Problem 3.48

An operator is defined not just by its *action* (what it *does* to the vector it is applied to) but its *domain* (the set of vectors on which it acts). In a *finite*-dimensional vector space the domain is the entire space, and we don't need to worry about it. But for most operators in Hilbert space the domain is restricted. In particular, only functions such that $\hat{Q}f(x)$ remains in Hilbert space are allowed in the domain of $\hat{Q}$. (As you found in Problem 3.2, the derivative operator can knock a function out of L^2.)

A hermitian operator is one whose *action* is the same as that of its adjoint[45] (Problem 3.5). But what is required to represent observables is actually something more: the *domains* of $\hat{Q}$ and $\hat{Q}^\dagger$ must *also* be identical. Such operators are called **self-adjoint**.[46]

(a) Consider the momentum operator, $\hat{p} = -i\hbar d/dx$, on the finite interval $0 \leq x \leq a$. With the infinite square well in mind, we might define its domain as the set of functions $f(x)$ such that $f(0) = f(a) = 0$ (it goes without saying that $f(x)$ and $\hat{p}f(x)$ are in $L^2(0, a)$). Show that $\hat{p}$ is hermitian: $\langle g|\hat{p}f\rangle = \langle \hat{p}^\dagger g|f\rangle$, with $\hat{p}^\dagger = \hat{p}$. But is it self-adjoint? *Hint:* as long as $f(0) = f(a) = 0$, there is no restriction on $g(0)$ or $g(a)$—the domain of $\hat{p}^\dagger$ is much larger than the domain of $\hat{p}$.[47]

(b) Suppose we *extend* the domain of $\hat{p}$ to include all functions of the form $f(a) = \lambda f(0)$, for some fixed complex number λ. What condition must we then impose on the domain of $\hat{p}^\dagger$ in order that $\hat{p}$ be hermitian? What value(s) of λ will render $\hat{p}$ self-adjoint? *Comment:* Technically, then, there *is* no momentum operator on the finite interval—or rather, there are infinitely many, and no way to decide which of them is "correct." (In Problem 3.34 we avoided the issue by working on the infinite interval.)

(c) What about the semi-infinite interval, $0 \leq x < \infty$? Is there a self-adjoint momentum operator in this case?[48]

[Capitalize the "a."]

Solution

[45] Mathematicians call them "symmetric" operators.

[46] Because the distinction rarely intrudes, physicists tend to use the word "hermitian" indiscriminately; technically, we should always say "self-adjoint," meaning $\hat{Q} = \hat{Q}^\dagger$ both in action and in domain.

[47] The domain of $\hat{Q}$ is something we *stipulate*; that *determines* the domain of $\hat{Q}^\dagger$.

[48] J. von Neumann introduced machinery for generating **self-adjoint extensions** of hermitian operators—or in some cases proving that they cannot exist. For an accessible introduction see G. Bonneau, J. Faraut, and B. Valent, *Am. J. Phys.* **69**, 322 (2001); for an interesting application see M. T. Ahari, G. Ortiz, and B. Seradjeh, *Am. J. Phys.* **84**, 858 (2016).

Part (a)

Define the domain of $\hat{p}$ to be the set of functions such that $f(0) = 0$ and $f(a) = 0$. Show that $\hat{p}$ is hermitian on the finite interval $0 \leq x \leq a$.

$$\begin{aligned}
\langle g \,|\, \hat{p} \,|\, f \rangle &= \int_0^a g^*(x)[\hat{p} f(x)]\, dx \\
&= \int_0^a g^*(x) \left(-i\hbar \frac{df}{dx} \right) dx \\
&= -i\hbar \int_0^a g^*(x) \frac{df}{dx}\, dx \\
&= -i\hbar \left[g^*(x) f(x) \bigg|_0^a - \int_0^a \frac{dg^*}{dx} f(x)\, dx \right] \\
&= -i\hbar \left[g^*(a) f(a) - g^*(0) f(0) - \int_0^a \frac{dg^*}{dx} f(x)\, dx \right] \\
&= -i\hbar \left[g^*(a)(0) - g^*(0)(0) - \int_0^a \frac{dg^*}{dx} f(x)\, dx \right] \\
&= i\hbar \int_0^a \frac{dg^*}{dx} f(x)\, dx \\
&= \int_0^a \left(-i\hbar \frac{dg}{dx} \right)^* f(x)\, dx \\
&= \int_0^a \left[\hat{p}^\dagger g(x) \right]^* f(x)\, dx
\end{aligned}$$

Since $\hat{p} = \hat{p}^\dagger$, $\hat{p}$ is a hermitian operator. There are no conditions on g, so the domain of $\hat{p}^\dagger$ is larger than that of $\hat{p}$; $\hat{p}$ is not self-adjoint.

Part (b)

Define the domain of $\hat{p}$ to be the set of functions such that $f(a) = \lambda f(0)$. Show that $\hat{p}$ is hermitian on the finite interval $0 \leq x \leq a$.

$$\begin{aligned}
\langle g \,|\, \hat{p} \,|\, f \rangle &= \int_0^a g^*(x)[\hat{p} f(x)]\, dx \\
&= \int_0^a g^*(x) \left(-i\hbar \frac{df}{dx}\right) dx \\
&= -i\hbar \int_0^a g^*(x) \frac{df}{dx}\, dx \\
&= -i\hbar \left[g^*(x) f(x) \Big|_0^a - \int_0^a \frac{dg^*}{dx} f(x)\, dx \right] \\
&= -i\hbar \left[g^*(a) f(a) - g^*(0) f(0) - \int_0^a \frac{dg^*}{dx} f(x)\, dx \right] \\
&= -i\hbar \left[\lambda g^*(a) f(0) - g^*(0) f(0) - \int_0^a \frac{dg^*}{dx} f(x)\, dx \right] \\
&= -i\hbar [\lambda g^*(a) f(0) - g^*(0) f(0)] + i\hbar \int_0^a \frac{dg^*}{dx} f(x)\, dx \\
&= -i\hbar [\lambda g^*(a) - g^*(0)] f(0) + \int_0^a \left(-i\hbar \frac{dg}{dx}\right)^* f(x)\, dx \\
&= -i\hbar [\lambda^* g(a) - g(0)]^* f(0) + \int_0^a \left[\hat{p}^\dagger g(x)\right]^* f(x)\, dx
\end{aligned}$$

In order for $\hat{p}$ to be hermitian,

$$-i\hbar [\lambda^* g(a) - g(0)]^* f(0) = 0 \quad \Rightarrow \quad \lambda^* g(a) - g(0) = 0 \quad \text{or} \quad f(0) = 0$$

$$g(a) = \frac{1}{\lambda^*} g(0) \quad \text{or} \quad f(0) = 0.$$

Therefore, the condition that must be imposed on the domain of $\hat{p}^\dagger$ in order for $\hat{p}$ to be hermitian is

$$g(a) = \frac{1}{\lambda^*} g(0).$$

For $\hat{p}$ to be self-adjoint, the conditions on f and g have to be the same, so

$$\lambda = \frac{1}{\lambda^*}$$

$$\lambda^* \lambda = 1$$

$$|\lambda|^2 = 1$$

λ must be a point on the unit circle in the complex plane: $\lambda = e^{i\phi}$.

Part (c)

On the semi-infinite interval $0 \leq x < \infty$, the functions f and g go to zero as $x \to \infty$. Show that $\hat{p}$ is hermitian on this interval.

$$\begin{aligned}
\langle g \,|\, \hat{p} \,|\, f \rangle &= \int_0^\infty g^*(x)[\hat{p}f(x)]\,dx \\
&= \int_0^\infty g^*(x)\left(-i\hbar\frac{df}{dx}\right)dx \\
&= -i\hbar\int_0^\infty g^*(x)\frac{df}{dx}\,dx \\
&= -i\hbar\left[g^*(x)f(x)\Big|_0^\infty - \int_0^\infty \frac{dg^*}{dx}f(x)\,dx\right] \\
&= -i\hbar\left[g^*(\infty)f(\infty) - g^*(0)f(0) - \int_0^\infty \frac{dg^*}{dx}f(x)\,dx\right] \\
&= -i\hbar[-g^*(0)f(0)] + i\hbar\int_0^\infty \frac{dg^*}{dx}f(x)\,dx \\
&= i\hbar g^*(0)f(0) + \int_0^a \left(-i\hbar\frac{dg}{dx}\right)^* f(x)\,dx \\
&= i\hbar g^*(0)f(0) + \int_0^a \left[\hat{p}^\dagger g(x)\right]^* f(x)\,dx
\end{aligned}$$

In order for $\hat{p}$ to be hermitian,

$$i\hbar g^*(0)f(0) = 0 \quad \Rightarrow \quad g(0) = 0 \quad \text{or} \quad f(0) = 0.$$

If we choose the domain of $\hat{p}$ to be the set of functions that satisfy $f(0) = 0$, then there is no restriction on $g(0)$. The domain of $\hat{p}^\dagger$ is larger than that of $\hat{p}$, so $\hat{p}$ is not self-adjoint on the semi-infinite interval.