Exponential Operators

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

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

We will see that these exponential operators act on a wavefunction to move it in time and space. 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

$$\hat{T} = e^{-i\hat{A}} = \sum_{n=0}^{\infty} \frac{(-i\hat{A})^n}{n!} = 1 - i\hat{A} - \frac{\hat{A}\hat{A}}{2} - \cdots \tag{1.1}$$

The most common one will be the time-propagator or time-evolution operator, $\hat{U}$, which is a function of the Hamiltonian and propagates the wavefunction forward in time

$$\hat{U} = \exp\left(-i\hat{H}t/\hbar\right) = 1 - \frac{i\hat{H}t}{\hbar} + \frac{1}{2!}\left(\frac{i\hat{H}t}{\hbar}\right)^2 - \cdots \tag{1.2}$$

Since we use them so frequently, let's review the properties of exponential operators that can be established with eq. (1.1). If the operator $\hat{A}$ is Hermetian, then $\hat{T} = e^{-i\hat{A}}$ is unitary, i.e. $\hat{T}^{\dagger} = \hat{T}^{-1}$. Thus the Hermetian conjugate of $\hat{T}$ reverses the action of $\hat{T}$. For the time-propagator $\hat{U}$, $\hat{U}^{\dagger}$ 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, given the eigenvalues and eigenvectors of $\hat{A}$, i.e., $\hat{A}\varphi_n = a_n\varphi_n$, you can show by expanding the function that

$$f\left(\hat{A}\right)\varphi_n = f\left(a_n\right)\varphi_n \tag{1.3}$$

Our most common application of this property will be to exponential operators in the Hamiltonian with eigenstates φ_n. Then $\hat{H}\left|\varphi_n\right\rangle = E_n\left|\varphi_n\right\rangle$ implies

$$e^{-i\hat{H}t/\hbar}\left|\varphi_n\right\rangle = e^{-iE_n t/\hbar}\left|\varphi_n\right\rangle \tag{1.4}$$

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

$$\left|\psi(x-\lambda)\right\rangle = \hat{D}(\lambda)\left|\psi(x)\right\rangle \tag{1.5}$$

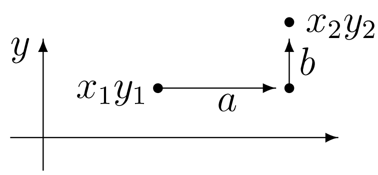
Also, applying $\hat{D}_x(\lambda)$ to a position operator shifts the operator by λ

$$\hat{D}^\dagger \hat{x} \hat{D} = \hat{x} + \lambda \tag{1.6}$$

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

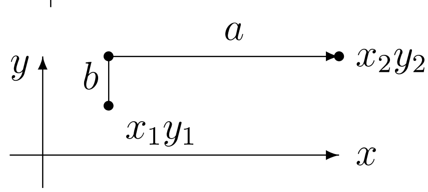
We know intuitively that linear displacements commute. For example, if we wish to shift a particle in two dimensions, *x* and *y*, the order of displacement doesn't matter. We end up at the same position. These displacement operators commute, as expected from $[p_x,p_y] = 0$.

$\left|x_2y_2\right\rangle = e^{-ibp_y/\hbar}e^{-iap_x/\hbar}\left|x_1y_1\right\rangle \Rightarrow$



first move along *x* by *a*, then along *y* by *b*.

$= e^{-iap_x/\hbar}e^{-ibp_y/\hbar}\left|x_1y_1\right\rangle \Rightarrow$

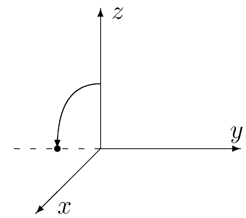


reverse order

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 $\hat{R}_x(\phi) = e^{-i\phi L_x/\hbar}$ 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, $|z_0\rangle$. Now the action of two rotations $\hat{R}_x$ and $\hat{R}_y$ by an angle of π/2 on this particle differs depending on the order of operation.

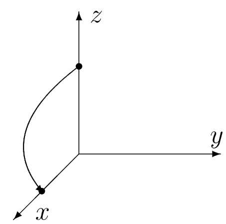
$$\underbrace{e^{-i\frac{\pi}{2}L_y/\hbar}}_{\substack{\text{rotation by } \frac{\pi}{2} \\ \text{about } y\text{-axis}}} \quad \underbrace{e^{-i\frac{\pi}{2}L_x/\hbar}\left|z_0\right\rangle}_{\substack{\text{rotation by } \frac{\pi}{2} \\ \text{about } x\text{-axis}}} \Rightarrow$$

particle on –*y* axis



$$\underbrace{e^{-i\frac{\pi}{2}L_x/\hbar}}_{\substack{\text{rotation by } \frac{\pi}{2} \\ \text{about } x\text{-axis}}} \quad \underbrace{e^{-i\frac{\pi}{2}L_y/\hbar}\left|z_0\right\rangle}_{\substack{\text{rotation by } \frac{\pi}{2} \\ \text{about } y\text{-axis}}} \Rightarrow$$

particle on +*x* axis



The results of these two rotations taken in opposite order differ by a rotation about the *z*–axis. Thus, because the rotations about different axes don't commute, we must expect the angular momentum operators, which generate these rotations, not to commute. Indeed, we know that $[L_x,L_y] = i\hbar L_z$, 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.

Finally, it is worth noting some relationships that are important in evaluating the action of exponential operators.

(1) The Baker-Hausdorff relationship:

$$\begin{aligned}\exp\left(i\hat{G}\lambda\right)\hat{A}\,\exp\left(-i\hat{G}\lambda\right) \;=\; & \hat{A}+i\lambda\left[\hat{G},\hat{A}\right] + \left(\frac{i^2\lambda^2}{2!}\right)\left[\hat{G},\left[\hat{G},\hat{A}\right]\right]+\ldots \\ & + \left(\frac{i^n\lambda^n}{n!}\right)\left[\hat{G},\left[\hat{G},\left[\hat{G}\ldots\left[\hat{G},\hat{A}\right]\right]\right]\ldots\right] + \ldots\end{aligned} \tag{1.7}$$

(2) If $\hat{A}$ and $\hat{B}$ do not commute, but $\left[\hat{A},\hat{B}\right]$ commutes with $\hat{A}$ and $\hat{B}$, then

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}\left[\hat{A},\hat{B}\right]} \tag{1.8}$$