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**Comments on Hermitian Operators**

In lecture I mentioned that whether an operator is hermitian or not depends not only on the form of the operator but also on the type of states on which it is allowed to act. You explored this on problem set 3, #4. Here is a bit more information on the subject.

We say an operator is hermitian if

$$\hat{A} = \hat{A}^\dagger. \tag{1}$$

However we defined  $\hat{A}^\dagger$  by its action on bras, if  $\hat{A}|\alpha\rangle = |\beta\rangle$  then  $\langle\alpha|\hat{A}^\dagger = \langle\beta|$ . To define  $\langle\alpha|\hat{A}$  we inserted the identity written with a complete set of states,  $\{|n\rangle\}$ , so  $\langle\alpha|\hat{A} = \sum_n \langle\alpha|\hat{A}|n\rangle\langle n|$ , and the action of the operator  $\hat{A}$  on bras is thus also defined by its action on kets,  $\hat{A}|n\rangle$ . In a similar manner we can also define the action of  $\hat{A}^\dagger$  on kets by inserting the identity operator,  $\hat{1}$ , on the left,

$$\hat{A}^\dagger|\alpha\rangle = \hat{1}\hat{A}^\dagger|\alpha\rangle = \sum_n |n\rangle\langle n|\hat{A}^\dagger|\alpha\rangle, \tag{2}$$

and using our knowledge of  $\langle n|\hat{A}^\dagger$ . The crucial point is that Equation (1) is really a statement about the equality of operators which *act on* bras or kets, and thus depends on the states allowed in the Hilbert space. For example the meaning of  $\hat{A} = \hat{B}$  is that  $\langle\psi|\hat{A}|\phi\rangle$  for any states  $|\psi\rangle$  and  $|\phi\rangle$  in the Hilbert space, so the validity of an operator equation depends on which states we allow the operators to act.

It is easiest to explore this on a space of functions. An operator could be hermitian on one function space, but not another. The wavefunctions of quantum mechanics are usually restricted to live in the space of functions that are complex valued and *square integrable*,

$$\int_{-\infty}^{\infty} dx |f(x)|^2 < \infty. \tag{3}$$

This way they can be normalized to unity ( $\int_{-\infty}^{\infty} dx |f(x)|^2 = 1$ ) so that  $|f(x)|^2$  can be interpreted as a probability. Such functions must vanish as  $x \rightarrow \pm\infty$ ,

$$\lim_{x \rightarrow \pm\infty} f(x) = 0 \tag{4}$$

in order for the integral (eq. (3)) to exist.

Now, consider the usual momentum operator,

$$\hat{p} \equiv -i\hbar \frac{d}{dx} \tag{5}$$

defined on this set of functions. We want to see if  $\hat{p}$  is hermitian – *i.e.* does  $\langle f|\hat{p}g\rangle = \langle \hat{p}f|g\rangle$ ? [ Remember, that on the space of functions we take  $\langle f|g\rangle \equiv \int_{-\infty}^{\infty} dx f^*(x)g(x)$ . Also the definition of the hermitian conjugate of  $\hat{p}$  can be written  $\langle \hat{p}^\dagger f|g\rangle \equiv \langle f|\hat{p}g\rangle$ , and  $\hat{p}$  is hermitian if  $\hat{p}^\dagger = \hat{p}$ . ] So we want to prove

$$\int_{-\infty}^{\infty} dx f^*(x) \left[ -i\hbar \frac{d}{dx} g(x) \right] = \int_{-\infty}^{\infty} dx \left[ -i\hbar \frac{d}{dx} f(x) \right]^* g(x). \quad (6)$$

All we have to do is write  $f^*(\frac{d}{dx}g) = \frac{d}{dx}(f^*g) - (\frac{d}{dx}f^*)g$ , substitute into  $\langle f|\hat{p}g\rangle$  and integrate the total derivative  $\frac{d}{dx}(f^*g)$ ,

$$\int_{-\infty}^{\infty} dx f^*(x) \left[ -i\hbar \frac{d}{dx} g(x) \right] = -i\hbar f^*(x)g(x)|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} dx \left[ -i\hbar \frac{d}{dx} f(x) \right]^* g(x). \quad (7)$$

The “surface term” at  $\pm\infty$  vanishes because of (4), and we have shown that  $\hat{p}$  is hermitian.

The same operator,  $\hat{p} = -i\hbar \frac{d}{dx}$ , is *not* Hermitian in the space of functions defined on the half-line  $x \in [0, \infty]$  unless the functions are required to obey some boundary condition at  $x = 0$ . The attempt to prove  $\hat{p}$  Hermitian, (7), now reads

$$\int_0^{\infty} dx f^*(x) \left[ -i\hbar \frac{d}{dx} g(x) \right] = -i\hbar f^*(x)g(x)|_0^{\infty} + \int_0^{\infty} dx \left[ -i\hbar \frac{d}{dx} f(x) \right]^* g(x). \quad (8)$$

The “surface term” at  $x = 0$  must vanish if  $\hat{p}$  is to be Hermitian. This can be assured if  $f(0) = g(0) = 0$ . So in order for  $\hat{p} = -i\hbar \frac{d}{dx}$  to be Hermitian on  $x \in [0, \infty]$ , we must supplement the definition of the Hilbert space with the boundary condition  $f(x)|_{x=0} = 0$  for all states, as you showed on the problem set.

Another interesting wrinkle on this subject, that goes beyond what you did on the problem set, concerns the operator  $\hat{p}^2$ , which appears in the Hamiltonian,  $\hat{H} = \frac{\hat{p}^2}{2m}$ . We want  $\hat{H}$  to be Hermitian, so the energy eigenvalues will be real. Suppose we confine the quantum system to an interval, say  $0 \leq x \leq L$ . Then showing  $\hat{H}$  to be Hermitian entails integrating by parts twice,

$$\int_0^{\infty} dx f^*(x) \left[ \frac{d^2}{dx^2} g(x) \right] = [f^*(x)g'(x) - f'^*(x)g(x)]_0^L + \int_0^{\infty} dx \left[ \frac{d^2}{dx^2} f(x) \right]^* g(x). \quad (9)$$

In this case the “surface term” will vanish if  $f(0) = cf'(0)$  and  $f(L) = cf'(L)$ , where  $c$  is any *real* constant, and likewise for the function  $g$ . Here  $c = 0$  is a familiar boundary condition from wave mechanics, corresponding to an infinitely high potential barrier at  $x = 0$  and  $L$ . Actually there is a simple interpretation for the general boundary condition. *It is exactly the condition that guarantees that the probability flux of any wavefunction is zero at  $x = 0$  and  $L$ .* Remember the flux is defined by

$$J(x) = \frac{\hbar}{2mi} (f^*(x)f'(x) - f'^*(x)f(x))$$

and it is easy to see that  $f' = cf$  implies  $S = 0$  if  $c$  is real. Thus the boundary condition that makes  $\hat{H} = \frac{\hat{p}^2}{2m}$  Hermitian makes sure that no probability escapes out the ends of the box. This is consistent with the interpretation of  $\hat{H}$  as the generator of time development (which we are discussing in lecture in part II). To conserve probability as time progresses, we need  $\mathcal{U} = e^{i\hat{H}t/\hbar}$  to be unitary and therefore require  $\hat{H}$  to be Hermitian!