16.2 Deriving the Schrödinger Equation

The time evolution of states has been specified in terms of a unitary operator □ assumed known. We now ask a “reverse engineering” question. What kind of differential equation do states satisfy for which the solution is unitary time evolution? The answer is simple and satisfying: the states satisfy the Schrödinger equation. The discussion that follows can be called a derivation of the Schrödinger equation.

We begin by taking the time derivative of the time evolution postulate (16.1.3) to find that

$$\frac{\partial}{\partial t}|\Psi, t\rangle = \frac{\partial \mathcal{U}(t, t_0)}{\partial t}|\Psi, t_0\rangle. \tag{16.2.1}$$

We want the right-hand side to involve the ket $|\Psi, t\rangle$ so we write

$$\frac{\partial}{\partial t}|\Psi, t\rangle = \frac{\partial \mathcal{U}(t, t_0)}{\partial t}\,\mathcal{U}(t_0, t)|\Psi, t\rangle. \tag{16.2.2}$$

This now looks like a differential equation for the state $|\Psi, t\rangle$. Let us introduce a name for the operator appearing on the right-hand side:

$$\frac{\partial}{\partial t}|\Psi, t\rangle = \Lambda(t, t_0)|\Psi, t\rangle, \quad \text{with} \quad \Lambda(t, t_0) \equiv \frac{\partial \mathcal{U}(t, t_0)}{\partial t}\,\mathcal{U}(t_0, t). \tag{16.2.3}$$

The operator Λ has units of inverse time. Note also that

$$\Lambda^\dagger(t, t_0) = \mathcal{U}(t, t_0)\,\frac{\partial \mathcal{U}(t_0, t)}{\partial t}, \tag{16.2.4}$$

since the adjoint operation reverses the order of the operators, changes the order of time arguments in each $\mathcal{U}$, and does not interfere with the time derivative.

We now want to prove two important facts about Λ:

1. $\Lambda(t, t_0)$ is anti-Hermitian. To prove this begin with $\mathcal{U}(t, t_0)\,\mathcal{U}(t_0, t) = \mathbb{1}$, and take a derivative with respect to time to find

   $$\frac{\partial \mathcal{U}(t, t_0)}{\partial t}\,\mathcal{U}(t_0, t) + \mathcal{U}(t, t_0)\,\frac{\partial \mathcal{U}(t_0, t)}{\partial t} = 0. \tag{16.2.5}$$

   Glancing at (16.2.3) and (16.2.4), we see that we got

   $$\Lambda(t, t_0) + \Lambda^\dagger(t, t_0) = 0, \tag{16.2.6}$$

   proving that $\Lambda(t, t_0)$ is indeed anti-Hermitian.

2. $\Lambda(t, t_0)$ is actually independent of t_0. This is important because in the differential equation (16.2.3) t_0 appears nowhere except in Λ. We will show that $\Lambda(t, t_0)$ is actually equal to $\Lambda(t, t_1)$ for any other time t_1 different from t_0. To prove this we begin with the expression for $\Lambda(t, t_0)$ in (16.2.3) and insert a suitable form of the unit operator in between the two factors:

   $$\Lambda(t, t_0) = \frac{\partial \mathcal{U}(t, t_0)}{\partial t}\big(\mathcal{U}(t_0, t_1)\mathcal{U}(t_1, t_0)\big)\,\mathcal{U}(t_0, t). \tag{16.2.7}$$

Since the time derivative ignores both t_0 and t_1, we have, as claimed,

$$\begin{aligned}\Lambda(t, t_0) &= \frac{\partial}{\partial t}\Big(\mathcal{U}(t, t_0)\mathcal{U}(t_0, t_1)\Big)\Big(\mathcal{U}(t_1, t_0)\mathcal{U}(t_0, t)\Big)\\ &= \frac{\partial \mathcal{U}(t, t_1)}{\partial t}\mathcal{U}(t_1, t) = \Lambda(t, t_1).\end{aligned} \tag{16.2.8}$$

It follows that we can write $\Lambda(t) \equiv \Lambda(t,\ t_0)$, and thus equation (16.2.3) becomes

$$\frac{\partial}{\partial t}|\Psi, t\rangle \;=\; \Lambda(t)|\Psi, t\rangle. \tag{16.2.9}$$

We define an operator $\hat{H}(t)$ by multiplication of Λ by $i\hbar$:

$$\boxed{\hat{H}(t) \;\equiv\; i\hbar\Lambda(t) \;=\; i\hbar\frac{\partial \mathcal{U}(t, t_0)}{\partial t}\mathcal{U}(t_0, t).} \tag{16.2.10}$$

Since Λ is anti-Hermitian and has units of inverse time, $\hat{H}(t)$ is a *Hermitian* operator with units of energy. $\hat{H}(t)$ is called the (quantum) Hamiltonian of the quantum system. Multiplying (16.2.9) by $i\hbar$, we find the

$$\boxed{\text{Schrödinger equation:}\quad i\hbar\frac{\partial}{\partial t}|\Psi, t\rangle \;=\; \hat{H}(t)\,|\Psi, t\rangle.} \tag{16.2.11}$$

This is our main result. Unitary time evolution implies this equation. In this derivation the Hamiltonian $\hat{H}(t)$ follows from the knowledge of □, as shown in (16.2.10). If you are handed the unitary operator that generates time evolution, you can quickly reconstruct the Hamiltonian. Most often, however, we know the Hamiltonian and wish to calculate the time evolution operator □.

The above equation for $|\Psi,\ t\rangle$ is the ket form of the Schrödinger equation. As discussed in example 14.15, the ordinary form of the Schrödinger equation for a wave function with coordinate dependence arises by writing $\Psi(x,\ t) \equiv \langle x|\Psi,\ t\rangle$.

There are basically two reasons why the quantity $\hat{H}(t)$ appearing in the above Schrödinger equation is called the Hamiltonian, or energy operator. First, in quantum mechanics the momentum operator is given by $\hbar/i$ times the derivative with respect to a spatial coordinate. In special relativity, energy corresponds to the time component of the momentum four-vector, and it is reasonable to view the energy operator as an operator proportional to a time derivative. The second argument is based on analogy to classical mechanics, as we explain now.

We have used the Schrödinger equation (16.2.11) to derive an equation for the time evolution of expectation values of observables. For a time-independent observable $\hat{Q}$, this took the form (15.3.5), which we rewrite as

$$\frac{d\langle\hat{Q}\rangle}{dt} = \left\langle \frac{1}{i\hbar}[\hat{Q}, \hat{H}] \right\rangle. \tag{16.2.12}$$

This equation is a natural generalization of the Hamiltonian equations in classical mechanics, and $\hat{H}$ plays a role analogous to that of the classical Hamiltonian. Indeed, in classical mechanics one has Poisson brackets $\{\cdot, \cdot\}_{\rm pb}$ defined for functions of x and p by

$$\{A, B\}_{\rm pb} = \frac{\partial A}{\partial x}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial x}. \tag{16.2.13}$$

Note that $\{x, p\}_{\rm pb} = 1$. Moreover, just like commutators, Poisson brackets are antisymmetric: $\{A, B\}_{\rm pb} = -\{B, A\}_{\rm pb}$. For any function $Q(x, p)$ without explicit time dependence, its time derivative is given by taking the Poisson bracket of Q with the classical Hamiltonian H. To see this begin with

$$\frac{dQ}{dt} = \frac{\partial Q}{\partial x}\dot{x} + \frac{\partial Q}{\partial p}\dot{p}, \tag{16.2.14}$$

where we used the chain rule for derivatives, and dots mean time derivatives. Hamilton's equations of motion state that

$$\dot{x} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial x}. \tag{16.2.15}$$

If you have not seen this before, you can at least quickly check that for a classical Hamiltonian $H(x, p) = \frac{p^2}{2m} + V(x)$ the equations above give exactly what you would expect. Using the values for $\dot{x}$ and $\dot{p}$ in (16.2.14), we now have

$$\frac{dQ}{dt} = \frac{\partial Q}{\partial x}\frac{\partial H}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial H}{\partial x}. \tag{16.2.16}$$

The right-hand side is indeed the Poisson bracket of Q with the Hamiltonian, so we have that

$$\frac{dQ}{dt} = \{Q, H\}_{\text{pb}}. \tag{16.2.17}$$

The similarity to the time derivative of the quantum expectation values (16.2.12) is quite striking and suggests that $\hat{H}$ is indeed a quantum version of the classical Hamiltonian H. Note also that this comparison suggests that quantum commutators behave as $i\hbar$ times Poisson brackets:

$$[\hat{A}, \hat{B}] \quad \Longleftrightarrow \quad i\hbar\{A, B\}_{\text{pb}}. \tag{16.2.18}$$

This correspondence is sometimes an equality: $\{x, p\}_{pb} = 1$ while $[\hat{x}, \hat{p}] = i\hbar$. But for general functions $A(x, p)$ and $B(x, p)$, there are ordering ambiguities in the quantum analogs $\hat{A}(\hat{x}, \hat{p})$ and $\hat{B}(\hat{x}, \hat{p})$ and in passing from the result of the Poisson bracket to its quantum analog. This is illustrated in the following exercise:

Exercise16.1. *Show that* $\{x^2, p^2\}_{\text{pb}} = 4xp$, *while* $[\hat{x}^2, \hat{p}^2] = i\hbar(2\hat{x}\hat{p} + 2\hat{p}\hat{x}) = i\hbar(4\hat{x}\hat{p} - 2i\hbar)$.

While the reasons discussed above justify our calling $\hat{H}$ the Hamiltonian, ultimately any Hermitian operator with units of energy has the right to be called a Hamiltonian regardless of any connection to a classical theory. The value of the classical theory is that it suggests potentially interesting quantum Hamiltonians, as we saw, for example, in setting up the quantum harmonic oscillator.