1.4: Exponential Operators

Throughout our work, we will make use of exponential operators of the form

$$\hat{T} = e^{-i\hat{A}} \tag{1.4.1}$$

We will see that these exponential operators act on a wavefunction to move it in time and space, and are therefore also referred to as propagators. Of particular interest to us is the time-evolution operator, $\hat{U} = e^{-i\hat{H}t/\hbar}$, which propagates the wavefunction in time. Note the operator $\hat{T}$ is a function of an operator, $f(\hat{A})$. A function of an operator is defined through its expansion in a Taylor series, for instance

$$\hat{T} = e^{-i\hat{A}} = \sum_{n=0}^{\infty} \frac{(-i\hat{A})^n}{n!} = 1 - i\hat{\hat{A}} - \frac{\hat{A}\hat{A}}{2} - \cdots \tag{1.4.2}$$

Since we use them so frequently, let's review the properties of exponential operators that can be established with Equation 1.4.2. If the operator $\hat{A}$ is Hermitian, then$\hat{T} = e^{-i\hat{A}}$ is unitary, i.e., $\hat{T}^{\dagger} = \hat{T}^{-1}$. Thus the Hermitian conjugate of $\hat{T}$ reverses the action of $\hat{T}$. For the time-propagator $\vec{U}$, $\vec{U}^{\dagger}$ is often referred to as the **time-reversal operator**.

The eigenstates of the operator $\hat{A}$ also are also eigenstates of $f(\hat{A})$, and eigenvalues are functions of the eigenvalues of $\hat{A}$. Namely, if you know the eigenvalues and eigenvectors of $\hat{A}$, i.e., $\hat{A}\varphi_n = a_n\varphi_n$,you can show by expanding the function

$$f(\hat{A})\varphi_n = f(a_n)\varphi_n \tag{1.4.3}$$

Our most common application of this property will be to exponential operators involving the Hamiltonian. Given the eigenstates φ_n, then $\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$ implies

$$e^{-i\hat{H}t/\hbar}|\varphi_n\rangle = e^{-iE_nt/\hbar}|\varphi_n\rangle \tag{1.4.4}$$

Just as $\hat{D}_x(\lambda)$ is the time-evolution operator that displaces the wavefunction in time, $\hat{D}_x = e^{-i\hat{p}_x x/h}$ is the spatial displacement operator that moves ψ along the x coordinate. If we define $\hat{D}_x = e^{-i\hat{p}_x x/h}$, then the action of is to displace the wavefunction by an amount λ

$$|\psi(x-\lambda)\rangle = \hat{D}_x(\lambda)|\psi(x)\rangle \tag{1.4.5}$$

Also, applying $\hat{D}_x(\lambda)$ to a position operator shifts the operator by λ

$$\hat{D}_x^{\dagger}\hat{x}\hat{D}_x = x + \lambda \tag{1.4.6}$$

Thus $e^{-i\hat{p}_x\lambda/\hbar}|x\rangle$ is an eigenvector of $\hat{x}$ with eigenvalue $x+\lambda$ instead of x. The operator

$\hat{D}_x = e^{-i\hat{p}_x\lambda/h}$ is a displacement operator for x position coordinates. Similarly, $\hat{D}_y = e^{-i\hat{p}_y\lambda/h}$ generates displacements in y and $\hat{D}_z$ in z. Similar to the time-propagator $\boldsymbol{U}$, the displacement operator $\boldsymbol{D}$ must be **unitary**, since the action of $\hat{D}^{\dagger}\hat{D}$ must leave the system unchanged. That is if $\hat{D}_x$ shifts the system to x from x_0, then $\hat{D}_x^{\dagger}$ shifts the system from x back to x_0.

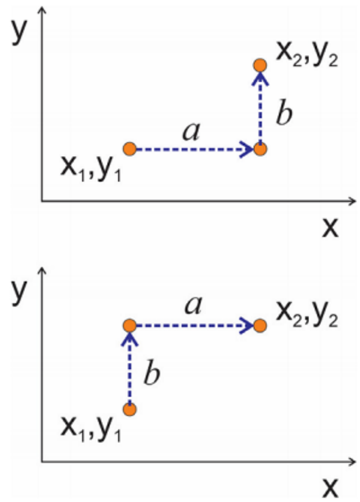

Figure 7. (Top) Displacement first along x by an amount a, then along y by b. (Bottom) Displacement in the reverse order yields the same state.

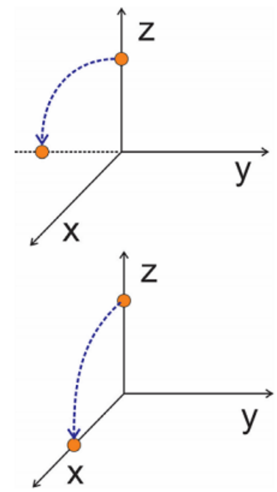

Figure 8. (Top) Rotation first about x by π/2, then about y by π/2, leaves the particle on the –y axis. (Bottom) Changing order by first rotating about y, then about x, leads to particle along +x axis.

Figure 1.4.1

We know intuitively that linear displacements commute. For example, if we wish to shift a particle in two dimensions, x and y, the order of displacement does not matter. We end up at the same position, whether we move along x first or along y, as illustrated in Figure 7. In terms of displacement operators, we can write

$$\begin{aligned} |x_2, y_2\rangle &= e^{-ibp_y/\hbar} e^{-iap_x/\hbar} |x_1, y_1\rangle \\ &= e^{-iap_x/\hbar} e^{-ibp_y/\hbar} |x_1, y_1\rangle \end{aligned}$$

These displacement operators commute, as expected from $[p_x, p_y] = 0$.

Similar to the displacement operator, we can define rotation operators that depend on the angular momentum operators, L_x, L_y, and L_z. For instance,

$$\hat{R}_x(\phi) = e^{-i\phi L_x/\hbar} \tag{1.4.7}$$

gives a rotation by angle ϕ about the x axis. Unlike linear displacement, rotations about different axes do not commute. For example, consider a state representing a particle displaced along the z axis, $|z0\rangle$. Now the action of two rotations $\hat{R}_x$ and $\hat{R}_y$ by an angle of $\phi = \pi/2$ on this particle differs depending on the order of operation, as illustrated in Figure 8. If we rotate first about x, the operation

$$e^{-i\frac{\pi}{2}L_y/\hbar} e^{-i\frac{\pi}{2}L_x/\hbar} |z_0\rangle \to |-y\rangle \tag{1.4.8}$$

leads to the particle on the –y axis, whereas the reverse order

$$e^{-i\frac{\pi}{2}L_x/\hbar} e^{-i\frac{\pi}{2}L_y/\hbar} |z_0\rangle \to |+x\rangle \tag{1.4.9}$$

leads to the particle on the +x axis. The final state of these two rotations taken in opposite order differ by a rotation about the z axis. Since rotations about different axes do not commute, we expect the angular momentum operators not to commute. Indeed, we know that

$$[L_x, L_y] = i\hbar L_z \tag{1.4.10}$$

where the commutator of rotations about the x and y axes is related by a z-axis rotation. As with rotation operators, we will need to be careful with time-propagators to determine whether the order of time-propagation matters. This, in turn, will depend on whether the Hamiltonians at two points in time commute.

Properties of exponential operators

1. If $\hat{A}$ and $\hat{B}$ do not commute, but $[\hat{A}, \hat{B}]$ commutes with $\hat{A}$ and $\hat{B}$, then

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-\frac{1}{2}[\hat{A},\hat{B}]} \tag{1.4.11}$$

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{B}} e^{\hat{A}} e^{-[\hat{B},\hat{A}]} \tag{1.4.12}$$

2. More generally, if $\hat{A}$ and $\hat{B}$ do not commute,

$$e^{\hat{A}} e^{\hat{B}} = \exp\left[\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{12}([\hat{A}, [\hat{A}, \hat{B}]] + [\hat{A}, [\hat{B}, \hat{B}]]) + \cdots\right] \tag{1.4.13}$$

3. The Baker–Hausdorff relationship:

$$\begin{aligned} \mathrm{e}^{i\hat{G}\lambda} \hat{A} \mathrm{e}^{-i\hat{G}\lambda} = \hat{A} + i\lambda[\hat{G}, \hat{A}] + \left(\frac{i^2\lambda^2}{2!}\right)[\hat{G}, [\hat{G}, \hat{A}]] + \ldots \\ + \left(\frac{i^n\lambda^n}{n!}\right)[\hat{G}, [\hat{G}, [\hat{G}, \hat{A}]]] \ldots] + \ldots \end{aligned} \tag{1.4.14}$$

where λ is a number.