Chapter 19
Symmetry and Transformations: Rotation Matrices

Now that I have looked at approximation techniques and scattering theory, I return to some more formal aspects of quantum mechanics. I begin with a discussion of symmetry and see how this leads to a somewhat more sophisticated picture of angular momentum. We have seen already that energy degeneracy arises in problems for which there is an associated symmetry. Moreover, in most of these cases, there is also a conserved dynamic variable that was connected with the symmetry (e.g., in central field potentials, angular momentum is conserved and the potential is spherically symmetric).

Symmetry is central to modern physics. When you learn about the standard model of particle physics, you will see the critical role symmetry plays in the classification of particles and forces. Even in elementary quantum mechanics, symmetry considerations are important. I will try to give you a very brief introduction to this topic. I might say from the outset that I often encounter sign problems in considering either active or passive transformations, but I have learned to live with it. I need to consider transformations of coordinates, vectors, scalar functions, vector functions, and operators. These quantities transform differently under symmetry operations. Before applying the ideas of symmetry operations to quantum mechanics, I review what happens to coordinates, vectors, and functions under translation and rotation.

19.1 Active Versus Passive Transformations

In general, it is possible to define scalar, vector, and tensor operators by their transformation properties under a given symmetry operation such as translation or rotation. To make matters confusing, one can look at changes from either a passive (coordinate axes change) or an active (axes remain fixed, but vectors and functions are transformed) point of view. I will review these concepts for translation in one-dimension and rotations in both two and three dimensions. The study of translations

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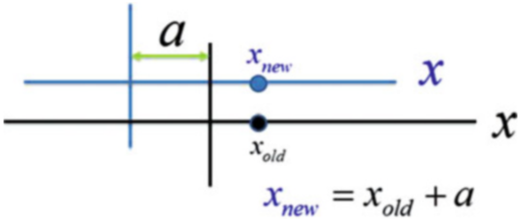

Fig. 19.1 Passive transformation of the coordinate axis to the left by a units. A point that has coordinate x_{old} in the original coordinate system has $x_{\text{new}} = x + a$ in the new coordinate system. The upper axis in the figure is the translated one

and rotations is important from a practical standpoint. For example, if you need to average collision cross sections over different orientations of the colliding particles, you can calculate the result for a given orientation of the colliding particles and then use rotation matrices to transform the result to account for arbitrary orientations.

19.1.1 Passive and Active Translations

19.1.1.1 Passive Translation

In a passive translation of the coordinate system the coordinate axes are translated. Imagine that the x-axis in Fig. 19.1 is translated a units to the *left*. If I label the coordinate of a point in the original coordinate system by x_{old} and in the new coordinate system by x_{new}, then $x_{\text{new}} = x_{\text{old}} + a$. I define a translation operator $\hat{T}^P(-a)$ for a passive transformation to the left by a units as one that changes the coordinate of a point from x_{old} to x_{new} according to

$$x_{\text{new}} = \hat{T}^P(-a)x_{\text{old}} = x_{\text{old}} + a. \tag{19.1}$$

Under this passive transformation, functions $f(x)$ are not translated; however, since the coordinate axis is translated, the *functional form* of $f(x)$ changes. The new functional form is denoted by $f_P(x; -a)$, where the minus sign is associated with a translation of the coordinate axis to the left. Since the value of the function at a fixed point in space is unchanged, the relationship between $f_P(x; -a)$ and $f(x)$ is given by

$$f_P(x; -a) = f\left[\left(\hat{T}^P(-a)\right)^{-1} x\right] = f\left[\hat{T}^P(a)x\right] = f(x - a), \tag{19.2}$$

where

$$\left(\hat{T}^P(-a)\right)^{-1} = \hat{T}^P(a) \tag{19.3}$$

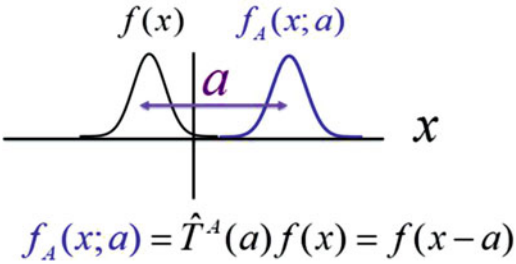

Fig. 19.2 Active transfomation of the function $f(x)$ to the right by a units

is the *inverse transformation*. For example, suppose the original function is $f(x) = e^{-x^2}$, which is centered at $x = 0$. The new function, $f_P(x; -a) = e^{-(x-a)^2}$, is now centered at $x = a$ since $x_{\text{new}} = a$ is the transformed coordinate of $x_{\text{old}} = 0$ in the original coordinate system. In effect, Eq. (19.2) defines the properties of a scalar function f_P under translation.

19.1.1.2 Active Translation

I *define* an active translation $\hat{T}^A(a)$ of a *function* to the right by a units as producing the same function I would get by translating the axis by a units to the *left* in a passive transformation (see Fig. 19.2), that is,

$$f_A(x; a) = \hat{T}^A(a)f(x) = f_P(x; -a) = f\left[\left(\hat{T}^P(a)\right)x\right] = f(x-a). \tag{19.4}$$

If the original function was centered at $x = 0$, the transformed function is centered at $x = a$. A translation of the function to the right is equivalent to a transformation of the coordinate axis to the left. Note that the passive transformation acts on coordinates while the active transformation acts on functions. In other words, $\hat{T}^A(a)$ translates functions to the right by a units while $\hat{T}^P(a)$ translates the coordinate axis to the right by a units.

19.1.2 Passive and Active Rotations

19.1.2.1 Passive Rotations

Consider a rotation of the coordinate axes in which the position vector $\mathbf{r}$ remains fixed. The axes are rotated by an angle $-\phi$ (see Fig. 19.3) about the z-axis. The unit vectors are denoted by $\mathbf{u}_1 = \mathbf{u}_x$, $\mathbf{u}_2 = \mathbf{u}_y$. Under the rotation, coordinates of the position vector change (even though the vector remains fixed in space) according to

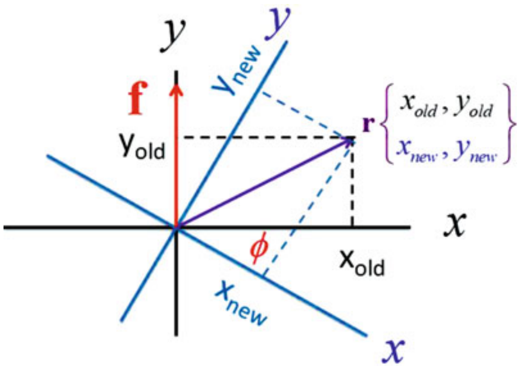

Fig. 19.3 A passive rotation of the coordinate axes by an angle $-\phi$ about the z axis. The position vector **r** and the constant vector **f** are unchanged in an absolute sense, but their coordinates change. On the other hand, the unit vectors, which are aligned along the coordinate axes change in this passive rotation. The position vector shown has coordinates $(x_{\text{old}}, y_{\text{old}})$ in the original coordinate system and $(x_{\text{new}}, y_{\text{new}})$ in the new coordinate system

$$\mathbf{r}_{\text{new}} = \begin{pmatrix} x_{\text{new}} \\ y_{\text{new}} \end{pmatrix} = \underset{\sim}{R}^P(-\phi)\mathbf{r}_{\text{old}} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} x_{\text{old}} \\ y_{\text{old}} \end{pmatrix}, \tag{19.5}$$

where

$$\underset{\sim}{R}^P(\phi) = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \tag{19.6}$$

is the *passive rotation matrix*. In other words, under this passive transformation of $-\phi$, the position vector $\mathbf{r}_{\text{old}} = (x_{\text{old}}, y_{\text{old}})$ in the old system has coordinates in the new system given by

$$x_{\text{new}} = x_{\text{old}} \cos\phi - y_{\text{old}} \sin\phi; \tag{19.7a}$$

$$y_{\text{new}} = x_{\text{old}} \sin\phi + y_{\text{old}} \cos\phi. \tag{19.7b}$$

Moreover, the basis vectors have also changed since they are aligned along the new axes, with

$$(\mathbf{u}_i)_{\text{new}} = \sum_{j=1}^{3} \underset{\sim}{R}^P_{ij}(-\phi)\,(\mathbf{u}_j)_{\text{old}}, \tag{19.8}$$

where $\underset{\sim}{R}^P_{ij}$ are elements of the passive rotation matrix (19.6).

The effect of a passive rotation on a scalar function is defined in an analogous manner to that for translations, namely

$$f_P(\mathbf{r}; -\phi) = f\left[\left(\underset{\sim}{R}^P(-\phi)\right)^{-1}\mathbf{r}\right] = f\left[\left(\underset{\sim}{R}^P(-\phi)\right)^{\dagger}\mathbf{r}\right] = f\left[\underset{\sim}{R}^P(\phi)\mathbf{r}\right], \tag{19.9}$$

where I used the fact that $\underset{\sim}{R}^P(\phi)$ is a unitary matrix whose inverse is simply its adjoint. Things can get a little more complicated when you look at the effect of rotations on vector functions (such as the electric field). For a vector function $\mathbf{E}(\mathbf{r})$, under a passive rotation of $-\phi$,

$$\mathbf{E}_P(\mathbf{r};-\phi) = \underset{\sim}{R}^P(-\phi)\mathbf{E}\left[\underset{\sim}{R}^P(\phi)\mathbf{r}\right], \tag{19.10}$$

the components are changed and they are evaluated at the new coordinates.

19.1.2.2 Active Rotations

As in the case of translations I can define an active rotation of a scalar function by an operator $\hat{R}^A(\phi)$ that, when acting on a function $f(\mathbf{r})$, produces a new function according to

$$f_A(\mathbf{r};\phi) = \hat{R}^A(\phi)f(\mathbf{r}) = f_P(\mathbf{r};-\phi) = f\left[\underset{\sim}{R}^P(\phi)\mathbf{r}\right]. \tag{19.11}$$

Now here's where things get really confusing. Note that $\hat{R}^A(\phi)$ is an *operator* while $\underset{\sim}{R}^P(\phi)$ is a matrix. The operator $\hat{R}^A(\phi)$ operates on functions and the matrix $\underset{\sim}{R}^P(\phi)$ operates on the position vector. However I can *define* an active transformation *matrix* by

$$\underset{\sim}{R}^A(\phi) = \underset{\sim}{R}^P(-\phi) = \left[\underset{\sim}{R}^P(\phi)\right]^\dagger = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix}. \tag{19.12}$$

With this definition, Eq. (19.11) becomes

$$f_A(\mathbf{r};\phi) = \hat{R}^A(\phi)f(\mathbf{r}) = f\left[\left(\underset{\sim}{R}^A(\phi)\right)^\dagger \mathbf{r}\right] = f\left[\left(\underset{\sim}{R}^A(\phi)\right)^{-1} \mathbf{r}\right]. \tag{19.13}$$

A vector function $\mathbf{E}(\mathbf{r})$ transforms under an active rotation by ϕ as

$$\mathbf{E}_A(\mathbf{r};\phi) = \hat{R}^A(\phi)\mathbf{E}(\mathbf{r}) = \underset{\sim}{R}^A(\phi)\mathbf{E}\left[\left(\underset{\sim}{R}^A(\phi)\right)^{-1} \mathbf{r}\right]. \tag{19.14}$$

The operation of $\hat{R}^A(\phi)$ on a vector function is to change the components and evaluate the coordinates at the rotated values, leaving the length of the vector unchanged. For a *constant* vector function $\mathbf{f}$,

$$\mathbf{f}_A(\phi) = \hat{R}^A(\phi)\mathbf{f} = \underset{\sim}{R}^A(\phi)\mathbf{f}. \tag{19.15}$$

For constant vectors, the rotation operator acts as a matrix and we can think of the rotation operator as rotating the vector (see Fig. 19.4).

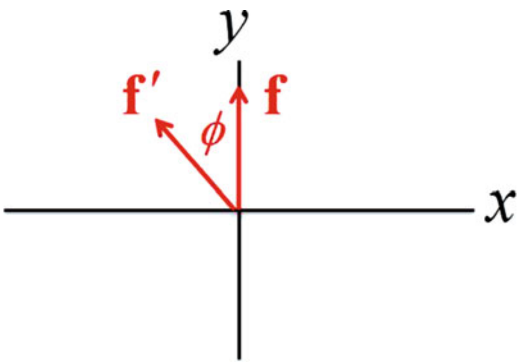

Fig. 19.4 An active rotation of a *constant* vector **f** by angle ϕ about the z axis. The axes and unit vectors remain constant, but the coordinates of the vector change

19.1.3 Extension to Three Dimensions

To specify a rotation in three dimensions, I need to specify the axis of rotation $\mathbf{u_n}(\theta,\phi)$ and the angle of rotation ω about this axis. The quantity $\mathbf{u_n}(\theta,\phi)$ is a unit vector in a spherical coordinate system having polar angle θ and azimuthal angle ϕ. Thus, *three* angles have to be specified.

Instead of specifying the axis of rotation and the rotation angle, I can equally well represent any rotation by the *Euler angles* (α,β,γ). The convention chosen for a passive rotation is one that takes the axes (x,y,z) into the axes (X,Y,Z) (see Fig. 19.5) using

- a rotation by α about the z axis
- a rotation by β about the *new* y axis
- a rotation by γ about the *new* z axis.

This leads to the passive rotation matrix

$$\begin{aligned}
\underset{\sim}{R}^P(\alpha,\beta,\gamma) &= \begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \\
&\quad \times \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\gamma\sin\alpha & \cos\gamma\cos\beta\sin\alpha + \cos\alpha\sin\gamma & -\sin\beta\cos\gamma \\ -\sin\gamma\cos\beta\cos\alpha - \sin\alpha\cos\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\gamma\cos\alpha & \sin\beta\sin\gamma \\ \cos\alpha\sin\beta & \sin\alpha\sin\beta & \cos\beta \end{pmatrix}.
\end{aligned} \tag{19.16}$$

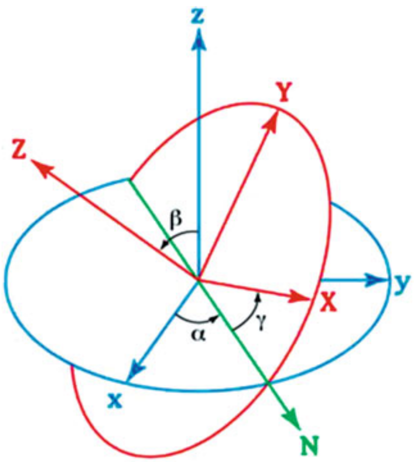

Fig. 19.5 Euler angles. A passive rotation of α about the z axis takes the axes (x, y, z) into (x', y', z). This is followed by a passive rotation of β about the y' axis that takes the axes (x', y', z) into (x'', y', Z) and a passive rotation of γ about the Z axis that takes the axes (x'', y', Z) into (X, Y, Z). The vector **N** that lies along the intersection of the xy and XY planes is referred to as the *line of nodes*

The active rotation *matrix* is defined as the inverse of this passive rotation matrix,

$$\underset{\sim}{R}^A(\alpha,\beta,\gamma) = \left[\underset{\sim}{R}^P(\alpha,\beta,\gamma)\right]^{-1} = \underset{\sim}{R}_z^A(\alpha)\underset{\sim}{R}_y^A(\beta)\underset{\sim}{R}_z^A(\gamma)$$
$$= \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\gamma\sin\alpha & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix}, \quad (19.17)$$

where the rotations are now relative to the *fixed* axes. The matrix $\underset{\sim}{R}_z^A(\alpha)$ is the active rotation matrix for a rotation about the z axis by an angle α given by Eq. (19.12); note that in active rotations, *the* γ *rotation is carried out first*. Under an active rotation,

$$f_A(\mathbf{r};\alpha,\beta,\gamma) = \hat{R}^A(\alpha,\beta,\gamma)f(\mathbf{r}) = f\left[\left[\underset{\sim}{R}^A(\alpha,\beta,\gamma)\right]^{-1}\mathbf{r}\right] \quad (19.18)$$

for scalar functions and

$$\mathbf{E}_A(\mathbf{r};\alpha,\beta,\gamma) = \hat{R}^A(\alpha,\beta,\gamma)\mathbf{E}(\mathbf{r}) = \underset{\sim}{R}^A(\alpha,\beta,\gamma)\mathbf{E}\left[\left[\underset{\sim}{R}^A(\alpha,\beta,\gamma)\right]^{-1}\mathbf{r}\right] \quad (19.19)$$

for vector functions. The rotation matrix acting on a vector must leave the length of the vector unchanged. Since the rotation matrix is real, the rotation matrix must be an orthogonal matrix to preserve the length of vectors. In fact, the matrix given in Eq. (19.17) is the most general orthogonal 3×3 matrix having determinant equal to $+1$.

For a *constant* vector field,

$$\mathbf{f}_A(\alpha,\beta,\gamma) = \hat{R}^A(\alpha,\beta,\gamma)\mathbf{f} = \underline{\mathrm{R}}^A(\alpha,\beta,\gamma)\mathbf{f}. \tag{19.20}$$

As a simple example consider the vector $\mathbf{f} = \left(\mathbf{u}_x + \mathbf{u}_y\right)/\sqrt{2}$. I want to rotate this vector so it is aligned along the z axis. I can do this by a passive transformation $(\alpha,\beta,\gamma) = (\pi/4, \pi/2, 0)$. Under such a passive transformation

$$\mathbf{f}_P(\pi/4,\pi/2,0) = \underline{\mathrm{R}}^P(\pi/4,\pi/2,0)\mathbf{f}\begin{pmatrix} 0 & 0 & -1 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{19.21}$$

The vector is now along the *new* z axis.

Alternatively I can use an active rotation with $(\alpha,\beta,\gamma) = (0,-\pi/2,-\pi/4)$ (recall in active rotations the γ rotation is carried out first). Under this active rotation,

$$\begin{aligned} \mathbf{f}_A\left(0,-\pi/2,-\pi/4\right) &= \underline{\mathrm{R}}^A\left(0,-\pi/2,-\pi/4\right)\mathbf{f} \\ &= \begin{pmatrix} 0 & 0 & -1 \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \end{aligned} \tag{19.22}$$

The vector has been rotated to lie along the (original) z axis. Additional examples are given below.

Although the unit vectors used to expand vectors are unchanged by an active transformation, I can nevertheless see how the unit vectors, *considered as vectors*, transform in this case. Since the unit vectors are constant vectors, they transform as

$$\mathbf{u}_A(\alpha,\beta,\gamma)_i = \underline{\mathrm{R}}^A(\alpha,\beta,\gamma)\mathbf{u}_i, \tag{19.23}$$

so that, for example,

$$\mathbf{u}_A(\alpha,\beta,\gamma)_1 = \underline{\mathrm{R}}^A(\alpha,\beta,\gamma)\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \underline{\mathrm{R}}^A_{11}(\alpha,\beta,\gamma) \\ \underline{\mathrm{R}}^A_{21}(\alpha,\beta,\gamma) \\ \underline{\mathrm{R}}^A_{31}(\alpha,\beta,\gamma) \end{pmatrix}. \tag{19.24}$$

In other words, the transformation can be written as

$$\mathbf{u}_A(\alpha,\beta,\gamma)_i = \sum_{j=1}^{3} \underline{\mathrm{R}}^A_{ji}(\alpha,\beta,\gamma)\mathbf{u}_j. \tag{19.25}$$

Note the order of the indices on the rotation matrix elements.

19.2 Quantum Mechanics

All these ideas can now be taken over to quantum mechanics. In fact we can use our understanding of the physics associated with Hamiltonians for the free particle and spherically symmetric potentials to obtain expressions for operators such as the translation and rotation operators. To this point, I have defined these operators only implicitly through Eqs. (19.4) and (19.11), in terms of their actions on functions.

Before starting any formalism, it might be helpful to remind you of what you already know about symmetry operations. For the moment I consider only continuous symmetry operations such as translation or rotation, but will discuss discrete symmetry operations as well. So what do you know?

1. If an operator commutes with the Hamiltonian, the expectation value of the physical observable associated with that operator is a constant of the motion.
2. If an operator $\hat{A}$ commutes with a Hamiltonian $\hat{H}$, and if $|E\rangle$ is an eigenket of $\hat{H}$ with eigenenergy E, then $\hat{A}\,|E\rangle$ is also an eigenket of $\hat{H}$ with eigenenergy E. We are guaranteed that $\hat{A}\,|E\rangle$ is equal to a constant times $|E\rangle$ *only* if there is no degeneracy in the eigenenergies of $\hat{H}$. When there is degeneracy, $\hat{A}\,|E\rangle$ is not *necessarily* equal to a constant times $|E\rangle$, this implies that there can be more than one eigenket with the same energy—when an operator commutes with the Hamiltonian, there is often energy degeneracy.
3. An operator $\hat{A}$ acting on an eigenket $|E\rangle$ of a given Hamiltonian $\hat{H}$ produces a new ket $|E\rangle'$, in general, that is not necessarily an eigenket of $\hat{H}$. Suppose that $\hat{A}$ corresponds to a symmetry operation such as a translation or rotation in Hilbert space. If the Hamiltonian $\hat{H}$ is invariant under this symmetry operation, the *eigenenergy* of the transformed state $|E\rangle'$ cannot change; it must also be an eigenket of $\hat{H}$. Since $|E\rangle' \neq |E\rangle$, in general, this again implies some energy degeneracy.
4. Combining these ideas, we see that if a Hamiltonian is invariant under some symmetry operation, there is associated with the symmetry operation a Hermitian operator that commutes with the Hamiltonian. As you will see, the operator is a generator of infinitesimal transformations on the wave function or eigenkets that leave the Hamiltonian invariant.

A simple example will serve to illustrate these ideas. Let us look at the case of a free particle having mass m in one-dimension for which the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} \tag{19.26}$$

where $\hat{p} = -i\hbar d/dx$. The (unnormalized) eigenfunctions can be taken as

$$\psi_k(x) = e^{\pm ikx} \tag{19.27}$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}} > 0. \tag{19.28}$$

Equally well, the eigenfunctions can be taken as

$$\psi_k(x) = \cos(kx)\,; \qquad \sin(kx)\,. \tag{19.29}$$

The eigenfunctions are two-fold degenerate.

How is all this related to the momentum operator? Since $\left[\hat{p}, \hat{H}\right] = 0$, if $\psi_k(x)$ is an eigenfunction, then $\hat{p}\psi_k(x)$ is also an eigenfunction having the same energy. If I take e^{ikx} as an eigenfunction, then $\hat{p}\psi_k(x) = \hbar k e^{ikx}$, which is the same eigenfunction. That is, if I use the *simultaneous* eigenfunctions of $\hat{p}$ and $\hat{H}$, I do not generate a new eigenfunction by applying $\hat{p}$ to an eigenfunction. On the other hand, if I choose $\cos(kx)$ as an eigenfunction of $\hat{H}$ then $\hat{p}\psi_k(x) = i\hbar k \sin(kx)$. It generates a *new* eigenfunction with the same energy, demonstrating the energy degeneracy.

19.2.1 Translation Operator

Since the momentum operator commutes with the Hamiltonian and since the free particle Hamiltonian is invariant under translation, we might expect that the momentum operator is somehow connected with the translation operator in quantum mechanics. To demonstrate that this is indeed the case, I start by considering an infinitesimal displacement ϵ of an arbitrary wave function $\psi(x)$, for which

$$\psi(x-\epsilon) \approx \left(1 - \epsilon\frac{d}{dx}\right)\psi(x) = \left(1 - \frac{i}{\hbar}\epsilon\hat{p}\right)\psi(x). \tag{19.30}$$

The momentum operator is said to be *the generator of infinitesimal translations.* I can build up a finite translation a by taking N infinitesimal translations, each having $\epsilon = a/N$, and then take the limit as $N \to \infty$. In this manner I obtain

$$\begin{aligned}
\psi(x;a)_T = \hat{T}(a)\psi(x) &= \lim_{N\to\infty}\left(1 - e^{-\frac{i}{\hbar}\frac{a}{N}\hat{p}}\right)^N \psi(x) \\
&= \lim_{N\to\infty}\left(1 - e^{-\frac{i}{\hbar}\frac{a}{N}\hat{p}}\right)^{N-1} \psi(x - a/N) \\
&= \lim_{N\to\infty}\left(1 - e^{-\frac{i}{\hbar}\frac{a}{N}\hat{p}}\right)^{N-2} \psi(x - a/N - a/N) = \cdots \\
&= \lim_{N\to\infty}\psi(x - Na/N) = \psi(x-a),
\end{aligned} \tag{19.31}$$

where

$$\hat{T}(a) = \lim_{N\to\infty}\left(1 - e^{-\frac{i}{\hbar}\frac{a}{N}\hat{p}}\right)^N = e^{-i\hat{p}a/\hbar} = e^{-a\frac{d}{dx}} \tag{19.32}$$

is the translation operator and $\psi(x;a)_T$ is the translated function. The translation operator is unitary.

If the exponential in Eq. (19.32) is expanded in a Taylor series about $a = 0$ and operates on a function $\psi(x)$, the following series is generated:

$$\begin{aligned} e^{-a\frac{d}{dx}}\psi(x) &= \left(1 - a\frac{d}{dx} + \frac{(-a)^2}{2!}\frac{d^2}{dx^2} - \cdots\right)\psi(x) \\ &= \psi(x) - a\frac{d\psi(x)}{dx} + \frac{(-a)^2}{2!}\frac{d^2\psi(x)}{dx^2} - \cdots . \end{aligned} \tag{19.33}$$

The right side of this equation is a Taylor expansion of $\psi(x-a)$ about $a = 0$, but the Taylor expansion *does not necessarily converge*. Thus,

$$e^{-i\hat{p}a/\hbar}\psi(x) = \psi(x-a) \tag{19.34}$$

only if the series expansion of $\psi(x-a)$ about $a = 0$ converges for *all* x. This is always the case for any infinitesimal translation if $\psi(x)$ is an analytic function, for polynomial $\psi(x)$, and for an $\psi(x)$ that is an exponential of an analytic function, but it is not true in general (see the Appendix for more details).

[Here is a simple example where it works. Take

$$\psi(x) = 2x^2 + x \tag{19.35}$$

and let the translation of the function be two units to the right. The function is transformed as

$$\begin{aligned} \psi(x;2)_T &= e^{-\frac{i}{\hbar}2\hat{p}}\psi(x) = e^{-2\frac{d}{dx}}\left(2x^2 + x\right) \\ &= \left(1 - 2\frac{d}{dx} + \frac{(-2)^2}{2!}\frac{d^2}{dx^2} - \cdots\right)\left(2x^2 + x\right) \\ &= 2x^2 + x - 8x - 2 + 8 = 2x^2 - 7x + 6, \end{aligned} \tag{19.36}$$

which can be written as

$$\psi(x;2)_T = 2(x-2)^2 + (x-2)\,; \tag{19.37}$$

the original function is simply translated to the right by two units.]

If the momentum operator commutes with the Hamiltonian, then the Hamiltonian is invariant under translation, $\hat{T}(a)\hat{H}\hat{T}^{\dagger}(a) = \hat{H}$. This is a general result, continuous operators that commute with a Hamiltonian are the generators of infinitesimal transformations under which the Hamiltonian remains invariant. In this case, the momentum operator generates infinitesimal translations. *By looking at the infinitesimal transformations that are generated by operators that commute with the Hamiltonian, we can determine the symmetry properties of the Hamiltonian!*

The situation is a bit different for discrete operators such as the parity operator defined by

$$\hat{\mathcal{P}}\psi(x) = \psi(-x). \tag{19.38}$$

There can be no infinitesimal transformations associated with a discrete operator of this form. On the other hand, if an operator commutes with the parity operator, this could imply degeneracy. You can see this if you choose the eigenfunctions of the free particle Hamiltonian that are *not* eigenfunctions of the parity operator, namely $e^{\pm ikx}$. Clearly,

$$\hat{\mathcal{P}}e^{ikx} = e^{-ikx} \tag{19.39}$$

produces a new eigenfunction with the same energy. Other discrete operators of importance are the *time-reversal operator* and the *charge-conjugation operator* (see problems). All physical processes are believed to be invariant under the product of the parity, charge-conjugation, and time-reversal operators (CPT theorem).

19.2.2 Rotation Operator

Now let us consider a Hamiltonian with a spherically symmetric potential. You know that the angular momentum operator commutes with this Hamiltonian so you can see what type of infinitesimal transformation it generates. Of course, you can probably guess that it will produce a rotation since the Hamiltonian is invariant under rotations, but let's see. I need only consider $\hat{L}_z$ since the results can be generalized for the other components. I look at

$$\begin{aligned}\left(1 - \frac{i}{\hbar}\delta\phi\hat{L}_z\right)\psi(\mathbf{r}) &= \left[1 - \frac{i}{\hbar}\delta\phi\left(x\hat{p}_y - y\hat{p}_x\right)\right]\psi(\mathbf{r}) \\ &= \left[1 - \delta\phi\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right]\psi(\mathbf{r}) \\ &= \psi(\mathbf{r}) - \delta\phi\left(x\frac{\partial\psi(\mathbf{r})}{\partial y} - y\frac{\partial\psi(\mathbf{r})}{\partial x}\right)\end{aligned}$$

$$= \psi(x,y,z) + \frac{\partial \psi(x,y,z)}{\partial x}(y\delta\phi) - \frac{\partial \psi(x,y,z)}{\partial y}(x\delta\phi)$$
$$\approx \psi(x + y\delta\phi, y - x\delta\phi, z), \tag{19.40}$$

where $\delta\phi$ is an infinitesimal angle. But under an active rotation $\hat{R}$ of the vector $\mathbf{r}$ by an infinitesimal angle $\delta\phi$ about the z axis,

$$\hat{R}_z(\delta\phi)\,\mathbf{r} = \underline{\mathrm{R}}_z(\delta\phi)\,\mathbf{r} = (x - y\delta\phi)\,\mathbf{u}_x + (y + x\delta\phi)\,\mathbf{u}_y + \mathbf{u}_z \tag{19.41}$$

Therefore,

$$\psi(\mathbf{r};\delta\phi)_R = \left(1 - \frac{i}{\hbar}\delta\phi\hat{L}_z\right)\psi(\mathbf{r}) \approx \psi(x + y\delta\phi, y - x\delta\phi, z) \approx \psi\left[\underline{\mathrm{R}}_z(\delta\phi)^{-1}\,\mathbf{r}\right], \tag{19.42}$$

where $\underline{\mathrm{R}}_z(\delta\phi)$ is a rotation matrix corresponding to a rotation about the z-axis and $\psi(\mathbf{r};\delta\phi)_R$ is the rotated function. A comparison with Eq. (19.13) allows us to conclude that the operator $\hat{L}_z$ is the generator of infinitesimal rotations about the z axis. For an arbitrary infinitesimal rotation $\delta\omega$ about the $\mathbf{u_n}$ direction,

$$\psi(\mathbf{r};\mathbf{u_n},\delta\omega)_R = \left(1 - \frac{i}{\hbar}\mathbf{u_n}\cdot\hat{\mathbf{L}}\delta\omega\right)\psi(\mathbf{r}) \approx \psi(\underline{\mathrm{R}}(\mathbf{u_n},\delta\omega)^{-1}\,\mathbf{r}) \tag{19.43}$$

and, for a finite rotation ω about the $\mathbf{u_n}$ direction, the rotation operator is

$$\hat{R}(\mathbf{u_n},\omega) = \lim_{N\to\infty}\left(1 - \frac{i}{\hbar}\mathbf{u_n}\cdot\hat{\mathbf{L}}\frac{\omega}{N}\right)^N = e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}}. \tag{19.44}$$

In this case, the transformed function is

$$\psi(\mathbf{r};\mathbf{u_n},\omega)_R = e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}}\psi(\mathbf{r}) = \psi(\underline{\mathrm{R}}(\mathbf{u_n},\omega)^{-1}\,\mathbf{r}). \tag{19.45}$$

We have seen already that rotations can be described as active rotations about the z, y, and z axes by the Euler angles (γ,β,α) ; as a consequence, the rotation operator can also be written as

$$\hat{R}(\alpha,\beta,\gamma) = e^{-\frac{i}{\hbar}\alpha\hat{L}_z}e^{-\frac{i}{\hbar}\beta\hat{L}_y}e^{-\frac{i}{\hbar}\gamma\hat{L}_z} \tag{19.46}$$

and the transformed wave function as

$$\psi(\mathbf{r})_{\alpha,\beta,\gamma} = e^{-\frac{i}{\hbar}\alpha\hat{L}_z}e^{-\frac{i}{\hbar}\beta\hat{L}_y}e^{-\frac{i}{\hbar}\gamma\hat{L}_z}\psi(\mathbf{r}) = \psi(\underline{\mathrm{R}}(\alpha,\beta,\gamma)^{-1}\,\mathbf{r}). \tag{19.47}$$

Since the $\exp\left(i\hat{H}\right)$ is unitary if $\hat{H}$ is Hermitian, the rotation operator is unitary; that is, the value of $|\psi(\mathbf{r})|$ is unchanged when acted upon by the rotation operator.

19.2.2.1 Transformation of Eigenkets Under Rotation

So far I have been looking at the effect of transformations on wave functions. In some sense, the eigenkets replace the unit vectors, since they can be represented as column vectors. However, I cannot simply use the three-dimensional rotation matrix to transform the infinite dimensional basis vectors in Hilbert space. Instead I need a generalization of Eq. (19.25). To do this I *define* an active rotation of the eigenkets $|\ell m\rangle$ by

$$\begin{aligned}|\ell m\rangle_R &= \hat{R}(\alpha,\beta,\gamma)\,|\ell m\rangle = \sum_{\ell',m'} \left|\ell' m'\right\rangle\left\langle \ell' m'\right| \hat{R}(\alpha,\beta,\gamma)\,|\ell m\rangle \\ &= \sum_{m'} \left|\ell m'\right\rangle\left\langle \ell m'\right| \hat{R}(\alpha,\beta,\gamma)\,|\ell m\rangle = \sum_{m'} \mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\left|\ell m'\right\rangle, \end{aligned} \tag{19.48}$$

where $|\ell m\rangle_R$ is the transformed basis ket and

$$\mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma) = \left\langle \ell m'\right| \hat{R}(\alpha,\beta,\gamma)\,|\ell m\rangle = \left\langle \ell m'\right| e^{-\frac{i}{\hbar}\alpha\hat{L}_z} e^{-\frac{i}{\hbar}\beta\hat{L}_y} e^{-\frac{i}{\hbar}\gamma\hat{L}_z}\,|\ell m\rangle \tag{19.49}$$

is a matrix element of the rotation operator in the $|\ell m\rangle$ basis, which is diagonal in the ℓ quantum number. Note the order of the subscripts in Eq. (19.48), which is consistent with Eq. (19.25). For a state vector

$$|\psi\rangle = \sum_{\ell' m'} a_{\ell m}\,|\ell m\rangle\,, \tag{19.50}$$

the rotated state vector is

$$\begin{aligned}|\psi\rangle_R &= \hat{R}(\alpha,\beta,\gamma)\,|\psi\rangle = \sum_{\ell,m} a_{\ell m}\hat{R}(\alpha,\beta,\gamma)\,|\ell m\rangle \\ &= \sum_{\ell,m,m'} a_{\ell m}\mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\left|\ell m'\right\rangle \\ &= \sum_{\ell,m,m'} (a_{\ell m'})_R\left|\ell m'\right\rangle, \end{aligned} \tag{19.51}$$

where

$$(a_{\ell m'})_R = \sum_{m'} \mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\,(a_{\ell m})\,. \tag{19.52}$$

The components of the state vector transform as would be expected for any vector.

I will usually refer to the $\mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)$ as *rotation matrices* (even though they are actually matrix elements of the rotation operator), to be distinguished from the three-dimensional rotation matrix $\underline{R}(\alpha, \beta, \gamma)$. Some properties of the rotation matrices are:

$$\mathcal{D}^{(\ell)}_{m'm}(\alpha, \beta, \gamma) = \left[\mathcal{D}^{(\ell)}_{mm'}(-\gamma, -\beta, -\alpha)\right]^*; \tag{19.53a}$$

$$\left[\mathcal{D}^{(\ell)}_{m'm}(\alpha, \beta, \gamma)\right]^* = (-1)^{m-m'}\mathcal{D}^{(\ell)}_{-m',-m}(\alpha, \beta, \gamma); \tag{19.53b}$$

$$\left[\mathcal{D}^{(\ell)}(\alpha, \beta, \gamma)\right]^{-1} = \left[\mathcal{D}^{(\ell)}(\alpha, \beta, \gamma)\right]^{\dagger} = \mathcal{D}^{(\ell)}(-\gamma, -\beta, -\alpha); \tag{19.53c}$$

$$\sum_m \mathcal{D}^{(\ell)}_{mm'}\left[\mathcal{D}^{(\ell)}_{mm''}\right]^* = \delta_{m',m''} = \sum_m \mathcal{D}^{(\ell)}_{m'm}\left[\mathcal{D}^{(\ell)}_{m''m}\right]^*; \tag{19.53d}$$

$$\begin{aligned}\mathcal{D}^{(\ell)}_{mm'}(\alpha, \beta, \gamma) &= \langle \ell m| e^{-\frac{i}{\hbar}\alpha\hat{L}_z} e^{-\frac{i}{\hbar}\beta\hat{L}_y} e^{-\frac{i}{\hbar}\gamma\hat{L}_z}\left|\ell m'\right\rangle; \\ &= e^{-im\alpha}e^{-im'\gamma} r^{(\ell)}_{mm'}(\beta),\end{aligned} \tag{19.53e}$$

where

$$r^{(\ell)}_{mm'}(\beta) = \langle \ell m| e^{-\frac{i}{\hbar}\beta\hat{L}_y}\left|\ell m'\right\rangle. \tag{19.53f}$$

The derivation of the explicit expressions for the matrix elements is not trivial, but can be obtained using recursion relations.[1] A Mathematica program to evaluate the $\mathcal{D}^{(\ell)}_{m'm}(\alpha, \beta, \gamma)$ is given on the book's web site. Since

$$\mathcal{D}^{(\ell)}_{m'm}(\alpha, \beta, \gamma) = \left\langle \ell m'\right| \hat{R}(\alpha, \beta, \gamma) |\ell m\rangle = \langle \ell m| \hat{R}^{\dagger}(\alpha, \beta, \gamma)\left|\ell m'\right\rangle^*, \tag{19.54}$$

it follows from Eq. (19.53a) that

$$\hat{R}^{\dagger}(\alpha, \beta, \gamma) = \hat{R}(-\gamma, -\beta, -\alpha) = \hat{R}^{-1}(\alpha, \beta, \gamma), \tag{19.55}$$

consistent with the fact that $\hat{R}(\alpha, \beta, \gamma)$ is a unitary operator.

The rotation matrices are important. You will learn more about them if you take a graduate course in quantum mechanics. Just as I defined a scalar function under translation, I can define a scalar function under rotation. Even more important is that vector and tensor *operators* can be defined under rotation by their transformation properties. Vector and tensor operators, as well as *irreducible tensor operators*, are described briefly in Chap. 20.

The way in which the spherical harmonics transform under rotation can also be calculated. Recall that

$$Y^m_\ell(\theta, \phi) = \langle \mathbf{u}_r(\theta, \phi) |\ell m\rangle. \tag{19.56}$$

The transformed spherical harmonics are defined by

[1]For example, see U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press, Inc, New York, 1959), appendices D and E.

$$Y_\ell^m(\theta,\phi)_R \equiv \langle \mathbf{u}_r(\theta,\phi)\,|\ell m\rangle' = \sum_{m'} \mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\,\langle \mathbf{u}_r(\theta,\phi)\,\left|\ell m'\right\rangle$$
$$= \sum_{m'} \mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)\,Y_\ell^{m'}(\theta,\phi)\,. \tag{19.57}$$

It is seen that the spherical harmonics transform in the same manner as the kets.

19.2.3 Extension to Include Spin Angular Momentum

The angular momentum operator is a unitary operator that preserves the length of state vectors. In other words,

$$_R\langle \ell m\,|\ell m\rangle_R = \langle \ell m|\,\hat{R}^\dagger\hat{R}\,|\ell m\rangle = \langle \ell m\,|\ell m\rangle\,. \tag{19.58}$$

Although I derived an expression for the rotation operator using spatial wave functions, I could equally well have derived it by considering the most general unitary operator that satisfies Eq. (19.58). If I follow the same procedure for the eigenkets $|sm_s\rangle = \left|\frac{1}{2}, m_s\right\rangle$ of the spin operator $\hat{\mathbf{S}}$, I find a spin rotation operator

$$\hat{R}_{\text{spin}}(\mathbf{u}_\mathbf{n},\omega) = e^{-\frac{i}{\hbar}\omega\mathbf{u}_\mathbf{n}\cdot\hat{\mathbf{S}}} = e^{-i\omega\mathbf{u}_\mathbf{n}\cdot\boldsymbol{\sigma}/2}, \tag{19.59}$$

or

$$\hat{R}_{\text{spin}}(\alpha,\beta,\gamma) = e^{-i\alpha\sigma_z/2}e^{-i\alpha\beta\sigma_y/2}e^{-i\gamma\sigma_z/2}, \tag{19.60}$$

where

$$\boldsymbol{\sigma} = \sigma_x\mathbf{u}_x + \sigma_y\mathbf{u}_y + \sigma_z\mathbf{u}_z, \tag{19.61}$$

σ_α $\{\alpha = x, y, z\}$ is a Pauli spin matrix, and $\{\alpha,\beta,\gamma\}$ are the Euler angles. The operator given by Eq. (19.59) or (19.60) is the most general operator that preserves the length of a two-component state vector. The effect of a rotation on the spin eigenkets is then given by

$$|sm_s\rangle_R = \hat{R}_{\text{spin}}\,|\ell m_s\rangle = \sum_{m_s'} \mathcal{D}^{(1/2)}_{m_s'm_s}(\alpha,\beta,\gamma)\,\left|sm_s'\right\rangle, \tag{19.62}$$

where $|sm_s\rangle_R$ is the transformed basis ket and

$$\mathcal{D}^{(1/2)}_{m_s'm_s}(\mathbf{u}_\mathbf{n},\omega) = \left\langle sm_s'\right|e^{-i\omega\mathbf{u}_\mathbf{n}\cdot\boldsymbol{\sigma}/2}\,|sm_s\rangle\,; \tag{19.63a}$$

$$\mathcal{D}^{(1/2)}_{m_s'm_s}(\alpha,\beta,\gamma) = \left\langle sm_s'\right|e^{-i\alpha\sigma_z/2}e^{-i\alpha\beta\sigma_y/2}e^{-i\gamma\sigma_z/2}\,|sm_s\rangle\,, \tag{19.63b}$$

with $s = 1/2$. Even though the spin wave functions are defined in an abstract space and *not* in coordinate space, their components are changed under rotation of coordinates. I have already emphasized this property in Chap. 12.

Somewhat surprisingly, Eqs. (19.63) can help in evaluating matrix elements of the rotation operator $\exp\left(-i\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}/\hbar\right)$ given in Eq. (19.44). To understand why, recall that there are closed form expressions available for the $\mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)$, which are matrix elements of the operator $e^{-\frac{i}{\hbar}\alpha\hat{L}_z}e^{-\frac{i}{\hbar}\beta\hat{L}_y}e^{-\frac{i}{\hbar}\gamma\hat{L}_z}$, but none for the matrix elements of $\exp\left(-i\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}/\hbar\right)$. The most straightforward way to evaluate such matrix elements is to calculate the Euler angles $\{\alpha,\beta,\gamma\}$ that correspond to the rotation specified by $\{\mathbf{u_n},\omega\}$, and then calculate the corresponding $\mathcal{D}^{(\ell)}_{m'm}(\alpha,\beta,\gamma)$. But up to this point, we have no simple prescription for relating the $\{\mathbf{u_n},\omega\}$ to the $\{\alpha,\beta,\gamma\}$. Equations (19.63) afford us this possibility.

To relate the $\{\mathbf{u_n},\omega\}$ to the $\{\alpha,\beta,\gamma\}$, I write

$$e^{-i\omega\mathbf{u_n}\cdot\boldsymbol{\sigma}/2} = \cos\left(\omega\mathbf{u_n}\cdot\boldsymbol{\sigma}/2\right) - i\sin\left(\omega\mathbf{u_n}\cdot\boldsymbol{\sigma}/2\right), \tag{19.64}$$

expand the sines and cosines, and use the identity

$$\left(\mathbf{u_n}\cdot\boldsymbol{\sigma}\right)\left(\mathbf{u_n}\cdot\boldsymbol{\sigma}\right) = \mathbf{1} \tag{19.65}$$

to show that

$$e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\boldsymbol{\sigma}/2} = \mathbf{1}\cos\left(\omega/2\right) - i\,\mathbf{u_n}\cdot\boldsymbol{\sigma}\sin\left(\omega/2\right), \tag{19.66}$$

where $\mathbf{1}$ is the 2×2 unit matrix. I then insert sums over complete sets of spin eigenkets between the exponential in Eq. (19.63b) to calculate

$$\mathcal{D}^{(1)}_{m_s'm_s}(\alpha,\beta,\gamma) = e^{-im_s'\alpha}e^{-im_s\gamma}\left\langle sm_s'\right| e^{-i\beta\sigma_y/2}\left|sm_s\right\rangle \tag{19.67}$$

and use Eq. (19.66) with $\mathbf{u_n} = \mathbf{u}_y$ and $\omega = \beta$ to arrive at

$$\mathcal{D}^{(1/2)}(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\left(\beta/2\right)e^{-i(\alpha+\gamma)/2} & -\sin\left(\beta/2\right)e^{-i(\alpha-\gamma)/2} \\ \sin\left(\beta/2\right)e^{i(\alpha-\gamma)/2} & \cos\left(\beta/2\right)e^{i(\alpha+\gamma)/2} \end{pmatrix}, \tag{19.68}$$

where, by convention, the matrix indices go from highest to lowest values of m. By equating Eqs. (19.66) and (19.68), you can calculate the Euler angles $\{\alpha,\beta,\gamma\}$ in terms of $\{\mathbf{u_n},\omega\}$.

The eigenkets of hydrogen consist of both orbital and spin angular momentum components. To determine how an eigenket of the form

$$\left|\ell,s;m_\ell,m_s\right\rangle = \left|\ell m_\ell\right\rangle\left|sm_s\right\rangle \tag{19.69}$$

transforms under rotation, you need only remember that the orbital and spin operators act in different Hilbert spaces. It then follows that the effect of a rotation on the ket $|\ell, s; m_\ell, m_s\rangle$ is to produce a new ket

$$|\ell, s; m_\ell, m_s\rangle_R = e^{-\frac{i}{\hbar}\omega \mathbf{u_n}\cdot\hat{\mathbf{L}}} |\ell m_\ell\rangle \, e^{-\frac{i}{\hbar}\omega \mathbf{u_n}\cdot\hat{\mathbf{S}}} |s m_s\rangle = e^{-\frac{i}{\hbar}\omega \mathbf{u_n}\cdot\hat{\mathbf{J}}} |\ell m_\ell\rangle \, |s m_s\rangle \,, \tag{19.70}$$

where

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}} \tag{19.71}$$

is the total angular momentum operator and I have used the fact that $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$ commute. As we have seen in Chap. 12, it is sometimes more convenient to use the eigenkets $|\ell, s; j, m\rangle$ instead of $|\ell, s; m_\ell, m_s\rangle$. The $|\ell, s; j, m\rangle$ basis is the natural one for evaluating matrix elements of the rotation operator,

$$\begin{aligned}
\mathcal{D}^{(j)}_{m'm}(\alpha, \beta, \gamma) &= \left\langle jm' \right| \hat{R}(\alpha, \beta, \gamma) \left| jm \right\rangle \\
&= \left\langle jm' \right| e^{-\frac{i}{\hbar}\alpha \hat{J}_z} e^{-\frac{i}{\hbar}\beta \hat{J}_y} e^{-\frac{i}{\hbar}\gamma \hat{J}_z} \left| jm \right\rangle \\
&= e^{-im'\alpha} e^{-im\gamma} \left\langle jm' \right| e^{-\frac{i}{\hbar}\beta \hat{J}_y} \left| jm \right\rangle ,
\end{aligned} \tag{19.72}$$

for reasons to be discussed in Chap. 20. Closed form expressions for the $\mathcal{D}^{(j)}_{m'm}(\alpha, \beta, \gamma)$ are given on the book's web site. Equations (19.53) remain valid when ℓ is replaced by j.

19.2.4 Transformation of Operators

Imagine there is an operator $\hat{A}$ such that

$$\psi_2(\mathbf{r}) = \hat{A}\psi_1(\mathbf{r}). \tag{19.73}$$

Under a unitary transformation $\hat{U}$ that transforms the wave function as

$$\psi_u(\mathbf{r}) = \hat{U}\psi(\mathbf{r}), \tag{19.74}$$

Eq. (19.73) is transformed into

$$\psi_{2u}(\mathbf{r}) = \hat{U}\psi_2(\mathbf{r}) = \hat{U}\hat{A}\psi_1(\mathbf{r}) = \hat{U}\hat{A}\hat{U}^\dagger\psi_2(\mathbf{r}) = \hat{A}_u\psi_2(\mathbf{r}), \tag{19.75}$$

where $\hat{A}_u$ is the transformed operator and I have used the fact that $\hat{U}^\dagger\hat{U} = \hat{1}$. Thus, under translation, an operator $\hat{A}$ is transformed into

$$\hat{A}_T = \hat{T}\hat{A}\hat{T}^\dagger, \tag{19.76}$$

while under rotation it is transformed into

$$\hat{A}_R = \hat{R}\hat{A}\hat{R}^{\dagger}. \tag{19.77}$$

It can be a bit confusing when one encounters a Hamiltonian of the form $\hat{H} = \alpha\hat{\mathbf{r}}\cdot\mathbf{E}$, where α is a constant and $\mathbf{E}$ is a (classical) electric field. Although conventional vectors are transformed under rotation, in quantum mechanics the only quantities that are transformed under rotation (and any other symmetry operation, for that matter) are quantum-mechanical *operators*. That is, under rotation, $\hat{H}_R = \alpha\hat{\mathbf{r}}_R \cdot \mathbf{E}$, where $\hat{\mathbf{r}}_R = \hat{R}\hat{\mathbf{r}}\hat{R}^{\dagger}$, only the operator is transformed. The electric field appearing in the Hamiltonian is taken to be an external field (*not* an operator) and is unaffected by the transformation. You can expand your quantum system to include the electric field (it is no longer an external field in this case), but to do so you must quantize the field. Once the field is quantized, the electric field becomes an operator that is also transformed under rotation.

19.3 Rotations: Examples

In dealing with rotations, I distinguish between the rotation matrix (all operations are for active transformations)

$$\underline{R}(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\gamma\sin\alpha & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix}, \tag{19.78}$$

the rotation operator

$$\hat{R}\left(\mathbf{u_n},\omega\right) = e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}}; \tag{19.79a}$$

$$\hat{R}\left(\alpha,\beta,\gamma\right) = e^{-\frac{i}{\hbar}\alpha\hat{L}_z}e^{-\frac{i}{\hbar}\beta\hat{L}_y}e^{-\frac{i}{\hbar}\gamma\hat{L}_z}, \tag{19.79b}$$

and the rotation matrices

$$\mathcal{D}^{(\ell)}_{mm'}\left(\mathbf{u_n},\omega\right) = \langle \ell m|\, e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}}\left|\ell m'\right\rangle \tag{19.80a}$$

$$\mathcal{D}^{(\ell)}_{mm'}\left(\alpha,\beta,\gamma\right) = \langle \ell m|\, e^{-\frac{i}{\hbar}\alpha\hat{L}_z}e^{-\frac{i}{\hbar}\beta\hat{L}_y}e^{-\frac{i}{\hbar}\gamma\hat{L}_z}\left|\ell m'\right\rangle. \tag{19.80b}$$

Each has a specific function which I now review.

19.3.1 Rotation Matrix

I start with the rotation matrix, Eq. (19.78). The rotation matrix tells you how the *coordinates* of a vector change under an active rotation of the vector. Remember in an active rotation the axes remain fixed and the vector is rotated, first by γ about the z axis, then by β around the y axis, and finally by α around the z axis. For example, the rotation $(\alpha = 0, \beta = -\pi/2, \gamma = 0)$ rotates a unit vector $\mathbf{f} = \mathbf{u}_x$ along the x axis into one along the z axis and I find accordingly

$$\begin{pmatrix} f_{Rx} \\ f_{Ry} \\ f_{Rz} \end{pmatrix} = \underline{R}(0, \pi/2, 0) \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{19.81}$$

A somewhat more complicated example is to rotate the vector

$$\mathbf{f} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \tag{19.82}$$

into the "negative" of itself

$$\mathbf{f}_R = -\frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \tag{19.83}$$

You can convince yourself that this is accomplished by the rotation

$$\begin{aligned} &\underline{R}(\alpha = -3\pi/4, \beta = \pi - 2\cos^{-1}(1/\sqrt{3}), \gamma = -\pi/4) \\ &= \frac{1}{3} \begin{pmatrix} -2 & 1 & -2 \\ 1 & -2 & -2 \\ -2 & -2 & 1 \end{pmatrix}. \end{aligned} \tag{19.84}$$

On the other hand, the *same* transformation is given simply by the matrix

$$\underline{M} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{19.85}$$

but this matrix *cannot* be obtained from the rotation matrix $\underline{R}(\alpha, \beta, \gamma)$. The reason for this is that the rotation matrices I am using are called *proper rotations* (having determinant $+1$), since they can be generated continuously from the unit matrix. The *improper* rotation matrices form another whole set of rotation matrices having determinant -1, that cannot be generated from the identity. Since there are two ways of generating rotations in this fashion, the rotation group (groups are discussed briefly in the following chapter) is not *simply connected*.

19.3.2 Rotation Operator

Now let me move on to the rotation operator. The rotation operator acts on *state vectors or wave functions*. In general you would expect the result to be very complicated since

$$\hat{R}(\alpha,\beta,\gamma)\,\psi(\mathbf{r}) = e^{-\frac{i}{\hbar}\alpha\hat{L}_z}e^{-\frac{i}{\hbar}\beta\hat{L}_y}e^{-\frac{i}{\hbar}\gamma\hat{L}_z}\psi(\mathbf{r}) \tag{19.86}$$

appears very difficult to evaluate. However, if you remember that the wave function is a scalar, then

$$\psi(\mathbf{r})_R = \hat{R}(\alpha,\beta,\gamma)\,\psi(\mathbf{r}) = \psi[\underset{\sim}{\mathrm{R}}(\alpha,\beta,\gamma)^{-1}\,\mathbf{r}], \tag{19.87}$$

where $\underset{\sim}{\mathrm{R}}(\alpha,\beta,\gamma)^{-1}$ is just the transpose of the (active) rotation matrix.

As an example, let us see how the spherical harmonic $Y_1^0(\theta,\phi)$ is transformed under a rotation of $-\pi/2$ about the y-axis, for which the Euler angles are $(\alpha,\beta,\gamma) = (0,-\pi/2,0)$. The transformed function is

$$Y_1^0(\theta,\phi)_R = Y_1^0(x,y,z)_R = \underset{\sim}{\mathrm{R}}(0,-\pi/2,0)\,Y_1^0(\theta,\phi) = e^{\frac{i}{2\hbar}\pi\hat{L}_y}Y_1^0(\theta,\phi)\,. \tag{19.88}$$

Recall that the spherical coordinates can be considered to be functions of x, y, and z. This looks a bit complicated, but using Eq. (19.87), I find

$$\begin{aligned} Y_1^0(x,y,z)_R &= e^{\frac{i}{2\hbar}\pi\hat{L}_y}Y_1^0(\theta,\phi) = \psi[\underset{\sim}{\mathrm{R}}(0,-\pi/2,0)^{-1}\,\mathbf{r}] \\ &= \psi\left[\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}\right] = Y_1^0(z,y,-x) \end{aligned} \tag{19.89}$$

The problem reduces to expressing Y_1^0 as a function of (x,y,z) instead of (θ,ϕ). To do this I write

$$Y_1^0(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} = Y_1^0(x,y,z)\,, \tag{19.90}$$

such that

$$\begin{aligned} Y_1^0(z,y,-x) &= -\sqrt{\frac{3}{4\pi}}\frac{x}{r} = -\sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi \\ &= -\sqrt{\frac{3}{4\pi}}\sin\theta\frac{e^{i\phi}+e^{-i\phi}}{2} = \frac{1}{\sqrt{2}}\left[Y_1^1(\theta,\phi) - Y_1^{-1}(\theta,\phi)\right]. \end{aligned} \tag{19.91}$$

Thus

$$\psi(\mathbf{r})_R = e^{\frac{i}{2\hbar}\pi\hat{L}_y} Y_1^0(\theta,\phi) = \frac{1}{\sqrt{2}}\left[Y_1^1(\theta,\phi) - Y_1^{-1}(\theta,\phi)\right], \tag{19.92}$$

a result I will derive now using the rotation matrices.

19.3.3 Rotation Matrices

The rotation matrices are defined by

$$\mathcal{D}_{mm'}^{(\ell)}(\alpha,\beta,\gamma) = \left\langle \ell m' \right| e^{-\frac{i}{\hbar}\alpha\hat{L}_z} e^{-\frac{i}{\hbar}\beta\hat{L}_y} e^{-\frac{i}{\hbar}\gamma\hat{L}_z} \left| \ell m \right\rangle. \tag{19.93}$$

The state vector transforms as

$$\left|\ell m\right\rangle_R = \sum_{m'} \mathcal{D}_{m'm}^{(\ell)}(\alpha,\beta,\gamma)\left|\ell m'\right\rangle, \tag{19.94}$$

as do the spherical harmonics,

$$Y_\ell^m(\theta,\phi)_R = \sum_{m'} \mathcal{D}_{m'm}^{(\ell)}(\alpha,\beta,\gamma)\, Y_\ell^{m'}(\theta,\phi). \tag{19.95}$$

Equations (19.93) and (19.94) remain valid when ℓ is replaced by the total angular momentum quantum number j, which can be integral or half-integral.

For $\ell = 1$,

$$\mathcal{D}^{(1)}(\alpha,\beta,\gamma) = \begin{pmatrix} \cos^2\left(\frac{\beta}{2}\right)e^{-i(\alpha+\gamma)} & -\frac{1}{\sqrt{2}}\sin\beta e^{-i\alpha} & \sin^2\left(\frac{\beta}{2}\right)e^{-i(\alpha-\gamma)} \\ \frac{1}{\sqrt{2}}\sin\beta e^{-i\gamma} & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta e^{i\gamma} \\ \sin^2\left(\frac{\beta}{2}\right)e^{i(\alpha-\gamma)} & \frac{1}{\sqrt{2}}\sin\beta e^{i\alpha} & \cos^2\left(\frac{\beta}{2}\right)e^{i(\alpha+\gamma)} \end{pmatrix} \tag{19.96}$$

and, for $j = 1/2$,

$$\mathcal{D}^{(1/2)}(\alpha,\beta,\gamma) = \begin{pmatrix} \cos(\beta/2)\,e^{-i(\alpha+\gamma)/2} & -\sin(\beta/2)\,e^{-i(\alpha-\gamma)/2} \\ \sin(\beta/2)\,e^{i(\alpha-\gamma)/2} & \cos(\beta/2)\,e^{i(\alpha+\gamma)/2} \end{pmatrix}. \tag{19.97}$$

I can check to see if Eq. (19.95) agrees with Eq. (19.92) when $(\alpha = 0, \beta = -\pi/2, \gamma = 0)$. In that case

$$\mathcal{D}^{(1)}(0,-\pi/2,0) = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix} \tag{19.98}$$

and

$$\begin{aligned} Y_1^0(\theta,\phi)_R &= \sum_{q'=-k}^{k} \mathcal{D}_{q'0}^{(k)}(\alpha,\beta,\gamma)\, Y_1^{q'}(\theta,\phi) \\ &= \frac{1}{\sqrt{2}}\left[Y_1^1(\theta,\phi) - Y_1^{-1}(\theta,\phi)\right] \end{aligned} \tag{19.99}$$

in agreement with Eq. (19.92).

19.4 Summary

In this chapter, a brief introduction was given of the role played by transformations and symmetry in quantum mechanics. The interplay between degeneracy, symmetry, and operators that commute with the Hamiltonian was elaborated. It was shown that the operators associated with conserved physical quantities can be used to generate transformations on the eigenfunctions that leave the Hamiltonian invariant. The transformations of the eigenfunctions and eigenkets under translation and rotation were derived. It was shown that the transformations of the eigenkets under rotation matrices could be expressed in terms of the rotation matrices, whose elements, $\mathcal{D}_{m'm}^{(\ell)}(\alpha,\beta,\gamma)$, are simply matrix elements of the rotation operator in the $|\ell m\rangle$ basis.

19.5 Appendix: Finite Translations and Rotations

19.5.1 Translation Operator

I can use a slightly different definition of the translation operator (in one-dimension), writing it as

$$\hat{T}(a) = \lim_{N\to\infty}\left(1 - e^{-\frac{i}{\hbar}\frac{a}{N}\hat{p}}\right)^N = \widehat{e^{-ipa/\hbar}}, \tag{19.100}$$

with the operator $\widehat{e^{-ipa/\hbar}}$ defined such that

$$\widehat{e^{-ipa/\hbar}}\left|p'\right\rangle = e^{-ip'a/\hbar}\left|p'\right\rangle. \tag{19.101}$$

Equation (19.101) is consistent with Eq. (5.64).

It is then straightforward to show that this operator produces the correct translations of kets. That is, with

$$|x\rangle = \int_{-\infty}^{\infty} dx \langle p' \; |x\rangle \left|p'\right\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp' e^{-ip'x/\hbar} \left|p'\right\rangle, \tag{19.102}$$

I find that

$$\begin{aligned} |x\rangle_T &= \widehat{e^{-ipa/\hbar}} \, |x\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp e^{-ipx/\hbar} \widehat{e^{-ipa/\hbar}} \, |p\rangle \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dp e^{-ipx/\hbar} e^{-ipa/\hbar} \left|x'\right\rangle \langle x' \; |p\rangle \\ &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dp' e^{-ipx/\hbar} e^{-ipa/\hbar} e^{ipx'/\hbar} \left|x'\right\rangle \\ &= \int_{-\infty}^{\infty} dx' \delta\left(x' - x - a\right) \left|x'\right\rangle = |x + a\rangle \, , \end{aligned} \tag{19.103}$$

Thus, the operator $\widehat{e^{-ipa/\hbar}}$ translate kets to the *left* by a.

To see the effect of this operator on functions, I use Eq. (5.66),

$$\widehat{e^{-ipa/\hbar}} f(x) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} dx' \, \tilde{B}(x - x') f(x'). \tag{19.104}$$

where

$$\tilde{B}(x) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} dp \, e^{-ipa/\hbar} e^{ipx/\hbar} = (2\pi\hbar)^{3/2} \, \delta\,(x - a) \tag{19.105}$$

is the Fourier transform of $e^{-ipa/\hbar}$. Combining Eqs. (19.104) and (19.105),

$$\widehat{e^{-ipa/\hbar}} f(x) = f(x - a); \tag{19.106}$$

the operator $\widehat{e^{-ipa/\hbar}}$ translates *functions* to the right by a.

In other words, the assumption that,

$$\widehat{e^{-ipa/\hbar}} g(p) = e^{-ipa/\hbar} g(p), \tag{19.107}$$

which led to Eq. (5.66) guarantees that the operator $\widehat{e^{-ipa/\hbar}}$ translates functions. On the other hand, when interpreted in terms of its series expansion,

$$e^{-i\hat{p}a/\hbar} f(x) = f(x - a) \tag{19.108}$$

only if the series expansion of $f(x - a)$ about $a = 0$ converges for all x.

19.5.2 Rotation Operator

Similar considerations hold for the rotation operator. I can define the rotation operator via

$$\hat{R}(\mathbf{u_n}, \omega) = \lim_{N\to\infty}\left(1 - \frac{i}{\hbar}\mathbf{u_n}\cdot\hat{\mathbf{L}}\frac{\omega}{N}\right)^N = \widehat{e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}}}. \tag{19.109}$$

In this case, however, I am not able to prove that

$$\widehat{e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}}}\psi(\mathbf{r}) = \psi(\underline{\mathrm{R}}(\mathbf{u_n}, \omega)^{-1}\,\mathbf{r}), \tag{19.110}$$

since the angular momentum operator is a function of both momentum and position and I have no simple prescription for the action of such an operator on functions such as $f(\mathbf{r})$ or $g(\mathbf{p})$. I can resort to setting

$$\widehat{e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}}} = e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}} \tag{19.111}$$

and define $e^{-\frac{i}{\hbar}\omega\mathbf{u_n}\cdot\hat{\mathbf{L}}}$ in terms of its Taylor expansion. Fortunately, when defined in this manner, the rotation operator acting on a spherical harmonic produces a series that is always convergent. Thus, for all cases of practical interest, I can take the rotation operator to be given by Eq. (19.44) or (19.46).

19.6 Problems

1. Explain in general terms why symmetry, energy degeneracy, and conserved dynamic variables are related concepts? Give several reasons why it is useful to identify operators that commute with the Hamiltonian.

2. The parity operator is defined such that

$$\hat{P}\psi(\mathbf{r}) = \psi(-\mathbf{r}).$$

Prove that $\hat{P}$ is a Hermitian operator having eigenvalues ± 1. Under what conditions does the parity operator commute with the Hamiltonian for a one-dimensional potential? For potentials $V(r)$, prove the parity operator commutes with the Hamiltonian, which implies that simultaneous eigenfunctions of the Hamiltonian and the parity operator can be found, namely

$$\psi_{E\ell m}(\mathbf{r}) = R_{E\ell}(r)Y_\ell^m(\theta, \phi).$$

Prove that the parity of these eigenfunctions is $(-1)^\ell$.

3. Starting from the operator

$$\hat{T}(\epsilon) = e^{-\frac{i}{\hbar}\epsilon\hat{p}} \approx 1 - \frac{i}{\hbar}\epsilon\hat{p}$$

which is the generator of infinitesimal translations ϵ, prove that that $\hat{T}(a) = e^{-ia\hat{p}/\hbar}$. To derive this result expand $\hat{T}(a+\epsilon)$ to obtain a differential equation for $\hat{T}(a)$. It is often stated that $\hat{T}(a)$ is the translation operator for a finite displacement a. As shown in the Appendix, however, this assignment is valid only when $\hat{T}(a)$ acts on functions $f(x)$ for which the series expansion of $f(x-a)$ about $a=0$ converges for all x.

4. Calculate

$$\left(1 - \epsilon\frac{d}{dx}\right)f(x)$$

and show that it corresponds to the function $f(x)$ translated ϵ units to the right in the limit that $\epsilon \to 0$, provided $f(x)$ is an analytic function. This implies that $\hat{T}(\epsilon)$ is the generator of infinitesimal translations for such functions.

Show, however, that the operator $\hat{T}(a) = e^{-\frac{i}{\hbar}a\hat{p}}$ acting on the function $f(x) = 1/\left(1+x^2\right)$ does *not* translate the function a units to the right.

5. Why does

$$e^{-\frac{i}{\hbar}\theta\mathbf{n}\cdot\hat{\mathbf{L}}}e^{-r^2} = e^{-r^2},$$

where $\mathbf{n}$ is a unit vector?

6. Evaluate

$$Y_1^0(\theta,\phi)_R = e^{-\frac{i}{\hbar}\frac{\pi}{4}\hat{L}_x}Y_1^0(\theta,\phi),$$

using the fact that

$$Y_1^0(\theta,\phi)_R = Y_1^0\left(\underline{\mathrm{R}}^{-1}\mathbf{r}\right),$$

where $\underline{\mathrm{R}}$ is the rotation matrix. (Hint: What Euler angles give you a rotation of $\pi/4$ about the x axis?).

7. Evaluate

$$e^{-\frac{i}{\hbar}\frac{\pi}{4}\hat{L}_x}Y_1^0(\theta,\phi),$$

using the fact that the $Y_\ell^m(\theta,\phi)$ transform under rotation as

$$\left[Y_\ell^m(\theta,\phi)\right]_R = \sum_{m'} \mathcal{D}^{(1)}_{m'm}(\alpha,\beta,\gamma) Y_\ell^{m'}(\theta,\phi)$$

Compare your answer with that of the previous problem.

8. If you apply the rotation operator to a state $|n,\ell,m\rangle$ of the hydrogen atom, how many distinct new eigenkets can you produce using different values of the rotation angles. Use four different sets of rotation angles to calculate the effect of a rotation on the state vector $|n=1,\ell=1,m=0\rangle$. Show that the four new eigenkets that are generated are not linearly independent. Why must this be the case? Do not take any angles equal to zero or integral or half integral values of π in choosing your angles.

9. Suppose that you are given a state vector

$$|\psi\rangle = |\uparrow\rangle$$

for a spin 1/2 quantum system. Find the transformed state vector

$$|\psi\rangle_R = |x\rangle$$

for a rotation that takes a vector along the z-axis to the x-axis and

$$|\psi\rangle_R = |y\rangle$$

for a rotation that takes a vector along the z-axis to the y-axis. Prove that

$$\langle x|\hat{S}_x|x\rangle = \langle y|\hat{S}_y|y\rangle = 1;$$
$$\langle y|\hat{S}_x|y\rangle = \langle x|\hat{S}_y|x\rangle = 0,$$

In other words, if the quantum system is in the state $|x\rangle$ ($|y\rangle$), a measurement of the spin along the $x(y)$-direction always yields a value of $\hbar/2$.

10. You might expect that, in the absence of any external interactions, the Schrödinger equation would be invariant under time reversal. Show, however, that the solution of the time-dependent Schrödinger equation *changes* under the substitution $t \to -t$, that is

$$i\hbar\frac{\partial\psi(\mathbf{r},-t)}{\partial t} \neq \hat{H}\psi(\mathbf{r},-t),$$

but, instead,

$$i\hbar\frac{\partial\left[\psi(\mathbf{r},-t)\right]^*}{\partial t} = \hat{H}\left[\psi(\mathbf{r},-t)\right]^*. \tag{19.112}$$

The *time-independent*, *time-reversal operator* $\hat{T}$ (not to be confused with the translation operator) is defined such that

$$\hat{T}\psi(\mathbf{r}) = \psi_t(\mathbf{r}) = [\psi(\mathbf{r})]^*$$

and

$$\hat{T}\sum_n a_n\psi(\mathbf{r}) = \sum_n a_n^*\hat{T}\psi(\mathbf{r}) = \sum_n a_n^*[\psi(\mathbf{r})]^*.$$

Prove that $\hat{T}^{-1} = \hat{T} = \hat{T}^\dagger$. Show that by applying the operator $\hat{T}$ to the time-dependent Schrödinger equation, you reproduce Eq. (19.112), provided the Hamiltonian is invariant under time reversal, $\hat{T}\hat{H}\hat{T}^{-1} = \hat{H}$.

11. Under the time reversal operation, $\hat{T}\hat{\mathbf{r}}\hat{T}^{-1} = \hat{\mathbf{r}}$, $\hat{T}\hat{\mathbf{p}}\hat{T}^{-1} = -\hat{\mathbf{p}}$, and $\hat{T}\hat{\mathbf{L}}\hat{T}^{-1} = -\hat{\mathbf{L}}$. Prove these transformation properties by considering the actions of the operators on a wave function $\psi(\mathbf{r})$, using $\hat{T}\psi(\mathbf{r}) = \hat{T}^{-1}\psi(\mathbf{r}) = [\psi(\mathbf{r})]^*$.

12. The transformation $\hat{T}\psi(\mathbf{r}) = [\psi(\mathbf{r})]^*$ equation holds only for wave functions corresponding to particles without spin. Prove that, in order to have $\hat{T}\hat{\mathbf{S}}\hat{T}^{-1} = -\hat{\mathbf{S}}$ for a spin 1/2 particle, you can take $\hat{T}\psi(\mathbf{r}) = \exp\left(-i\pi\hat{S}_y/\hbar\right)[\psi(\mathbf{r})]^*$. This definition also extends to the total angular momentum operator $\hat{\mathbf{J}}$. The operator corresponds to a rotation of π about the y-axis.

13. For a time-reversal invariant Hamiltonian $\hat{H}$, prove that, if $|\alpha\rangle$ is an eigenket of $\hat{H}$, then $\hat{T}|\alpha\rangle$ is also an eigenket with the same energy eigenvalue. As a consequence if $\hat{T}|\alpha\rangle \neq |\alpha\rangle$, then there is a degeneracy related to time-reversal invariance that is referred to as *Kramers degeneracy* (after Hans Kramers). Show that for a spinless particle, there is no Kramers degeneracy but, for a particle having spin 1/2, $\hat{T}|\uparrow\rangle = |\downarrow\rangle$; there is a two-fold Kramers degeneracy.

14. For a single-particle system, the charge conjugation operator $\hat{C}$ changes the particle into its antiparticle—it effectively changes the sign of the particle's charge without affecting its other properties. The equations of physics are believed to be invariant under the combined action of the parity, time-reversal, and charge conjugation operators. Explain why the interaction potentials $-\hat{\mathbf{p}}_e \cdot \mathbf{E}$ and $-\hat{\boldsymbol{\mu}} \cdot \mathbf{B}$ are invariant under $\hat{C}\hat{P}\hat{T}$ by considering the action of each of these operators separately on the atomic dipole moment $\mathbf{p}_e = -e\hat{\mathbf{r}}$ and the magnetic dipole moment operator $\hat{\boldsymbol{\mu}} = -e\hat{\mathbf{L}}/2m_e$. The electric and magnetic fields appearing in these equations are taken to be external fields (not operators) and are unaffected by the transformations. Also determine if these interactions preserve parity and if they are time-reversal invariant.

15. Prove that the Bell state $|\Psi_-\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ of two electrons is invariant under an arbitrary rotation. Prove that the Bell state $|\Phi_+\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$ is unchanged under a rotation that takes the z-axis into the x-axis, but that it is

transformed (to within a phase) into the Bell state $|\Phi_-\rangle = (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) / \sqrt{2}$ under a rotation that takes the z-axis into the y-axis.

16. Prove that

$$(\mathbf{u_n} \cdot \boldsymbol{\sigma}) (\mathbf{u_n} \cdot \boldsymbol{\sigma}) = \mathbf{1},$$

where $\mathbf{u_n}$ is a unit vector, and use this identity to prove that

$$\cos(\omega \mathbf{u_n} \cdot \boldsymbol{\sigma}/2) - i \sin(\omega \mathbf{u_n} \cdot \boldsymbol{\sigma}/2) = \mathbf{1} \cos(\omega/2) - i \mathbf{u_n} \cdot \boldsymbol{\sigma} \sin(\omega/2).$$

In turn, use this expression to show that

$$e^{-i\beta\sigma_y/2} = \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix}.$$

17–18. Use Eqs. (19.66) and (19.68) to express the Euler angles in terms of $\mathbf{u_n}$ and ω. Verify that your solution is correct for $\mathbf{u_n} = \mathbf{u}_x$, $\mathbf{u_n} = \mathbf{u}_y$, and $\mathbf{u_n} = \mathbf{u}_z$ by calculating the rotation matrix $\underline{\mathrm{R}}(\alpha, \beta, \gamma)$ in each case.

19–21. In Problem 12.7–8 you were asked to obtain the electron spin eigenkets for a quantization axis in the direction of the unit vector

$$\mathbf{u}(\theta, \phi, \psi) = \cos\psi \, \mathbf{u}_\theta + \sin\psi \, \mathbf{u}_\varphi.$$

The angles θ and ϕ are the polar and azimuthal angles of a spherical coordinate system, while ψ is the angle of the quantization axis relative to the $\mathbf{u}_\theta$ direction in a plane perpendicular to $\mathbf{u}_r$. To obtain the eigenkets using the rotation matrices, find the Euler angles that correspond to a rotation that takes the unit vector $\mathbf{v} = \mathbf{u}_z$ to the direction $\mathbf{u}(\theta, \phi, \psi)$ (since this takes the original quantization axis into the new one). Then use Eqs. (19.48) and (19.97) to calculate the eigenkets. Show that, to within a phase factor, they agree with the ones given in Problem 12.7–8. [Hint: Since $\mathbf{v} = \mathbf{u}_z$, the first rotation does not affect the vector $\mathbf{v} = \mathbf{u}_z$; that is, $\gamma = 0$. To get the remaining Euler angles, set $\mathbf{u}(\theta, \phi, \psi) = \underline{\mathrm{R}}(\alpha, \beta, \gamma)\mathbf{u}_z$.]

22. Using Eq. (5.86),

$$e^{\hat{A}} \hat{O} e^{-\hat{A}} = \hat{O} + \left[\hat{A}, \hat{O}\right] + \frac{1}{2!}\left[\hat{A}, \left[\hat{A}, \hat{O}\right]\right] + \cdots,$$

prove that, under an active translation produced by the operator $\hat{T}(a) = e^{-ia\hat{p}_x/\hbar}$, the operators $\hat{x}$ and $\hat{x}^2$ are transformed as

$$\hat{x}_T = \hat{x} - a; \qquad \hat{x}^2_T = (\hat{x} - a)^2,$$

and that under an active *momentum boost* produced by the *momentum translation* operator $\hat{B}(q) = e^{iq\hat{x}/\hbar}$, the operators $\hat{p}_x$ and $\hat{p}_x$ are transformed as

$$(\hat{p}_x)_T = \hat{p}_x - q; \qquad \left(\hat{p}_x^2\right)_T = (\hat{p}_x - q)^2 .$$

23. Consider one-dimensional motion with $\hat{p} = \hat{p}_x$. The combined operation of a translation and a momentum boost of the previous problem,

$$\hat{B}(q)\hat{T}(a) = e^{iq\hat{x}/\hbar}e^{-ia\hat{p}_x/\hbar}$$

translates both the momentum and position wave functions. If $a = v_b t$ and $q = mv_b$ for a particle having mass m, this combined operation would seem to constitute a Galilean transformation. Of course, we are free to multiply this operator by any phase factor that does not contain any operators. Show that the free particle Hamiltonian is changed under the transformation produced by the operator

$$\hat{G}(v_b, t) = e^{-imv_b^2 t/2}\hat{B}(mv_b)\hat{T}(v_b t)$$

but the wave function

$$\psi(x,t)_G = \hat{G}(v_b, t)\psi(x,t)$$

still satisfies the Schrödinger equation. This result proves that the free particle Schrödinger equation is invariant under a Galilean transformation. It can be generalized to many-particle systems whose interaction energies depend only on the relative position vectors of the particles. In that case, the transformation is made with respect to center-of-mass variables. In solving this problem, it may prove helpful to use Eq. (5.85),

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-[\hat{A},\hat{B}]/2}.$$

24. Prove that under the Galilean transformation,

$$\hat{G}(v_b, t) = e^{-imv_b^2 t/2}e^{imv_b\hat{x}/\hbar}e^{-iv_b t\hat{p}_x/\hbar},$$

the free particle spatial wave function,

$$\psi(x,t) = \exp(ip_0/\hbar)\exp\left(-ip_0^2 t/2m\hbar\right),$$

and free particle momentum wave function,

$$\Phi(p,t) = \delta(p - p_0)\exp\left(-ip^2 t/2m\hbar\right),$$

transform as you would expect.