right\rangle^* = \left\langle \hat{Q} \right\rangle$.

The wavefunction representation is nice and familiar, but it is important to stress that we did not *have* to use any representation *at all* to accomplish this proof. We could instead have used one of the three defining properties of the inner product, which are recapped on the last page of this discussion :

conjugate symmetry : $\left\langle y \middle| x \right\rangle = \left\langle x \middle| y \right\rangle^*$

The representation-free proof is even shorter:

$\left\langle \hat{Q} \right\rangle \equiv \left\langle \psi \middle| \hat{Q}\, \psi \right\rangle$ and $\left\langle \hat{Q} \right\rangle^* \equiv \left\langle \psi \middle| \hat{Q}\, \psi \right\rangle^* = \left\langle \hat{Q}\, \psi \middle| \psi \right\rangle$ by conjugate symmetry

$\therefore \left\langle \hat{Q} \right\rangle = \left\langle \hat{Q} \right\rangle^*$ is equivalent to $\boxed{\left\langle \psi \middle| \hat{Q} \psi \right\rangle = \left\langle \hat{Q} \psi \middle| \psi \right\rangle}$

That last expression, in the box, is *almost* the same as the self-adjoint definition. To finish the proof that "all expectation values of Q must be real" is equivalent to "Q must be self-adjoint", one must show that the boxed expression is equivalent to this :

$\boxed{\left\langle f \middle| \hat{Q}\, g \right\rangle = \left\langle \hat{Q}\, f \middle| g \right\rangle}$ where f and g are any *two* elements in your Hilbert space.

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[1] **Q1 (b)** evaluate $\left\langle Q \right\rangle$ and $\left\langle Q^2 \right\rangle$ for the eigenstate ψ_q with eigenvalue q … it is really easy to show that $\left\langle Q^n \right\rangle = q^n$ in an eigenstate! **(c)** What do you want to show? Write it down. … You want to show $< f_1 \mid f_2 > = 0$ … 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)** yes **(g)** hermiticity condition is $[\hat{A}, \hat{B}] = 0$.

This last piece of the proof is problem 2 below. But first, let's learn more about Hermitian operators and their eigenstates.

(a) Prove that **all eigenvalues** of a Hermitian operator are **REAL**. Recall the definition of eigen-things[2]: if

$$\hat{Q} f_q = q f_q$$

for some function f_q and some scalar q, then f_q is an **eigenfunction** of $\hat{Q}$ with **eigenvalue** q.

▶ HINTS: Apply the Hermitian condition in the form $\langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle$ to an eigenfunction f_q of Q … use the conjugate symmetry of the inner product … what condition do you get on the eigenvalue q?

(b) It is *really* important that those eigenvalues are real because they represent measurable values! We need to be 100% clear on something else too : an **eigenfunction** ψ_q of $\hat{Q}$ with eigenvalue q is **a state of definite *Q*** i.e. <u>the only possible value that the quantity *Q* can take</u> if it is <u>measured</u> is the <u>eigenvalue *q*</u>. To prove this, show that the variance $\sigma_Q^2 = \langle Q^2 \rangle - \langle Q \rangle^2$ is <u>zero</u> 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 <u>eigenfunctions</u> of the <u>momentum operator</u>? 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 "Fourier" representation of the Dirac δ function :

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{iKx} \, dx = \delta(K)$$

Note: we wrote down the normalization constant in class, but we didn't actually derive it … time to fix that! ☺

(e) What are the <u>eigenfunctions</u> of the <u>position operator</u> $\hat{x} = x$? We presented them in class, but they are fairly strange, and we didn't check their normalization. First, show that $\psi_{x_0}(x) = B_0 \, \delta(x - x_0)$ works, with eigenvalue x_0. Next, 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) On your homework, you showed explicitly that $\hat{x} = x$ and $\hat{p}_x = -i\hbar \partial / \partial x$ are Hermitian operators. Additional operators can be formed by adding and/or multiplying other operators together, e.g. kinetic energy $\hat{T} = \hat{p}^2 / 2m$, or the angular momentum operator $\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$ that is coming up very soon. We'd better find out if such combinations of Hermitian operators are also Hermitian.
First consider **addition**. If $\hat{A}$ and $\hat{B}$ are Hermitian operators, is $\hat{A} \pm \hat{B}$ Hermitian?

(g) And now **multiplication**: 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 <u>only if a certain condition is met</u>. What is that condition?

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[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. ☺

Problem 2 : Equivalent Definitions of a Hermitian Operator *adapted from Griffiths 3.3*

For this question, you will need the **defining properties of an inner product**. They were presented in lecture, and can be found in Griffiths Appendix A.2 (or Wikipedia, or a linear algebra text). Here they are again:

> Let x, y, and z be members of a linear vector space $\mathbb{V}$ over the field of scalars $\mathbb{F}$ (which can be the real numbers $\mathbb{R}$ or the complex numbers $\mathbb{C}$). Let c be a scalar within $\mathbb{F}$. Any valid inner product $\langle x|y\rangle$ (which, by construction, maps two elements of $\mathbb{V}$ onto a scalar from $\mathbb{F}$) must have these properties:
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> 1. **positive definiteness** of the norm : $\langle x|x\rangle \geq 0$ and $\{\ \langle x|x\rangle = 0 \Rightarrow |x\rangle = |0\rangle =$ zero element[3] $\}$
> 2. **conjugate** symmetry : $\langle y|x\rangle = \langle x|y\rangle^*$
> 3. **linearity** in the 2nd argument : $\langle x|y+z\rangle = \langle x|y\rangle + \langle x|z\rangle$ and $\langle x|c\,y\rangle = c\langle x|y\rangle$
>
> $\rightarrow$ together, 2&3 imply that : $\langle x+y|z\rangle = \langle x|z\rangle + \langle y|z\rangle$ and $\langle c\,x|y\rangle = c^*\langle x|y\rangle$

Now on to our question. As you showed in problem 1, the physics definition of a Hermitian operator $\hat{Q}$ can be written in two equivalent ways :

$$\langle \hat{Q}\rangle^* = \langle \hat{Q}\rangle \quad \text{and} \quad \langle f|\hat{Q}f\rangle = \langle \hat{Q}f|f\rangle .$$

That second expression is not *quite* equivalent to our mathematical definition, which is self-adjointness:

$$\langle g|\hat{Q}h\rangle = \langle \hat{Q}g|h\rangle .$$

for any *two* elements g and h of an inner product space. This seems like a *stronger* condition on $\hat{Q}$ …
but no, this third expression is equivalent to the other two expressions. Using the last two defining properties of the inner product and the fact that $\hat{Q}$ is linear (see footnote [4]), show that

$$\langle f|\hat{Q}f\rangle = \langle \hat{Q}f|f\rangle \text{ for any element } f \quad \underline{\text{implies}} \quad \langle g|\hat{Q}h\rangle = \langle \hat{Q}g|h\rangle \text{ for any } two \text{ elements } g, h.$$

▶ GUIDANCE : Let $f = g + h$ and plug it into the left-hand condition, … then let $f = g + ih$ and plug that into the left-hand condition … and manipulate things until you arrive at the right-hand condition.

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[3] The **zero element** $|0\rangle$ of a vector space is the element you get when you multiply any element $|x\rangle$ by the scalar 0. It must be part of the vector space because all linear combinations of the basis elements are included, by construction, so all linear combinations of all elements are included too, and that includes scalar multiples of a single element.

[4] A **linear operator** $\hat{A}$ is one that preserves addition and scalar multiplication: $\hat{A}(x+y) = \hat{A}x + \hat{A}y$ and $\hat{A}(cx) = c\hat{A}x$ if c is a scalar.