Problem 3.4

(a) Show that the *sum* of two hermitian operators is hermitian.

(b) Suppose $\hat{Q}$ is hermitian, and α is a complex number. Under what condition (on α) is $\alpha\hat{Q}$ hermitian?

(c) When is the *product* of two hermitian operators hermitian?

(d) Show that the position operator ($\hat{x}$) and the Hamiltonian operator $\left(\hat{H} = -\left(\hbar^2/2m\right) d^2/dx^2 + V(x)\right)$ are hermitian.

Solution

Let $\hat{Q}$ and $\hat{R}$ be hermitian operators: $\hat{Q}^\dagger = \hat{Q}$ and $\hat{R}^\dagger = \hat{R}$.

Part (a)

The aim is to show that $\langle f \,|\, (\hat{Q}+\hat{R})f\rangle = \langle(\hat{Q}+\hat{R})f \,|\, f\rangle$ for all $f(x)$.

$$\begin{aligned}
\langle f \,|\, (\hat{Q}+\hat{R})f\rangle &= \langle f \,|\, (\hat{Q}+\hat{R}) \,|\, f\rangle \\
&= \int_{-\infty}^{\infty} f^*(x)\left[(\hat{Q}+\hat{R})f(x)\right] dx \\
&= \int_{-\infty}^{\infty} f^*(x)[\hat{Q}f(x)+\hat{R}f(x)]\, dx \\
&= \int_{-\infty}^{\infty} [f^*(x)\hat{Q}f(x)+f^*(x)\hat{R}f(x)]\, dx \\
\langle f \,|\, \hat{Q}f\rangle + \langle f \,|\, \hat{R}f\rangle &= \int_{-\infty}^{\infty} f^*(x)[\hat{Q}f(x)]\, dx + \int_{-\infty}^{\infty} f^*(x)[\hat{R}f(x)]\, dx \\
&= \int_{-\infty}^{\infty} f^*(x)\hat{Q}^\dagger f(x)\, dx + \int_{-\infty}^{\infty} f^*(x)\hat{R}^\dagger f(x)\, dx \\
\langle \hat{Q}f \,|\, f\rangle + \langle \hat{R}f \,|\, f\rangle &= \int_{-\infty}^{\infty} [\hat{Q}f(x)]^* f(x)\, dx + \int_{-\infty}^{\infty} [\hat{R}f(x)]^* f(x)\, dx \\
&= \int_{-\infty}^{\infty} \left\{[\hat{Q}f(x)]^* f(x) + [\hat{R}f(x)]^* f(x)\right\} dx \\
&= \int_{-\infty}^{\infty} \left\{[\hat{Q}f(x)]^* + [\hat{R}f(x)]^*\right\} f(x)\, dx \\
&= \int_{-\infty}^{\infty} \left[\hat{Q}f(x)+\hat{R}f(x)\right]^* f(x)\, dx \\
\langle(\hat{Q}+\hat{R})f \,|\, f\rangle &= \int_{-\infty}^{\infty} \left[(\hat{Q}+\hat{R})f(x)\right]^* f(x)\, dx
\end{aligned}$$

Therefore, the sum of two hermitian operators is hermitian.

Part (b)

Suppose that $\hat{Q}$ is hermitian.

$$\langle f \,|\, \hat{Q}f\rangle = \langle \hat{Q}f \,|\, f\rangle$$

$$\int_{-\infty}^{\infty} f^*(x)[\hat{Q}f(x)]\,dx = \int_{-\infty}^{\infty} [\hat{Q}f(x)]^* f(x)\,dx$$

Multiply both sides by α, a complex constant.

$$\alpha\int_{-\infty}^{\infty} f^*(x)[\hat{Q}f(x)]\,dx = \alpha\int_{-\infty}^{\infty} [\hat{Q}f(x)]^* f(x)\,dx$$

$$\int_{-\infty}^{\infty} \alpha f^*(x)[\hat{Q}f(x)]\,dx = \int_{-\infty}^{\infty} \alpha[\hat{Q}f(x)]^* f(x)\,dx$$

Provided that $\alpha = \alpha^*$, α can be brought inside the square brackets on the right side.

$$\int_{-\infty}^{\infty} f^*(x)[\alpha\hat{Q}f(x)]\,dx = \int_{-\infty}^{\infty} [\alpha\hat{Q}f(x)]^* f(x)\,dx$$

$$\langle f \,|\, \alpha\hat{Q}f\rangle = \langle \alpha\hat{Q}f \,|\, f\rangle$$

Therefore, $\alpha\hat{Q}$ is hermitian if α is real.

Part (c)

Here the aim is to find the conditions for when $\langle f \,|\, \hat{Q}\hat{R}f\rangle = \langle \hat{Q}\hat{R}f \,|\, f\rangle$ is true.

$$\begin{aligned}
\langle f \,|\, \hat{Q}\hat{R}f\rangle = \langle f \,|\, \hat{Q}\hat{R} \,|\, f\rangle &= \int_{-\infty}^{\infty} f^*(x)\hat{Q}\hat{R}f(x)\,dx \\
&= \int_{-\infty}^{\infty} f^*(x)\left\{\hat{Q}\left[\hat{R}f(x)\right]\right\}dx \\
&= \int_{-\infty}^{\infty} f^*(x)\hat{Q}^\dagger\left[\hat{R}f(x)\right]dx \\
&= \int_{-\infty}^{\infty} [\hat{Q}f(x)]^*\left[\hat{R}f(x)\right]dx \\
&= \int_{-\infty}^{\infty} [\hat{Q}f(x)]^*\hat{R}^\dagger f(x)\,dx \\
&= \int_{-\infty}^{\infty} \left\{\hat{R}\left[\hat{Q}f(x)\right]\right\}^* f(x)\,dx \\
&= \int_{-\infty}^{\infty} \left[\hat{R}\hat{Q}f(x)\right]^* f(x)\,dx \\
&= \int_{-\infty}^{\infty} \left[\hat{Q}\hat{R}f(x)\right]^* f(x)\,dx \\
&= \langle \hat{Q}\hat{R}f \,|\, f\rangle
\end{aligned}$$

Therefore, provided that two hermitian operators commute, their product is hermitian.

Part (d)

Show that the position operator is hermitian. Note that x is a real number that takes values between $-\infty$ and ∞, so $x = x^*$.

$$\begin{aligned}
\langle f \mid \hat{x} f \rangle &= \langle f \mid \hat{x} \mid f \rangle \\
&= \int_{-\infty}^{\infty} f^*(x) x f(x)\, dx \\
&= \int_{-\infty}^{\infty} x f^*(x) f(x)\, dx \\
&= \int_{-\infty}^{\infty} x^* f^*(x) f(x)\, dx \\
&= \int_{-\infty}^{\infty} [x f(x)]^* f(x)\, dx \\
&= \langle \hat{x} f \mid f \rangle
\end{aligned}$$

Now show that the Hamiltonian operator is hermitian. Note that the potential energy function $V(x)$ is a real-valued function $[V(x) = V^*(x)]$, whereas $f(x)$ is a complex-valued function $[f(x) = u(x) + iv(x)$, where $u(x)$ and $v(x)$ are real-valued functions$]$. Additionally, $f(x)$ is assumed to tend to zero as $x \to \pm\infty$.

$$\begin{aligned}
\langle f \mid \hat{H} f \rangle &= \langle f \mid \hat{H} \mid f \rangle \\
&= \int_{-\infty}^{\infty} f^*(x) \hat{H} f(x)\, dx \\
&= \int_{-\infty}^{\infty} f^*(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] f(x)\, dx \\
&= \int_{-\infty}^{\infty} f^*(x) \left[-\frac{\hbar^2}{2m} \frac{d^2 f}{dx^2} + V(x) f(x) \right] dx \\
&= \int_{-\infty}^{\infty} \left[-\frac{\hbar^2}{2m} f^*(x) \frac{d^2 f}{dx^2} + f^*(x) V(x) f(x) \right] dx \\
&= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} f^*(x) \frac{d^2 f}{dx^2}\, dx + \int_{-\infty}^{\infty} f^*(x) V(x) f(x)\, dx \\
&= -\frac{\hbar^2}{2m} \left[\underbrace{f^*(x) \frac{df}{dx} \bigg|_{-\infty}^{\infty}}_{=0} - \int_{-\infty}^{\infty} \frac{df^*}{dx} \frac{df}{dx}\, dx \right] + \int_{-\infty}^{\infty} V(x) f^*(x) f(x)\, dx \\
&= \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \frac{df^*}{dx} \frac{df}{dx}\, dx + \int_{-\infty}^{\infty} V^*(x) f^*(x) f(x)\, dx \\
&= \frac{\hbar^2}{2m} \left[\underbrace{\frac{df^*}{dx} f(x) \bigg|_{-\infty}^{\infty}}_{=0} - \int_{-\infty}^{\infty} \frac{d^2 f^*}{dx^2} f(x)\, dx \right] + \int_{-\infty}^{\infty} V^*(x) f^*(x) f(x)\, dx
\end{aligned}$$

Integration by parts was used twice in the first integral to transfer the derivatives from $f(x)$ to $f^*(x)$. Continue the simplification.

$$\begin{aligned}
\langle f \mid \hat{H} f\rangle &= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{d^2 f^*}{dx^2} f(x)\,dx + \int_{-\infty}^{\infty}[V(x)f(x)]^* f(x)\,dx \\
&= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left\{\frac{d^2}{dx^2}[u(x)+iv(x)]^*\right\} f(x)\,dx + \int_{-\infty}^{\infty}[V(x)f(x)]^* f(x)\,dx \\
&= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left\{\frac{d^2}{dx^2}[u(x)-iv(x)]\right\} f(x)\,dx + \int_{-\infty}^{\infty}[V(x)f(x)]^* f(x)\,dx \\
&= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\frac{d^2 u}{dx^2} - i\frac{d^2 v}{dx^2}\right) f(x)\,dx + \int_{-\infty}^{\infty}[V(x)f(x)]^* f(x)\,dx \\
&= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\frac{d^2 u}{dx^2} + i\frac{d^2 v}{dx^2}\right)^* f(x)\,dx + \int_{-\infty}^{\infty}[V(x)f(x)]^* f(x)\,dx \\
&= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left\{\frac{d^2}{dx^2}[u(x)+iv(x)]\right\}^* f(x)\,dx + \int_{-\infty}^{\infty}[V(x)f(x)]^* f(x)\,dx \\
&= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\frac{d^2 f}{dx^2}\right)^* f(x)\,dx + \int_{-\infty}^{\infty}[V(x)f(x)]^* f(x)\,dx \\
&= \int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}\right)^* f(x)\,dx + \int_{-\infty}^{\infty}[V(x)f(x)]^* f(x)\,dx \\
&= \int_{-\infty}^{\infty}\left\{\left(-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}\right)^* f(x) + [V(x)f(x)]^* f(x)\right\} dx \\
&= \int_{-\infty}^{\infty}\left\{\left(-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}\right)^* + [V(x)f(x)]^*\right\} f(x)\,dx \\
&= \int_{-\infty}^{\infty}\left[-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2} + V(x)f(x)\right]^* f(x)\,dx \\
&= \int_{-\infty}^{\infty}\left\{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right] f(x)\right\}^* f(x)\,dx \\
&= \int_{-\infty}^{\infty}\left[\hat{H} f(x)\right]^* f(x)\,dx \\
&= \langle \hat{H} f \mid f\rangle
\end{aligned}$$

Therefore, the Hamiltonian operator is hermitian.