Special Topic
Generators of Transformations in Hilbert Space

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Arbitrary States

- Our goal in this lecture to describe the action of operators on quantum states.
- We have seen that when an operator $\hat{A}$ acts on a arbitrary state $|\psi\rangle$ that is not an eigenstate of the operator it produces a new state $|\psi'\rangle$.

$$|\psi\rangle = \sum_n c_n |a_n\rangle$$

$$|\psi'\rangle = \hat{A}|\psi\rangle = \sum_n c_n a_n |a_n\rangle \neq \text{const.}\, |\psi\rangle$$

- We will study the new state that is produced in the context of spin-1/2 system.
- We will start by constructing the spin operator in an arbitrary direction $\hat{n}$.

$$\hat{n} = \cos\varphi \sin\theta\, \hat{x} + \sin\varphi \sin\theta\, \hat{y} + \cos\theta\, \hat{z}$$

- where (φ, θ) are the polar angles.
- We define the spin-1/2 operator in an arbitrary direction as

$$\hat{S}_n := \hat{\mathbf{S}} \cdot \hat{n} = \hat{S}_x \cos\varphi \sin\theta + \hat{S}_y \sin\varphi \sin\theta + \hat{S}_z \cos\theta$$

Arbitrary States

$$\hat{S}_n := \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\cos\varphi\sin\theta + \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\sin\varphi\sin\theta + \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\cos\theta$$

$$\hat{S}_n = \frac{\hbar}{2}\begin{pmatrix}\cos\theta & e^{-i\varphi}\sin\theta\\ e^{i\varphi}\sin\theta & -\cos\theta\end{pmatrix}$$

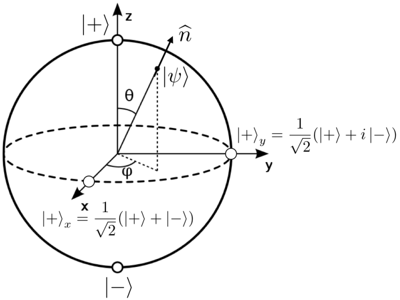
- The eigenvalues of $\hat{S}_n$ are $\pm\frac{\hbar}{2}$ with corresponding eigenstates:

$$|\psi_+(\theta,\phi)\rangle = \cos\left(\frac{\theta}{2}\right)|+\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}|-\rangle$$

$$|\psi_-(\theta,\phi)\rangle = \sin\left(\frac{\theta}{2}\right)|+\rangle - \cos\left(\frac{\theta}{2}\right)e^{i\phi}|-\rangle$$

Bloch Sphere

- The 2-dimensional Hilbert space of the spin-1/2 system can be represented as a the points on the surface of a sphere of radius 1 in 3-dimensional Euclidean space.
- This representation is referred to as the Bloch Sphere, named after the Physicist Felix Bloch.



Rotated States

- Let $|\psi'\rangle = S_n |\psi\rangle$, which is another state in the 2-dimensional Hilbert space of the spin-$\frac{1}{2}$ system.
- What is the relationship between $|\psi\rangle$ and $|\psi'\rangle$?
- Let's consider the following example:

$$\hat{S}_x |+\rangle = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}|-\rangle$$

- We see that up to a multiplicative factor of $\frac{\hbar}{2}$ the action of $\hat{S}_x$ on the state $|+\rangle$ rotates the state by an angle π about the $x-$axis.
- We can also consider another example:

$$\hat{S}_z |+\rangle_y = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{\hbar}{2}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{\hbar}{2}|-\rangle_y$$

- We see again that the state $|\psi'\rangle$ is a rotated version of the state $|+\rangle_y$ by an angle π about the $z-$axis.

Infinitesimal Rotation

- We see that angular momentum operators "generate" rotations of states on the Bloch sphere.
- The rotation axis is defined by the direction of the spin operator.
- The component of the state vector that is perpendicular to the rotation axis rotates by π.
- It is also possible to generate arbitrary rotations about any axis. To do this we start by first constructing an operator that generates an infinitesimal rotation.
- We begin by considering an infinitesimal rotation $d\phi$ about the $z-$axis.

$$\hat{R}_z(d\phi) := \mathbb{1} - \frac{i}{\hbar}\hat{S}_z d\phi \tag{1}$$

- The matrix representation of $\hat{R}_z(d\phi)$ in the $z-$basis is

$$\hat{R}_z(d\phi) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{id\phi}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 - i\frac{d\phi}{2} & 0 \\ 0 & 1 + i\frac{d\phi}{2} \end{pmatrix} \tag{2}$$

Infinitesimal Rotation

- Let $\zeta = 1 - i\frac{d\phi}{2}$.

$$\hat{R}_z(d\phi) = \begin{pmatrix} \zeta & 0 \\ 0 & \zeta^* \end{pmatrix}$$

$$\zeta = e^{-i\gamma}\sqrt{1 + \left(\frac{d\phi}{2}\right)^2}, \qquad \gamma = \tan^{-1}\left(\frac{d\phi}{2}\right)$$

- We take the limit $d\phi \to 0$

$$\lim_{d\phi \to 0} \zeta = e^{-id\phi/2}$$

$$\hat{R}_z(d\phi) \to \begin{pmatrix} e^{-i\frac{d\phi}{2}} & 0 \\ 0 & e^{i\frac{d\phi}{2}} \end{pmatrix} \tag{3}$$

$$\hat{R}_z(d\phi)\left|\psi_+(\theta,\phi)\right\rangle = e^{-i\frac{d\phi}{2}}\begin{pmatrix}1 & 0\\ 0 & e^{id\phi}\end{pmatrix}\begin{pmatrix}\cos\left(\frac{\theta}{2}\right)\\ \sin\left(\frac{\theta}{2}\right)e^{i\phi}\end{pmatrix}$$

$$= e^{-i\frac{d\phi}{2}}\begin{pmatrix}\cos\left(\frac{\theta}{2}\right)\\ \sin\left(\frac{\theta}{2}\right)e^{i(\phi+d\phi)}\end{pmatrix}$$

$$\hat{R}_z(d\phi)\left|\psi_+(\theta,\phi)\right\rangle = e^{-i\frac{d\phi}{2}}\left|\psi_+(\theta,\phi+d\phi)\right\rangle \tag{4}$$

$$\hat{R}_z(d\phi)\left|\psi_-(\theta,\phi)\right\rangle = e^{-i\frac{d\phi}{2}}\left|\psi_-(\theta,\phi+d\phi)\right\rangle \tag{5}$$

- We see that up to an overall phase factor $\hat{R}_z(d\phi)$ rotates the states $\left|\psi_\pm(\theta,\phi)\right\rangle$ counterclockwise about the $z-$axis by an angle $d\phi$.

Infinitesimal Rotation

- The operator $\hat{R}_z^\dagger(d\phi)$ is the inverse of $\hat{R}_z(d\phi)$ up to order $\mathcal{O}\big((d\phi)^2\big)$.

$$\hat{R}_z^\dagger(d\phi) = \mathbb{1} + \tfrac{i}{\hbar}\hat{S}_z d\phi \tag{6}$$

- We note that $\hat{S}_z$ is a Hermitian operator, therefore $\hat{S}_z^\dagger = \hat{S}_z$.

$$\begin{aligned}\hat{R}_z(d\phi)\,\hat{R}_z^\dagger(d\phi) &= \Big(\mathbb{1} - \tfrac{i}{\hbar}\hat{S}_z d\phi\Big)\Big(\mathbb{1} + \tfrac{i}{\hbar}\hat{S}_z d\phi\Big) \\ &= \mathbb{1} + \left(\frac{d\phi}{\hbar}\right)^2 S_z^2\end{aligned}$$

$$\lim_{d\phi\to 0} \hat{R}_z(d\phi)\,\hat{R}_z^\dagger(d\phi) \to \mathbb{1}$$

- In the limit that $d\phi \to 0$, $\hat{R}_z^\dagger(d\phi)$ produces a clockwise rotation by and angle $d\phi$ about the $z-$axis.

Angular Momentum – Generator of Rotation

- We can produce a larger rotation by an angle ϕ, by applying $\hat{R}_z(d\phi)$ back-to-back a large number N times.

$$\hat{R}_z(\phi) = \lim_{N\to\infty}\left(\mathbb{1} - \frac{i}{\hbar}\left[\frac{\phi}{N}\right]\hat{S}_z\right)^N \tag{7}$$

- To evaluate eq.(7), consider the Taylor series expansion of the following polynomial for $x/N < 1$.

$$\left(1+\frac{x}{N}\right)^N = 1 + x + \frac{1}{2!}\left(\frac{N-1}{N}\right)x^2 + \frac{1}{3!}\left(\frac{(N-1)(N-2)}{N^2}\right)x^3 + \cdots$$

- In the limit $N \to \infty$, the above expression reduces to the following

$$\lim_{N\to\infty}\left(1+\frac{x}{N}\right)^N \to 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{n=0}^{\infty}\frac{x^n}{n!} = e^x \tag{8}$$

Angular Momentum – Generator of Rotation

- If we replace the term x in eq.(8) by $-\frac{i\phi}{\hbar}\hat{S}_z$, then eq.(7) may be written as

$$\hat{R}_z(\phi) = \mathbb{1} - i\left(\frac{\phi}{\hbar}\right)\hat{S}_z - \frac{1}{2!}\left(\frac{\phi}{\hbar}\right)^2\hat{S}_z^2 + \frac{i}{3!}\left(\frac{\phi}{\hbar}\right)^3\hat{S}_z^3 + \cdots \tag{9}$$

$$= e^{-i\phi\hat{S}_z/\hbar} \tag{10}$$

- The exponential of an operator may look a bit strange, however we can use the power series expansion form of the exponential (eq.(9)) to evaluate its action on a state vector.

$$e^{-i\phi\hat{S}_z/\hbar}\left|+\right\rangle = \left[\mathbb{1} - i\left(\frac{\phi}{\hbar}\right)\hat{S}_z - \frac{1}{2!}\left(\frac{\phi}{\hbar}\right)^2\hat{S}_z^2 + \frac{i}{3!}\left(\frac{\phi}{\hbar}\right)^3\hat{S}_z^3 + \cdots\right]\left|+\right\rangle$$

Note: $\hat{S}_z^n\left|\pm\right\rangle = \left(\pm\frac{\hbar}{2}\right)^n\left|\pm\right\rangle$

Angular Momentum – Generator of Rotation

$$= \left[\mathbb{1} - i\left(\frac{\phi}{\hbar}\right)\frac{\hbar}{2} - \frac{1}{2!}\left(\frac{\phi}{\hbar}\right)^2\left(\frac{\hbar}{2}\right)^2 + \frac{i}{3!}\left(\frac{\phi}{\hbar}\right)^3\left(\frac{\hbar}{2}\right)^3 + \cdots\right]|+\rangle$$

$$= e^{-i\phi/2}\,|+\rangle$$

- We see that if the exponential operator acts on an eignenvector of the operator in the exponent, then we simply replace the operator by the corresponding eigenvalue.

$$\therefore\; e^{-i\phi\hat{S}_z/\hbar}\,|+\rangle = e^{-i\phi/2}\,|+\rangle$$

- We can now see what happens when $\hat{R}_z(\phi)$ acts on the state $|\psi_+(\theta,\phi)\rangle$.

$$\hat{R}_z(\phi)\,|\psi_+(\theta,\phi)\rangle = e^{-i\phi\hat{S}_z/\hbar}\left[\cos\left(\frac{\theta}{2}\right)|+\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\phi}\,|-\rangle\right]$$

Angular Momentum – Generator of Rotation

$$= \left[\cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} \left|+\right\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} e^{i\phi} \left|-\right\rangle\right]$$

$$= e^{-i\phi/2} \left[\cos\left(\frac{\theta}{2}\right) \left|+\right\rangle + \sin\left(\frac{\theta}{2}\right) e^{i(\phi+\phi)} \left|-\right\rangle\right]$$

$$\Rightarrow \quad \hat{R}_z(\phi) \left|\psi_+(\theta, \phi)\right\rangle = e^{-i\phi/2} \left|\psi_+(\theta, \phi + \phi)\right\rangle$$

- We see that up to an overall phase factor the operator $\hat{R}_z(\phi)$ produces a rotation of the state by an angle ϕ about the $z-$axis.
- Furthermore, $\hat{R}_z(\phi)$ corresponds to an unitary operator:

$$\hat{R}_z(\phi)\, \hat{R}_z^\dagger(\phi) = e^{-i\phi \hat{S}_z/\hbar}\, e^{i\phi \hat{S}_z/\hbar} = \mathbb{1} \tag{11}$$

$$\hat{R}_z^\dagger(-\phi) = \hat{R}_z(\phi) \tag{12}$$

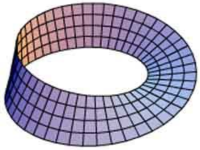
- Matrix representation of $\hat{R}_z(\phi)$ See the appendix at the end of the lecture for the derivation.

$$\boxed{e^{-i\phi \hat{S}_z/\hbar} = \mathbb{1} \cos\left(\frac{\phi}{2}\right) - \frac{2i\hat{S}_z}{\hbar} \sin\left(\frac{\phi}{2}\right)} \tag{13}$$

- I will end this lecture by making an interesting observation.
- A 2π rotation of the spin-1/2 state vector, does not reproduce the original state. Rather, it produces the negative of the state.

$$\hat{R}_z(\phi = 2\pi)\,|\psi_+(\theta,\phi)\rangle = e^{-i\pi}\,|\psi_+(\theta,\phi)\rangle = -\,|\psi_+(\theta,\phi)\rangle$$

- A 4π rotation is required to recover the original state. This property of the quantum state of a spin-1/2 particles is referred to as the "spinor" property.
- We can make a correspondence with spinors and a Möbius strip.



Interesting Observations

- We have said many times in this course that the overall phase factor of a quantum state does not change the probability of measurement outcomes.
- While strictly speaking this is true, it is also possible to measure this overall phase if we devise an experiment that interferes two quantum states with different overall phase factors. Such an experiment has been done using the technique of magnetic resonance. We will study how magnetic resonance works when we discuss time-dependent quantum processes.

Appendix A: Matrix Representation of the Rotation Operator

- We seek to find a matrix representation of the rotation operator.
- I will use the following notation for the operator $\hat{S}_z$ in this derivation

$$\hat{S}_z = \frac{\hbar}{2}\sigma_z, \qquad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}$$

$$e^{-i\phi\hat{S}_z/\hbar} = e^{-i\phi\sigma_z/2} =$$

$$= \mathbb{1} - i\left(\frac{\phi}{2}\right)\sigma_z - \tfrac{1}{2!}\left(\tfrac{\phi}{2}\right)^2\sigma_z^2 + \tfrac{i}{3!}\left(\tfrac{\phi}{2}\right)^3\sigma_z^3 + \tfrac{1}{4!}\left(\tfrac{\phi}{2}\right)^4\sigma_z^4$$

$$= \mathbb{1} - i\left(\frac{\phi}{2}\right)\sigma_z - \tfrac{1}{2!}\left(\tfrac{\phi}{2}\right)^2\mathbb{1} + \tfrac{i}{3!}\left(\tfrac{\phi}{2}\right)^3\sigma_z + \tfrac{1}{4!}\left(\tfrac{\phi}{2}\right)^4\mathbb{1}$$

$$= \mathbb{1} \underbrace{\left\{1 - \frac{1}{2!}\left(\frac{\phi}{2}\right)^2 + \frac{1}{4!}\left(\frac{\phi}{2}\right)^4 + \cdots\right\}}_{\sum_{n=0}^{\infty} \frac{(-1)^n (\phi/2)^{2n}}{(2n)!} = \cos\left(\frac{\phi}{2}\right)}$$

$$- i\sigma_z \underbrace{\left\{\frac{\phi}{2} - \frac{1}{3!}\left(\frac{\phi}{2}\right)^3 + \frac{1}{5!}\left(\frac{\phi}{2}\right)^5 + \cdots\right\}}_{\sum_{n=0}^{\infty} \frac{(-1)^n (\phi/2)^{2n+1}}{(2n+1)!} = \sin\left(\frac{\phi}{2}\right)}$$

$$e^{-i\phi \hat{S}_z/\hbar} = e^{-i\phi\sigma_z/2} = \mathbb{1}\cos\left(\frac{\phi}{2}\right) - i\sigma_z \sin\left(\frac{\phi}{2}\right)$$

$$= \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix}$$

Appendix B: Generators of Infinitesimal Transformations

- Operators corresponding to observables, such as angular momentum, linear momentum, position and energy all generate transformations on states in Hilbert space.
- Angular momentum, for example rotates kets. We will see later that the linear momentum operator will produce translations, and the energy operator will produce a translation of states in time.
- We can build continuous transformations by applying a series of infinitesimal transformations.
- The infinitesimal transformation operator has the basic form

$$U(\epsilon) = \mathbb{1} - i\epsilon G$$

where G is a Hermitian operator corresponding to the particular observable in question, e.g., angular momentum, and ϵ is the infinitesimal quantity, e.g., $d\phi$ for the case of rotations.

- There are two reasons for choosing $U(\epsilon)$ to have this mathematical form.
- First, we require
$$\lim_{\epsilon \to 0} U(\epsilon) = \mathbb{1}$$
- Second, $U(\epsilon)$ should be unitary, that is, it should transform a state without changing its norm. Another way of saying this is that it should conserve probability. We therefore require that $UU^\dagger = \mathbb{1}$.

$$\begin{gathered} UU^\dagger = (\mathbb{1} - i\epsilon G)(\mathbb{1} + i\epsilon G^\dagger) \\ U = U^\dagger \quad G \text{ is a Hermitian operator} \\ = \mathbb{1} + i\epsilon G - i\epsilon G + \epsilon^2 G^2 \end{gathered}$$

We see that terms of $\mathcal{O}(\epsilon)$ cancel. Neglecting terms of order $\mathcal{O}(\epsilon^2)$, $UU^\dagger = \mathbb{1}$, as required.