Symmetries, conservation laws

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In classical mechanics, arbitrarily complicated physical situations nonetheless obey a simple set of rules: conservation of energy, momentum, and angular momentum. Such conservation laws follow from *symmetries*: when the system is invariant under certain transformations (i.e., symmetric), physical quantities are conserved. This makes understanding the symmetries of a classical sysem incredibly powerful, since they give rise to universal rules that vastly simplify the dynamics.

We are now in a position to understand a similar set of statements in quantum mechanics. In doing so, we have two goals: First, to see how the conservation laws of classical mechanics emerge from quantum mechanics. Second, to understand the analogues of these classical conservation laws in intrinsically quantum systems, and connect them to symmetries of the quantum theory.

Classically, if you want to figure out the symmetries of a system, you transform it in various ways and see which transformations leave the dynamics unchanged. Since the classical variables are the positions of particles as functions of time, these transformations include translations in space (i.e. move it), rotations, reflections (i.e. flip it), and translations in time. Quantum mechanically, the information about the system is encoded in the state. It follows that transformations in quantum mechanics should take the form of operators that act on states. As we will see, there are operators that serve as the quantum analogs of all of the classical transformations: spatial translations, rotations, reflections, and time translations. Our goal will be to study each operator in turn, and use these operators to identify the possible symmetries of quantum states. These symmetries, in turn, will give rise to conservation laws. These conservation laws will drastically simplify our ability to answer questions in quantum mechanics, because they will tell us what things can or cannot be changed as a result of the dynamics.

In what follows, our treatment of the material will parallel Griffiths, but as is often the case, we will try to be more careful in defining the action of operators at

the level of states in Hilbert space, rather than jumping directly into position-space representations as Griffiths does. This will make it much clearer how the operators and transformations are defined. Let's begin with spatial translations.

1 Spatial Translations

Perhaps the simplest transformation is translation in space. Classically, this just means moving a particle from one point in space to another. Quantum mechanically, this corresponds to an operator that takes a state and shifts it by some amount in space. This operator must involve a parameter which tells us how much to shift by. Thus we define the *translation operator* $T(a)$, where a is the amount of displacement. Its action is defined by how it acts on eigenstates of position. In one dimension, it is simply defined by

$$T(a)\,|x\rangle = |x+a\rangle$$

This makes sense – the translation operator (by an amount a) takes a position eigenstate peaked somewhere in x, and turns it into one peaked at $x+a$. But what does this operator do to *states*? That is to say, what is $T(a)\,|\psi\rangle$ for some state $|\psi\rangle$ that is not a position eigenstate?

Well, before acting with $T(a)$, we have the state $|\psi\rangle$ with position-space wavefunction $\psi(x) = \langle x|\psi\rangle$. After acting with $T(a)$, we have some new state $|\phi\rangle = T(a)\,|\psi\rangle$ with position-space wavefunction $\phi(x) = \langle x|\phi\rangle$. So this amounts to figuring out the relationship between $\psi(x)$ and $\phi(x)$. We have

$$\phi(x) \equiv \langle x|\phi\rangle = \langle x|\,T(a)\,|\psi\rangle = \int dx'\,\langle x|\,T(a)\,|x'\rangle\,\langle x'|\psi\rangle = \int dx'\,\langle x|x'+a\rangle\,\langle x'|\psi\rangle \quad (1)$$

$$= \int dx'\delta(x-x'-a)\psi(x') = \psi(x-a) \quad (2)$$

where we have inserted a complete set of position eigenstates, used the definition of $T(a)$ on position eigenstates, used Dirac orthogonality of position eigenstates, and integrated. Thus we find

$$\phi(x) = (T(a)\psi)(x) = \psi(x-a)$$

This might seem a little counterintuitive – $T(a)$ shifted position eigenstates via $|x\rangle \to |x+a\rangle$, but shifts wavefunctions via $\psi(x) \to \psi(x-a)$. But ultimately this

makes sense – the minus sign is necessary to get a wavefunction that translates forward under displacement. The intuition is that the value of the new wavefunction at the new point is equal to the value of the old wave funciton at the old point.

A variety of properties of the translation operator follow from our definition, including

$$T(0) = 1 \tag{3}$$
$$T(a)T(b) = T(a+b) = T(b)T(a) \tag{4}$$
$$T(a)^{-1} = T(-a) \tag{5}$$
$$T(a)^{-1} = T(a)^\dagger \tag{6}$$

This last property tells us that the translation operator is unitary, which means $T(a)^\dagger T(a) = 1$ – this implies that it preserves probability, which it must to have a sensible interpretation in quantum mechanics. That is, if you have a normalized state $|\psi\rangle$ such that $\langle\psi|\psi\rangle = 1$, then the translated state $T(a)\,|\psi\rangle$ is also normalized, since

$$\langle T(a)\psi|T(a)\psi\rangle = \big\langle\psi\big|T(a)^\dagger T(a)\psi\big\rangle = \langle\psi|\psi\rangle = 1$$

But note that $T(a)$ is not *Hermitian*, so it is not itself an observable. This will turn out to be a general property of the transformation operators we encounter in the next few lectures that reveal the symmetries of quantum mechanics – they are unitary, and so preserve probabilities, but not Hermitian.

This last property is also the key to remembering that $T(a)\,|x\rangle = |x+a\rangle$ but $T(a)\psi(x) = \psi(x-a)$ – in the latter definition, we can think of $T(a)$ as acting to the left in $T(a)\psi(x) = \langle x|T(a)\psi\rangle$, i.e.

$$T(a)\psi(x) = \langle x|T(a)\psi\rangle = \big\langle T(a)^\dagger x\big|\psi\big\rangle = \langle T(-a)x|\psi\rangle = \langle x-a|\psi\rangle = \psi(x-a)$$

Although we will not make much use of it here, the translation operator in one dimension generalizes naturally to three dimensions. Now the operator is labeled by three parameters (the translations in x, y, z), which we can write as a vector $\vec{a}$, and the operator is defined by

$$T(\vec{a})\,|\vec{r}\rangle = |\vec{r}+\vec{a}\rangle$$

2 Generating Spatial Translations

Now let's focus on another consequence of the properties we just discussed. The property

$$T(a+b) = T(a)T(b)$$

means that we can build up larger translations by acting with multiple smaller ones. We can take this to the natural conclusion, namely that any finite translation can be built up out of infinitely many infinitesimal translations. As it turns out, in quantum mechanics the infinitesimal versions of unitary symmetry transformations can be expressed in terms of certain Hermitian operators – ones we have already encountered during our adventures in quantum mechanics. Because a finite symmetry transformation can be built out of the composition of many infinitesimal ones involving Hermitian operators, we call these operators *generators* of the symmetry. They "generate" the transformations of interest, as least infinitesimally.

This is perhaps easiest to see for spatial translations. Consider translation by some tiny distance a. In this case, we can imagine Taylor expanding $T(a)$ in small a around $a = 0$. This is just the form of a normal Taylor expansion,

$$T(a) = T(0) + a \left.\frac{dT(a)}{da}\right|_{a=0} + \dots$$

We know the first term is $T(0) = 1$, and the second term does not itself depend on a (because it is evaluated at a specific point, $a = 0$). Thus it must be some operator with no free parameters. Let's call this operator $\hat{k}$, where we will try to remember to explicitly use the hat to denote an operator. Right now we don't know what $\hat{k}$ is, but as we will see, it is something we have seen before. We'll define $\hat{k}$ with a factor of i, i.e.

$$\hat{k} \equiv i \left.\frac{dT(a)}{da}\right|_{a=0}$$

The factor of i guarantees that $\hat{k}$ is Hermitian, since $T(a) = 1 - ia\hat{k} + \dots$ and so

$$T(a)^\dagger = 1 + ia\hat{k}^\dagger + \dots = T(-a) = 1 + ia\hat{k} + \dots$$

which tells us $\hat{k} = \hat{k}^\dagger$. As a Hermitian operator that translates states by an infinitesimal amount, $\hat{k}$ is a generator of spatial translations in one dimension.

We have only written out the first two terms in the Taylor expansion of $T(a)$, but we can sum the entire series into a simple form. Recall the definition of the derivative as a limit,

$$\frac{dT(a)}{da} = \lim_{\epsilon\to 0}\frac{T(a+\epsilon)-T(a)}{\epsilon} = \lim_{\epsilon\to 0}\frac{T(\epsilon)T(a)-T(a)}{\epsilon} = \left[\lim_{\epsilon\to 0}\frac{T(\epsilon)-1}{\epsilon}\right]T(a)$$

We recognize the limit term in brackets as the definition of the derivative evaluated at $a = 0$, i.e.

$$\lim_{\epsilon\to 0}\frac{T(\epsilon)-1}{\epsilon} = \left.\frac{dT(a)}{da}\right|_{a=0} = -i\hat{k}$$

and so from this we can conclude

$$\frac{dT(a)}{da} = -i\hat{k}T(a)$$

This is just a simple first-order ODE, and we know the boundary condition $T(0) = 1$, so we can integrate to find

$$T(a) = \exp\left[-ia\hat{k}\right]$$

The exponential of an operator is really formally defined in terms of its Taylor series,

$$T(a) = 1 - ia\hat{k} - \frac{1}{2}a^2\hat{k}^2 + \ldots$$

and we see that a general translation by a can, indeed, be built up by acting repeatedly with the generator $\hat{k}$.

Now we can figure out what $\hat{k}$ does to states in Hilbert space. Here it is clearest to work in position space, and act directly on position-space eigenstates $\psi(x)$. We have

$$\hat{k}\psi(x) = i\left(\frac{dT(a)}{da}\psi\right)(x)\bigg|_{a=0} = i\frac{d}{da}\psi(x-a)\bigg|_{a=0} = -i\frac{d}{dx}\psi(x)$$

If that last step lost you, just think of doing the derivative by changing variables to $y = x - a$, so $d/da = -d/dy$.

Thus we conclude in position space, $\hat{k}$ is represented by $-i\frac{d}{dx}$. But this looks familiar! Indeed,

$$\hbar\hat{k} = -i\hbar\frac{d}{dx} = \hat{p}$$

From this we could simply go back to write

$$T(a) = \exp\left[-ia\hat{p}/\hbar\right]$$

and conclude that *momentum is the generator of spatial translations.*

3 Transforming Operators

Thus far have defined our first transformation operator, corresponding to spatial translations, seen how it acts on states, and observed that momentum is the generator of translations. But our ultimate goal is to use transformations to reveal the symmetries of a quantum system. Although we could figure this out by looking at how transformations act on all of the eigenstates of an operator, it is much easier to relate the transformations to the operators themselves.

The key idea here is to recognize that we have chosen to define observables (like expectation values) by having operators act on states, while the operators are themselves fixed. But, remarkably, we could arrive at equivalent physical conclusions by treating the states as fixed, and have the operators act on each other. For example, consider being in a state $|\psi\rangle$, and acting on the state with the transformation operator $T(a)$, so $|\psi\rangle \to |T(a)\psi\rangle$. Then the expectation value of some operator $\mathcal{O}$ in the transformed state would simply be

$$\langle T\psi| \mathcal{O} |T\psi\rangle = \langle\psi| T^\dagger \mathcal{O} T |\psi\rangle$$

We would get the same answer for the expectation value by imagining that we had not changed the state at all, but instead changed the operator

$$\mathcal{O} \to T^\dagger \mathcal{O} T$$

The two transformations (on states, defined by $|\psi\rangle \to T|\psi\rangle$, and on operators, defined by $\mathcal{O} \to T^\dagger \mathcal{O} T$) are equivalent, and correspond to active transformations (shifting the state over some distance) or passive transformations (leaving the state in place but shifting the coordinate system in the opposite direction).

By studying how transformations act on operators, we are now in a position to see how transformations relate to the symmetries of a system. In the case of spatial transformations, it is possible for operators to be unaffected by a translation,

$$T^\dagger \mathcal{O} T = \mathcal{O}$$

The most interesting such operator is, of course, the Hamiltonian, since the Hamiltonian is the operator that determines the dynamics of a system. If a Hamiltonian is unaffected by a translation,

$$T^\dagger H T = H$$

then the system is *translationally invariant*; the energy eigenstates don't change if the system is translated. Note that since $T^\dagger = T^{-1}$, we have

$$T^\dagger HT = H \rightarrow HT = TH \rightarrow [H, T] = 0$$

For physical systems in one dimension, translational invariance implies $V(x) = V(x + a)$. There are two classes of interesting translational invariance: those with *continuous* translational symmetry where $V(x) = V(x + a)$ for any a, which are boring (the potential is simply flat), and those with *discrete* translational symmetry, for which $V(x) = V(x + a)$ only for discrete choices of a. Each case has some remarkable physical consequences, though we will only discuss the continuous case today.

4 Conservation Laws

In the case of a continuous symmetry, $[H, T(a)] = 0$ for any a, including infinitesimal ones. For a tiny translation $a = \epsilon$, we have $T(\epsilon) \approx 1 - i\epsilon\hat{p}/\hbar$. Then

$$[H, T(\epsilon)] = 0 \rightarrow [H, p] = 0$$

So a Hamiltonian that is translationally invariant commutes with the momentum operator. And as you learned in 115A, the expectation value of any operator that commutes with the Hamiltonian must be constant in time. This follows from the generalized version of Ehrenfest's theorem,

$$\frac{d}{dt}\langle \mathcal{O} \rangle = \frac{i}{\hbar} \langle [H, \mathcal{O}] \rangle$$

(here we are assuming that $\mathcal{O}$ is not itself a function of time, as is the case for most operators of interest). If the expectation values are constant, we say the quantity is conserved. Thus we see that *translational invariance (a symmetry) implies momentum conservation*. This is the simplest example of symmetries implying conservation laws. Since expectation values are classical quantities (they are independent of $\hbar$), this immediately shows us how classical conservation of momentum arises from translational invariance, and that at the quantum level it corresponds to $[H, T(a)] = 0$ for any a.

Note that the constancy of expectation values is apparently not as strong as the classical statement of conservation – classical conservation of momentum, for example, means that the momentum is the same before and after the dynamics of interest.

Quantum mechanically, it might seem possible for the likelihood of obtaining certain values of the momentum could change before and after the dynamics of interest, as long as the expectation value is constant.

However, we can make a stronger statement of conservation in quantum mechanics: if an operator $\mathcal{O}$ commutes with the Hamiltonian, then not only is its expectation value independent of time, but also the probability for obtaining any specific eigenvalue is independent of time. To see this, consider the eigenstates $|f_n\rangle$ of the operator $\mathcal{O}$, with eigenvalues λ_n (for simplicity, let's consider an operator with discrete spectrum and no degeneracies, though the result holds more generally). If we are in a state $\Psi(t)$, the probability of getting a specific eigenvalue λ_n is of course

$$P(\lambda_n) = |\langle f_n|\Psi(t)\rangle|^2$$

Now can always decompose $\Psi(t)$ in terms of eigenstates $|\psi_m\rangle$ of H,

$$|\Psi(t)\rangle = \sum_m e^{-iE_m t/\hbar} c_m |\psi_m\rangle$$

so that

$$P(\lambda_n) = \left|\sum_m e^{-iE_m t/\hbar} c_m \langle f_n|\psi_m\rangle\right|^2$$

But if $\mathcal{O}$ and H commute, we can pick a simultaneous set of eigenstates for the two. In this basis, $|f_n\rangle = |\psi_n\rangle$, so we simply have

$$P(\lambda_n) = \left|\sum_m e^{-iE_m t/\hbar} c_m \langle \psi_n|\psi_m\rangle\right|^2 = |c_n|^2$$

which is independent of time. So for the quantum mechanical version of conservation laws, an operator commuting with the Hamiltonian has both constant expectation values in any state, and the probability that a measurement yields a given eigenvalue is independent of time.

5 Parity

Now let's turn to our next interesting spatial transformation: *parity*. Parity transformations implement the operation of *spatial inversion*, which inverts vectors through the origin. In one dimension, this amounts to taking $x \to -x$. In three dimensions,

it corresponds to $\vec{r} \to -\vec{r}$. Although this is a relatively simple transformation, it can have powerful implications.

As with spatial translations, we can define the parity operator $\hat{\Pi}$ by how it acts on position eigenstates. To implement spatial inversions, in one dimension we should have

$$\Pi |x\rangle = |-x\rangle$$

The action on wavefunctions is then clear: if we have $|\phi\rangle = \Pi |\psi\rangle$, then

$$\phi(x) = \langle x|\phi\rangle = \langle x| \Pi |\psi\rangle = \int dx' \langle x| \Pi |x'\rangle \langle x'|\psi\rangle = \int dx' \langle x|-x'\rangle \langle x'|\psi\rangle \tag{7}$$

$$= \int dx' \delta(x' + x)\psi(x') = \psi(-x) \tag{8}$$

From this we conclude that

$$\Pi\psi(x) = \psi(-x)$$

Several properties follow immediately. Clearly, Π is its own inverse, since

$$\Pi^2\psi(x) = \Pi\psi(-x) = \psi(x) \to \Pi^2 = 1 \to \Pi^{-1} = \Pi$$

Moreover, Π must be unitary, since

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\psi(x) = \int_{\infty}^{-\infty} d(-x)\, \psi^*(-x)\psi(-x) \tag{9}$$

$$= \int_{-\infty}^{\infty} dx\, [\Pi\psi(x)]^*[\Pi\psi(x)] = \langle\psi| \Pi^\dagger\Pi |\psi\rangle \to \Pi^\dagger\Pi = 1 \tag{10}$$

These two properties then imply that Π is also Hermitian (unlike translations $T(a)$), since

$$\Pi^2 = 1 = \Pi^\dagger\Pi \to \Pi^\dagger = \Pi^{-1} = \Pi$$

In position space, the eigenstates of parity are simply even and odd functions of x. This is because, since $\Pi^2 = 1$, its eigenvalues must be ± 1 (exactly as we showed for the permutation operator). The corresponding eigenstates $\psi(x)$ are ones for which

$$\Pi\psi(x) = \pm\psi(x) = \psi(-x)$$

where the first equality uses the definition of the eigenstates with eigenvalues ± 1, and the second uses the definition of Π.

Just as it was useful to think about translations acting on operators, we can think about how parity transformations act on operators; in this case operators transform as

$$\mathcal{O} \to \Pi^\dagger \mathcal{O} \Pi$$

As you will show on the homework, both the position and momentum operators are odd under parity, i.e.

$$\hat{x} \to \Pi^\dagger \hat{x} \Pi = -\hat{x} \qquad \hat{p} \to \Pi^\dagger \hat{p} \Pi = -\hat{p}$$

and from this we can figure out how any operator in one dimension transforms by writing it in terms of $\hat{x}$ and $\hat{p}$.

A system is symmetric under inversions *if* the Hamiltonian is invariant under a parity transformation, in which case

$$H \to \Pi^\dagger H \Pi = H$$

which (because Π is unitary) corresponds to

$$[H, \Pi] = 0$$

In one dimension, the kinetic term is automatically parity invariant, so invariance of the Hamiltonian corresponds to potentials that are even in x,

$$V(-x) = V(x)$$

and parity is conserved.

As you already learned in 115A, the eigenstates of a 1d Hamiltonian with an even potential can be taken to be either even or odd in x. Now we have a more systematic way of understanding this statement: if $V(x)$ is even, then $[H, \Pi] = 0$ and we can choose a simultaneous set of eigenstates of the two operators, namely even or odd functions of x.

This all generalizes naturally to three dimensions, where

$$\Pi \left|\vec{r}\right\rangle = \left|-\vec{r}\right\rangle$$

and so

$$\Pi \psi(\vec{r}) = \psi(-\vec{r})$$

As in one dimension, the operators $\vec{r}$ and $\vec{p}$ are odd under parity transformations. From this it follows that $\vec{L}$ is even under parity, since

$$\vec{L} = \vec{r} \times \vec{p} \to \Pi^\dagger \vec{L} \Pi = (-\vec{r}) \times (-\vec{p}) = \vec{r} \times \vec{p} = \vec{L}$$

(You might also wonder what parity does to intrinsic spin, i.e. what happens to $\vec{S}$ under parity. The answer is that, as another form of angular momentum, $\vec{S}$ is also even under parity. Eigenstates of spin operators can be taken to be either even or odd, and are fixed for various particles only when relativity is taken into account.)

Parity is particularly interesting for spherically symmetric potentials, since for these

$$V(\vec{r}) = V(r) = V(-\vec{r})$$

which means they have inversion symmetry. As such, parity is again conserved, and the eigenstates of the Hamiltonian can be chosen to be simultaneous eigenstates of parity. As you will show on the problem set, the eigenstates for a central potential are eigenstates of parity with

$$\Pi \psi_{n,\ell,m}(r,\theta,\phi) = (-1)^\ell \psi_{n,\ell,m}(r,\theta,\phi)$$

This is the three-dimensional analogue of parity-even and parity-odd states for spherically symmetric potentials; states with even ℓ are parity even, and states with odd ℓ are parity odd. This turns out to have magnificently powerful implications, giving rise to *parity selection rules*. In general, *selection rules* tell you that certain matrix elements vanish due to the symmetries of the theory, without even requiring an explicit calculation.

A particularly relevant example is the electric dipole moment operator,

$$\vec{d_e} = q\vec{r}$$

This is odd under parity. As you will learn in 115C, this operator is very interesting because it is involved in transitions between atomic energy levels. Such transitions occur because an electron in some energy level emits or absorbs a photon, ending up in a different energy level. The probability for such a transition to occur is proportional to the square of the matrix element of the dipole operator, i.e. the rate for transitions between states $|n,\ell,m\rangle$ and $|n',\ell',m'\rangle$ is proportional to the square of

$$\langle n',\ell',m'| \, \vec{d_e} \, |n,\ell,m\rangle$$

If you tried to calculate these explicitly, it would involve doing many painful integrals, and you would find that most of your answers were zero. Any time you get zero in physics, there is usually a symmetry at play, and in this case it is parity. To see this, note that

$$\langle n', \ell', m' | \, \vec{d}_e \, | n, \ell, m \rangle = - \langle n', \ell', m' | \, \Pi^\dagger \vec{d}_e \Pi \, | n, \ell, m \rangle = - \langle n', \ell', m' | \, (-1)^{\ell'} \vec{d}_e (-1)^{\ell} \, | n, \ell, m \rangle \quad (11)$$

$$= (-1)^{\ell + \ell' + 1} \langle n', \ell', m' | \, \vec{d}_e \, | n, \ell, m \rangle \quad (12)$$

But if $\ell + \ell'$ is even, this implies that $\langle n', \ell', m' | \, \vec{d}_e \, | n, \ell, m \rangle = 0$. Lo and behold, parity tells you that matrix elements of the electric dipole moment operator vanish unless $\ell + \ell'$ is odd. Selection rules are powerful!

6 Rotational Symmetry

There is one more spatial transformation of interest: rotations. Rather than developing the operator picture of rotations in one fell swoop, I would like to build up intuition based on how rotations act on 3-vectors, then make the appropriate generalization to states.

You are hopefully familiar with how to rotate vectors in three Euclidean dimensions. A 3-vector can be rotated by an angle θ about the x, y, or z axes by acting on it with rotation matrices

$$R_x(\theta_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_x & -\sin\theta_x \\ 0 & \sin\theta_x & \cos\theta_x \end{pmatrix} \quad (13)$$

$$R_y(\theta_y) = \begin{pmatrix} \cos\theta_y & 0 & \sin\theta_y \\ 0 & 1 & 0 \\ -\sin\theta_y & 0 & \cos\theta_y \end{pmatrix} \quad (14)$$

$$R_z(\theta_z) = \begin{pmatrix} \cos\theta_z & -\sin\theta_z & 0 \\ \sin\theta_z & \cos\theta_z & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (15)$$

We could make a more general rotation in three dimensions about an arbitrary axis by multiplying these three matrices together, with respective angles $\theta_x, \theta_y, \theta_z$, keeping in mind that the order matters, i.e. a rotation by an angle θ around an axis $\hat{n}$ can be written as

$$R(\hat{n}, \theta) = R_x(\theta_x) R_y(\theta_y) R_z(\theta_z)$$

In the language of quantum mechanics, such a rotation is clearly a matrix representation of a rotation operator acting on position vectors $\vec{r}$.

Now consider doing a rotation around the axis $\hat{n}$ by only an infinitesimal angle, so that $\theta_x, \theta_y, \theta_z$ are tiny. A matrix implementing this infinitesimal rotation can be written as

$$R_\epsilon(\hat{n}, \theta) = 1 + \theta_x \mathcal{L}_x + \theta_y \mathcal{L}_y + \theta_z \mathcal{L}_z$$

where

$$\mathcal{L}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \mathcal{L}_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad \mathcal{L}_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{16}$$

We arrive at these matrices just by Taylor expanding the $R_{x,y,z}$ matrices above in small θ. An equivalent way to write this infinitesimal rotation is as

$$R_\epsilon(\hat{n}, \theta) = I + \theta\, \hat{n} \cdot \vec{\mathcal{L}}$$

where $\theta \hat{n} = \vec{\theta} \equiv (\theta_x, \theta_y, \theta_z)$, so $\theta = |\vec{\theta}|$ and $\hat{n} = \vec{\theta}/|\vec{\theta}|$.

When discussing translations, we noted that an infinitesimal translation could be *generated* by a Hermitian operator with no free parameters, and this generator could be exponentiated to give an arbitrarily large translation. The same logic applies here: a rotation by a larger angle can be obtained by exponentiating infinitesimal rotations. Exponentiating the above, we can write a rotation by a larger angle θ around the axis $\hat{n}$ as

$$R(\hat{n}, \theta) = e^{\theta \hat{n} \cdot \vec{\mathcal{L}}}$$

But note that the operators $\mathcal{L}_{x,y,z}$ are not Hermitian – in fact, they are anti-hermitian (flipping sign under Hermitian conjugation). So to make the analogy with translations more precise, let us instead parameterize our infinitesimal rotations in terms of Hermitian matrices, which we can get by multiplying the above matrices by i. With some malice aforethought, let's scale them by an additional factor of $\hbar$, so that our generators are

$$L_x = i\hbar \mathcal{L}_x \qquad L_y = i\hbar \mathcal{L}_y \qquad L_z = i\hbar \mathcal{L}_z$$

Then our general rotation by an angle θ around the axis $\hat{n}$ in three dimensions is

$$R(\hat{n}, \theta) = \exp\left[-\frac{i\theta}{\hbar} \hat{n} \cdot \vec{L} \right] \tag{17}$$

Now our choice of notation brings to mind angular momentum. We know the matrices L_x, L_y, L_z, so we can go ahead and compute their commutators. Lo and behold, we have

$$[L_x, L_y] = i\hbar L_z \qquad [L_y, L_z] = i\hbar L_x \qquad [L_z, L_x] = i\hbar L_y$$

which are precisely the commutators of the angular momentum operators.

To arrive at this conclusion, we started with a classical problem, thinking about rotations as matrices acting on vectors in a particular basis. In this case, the vector was represented in terms of basis vectors $\hat{x}, \hat{y}, \hat{z}$. Having done so, the natural way to get to quantum mechanics is to promote these matrices to operators, in which the $\vec{L}$ are truly the angular momentum operators. The difference, of course, is that the operators $\vec{L}$ in quantum mechanics are not necessarily 3×3 matrices.

Unsurprisingly, the rotation operators $\hat{R}$ are unitary, in the sense that $\hat{R}^\dagger \hat{R} = 1$ (as you can check, and in fact showed generally on the problem set for complex exponentials of Hermitian operators). Working again in the language of passive transformations, we can classify various operators in quantum mechanics depending on what happens to them under rotations. Those left invariant under rotations are called *scalar operators*, and are ones for which

$$\mathcal{O}_s \to \hat{R}^\dagger \mathcal{O}_s \hat{R} = \mathcal{O}_s$$

For an infinitesimal rotation, this implies

$$[\vec{L}, \mathcal{O}_s] = 0$$

for scalar operators.

But we can also begin to classify operators that are *not* invariant by how they transform. The next simplest case are operators who transform "like a vector". This means the operator is really a vector of operators $\mathcal{O}_v = \vec{V}$, whose components transform as

$$V_i \to \hat{R}^\dagger V_i \hat{R} = \sum_j R_{ij} V_j$$

The first bit is just the rule for the transformation of the operator; the last equality says this transformation takes the form of the rotation of a vector, where R_{ij} is the 3×3 matrix corresponding to the rotation R. For an infinitesimal transformation we have

$$\hat{R} = 1 - \frac{i\epsilon}{\hbar} \hat{n} \cdot \vec{L},$$

so the above transformation is of the form

$$V_i \to V_i + \frac{\epsilon}{i\hbar}[V_i, \hat{n} \cdot \vec{L}] = \sum_j R_{ij}(\hat{n}, \epsilon) V_j$$

To see what this implies, let's take (say) $\hat{n} = \hat{z}$. Then, as we found last lecture, the matrix on the RHS is of the form

$$R(\hat{z}, \epsilon) = I + \epsilon \mathcal{L}_z$$

where

$$\mathcal{L}_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Again, to be definite, let's also consider (say) $i = x$. Putting it all together, our equation is

$$V_x + \frac{\epsilon}{i\hbar}[V_x, L_z] = V_x - \epsilon V_y$$

hence

$$[L_z, V_x] = i\hbar V_y$$

Interestingly, this means that the commutator of V_x with L_z is structurally similar to the commutator of L_x with L_z. Indeed, repeating the exercise for different choices of component i and rotation axis $\hat{n}$, the general rule is that a vector operator $\vec{V}$ is one whose commutators with $\vec{L}$ are the same as $\vec{L}$ itself, i.e. operators $\vec{V}$ such that

$$[L_x, V_y] = i\hbar V_z \qquad [L_y, V_z] = i\hbar V_x \qquad [L_z, V_x] = i\hbar V_y$$

These *vector* operators include $\vec{r}$, $\vec{p}$, and $\vec{L}$ itself. You will further refine this classification using transformation under parity on the problem set.

As with translational invariance, we can work out which conservation law follows from rotational invariance of the Hamiltonian. The operator p^2 is a scalar operator, and so rotationally invariant. In general $V(\vec{r})$ is only rotationally invariant for spherically symmetric potentials, $V(\vec{r}) = V(r)$. In that case,

$$[H, R(\hat{n}, \theta)] = 0$$

and for infinitesimal rotations this corresponds to

$$[H, \vec{L}] = 0$$

From the generalized Ehrenfest's theorem, we see that

$$\frac{d}{dt}\langle \vec{L} \rangle = 0$$

for such Hamiltonians, from which we conclude that *angular momentum conservation is a consequence of rotational invariance.*

7 Time translations

Finally, in addition to our spatial transformations, there is one more interesting transformation to consider: translations in time. Given the Schrödinger equation,

$$H\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$$

we can formally "solve" the equation by treating H as a number and integrating both sides:

$$\int \frac{d\Psi}{\Psi} = -\frac{iH}{\hbar}\int dt \Rightarrow \Psi(x,t) = e^{-iHt/\hbar}\Psi(x,0)$$

Formally, the exponential of an operator is defined through its Taylor series. Obviously this is only possible if H is independent of time, but this is the case for most scenarios of interest (and almost all that can be solved in closed form).

You can check that this proposed solution works by plugging it back in to the SE:

$$He^{-iHt/\hbar}\Psi(x,0) = i\hbar\left(\frac{\partial}{\partial t}e^{-iHt/\hbar}\right)\Psi(x,0) = He^{-iHt/\hbar}\Psi(x,0)$$

We can identify the exponential of the Hamiltonian with a unitary operator,

$$U(t) = \exp\left[-iHt/\hbar\right]$$

and have seen that this operator generates time translations, in the sense that

$$\Psi(x,t) = U(t)\Psi(x,0)$$

Thus we say that the Hamiltonian is the generator of time translations. In fact, you can think of the Schrödinger equation as a *consequence* of this statement. That is, Taylor expanding $U(t+dt)$ for small dt tells us

$$U(t+dt) = U(t)(1 - \frac{i}{\hbar}Hdt) \rightarrow \frac{U(t+dt)-U(t)}{dt} = -\frac{i}{\hbar}HU(t) \rightarrow i\hbar\frac{d}{dt}U(t) = HU(t)$$

From this, the Schrödinger equation itself follows immediately:

$$i\hbar\frac{d}{dt}\Psi(x,t) = i\hbar\frac{d}{dt}U(t)\Psi(x,0) = HU(t)\Psi(x,0) = H\Psi(x,t)$$

so one can think of the Schrödinger equation as simply following from the statement that the Hamiltonian generates time translations. There is a reasonable argument for teaching you quantum mechanics this way from the beginning!

Although our discussion has assumed H is independent of time, the Hamiltonian remains the generator of time translations even when it is itself time-dependent. The unitary operator becomes more complicated,

$$U(t) = \hat{T}\exp\left[-\frac{i}{\hbar}\int_0^t dt' H(t')\right]$$

where $\hat{T}$ denotes time-ordering of the terms in the Taylor expansion of the exponential. But the basic physical picture still holds.

8 Heisenberg Picture

Just as we moved from considering spatial transformations acting on states to spatial transformations acting on operators, we can do the same for time translations. This actually transforms us from a picture of quantum mechanics in which the states depend on time and the operators are time-independent, to one in which the operators are time-dependent and the states are fixed. This is known as the *Heisenberg picture*, where the states are defined via

$$|\Psi_H(t)\rangle = U_S^\dagger(t)|\Psi_S(t)\rangle = |\Psi_S(0)\rangle$$

where I am attaching the subscript S to all of the statements in our usual picture, which is known as the *Schrödinger picture*. In the last step we have used unitarity of U_S. Requiring expectation values (which are observables) to be unchanged by this definition tells us how the operators must transform,

$$\langle\Psi_S(t)|\mathcal{O}_S|\Psi_S(t)\rangle = \langle\Psi_S(0)|e^{iHt/\hbar}\mathcal{O}_S e^{-iHt/\hbar}|\Psi_S(0)\rangle = \langle\Psi_H|e^{iHt/\hbar}\mathcal{O}_S e^{-iHt/\hbar}|\psi_H\rangle$$

This suggests we should define operators in the Heisenberg picture as

$$\mathcal{O}_H = e^{iHt/\hbar}\mathcal{O}_S e^{-iHt/\hbar}$$

so that expectation values are equivalent in the two pictures. The time-variation of expectation values in this picture is now given by

$$\frac{d}{dt}\mathcal{O}_H = \frac{de^{iHt/\hbar}}{dt}\mathcal{O}_S e^{-iHt/\hbar} + e^{iHt/\hbar}\mathcal{O}_S\frac{de^{-iHt/\hbar}}{dt} \tag{18}$$

$$= \frac{i}{\hbar}\left(e^{iHt/\hbar}H\mathcal{O}_S e^{-iHt/\hbar} - e^{iHt/\hbar}\mathcal{O}_S H e^{-iHt/\hbar}\right) = \frac{i}{\hbar}[H, \mathcal{O}_H] \tag{19}$$

which is in precise agreement with our results in the Schrödinger picture, though here the time evolution is associated with the operators rather than the states.

Although it's not obvious that this picture is particularly better than the Schrödinger picture for nonrelativistic quantum mechanics, it turns out to be the natural framework for relativistic settings, and hence quantum field theory.

9 Time translation invariance

As with our spatial transformations, we can now describe operators that are time-translation invariant. Time-translation invariant operators are those for which

$$\mathcal{O} \to e^{iHt/\hbar}\mathcal{O}e^{-iHt/\hbar} = \mathcal{O}$$

For infinitesimal transformations, this amounts to

$$[H, \mathcal{O}] = 0$$

The most notable choice is $\mathcal{O} = H$ itself, for which we conclude that the conservation of energy follows from time-translation invariance as long as H itself is independent of time. Note that if H did depend on time, then this would no longer hold in general.

10 Symmetry and degeneracy

We have spent the last few lectures discussing the role of symmetry in quantum mechanics and its connection to conservation laws. Let's now bring the course to a close by revisiting one of the first things we discussed in 115B: degeneracy. If you recall, in 115A you learned that there are no distinct, normalizable energy eigenstates with the same energy in one dimension. We began our discussion of three-dimensional

quantum mechanics in 115B with the observation that this is no longer true, and in fact have observed a whole host of degenerate energy eigenstates – the most famous being the n^2-degenerate energy eigenstates $\psi_{n,\ell,m}$ of the hydrogen atom.

We are now in a position to understand where these degeneracies came from: symmetry. As we have seen, a symmetry of a quantum mechanical system implies there is an operator $\mathcal{O}$ that commutes with the Hamiltonian,

$$[\mathcal{O}, H] = 0$$

Among other things, this implies that if we have an energy eigenstate ψ_n of the Hamiltonian H with energy E_n (i.e., $H|\psi_n\rangle = E_n|\psi_n\rangle$), then the state $\mathcal{O}\psi_n$ is also an energy eigenstate with energy E_n:

$$H(\mathcal{O}|\psi_n\rangle) = \mathcal{O}H|\psi_n\rangle = E_n(\mathcal{O}|\psi_n\rangle)$$

Now, this does not necessarily imply degeneracy, which occurs when there are multiple *distinct* states with the same energy. It could well be the case that $|\psi_n\rangle$ and $\mathcal{O}|\psi_n\rangle$ are actually the same state.

In fact, that is always the case if there is only one operator $\mathcal{O}$ involved in the symmetry in question – $|\psi_n\rangle$ and $\mathcal{O}|\psi_n\rangle$ are actually the same state and there is no degeneracy. The reason is that $[\mathcal{O}, H] = 0$ and so the two operators share a common basis of eigenstates. Then $\mathcal{O}|\psi_n\rangle = \lambda_n|\psi_n\rangle$ (where λ_n is the eigenvalue w.r.t $\mathcal{O}$), the same state (up to a scaling) as $|\psi_n\rangle$.

But we *do* obtain degeneracies if there are multiple operators $\mathcal{O}_i$ generating the symmetry, provided they do not all commute with each other. The simplest example is rotational symmetry, which we now know is generated by the angular momentum operators L_x, L_y, and L_z. Since they do not commute with each other, there is not a complete set of simultaneous eigenstates of H and L_x, L_y, L_z (even if H commutes with each L_i). Therefore there must be some states $L_i|\psi_n\rangle \neq |\psi_n\rangle$ with the same energies.

For example, given the hydrogen energy eigenstate $|2,1,0\rangle$, we have

$$L_+|2,1,0\rangle = (L_x + iL_y)|2,1,0\rangle = \sqrt{2}\hbar|2,1,1\rangle$$

which has the same principle number n and hence the same energy, but is orthogonal.

Thus we learn the general lesson that symmetries generated by multiple non-commuting operators will lead to energy degeneracies. This does not generally occur in 1 dimension but certainly occurs in 3 dimensions (due to rotational symmetry), explaining the emergence of degeneracy as we go to higher dimensions.