16.3 Calculating the Time Evolution Operator

Typically, the Hamiltonian $\hat{H}(t)$ is known, and we wish to calculate the unitary operator $\mathcal{U}$ that implements time evolution. For this it is useful to find an equation for $\mathcal{U}$. Multiplying equation (16.2.10) from the right by $\mathcal{U}(t, t_0)$ gives

$$i\hbar \frac{\partial \mathcal{U}(t, t_0)}{\partial t} = \hat{H}(t)\,\mathcal{U}(t, t_0). \tag{16.3.1}$$

This is indeed a differential equation for the *operator* □. Note also that letting both sides of this equation act on $|\Psi, t_0\rangle$ gives us back the Schrödinger equation.

Since there is no possible confusion with the time derivatives, we do not need to write them as partial derivatives. Then the above equation takes the form

$$\frac{d\mathcal{U}}{dt} = -\frac{i}{\hbar}\hat{H}(t)\mathcal{U}(t). \tag{16.3.2}$$

If we view operators as matrices, this is a differential equation for the *matrix* □, involving the matrix $\hat{H}$. Solving this equation is in general quite difficult. We will consider three cases of increasing complexity.

Case 1. $\hat{H}$ is time independent. In this case, equation (16.3.2) is structurally of the form

$$\frac{d\mathcal{U}}{dt} = \hat{K}\mathcal{U}(t), \quad \text{with } \hat{K} = -\frac{i}{\hbar}\hat{H}. \tag{16.3.3}$$

Here, $\hat{K}$ is a time-independent matrix. If the matrices were 1×1, this would reduce to the plain differential equation

$$\frac{du}{dt} = ku(t) \quad \Rightarrow \quad u(t) = e^{kt}u(0). \tag{16.3.4}$$

For the matrix case (16.3.3), we claim that

$$\mathcal{U}(t) = e^{t\hat{K}}\mathcal{U}(0). \tag{16.3.5}$$

Here, the exponential of $t\hat{K}$ is multiplied from the right by the matrix □(0). The ansatz clearly works at time equal zero. The exponential of a matrix, as usual, is defined by the Taylor series of the exponential function (section 13.7). With $\hat{K}$ time independent, we have the derivative

$$\frac{d}{dt}e^{t\hat{K}} = \hat{K}e^{t\hat{K}} = e^{t\hat{K}}\hat{K}. \tag{16.3.6}$$

With this result we readily verify that (16.3.5) solves (16.3.3):

$$\frac{d\mathcal{U}}{dt} = \frac{d}{dt}(e^{t\hat{K}}\mathcal{U}(0)) = \hat{K}e^{t\hat{K}}\mathcal{U}(0) = \hat{K}\mathcal{U}(t). \tag{16.3.7}$$

Using the explicit form of the matrix $\hat{K}$, the solution (16.3.5) is therefore

$$\mathcal{U}(t,t_0) \;=\; e^{-\frac{i}{\hbar}\hat{H}t}\,\mathcal{U}_0, \tag{16.3.8}$$

where □$_0$ is a constant matrix. Recalling that □$(t_0,\ t_0) = \mathbb{1}$, we have $\mathbb{1} = e^{-\frac{i}{\hbar}\hat{H}t_0}\,\mathcal{U}_0$, and therefore $\mathcal{U}_0 = e^{\frac{i}{\hbar}\hat{H}t_0}$. The two exponentials can be combined into a single one, and the full solution becomes

$$\boxed{\mathcal{U}(t,t_0) \;=\; \exp\Big[-\frac{i}{\hbar}\hat{H}(t-t_0)\Big], \quad \text{time-independent } \hat{H}.} \tag{16.3.9}$$

Exercise 16.2. *Verify that the ansatz* □(t) = □$(0)e^{tK}$, *consistent for* $t = 0$, *would not have provided a solution of (16.3.3).*

Case 2. $[\hat{H}(t_1),\ \hat{H}(t_2)\ ] = 0$ for all t_1, t_2. Here the Hamiltonian is time dependent, but, despite this, the Hamiltonians at different times commute. Of course, they trivially commute when both are evaluated at the same time. One example is provided by the Hamiltonian for a spin in a magnetic field of time-dependent magnitude but constant direction. We claim that the time evolution operator is now given by

$$\boxed{\mathcal{U}(t,t_0) \;=\; \exp\Big[-\frac{i}{\hbar}\int_{t_0}^{t} dt'\hat{H}(t')\Big], \quad \hat{H} \text{ at different times commute.}} \tag{16.3.10}$$

If the Hamiltonian is time independent, the integral in the exponent is easily done, and the above solution reduces correctly to (16.3.9). To prove that (16.3.10) solves the differential equation (16.3.2), we streamline notation by writing

$$\hat{R}(t) \;\equiv\; -\frac{i}{\hbar}\int_{t_0}^{t} dt'\hat{H}(t') \quad\Rightarrow\quad \hat{R}' \;=\; -\frac{i}{\hbar}\hat{H}(t), \tag{16.3.11}$$

where primes denote time derivatives. We claim that $\hat{R}'(t)$ and $\hat{R}(t)$ commute. Indeed

$$[\hat{R}'(t),\hat{R}(t)] = -\frac{1}{\hbar^2}\Big[\hat{H}(t), \int_{t_0}^{t} dt'\hat{H}(t')\Big] = -\frac{1}{\hbar^2}\int_{t_0}^{t} dt'\,[\hat{H}(t),\hat{H}(t')] = 0, \tag{16.3.12}$$

recalling that Hamiltonians at different times commute. The claimed solution is

$$\mathcal{U} = \exp \hat{R}(t). \tag{16.3.13}$$

Since $\hat{R}$ and $\hat{R}'$ commute, it follows that for any $n \geq 1$,

$$(\hat{R}^n)' = n\hat{R}'\hat{R}^{n-1} \tag{16.3.14}$$

because in all n terms produced by the derivative the $\hat{R}'$ factor can be moved to the left without impediment. Since first-order derivatives thus work as usual, we find that

$$\frac{d\mathcal{U}}{dt} = \frac{d}{dt}\exp \hat{R} = \hat{R}' \exp \hat{R} = -\frac{i}{\hbar}\hat{H}(t)\,\mathcal{U}, \tag{16.3.15}$$

which is exactly what we wanted to show.

Case 3. $[\hat{H}(t_1), \hat{H}(t_2)\,] \neq 0$. This is the most general situation, and there is only a series solution. The solution for □ is given by the so-called time-ordered exponential, denoted by the symbol T in front of an exponential:

$$\begin{aligned}
\mathcal{U}(t, t_0) &= \mathrm{T}\exp\Big[-\frac{i}{\hbar}\int_{t_0}^{t} dt'\hat{H}(t')\Big] = \mathrm{T}\sum_{n=0}^{\infty}\frac{1}{n!}\Big(-\frac{i}{\hbar}\Big)\int_{t_0}^{t} dt_1\hat{H}(t_1)\cdots\int_{t_0}^{t} dt_n\hat{H}(t_n) \\
&\equiv \mathbb{1} + \Big(-\frac{i}{\hbar}\Big)\int_{t_0}^{t} dt_1\hat{H}(t_1) \\
&\quad + \Big(-\frac{i}{\hbar}\Big)^2\int_{t_0}^{t} dt_1\hat{H}(t_1)\int_{t_0}^{t_1} dt_2\hat{H}(t_2) \\
&\quad + \Big(-\frac{i}{\hbar}\Big)^3\int_{t_0}^{t} dt_1\hat{H}(t_1)\int_{t_0}^{t_1} dt_2\hat{H}(t_2)\int_{t_0}^{t_2} dt_3\hat{H}(t_3) \\
&\qquad \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
&\quad + \Big(-\frac{i}{\hbar}\Big)^n\int_{t_0}^{t} dt_1\hat{H}(t_1)\int_{t_0}^{t_1} dt_2\hat{H}(t_2)\ \cdots\ \int_{t_0}^{t_{n-1}} dt_n\hat{H}(t_n) \\
&\qquad \vdots \qquad\qquad \vdots \qquad\qquad \vdots
\end{aligned} \tag{16.3.16}$$

The action of time ordering T on each term of the exponential is defined by the above expression. The time ordering refers to the fact that in the nth term of the series we have a product $\hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_n)$ of *noncommuting* operators with integration ranges that force ordered times $t_1 \geq t_2 \geq t_3 \cdots \geq t_n$.

Note also that the nth term in the time-ordered exponential does not have the $1/n!$ combinatorial factor of the exponential. In the exponential, all t_1, …, t_n are integrated from t_0 to t, and the full region of integration splits over $n!$ subregions, each with a different ordering of the times. Effectively, the T operator reorders the operators within each region, giving the same integral for each. Thus, the $1/n!$ is canceled by the $n!$ contributions. Some aspects of this construction are explored in problem 16.4.