Chapter 1

Symmetric, Hermitian and Self-adjoint operators

Introduction

The usual definition for an $n \times n$ operator A is

$$A \text{ is } \begin{cases} \text{symmetric} & \text{if } a_{ij} = a_{ji} \text{ for all } i, j = 1, \dots, n \\ \\ \text{hermitian/self-adjoint} & \text{if } a_{ij} = a^{\dagger}_{ji} \text{ for all } i, j = 1, \dots, n \end{cases}$$

This definition, however, does not lead us lead us anywhere in the case of differential operators. In that case, we need to be more careful with our words and precise in our definitions.

Definition 1. *Given two operators (differential or otherwise) A and B and space L on which they act, if for all $\langle\psi|,\ \langle\chi| \in L$, we find that*

$$\langle\chi|A\psi\rangle = \langle B\chi|\psi\rangle$$

*then B is called the **adjoint** of A, and is denoted by $A^{\dagger}$.*

Lets take an example: the case of the momentum operator $\hat{p}$. In this case, $L = \mathcal{L}_2(-\infty, \infty)$, that is, the space of square integrable functions in the domain $(-\infty, \infty)$. The position space representation for the operator

$$\begin{array}{l|l} \hat{x} = x & \hat{x} = \iota\hbar\frac{\partial}{\partial y} \\ \hat{p} = -\iota\hbar\frac{\partial}{\partial x} & \hat{p} = p \end{array}$$

Let $A = -\iota\hbar\frac{\partial}{\partial x}$

$$\begin{aligned}
\langle f|g\rangle &= \int_{-\infty}^{\infty} dx f(x)^* g(x) \\
\langle f|Ag\rangle &= \int_{-\infty}^{\infty} dx f(x)^* \left(-\iota\hbar\frac{\partial g(x)}{\partial x}\right) \\
&= \iota\hbar f(x)^* g(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dx \left(-\iota\hbar\frac{\partial f(x)}{\partial x}\right)^* g(x) \\
&= \langle A^\dagger f|g\rangle
\end{aligned}$$

Note that the term evaluated at $-\infty$ and ∞ vanishes only because the functions lie in $\mathcal{L}_2(-\infty,\infty)$ and therefore must be vanish at infinity.

Hence, the momentum operator is the same as its adjoint operator and is called **self-adjoint.**

But something more interesting happens when the space is instead $\mathcal{L}(a,b)$ with $a,b \in \mathbb{R}$. We then get

$$\langle f|Ag\rangle = \langle A^\dagger f|g\rangle + \Delta(a,b)$$

where

$$\Delta(a,b) = \iota(f^*(a)g(a) - f^*(b)g(b)).$$

Now, if we want the operator A to be self-adjoint, it is easily seen that we must restrict the class of allowed functions to the ones such that $\Delta(a,b) = 0$. Two ways to make this happen immediately strike us:

1. Choose the domain of $A^\dagger$, to be all functions that vanish at the end points, that is,

   $$\mathcal{D}_{A^\dagger} = \{f(x) \in \mathcal{L}_2(a,b) \mid f(a) = f(b) = 0\}$$

   But since the domain of A still remains $\mathcal{L}_2(a,b)$, $A \neq A^\dagger$! Such a pair of operators which have the same functional representation but different domains are called **symmetric**.

2. Choose the domain of A to be

   $$\mathcal{D}_A = \{g(x) \in \mathcal{L}_2(a,b) \mid g(a) = e^{\iota\theta} g(b)\}$$

   for some fixed θ. Now

   $$\begin{aligned}
   0 &= \Delta(a,b) \\
   &= \iota(f^*(a)g(a) - f^*(b)g(b)) \\
   &= g(a)(f^*(a) - f^*(b)e^{-\iota\theta}) \qquad \forall g(a) \\
   \implies f(a) &= f(b)e^{\iota\theta}
   \end{aligned}$$

which means that the domain of $A^\dagger$ that now makes $\Delta(a, b) = 0$ is the same as that of A. Since $\mathcal{D}_A = \mathcal{D}_{A^\dagger}$ and $\langle A^\dagger f|g\rangle = \langle f|Ag\rangle$ for all $f, g \in \mathcal{D}_A$, we may call A and $A^\dagger$ to be **self-adjoint**. But there's another interesting twist here. We do not just have one self-adjoint extension of the operator, but a *one parameter* (θ) *family of self-adjoint extensions*! That means that for each value of θ, we can a self-adjoint extension of the operator.

If there's a *unique* self-adjoint extension for an operator, the operator is said to be **essentially self-adjoint.**

An operator is called **Hermitian** if it is symmetric and bounded.

Test for self-adjointness

Let $n_\pm$ be number of solutions to the pair of equations

$$A\langle f_\pm| = \pm\iota\langle f_\pm|$$

1. if $n_+ = n_- = 0$, then A is essentially self-adjoint
2. if $n_+ = n_- = n \neq 0$, then there is a n parameter family of self-adjoint extensions.
3. if $n_+ \neq n_-$, then there is no self-adjoint extension of the operator A.

An example of case (3): Take the momentum operator on the space $\mathcal{L}_2[0, \infty)$:

$$\Delta(0, \infty) = \iota f^*(0)g(0)$$

and therefore,

$$\mathcal{D}_{A^\dagger} = \{f(x) \in \mathcal{L}_2[0, \infty) \mid f(0) = 0\}$$

Notice that in this case, $\mathcal{D}_A \subset \mathcal{D}_{A^\dagger}$ always! So there is no self-adjoint extension. If we use the criterion given above,

$$\begin{aligned} -\iota f'(x) &= \iota f(x) \\ f'(x) &= -f(x) \\ f(x) &= e^{-x} \quad \in L_2[0, \infty) \end{aligned}$$

So $n_+ = 0$. The other equation

$$\begin{aligned} -\iota f'(x) &= -\iota f(x) \\ f'(x) &= f(x) \\ f(x) &= e^{x} \quad \notin L_2[0, \infty) \end{aligned}$$

So, $n_- = 0$. Since $n_- \neq n_+$, there exists no self-adjoint extension for A on the space $\mathcal{L}_2[0, \infty)$.

Exercises

1. Prove that the operator

$$\hat{p}_r = -\iota \left(\frac{\partial}{\partial r} + \frac{d-1}{2r} \right),$$

   where d is the number of dimensions of the physical space, is self adjoint on the space $\mathcal{L}_2[0,\infty)$. Note that the inner product for this is

$$\langle f|g\rangle = \int_0^\infty dr\ r^{d-1} f^*(r) g^*(r)$$

Chapter 2

Symmetries in Quantum Mechanics

2.1 Spatial Translation

Consider the state $|\alpha(t)\rangle$ and the position space wavefunction $\psi_\alpha(x,t) = \langle x|\alpha(t)\rangle$ associated with it.

If we spatially translate the state by an amount $\Delta x = \rho$, we get the new state

$$\begin{aligned} \psi'(x,t) &= \psi(x-\rho,t) \\ &= \psi(x,t) - \frac{\rho}{1!}\frac{\partial}{\partial x}\psi(x,t) + \frac{\rho^2}{2!}\frac{\partial^2}{\partial x^2}\psi(x,t) + \cdots \end{aligned}$$

Amazingly, the above taylor series can be very succintly expressed with the exponential:

$$\psi'(x,t) = \exp\left(-\rho\,\frac{\partial}{\partial x}\right)\psi(x,t)$$

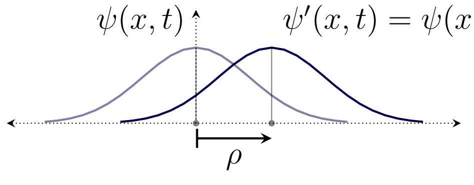

Figure 2.1: Active transformation of the state vector.

Ofcourse, in three dimensions,

$$\begin{aligned}\psi'(\mathbf{r},t) &= \exp\left(-\boldsymbol{\rho}\cdot\boldsymbol{\nabla}\right)\psi(\mathbf{r},t)\\ &= U_r(\rho)\psi(\mathbf{r},t)\end{aligned}$$

Recall that the momentum operator is just

$$\hat{\mathbf{p}} = -\iota\hbar\boldsymbol{\nabla}$$

So we get the **translation operator** to be

$$\hat{U}_r(\rho) = \exp\left(-\frac{\iota}{\hbar}\boldsymbol{\rho}\cdot\hat{\mathbf{p}}\right)$$

which is easily seen to be unitary, since $\hat{\mathbf{p}}$ is hermitian. It is in this sense that *momentum is the generator of translations*.

2.1.1 Spatial homogeniety of Schrödinger equation

Imposing homogeniety of space on the Schrödinger equation means that the temporal evolution should be same for $\psi(\mathbf{r},t)$ and $\psi'(\mathbf{r},t)$.

$$\begin{aligned}\iota\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} &= \hat{H}\psi(\mathbf{r},t)\\ \implies \iota\hbar\frac{\partial}{\partial t}\hat{U}_r^{\dagger}(\boldsymbol{\rho})\psi'(\mathbf{r},t) &= \hat{H}\hat{U}_r^{\dagger}(\boldsymbol{\rho})\psi'(\mathbf{r},t)\\ \implies \iota\hbar\;\hat{U}_r^{\dagger}(\boldsymbol{\rho})\frac{\partial}{\partial t}\psi'(\mathbf{r},t) &= \hat{H}\hat{U}_r^{\dagger}(\boldsymbol{\rho})\psi'(\mathbf{r},t)\\ \implies \iota\hbar\;\frac{\partial}{\partial t}\psi'(\mathbf{r},t) &= \hat{U}_r(\boldsymbol{\rho})\hat{H}\hat{U}_r^{\dagger}(\boldsymbol{\rho})\psi'(\mathbf{r},t)\end{aligned}$$

Now, if the $\psi'(\mathbf{r},t)$

$$\begin{aligned}\hat{U}_r(\boldsymbol{\rho})\hat{H}\hat{U}_r^{\dagger}(\boldsymbol{\rho}) &= \hat{H}\\ \implies [\hat{H},\hat{U}_r(\rho)] &= 0\end{aligned}$$

Since ρ is an arbitrary vector, we must have [Todo] elaborate this

$$[\hat{H},\hat{\mathbf{p}}] = 0$$

Hence, the momentum $\mathbf{p}$ is a constant of motion.