Symmetry and Degeneracy

Notes for PHYS 4702 Intro Quantum Mechanics II

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These notes are meant to complement the discussion in Modern Quantum Mechanics Third Edition, Section 4.1. Equation references are to those in that textbook.

Symmetry Operators

Consider some unitary operator $\mathcal{S}$ which turns an arbitrary state $|\alpha\rangle$ into a different state $|\beta\rangle$. That is, $\mathcal{S}|\alpha\rangle = |\beta\rangle$ which of course implies that $\langle\beta| = \langle\alpha|\mathcal{S}^\dagger$. We refer to $\mathcal{S}$ as a "symmetry operator", or just "symmetry", if the expectation value of the Hamiltonian H is the same for $|\alpha\rangle$ and $|\beta\rangle$. In other words

$$\langle\alpha|H|\alpha\rangle = \langle\beta|H|\beta\rangle = \langle\alpha|\mathcal{S}^\dagger H\mathcal{S}|\alpha\rangle$$

Since $|\alpha\rangle$ is arbitrary, this means that H is unchanged by what mathematicians call a "similarity transformation" based on $\mathcal{S}$, that is

$$\mathcal{S}^\dagger H\mathcal{S} = H \qquad \text{so} \qquad H\mathcal{S} = \mathcal{S}H$$

and the two operators commute. This should jive with your intuition about what a "symmetry" should mean. Different Hamiltonians, of course, are likely to have different, if any, symmetries.

Conserved Quantities

In classical mechanics, you learned that a symmetry of the Hamiltonian (or Lagrangian) implied that there was some conserved quantity associated with it. That wasn't so easy to prove, but it is simple to prove in quantum mechanics.

A measurable quantity in quantum mechanics corresponds to some Hermitian operator. Consider the case of a continuous symmetry $\mathcal{S} = \mathcal{S}(\lambda)$ where λ is some continuous parameter. Then you know that we can associate a Hermitian operator G, called the "generator", with the unitary operator $\mathcal{S}$ using Weyl's trick, namely

$$\mathcal{S}(d\lambda) = 1 - \frac{i}{\hbar}G\,d\lambda$$

where $d\lambda$ is infinitesimal. Therefore the similarity transformation implies that

$$\left(1 + \frac{i}{\hbar}G\,d\lambda\right) H \left(1 - \frac{i}{\hbar}G\,d\lambda\right) = H + \frac{i}{\hbar}(GH - HG)d\lambda = H \qquad \text{so} \qquad [G, H] = 0$$

Recalling the Heisenberg Equation of Motion (2.93) for observables in the Heisenberg picture, namely

$$\frac{dG}{dt} = \frac{1}{i\hbar}[G, H]$$

it is clear that the observables associated with the generator of a symmetry operator are conserved quantities.

For a discrete symmetry where $\mathcal{S}$ is also Hermitian, then the similarity transformation property directly implies that $\mathcal{S}$ corresponds to some conserved quantity. Parity is the usual example.

Degeneracies

If different eigenstates of the Hamiltonian have the same energy, then we refer to those states as *degenerate*. We will now show that a symmetry of a Hamiltonian implies that there will be degenerate eigenstates.

The proof is simple. Suppose $H|n\rangle = E_n|n\rangle$, so that $|n\rangle$ is an eigenstate of the Hamiltonian with energy eigenvalue E_n. Typically the state $|n'\rangle = \mathcal{S}|n\rangle$ is a different state than $|n\rangle$, but

$$H|n'\rangle = H\mathcal{S}|n\rangle = \mathcal{S}H|n\rangle = E_n|n'\rangle$$

so the state $|n'\rangle$ is degenerate with $|n\rangle$.

This is an extremely important concept. Experimentally, when eigenstates are discovered that have the same (or very close) energies, this points to some symmetry (perhaps only approximate) of the Hamiltonian. Great strides have been made in understanding the physical universe by observing degeneracies in nature and then building a theory that incorporates a symmetry to explain them. In this class, we will spend some time on the hydrogen atom, showing where the degeneracies are and what symmetries give rise to them, and then how small perturbations can break those symmetries.

Example: Translational Symmetry

You know that the translation operator in three dimensions is $\mathcal{T}(\vec{a}) = \exp(-i\vec{p}\cdot\vec{a}/\hbar)$. For the free particle Hamiltonian $H = \vec{p}^{\,2}/2m$, this clearly satisfies $\mathcal{T}(\vec{a})H = H\mathcal{T}(\vec{a})$, so the free particle Hamiltonian is translationally invariant. Indeed, the generator of translations, namely $\vec{p}$, obviously commutes with this Hamiltonian.

Unfortunately, we cannot illustrate degeneracies with this symmetry operator and Hamiltonian because there aren't any. Indeed, an energy eigenstate $|\vec{p}\,'\rangle$, that has energy eigenvalue $E_{\vec{p}\,'} = \vec{p}\,'^2/2m$, is not transformed by $\mathcal{T}(\vec{a})$. The Hamiltonian is rotationally invariant, but that's a different symmetry operator, which we'll get to later.

Example: Parity Symmetry

We'll talk about parity in more detail later in the course, but for now, this is a brief introduction for the sake of illustrating the connection with degeneracy.

Parity means "space inversion." That is, any position coordinate $\vec{r}$ becomes $-\vec{r}$. We express this quantitatively by requiring that the expectation value of $\vec{r}$ in any state $|\alpha\rangle$ reverses sign for the state $\mathcal{P}|\alpha\rangle$, where $\mathcal{P}$ is the (unitary) parity operator. That is

$$\langle\alpha|\mathcal{P}^\dagger\vec{r}\,\mathcal{P}|\alpha\rangle = -\langle\alpha|\vec{r}|\alpha\rangle \qquad \text{so} \qquad \mathcal{P}^\dagger\vec{r}\,\mathcal{P} = -\vec{r}$$

and we refer to position as "parity odd." It makes sense that $\mathcal{P}^2|\alpha\rangle = |\alpha\rangle$, so we have

$$\mathcal{P} = \mathcal{P}^{-1} = \mathcal{P}^\dagger$$

and the parity operator is Hermitian as well as unitary. It therefore corresponds to an observable with eigenvalues ± 1.

Momentum is also parity odd, that is

$$\mathcal{P}^\dagger\vec{p}\,\mathcal{P} = -\vec{p}$$

This makes sense because, classically, it is just the time derivative of position, but it's not hard to formally prove this using the translation operator. It follows directly that $\vec{p}\,\mathcal{P} = -\mathcal{P}\vec{p}$ so for an eigenstate $|\vec{p}\,'\rangle$ of momentum, $\vec{p}\,\mathcal{P}|\vec{p}\,'\rangle = -\vec{p}\,'\mathcal{P}|\vec{p}\,'\rangle$, that is $\mathcal{P}|\vec{p}\,'\rangle = |-\vec{p}\,'\rangle$.

Now consider the free particle again, with $H = \vec{p}^{\,2}/2m$. Parity is a symmetry operator, since

$$\mathcal{P}^\dagger H\mathcal{P} = \frac{1}{2m}\mathcal{P}^\dagger\vec{p}\cdot\vec{p}\,\mathcal{P} = \frac{1}{2m}\mathcal{P}^\dagger\vec{p}\,\mathcal{P}\cdot\mathcal{P}^\dagger\vec{p}\,\mathcal{P} = \frac{1}{2m}(-\vec{p}\,)\cdot(-\vec{p}\,) = H$$

The energy degeneracy that is created by $\mathcal{P}$ is now obvious, since $|\pm\vec{p}\,'\rangle$ are both eigenstates of the Hamiltonian with the same energy.

Example: Rotational Symmetry

The first two example are pretty simple, but not particularly interesting. Rotational symmetry is more interesting, but also a bit more complicated, so let's take this example slowly.

You've actually seen an important example of degeneracy due to rotational symmetry. The Hamiltonian for a particle in a central potential, like the hydrogen atom or the isotropic harmonic oscillator, has eigenvalues that depend on l and some principle quantum number n, but not m. Therefore, for any l, there is a $2l+1$ degeneracy.

You know that the unitary operator that describes rotations about an axis $\hat{n}$ through an angle ϕ is

$$\mathcal{D}(\hat{n},\phi) = \exp\left(-i\frac{\hat{n}\cdot\vec{J}}{\hbar}\phi\right)$$

where the generator $\vec{J}$ has the commutation relations of angular momentum. This is not a generally useful expression because it can only be expressed in a simple Taylor expansion if we stick to the component $J_n = \hat{n}\cdot\vec{J}$, so we can't write things in terms of the Cartesian components. However, it does show clearly that rotation is a symmetry operator for any term in a Hamiltonian proportional to $\vec{J}^2$.

In fact, although we didn't prove it in class, a consistent definition of a vector operator is one that obeys the same commutation relations with $\vec{J}$. In this way, you can show that any term that is the square of some vector, for example $\vec{p}^2$, is also rotationally invariant.

An important, but simple, physical example of this is the so-called "rigid rotor" Hamiltonian. An object with moment of inertia I and angular momentum $\vec{L}$ has the Hamiltonian

$$H = \frac{\vec{L}^2}{2I} \qquad \text{so} \qquad E_l = \frac{l(l+1)\hbar^2}{2I}$$

are the energy eigenvalues, and each energy level has a $2l + 1$ degeneracy. This kind of situation appears in nature in many places. For example, see the discussion of the HCl molecule in Townsend, Section 9.7. (The molecule also vibrates, and the two degrees of freedom are coupled.)

Nuclei provide more examples. The energy levels of ^{160}Dy, for example, show a clear rotational pattern with $l = 0, 2, 4, 6, 8$ before other degrees of freedom creep in. (This is a "symmetric rotor" so only even values of l are possible. Do you see why? Think about parity.) If you want to see these energy levels, try exploring the ENSDF database at Brookhaven National Laboratory.

Now let's see how the rotation operator creates degenerate states. The operator $\mathcal{D}(\hat{n}, \phi)$ is hard to decompose into Cartesian operators, but you know it will be some messy infinite expression involving $J_\pm$, along with J_z, and these will change the m values of the states.

More simply, though, just think about what the rotation operator does. For spin-1/2, for example, it can be used to turn a $|\uparrow\rangle$ state into $|\downarrow\rangle$ state. That is, it turns one eigenstate of J_z into another eigenstate of J_z, changing the value of m but leaving j unchanged. We haven't explicitly written down the rotation operator for $j > 1/2$, but the principle would be the same.