Energy and time evolution

Perhaps the most important physical transformation in quantum mechanics is the operation of *time evolution* that takes us from the state of the system at some time t_0 to the state of the system at some later time $t_0 + \delta t$. This is a unitary operator that we will call

$$\hat{\mathcal{T}}(\delta t, t_0) \ . \tag{1}$$

In many cases, we have a system with *time-translation invariance*: this means that the evolution operator is the same for any time t_0, so $\hat{\mathcal{T}}$ is only a function of δt.

As above, we can think of an infinitesimal version of this operator, where δt is taken to be very small. In this case, we can write

$$\hat{\mathcal{T}}(\delta t, t_0) = \mathbf{1} - i\delta t \frac{\hat{H}}{\hbar} + \dots \tag{2}$$

where $\hat{H}$ is a Hermitian operator that we call the *Hamiltonian*; in general, it can depend on t_0. We will see below that in the time-translation invariant case where it does not, the physical quantity associated with $\hat{H}$ is always conserved, this conserved quantity is what we call *energy*. The constant $\hbar$ introduced above is included so that $\hat{H}$ will have the ordinary units of energy instead of inverse time.

The result (2) gives the infinitesimal form of the time evolution operator. Applying this to a state, we learn that

$$|\Psi(t_0 + \delta t)\rangle = (\mathbf{1} - i\delta t \frac{\hat{H}}{\hbar} + \dots)|\Psi(t_0)\rangle \tag{3}$$

Rearranging this, we get

$$\frac{1}{\delta t}(|\Psi(t_0 + \delta t) - |\Psi(t_0)\rangle) = -i\frac{\hat{H}}{\hbar}|\Psi(t_0)\rangle + \dots \ , \tag{4}$$

where the dots indicate terms of order δt and higher. Finally, in the limit $\delta t \to 0$, the left side becomes the derivative of the state, so we obtain a differential equation for the time evolution of a state

$$i\hbar\frac{d}{dt}|\Psi\rangle = \hat{H}|\Psi\rangle \tag{5}$$

This is known as the *Schrödinger equation.* In this general form, it applies to any quantum system.

Conserved quantities in quantum mechanics

Now that we have some understanding of time evolution, we can discuss what is meant by a conserved quantity in quantum mechanics. Since physical observables don't even have definite values for most states, it is less obvious what we might mean by something being conserved. However, we might consider the following possibilities

- A physical observable $\mathcal{O}$ is conserved if and only if its expectation value is unchanging in time for all states of the system.
- A physical observable $\mathcal{O}$ is conserved if and only if for any state of the system, the probabilities of finding the various eigenvalues λ_n are all unchanging in time.

The latter statement clearly implies the former and appears to be a stronger condition, but we will see that they are equivalent (this is an exercise on the next homework; the proof will appear on the solutions).

Furthermore both are equivalent to the statement that the operator $\hat{\mathcal{O}}$ associated with $\mathcal{O}$ commutes with the Hamiltonian operator, i.e.

$$[\hat{\mathcal{O}}, \hat{H}] = 0 \ . \tag{6}$$

We are assuming here that $\mathcal{O}$ itself is some fixed physical quantity with no inherent time dependence (i.e, we assume $d\hat{\mathcal{O}}/dt = 0$).

Symmetries in quantum mechanics

A *symmetry* in quantum mechanics is a physical transformation represented by some unitary operator $\hat{\mathcal{T}}$ with the property that if $|\Psi(t)\rangle$ is any solution to the Schrödinger equation, then $\hat{\mathcal{T}}|\Psi(t)\rangle$ is a solution to the Schrödinger equation. This definition is in line with our intuition that symmetries acting on a system give us configurations "equivalent" to the original configuration.

To understand which physical transformations have this property, consider any $|\Psi(t)\rangle$ satisfying the Schrödinger equation (5). Then $\hat{\mathcal{T}}|\Psi(t)\rangle$ will also satisfy the Schrödinger equation for some specific operator $\hat{\mathcal{T}}$ if and only if

$$\begin{aligned} & i\hbar\frac{d}{dt}(\hat{\mathcal{T}}|\Psi\rangle) = \hat{H}(\hat{\mathcal{T}}|\Psi\rangle) \\ \iff \quad & i\hbar\hat{\mathcal{T}}\frac{d}{dt}|\Psi\rangle = \hat{H}\hat{\mathcal{T}}|\Psi\rangle \\ \iff \quad & \hat{\mathcal{T}}\hat{H}|\Psi\rangle = \hat{H}\hat{\mathcal{T}}|\Psi\rangle \\ \iff \quad & [\hat{\mathcal{T}}, \hat{H}]|\Psi\rangle = 0 \ . \end{aligned} \tag{7}$$

This will be true for any possible state $|\Psi\rangle$ if and only if

$$[\hat{\mathcal{T}}, \hat{H}] = 0 \ . \tag{8}$$

Thus, a physical transformation is a symmetry if and only if the corresponding unitary operator commutes with the Hamiltonian.

If we have a continuous family of symmetries such as rotations around an axis or translations, the operators $\hat{\mathcal{T}}(\epsilon)$ representing infinitesimal transformations must also obey the relation (8). From the expression

$$\hat{\mathcal{T}}(\epsilon) = \mathbf{1} - i\epsilon\hat{\mathcal{O}} + \ldots \tag{9}$$

we see that this will be true if and only if the Hermitian operator $\hat{\mathcal{O}}$ associated with this transformation also commutes with the Hamiltonian. Thus, the condition that a Hermitian operator gives an infinitesimal transformation that is a symmetry is

$$[\hat{\mathcal{O}}, \hat{H}] = 0 \ . \tag{10}$$

Symmetries ↔ conservation laws

We have already seen that any Hermitian operator can be associated with a physical observable and also a physical transformation. We now see that the condition (6) that the physical observable associated with $\hat{\mathcal{O}}$ is conserved is the same as the condition (10) that the physical transformation associated with $\hat{\mathcal{O}}$ is a symmetry. This establishes the relation between symmetries and conservation laws in quantum mechanics.

Time translations and energy

The most universal example of a operator that commutes with the Hamiltonian is the Hamiltonian itself. Thus, for any quantum mechanical system with time-translation invariance (i.e. for which a single time-independent operator governs the time evolution at all times), the observable associated with the Hamiltonian operator must be conserved. From our experience with classical mechanics, we know that the conserved quantity associated with time-translation invariance is the *total energy* of the system. Thus, the Hamiltonian operator appearing in the Schrödinger equation is the energy operator.