Chapter 3

Unitary Time Evolution

3.1 Introduction

An important part of any physical theory is the dynamics (time-evolution) that it predicts. According to Postulate 2, we can study the dynamics of isolated quantum systems by solving the Schrödinger equation

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle. \tag{3.1}$$

where H is the Hamiltonian, the Hermitian observable which represents the energy of the system. In this chapter of the course, we will study some of the general properties of solutions to the Schrödinger equation, and learn about some approximate methods for integrating this equation. We will close the chapter by introducing the Heisenberg picture, an alternative (and equivalent) formulation of time-evolution in quantum mechanics, in which the dynamics is captured by the evolution of observables, rather than states.

3.2 Evolution operator

When we integrate the Schrödinger equation, we need to specify, as a boundary condition, the state of the system at a certain time, e.g. time $t = 0$. The Schrödinger equation then allows us to calculate, given $|\psi(0)\rangle$, the state of the system at any other time time t, $|\psi(t)\rangle$. This evolution is a map from one state to another state, and can therefore be described in terms of an operator $U(t)$, which

we call the *evolution operator*.

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{3.2}$$

We write the evolution operator $U(t)$ since, as we shall show here, it is always unitary, regardless of the form of the Hamiltonian, and whether or not the Hamiltonian is time-dependent. When the Hamiltonian is constant in time, $U(t)$ has a particularly simple form

$$U(t) = \exp\left[-i\frac{H}{\hbar}t\right]. \tag{3.3}$$

Aside: Exponentiating operators

In equation (3.3), we are exponentiating the linear operator $-iHt/\hbar$. Exponentiated operators or matrices are defined using the power-series definition of e^x, i.e.

$$e^x = \sum_j \frac{x^j}{j!} \tag{3.4}$$

In analogy with this, we define, for operator (or square matrix) $\hat{A}$,

$$e^{\hat{A}} = \sum_j \frac{\hat{A}^j}{j!}. \tag{3.5}$$

where powers of $\hat{A}$ are defined as follows $\hat{A}^0 = \mathbb{1}$, $\hat{A}^1 = \hat{A}$, $\hat{A}^2 = \hat{A}\hat{A}$, etc.

For example, consider the following diagonal matrix B

$$B = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}. \tag{3.6}$$

It is easy to take powers of diagonal matrices,

$$B^j = \begin{bmatrix} \lambda_1^j & 0 \\ 0 & \lambda_2^j \end{bmatrix}. \tag{3.7}$$

and thus

$$e^B = \sum_j \begin{bmatrix} \lambda_1^j/j! & 0 \\ 0 & \lambda_2^j/j! \end{bmatrix} = \begin{bmatrix} e^{\lambda_1} & 0 \\ 0 & e^{\lambda_2} \end{bmatrix}. \tag{3.8}$$

In general, diagonal matrices are easy to exponentiate, however non-diagonal matrices do not share this, e.g. in general

$$\exp\left[\begin{bmatrix} a & b \\ c & d \end{bmatrix}\right] \neq \begin{bmatrix} e^a & e^b \\ e^c & e^d \end{bmatrix} \tag{3.9}$$

and the power-series definition must be directly employed.

Exponentiated operators share many, but not all, properties and identities of exponentiated numbers. In particular, for two operators $\hat{A}$ and $\hat{B}$, the identity

$$e^{a+b} = e^a e^b \tag{3.10}$$

which holds for any number a, b **does not hold** in general for matrices and operators. One can show, via the power-series definition that this identity does however hold in the special case that the matrices or operators commute, i.e. if $[\hat{A}, \hat{B}] = 0$

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}}. \tag{3.11}$$

If $\hat{A}$ and $\hat{B}$ do not commute then this identity usually does not hold.

Time-independent Hamiltonians

Above, we asserted that, if Hamiltonian H is time-independent then the evolution operator takes the form:

$$U(t) = \exp\left[-i\frac{H}{\hbar}t\right] \tag{3.12}$$

Let us now verify that this is indeed the case, by verifying that the state $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ with $U(t)$ defined according to (3.12) satisfies the Schrödinger equation. We will need to compute

$$\frac{\partial}{\partial t}|\psi(t)\rangle = \frac{\partial}{\partial t}\left(U(t)|\psi(0)\rangle\right) \tag{3.13}$$

Since $|\psi(0)\rangle$ is time invariant, we proceed by calculating

$$\frac{\partial}{\partial t}U(t) = \frac{\partial}{\partial t}\exp\left[-i\frac{H}{\hbar}t\right] \tag{3.14}$$

To differentiate an exponentiated operator, we use the power-series definition

$$\begin{aligned}\frac{\partial}{\partial t}\exp\left[-i\frac{H}{\hbar}t\right] &= \frac{\partial}{\partial t}\sum_{j=0}^{\infty}\left(\frac{-iH}{\hbar}\right)^j t^j/j! \\ &= \sum_{j=1}^{\infty}\left(\frac{-iH}{\hbar}\right)^j jt^{j-1}/j! \\ &= \frac{-iH}{\hbar}\sum_{j=1}^{\infty}\left(\frac{-iH}{\hbar}\right)^{j-1} t^{j-1}/(j-1)! \\ &= \frac{-iH}{\hbar}\exp\left[-i\frac{H}{\hbar}t\right]\end{aligned} \tag{3.15}$$

where the $j = 0$ term disappeared in the differentiation since it is constant in time.

This implies directly that

$$\frac{\partial}{\partial t}|\psi(t)\rangle = \frac{-i}{\hbar}HU(t)|\psi(0)\rangle = \frac{-i}{\hbar}H|\psi(t)\rangle \tag{3.16}$$

as required.

Unitarity

We can use equation (3.12) directly to show that for time-independent H, $U(t)$ is unitary. We shall argue below that this unitarity holds for quantum evolution operators, even if H is time-varying. Taking the Hermitian conjugate of equation (3.12)

$$U(t)^\dagger = \exp\left[i\frac{H}{\hbar}t\right] \tag{3.17}$$

since H is Hermitian, and multiplying with $U(t)$, we obtain

$$U(t)U(t)^\dagger = \exp\left[-i\frac{H}{\hbar}t\right]\exp\left[i\frac{H}{\hbar}t\right] = \exp\left[i\frac{H-H}{\hbar}t\right] = \mathbb{1} \tag{3.18}$$

We are allowed to combine the exponentials via equation (3.11) because H and $-H$ (trivially) commute. Note that $U(t)^\dagger$ is therefore the inverse of $U(t)$, which, is also equal to $U(-t)$.

Tracking evolution from other times

We have defined our evolution operator $U(t)$ as the operator which transforms state $|\psi(0)\rangle$ to $|\psi(t)\rangle$, but it is easy to derive evolution operators which track evolution from states at other times, e.g. $|\psi(t_1)\rangle$.

$$|\psi(t_1)\rangle = U(t_1)|\psi(0)\rangle \tag{3.19}$$

and hence

$$|\psi(0)\rangle = U(t_1)^\dagger|\psi(t_1)\rangle = U(-t_1)|\psi(t_1)\rangle \tag{3.20}$$

and hence, we can write the state at any time t in terms of $|\psi(t_1)\rangle$.

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = U(t)U(-t_1)|\psi(t_1)\rangle = U(t-t_1)|\psi(t_1)\rangle \tag{3.21}$$

where we use the fact that $U(x)U(y) = U(x+y)$.

Step-wise changing Hamiltonian

We can use evolution operators to solve the Schrödinger equation for a Hamiltonian which evolves step-wise, i.e. one which is constant over finite periods of time and changes discontinuously at certain points.

For example, consider a Hamiltonian which between times $0 \leq t \leq t_1$ the Hamiltonian is H_1 and between times $t_1 \leq t \leq t_2$ the Hamiltonian is H_2. Let us define $U_1(t) = \exp\left[-i\frac{H_1}{\hbar}t\right]$ and $U_2(t) = \exp\left[-i\frac{H_2}{\hbar}t\right]$. Using the reasoning in the previous section, for all times $0 \leq t \leq t_1$, the evolution operator will be simply $U_1(t)$, but for times $t_1 \leq t \leq t_2$, the evolution operator is $U_2(t-t_1)U_1(t_1)$, i.e. the first unitary operator applies for the first segment of time, of length t_1, and the second applies for the segment of length $t - t_1$.

This approach can be generalised to a Hamiltonian with any number of discrete changes in time. Since the product of two (or any number of) unitary operators is always unitary (check this), this evolution operator remains unitary.

Continuously changing Hamiltonian

Consider now a Hamiltonian $H(t)$ which varies constantly in time. We can approximate it by a series of n discrete slices, each applied for time $\delta t = t/n$, for each of which the Hamiltonian takes the constant value $H(j\delta t) = H(jt/n)$ where $j = 1, 2, \ldots, n$ is an integer which indexes each slice. This is equivalent to when

we approximate an integral by a sum of the areas of constant slices. An approximate evolution operator will be given by

$$U(t) \approx \prod_{j=1}^{n} \exp\left[-i\frac{H(jt/n)}{\hbar}\frac{t}{n}\right] \tag{3.22}$$

This operator is unitary for the reasons given above.

We can obtain an exact evolution operator, in the limit $n \to \infty$ (this is analogous to obtaining an exact integral by allowing the width of the slices to go to zero).

$$U(t) = \lim_{n\to\infty} \prod_{j=1}^{n} \exp\left[-i\frac{H(jt/n)}{\hbar}\frac{t}{n}\right] \tag{3.23}$$

The unitarity of this operator survives in the limit, hence, evolution operators are unitary also in this general case. Note that there are many similarities between the limits we have taken here, and the limits you are familiar with for standard calculus.

In practice, it is often not possible to exactly solve the Schrödinger equation for time-varying Hamiltonians, and find a closed form for this limit. For that reason approximation methods are very important. One of the most important of these is time-dependent perturbation theory, which we introduce in chapter 5 of this course.

Off-syllabus remark: The limit in equation (3.23) is sometimes known in the literature as a *time-ordered integral* and written

$$U(t) = \lim_{n\to\infty} \prod_{j=1}^{n} \exp\left[-i\frac{H(jt/n)}{\hbar}\frac{t}{n}\right] = \mathcal{T}\exp\left[-i\int_0^t dt'\frac{H(t')dt'}{\hbar}\right] \tag{3.24}$$

where the limit is to be understood as the definition of the expression on the right. (The notation is rather unconventional, as the integral sign goes up into the exponent. We shall not use this notation for this lecture course, but you may come across it in some advanced textbooks and research papers).

3.3 Suzuki-Trotter Decomposition

In physics, we often encounter Hamiltonians of the form

$$H = H_1 + H_2 \tag{3.25}$$

where the operators H_1 and H_2 do not commute, E.g.

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{3.26}$$

It is also often the case that the individual terms in such Hamiltonians can be solved individually (e.g. we can calculate a simple expression for $\exp[-iH_1t/\hbar]$ and $\exp[-iH_2t/\hbar]$, as in the above example), but the full Hamiltonian cannot be solved exactly (which is common in this example, unless $V(\hat{x})$ has a very special form).

In such cases, we can make use of a so-called Suzuki-Trotter decomposition. This derives from the following result, first shown by Trotter in 1959 and generalised by Suzuki in 1976. For any operators (or square matrices) $\hat{A}$ or $\hat{B}$, the following identity holds:

$$e^{\hat{A}+\hat{B}} = \lim_{n\to\infty} \left(e^{\hat{A}/n} e^{\hat{B}/n}\right)^n = \lim_{n\to\infty} \left(e^{\hat{B}/n} e^{\hat{A}/n}\right)^n \tag{3.27}$$

which, for quantum evolution operators, implies

$$U(t) = e^{\frac{-it}{\hbar}(H_1+H_2)} = \lim_{n\to\infty} \left(U_1(t/n)U_2(t/n)\right)^n \tag{3.28}$$

where $U_1(t) = \exp\left[-i\frac{H_1}{\hbar}t\right]$ and $U_2(t) = \exp\left[-i\frac{H_2}{\hbar}t\right]$. We can interpret this as follows. The full evolution under $H_1 + H_2$ is approximated by splitting time into discrete slices and then alternating between Hamiltonians H_1 and H_2 for successive slices. In the limit that the slices become infinitessimal the approximation becomes exact.

Equation (3.28) implies that we can construct a family of approximations to $U(t)$, where instead of taking the infinite limit, we keep a finite n.

Suzuki-Trotter approximations

Here we shall study the validity of Suzuki-Trotter approximations for small n. To gauge the effectiveness of the approximation, let us first write an expression for the exact operator. To avoid overloading our calculation with $\hbar$s, we shall consider

the following operator, and expand it as a power series

$$\begin{aligned} e^{(\hat{A}+\hat{B})t} &= \sum_j \frac{(\hat{A}+\hat{B})^j t^j}{j!} \\ &= \mathbb{1} + (\hat{A}+\hat{B})t + \frac{(\hat{A}+\hat{B})^2 t^2}{2} + \cdots \\ &= \mathbb{1} + (\hat{A}+\hat{B})t + \frac{(\hat{A}^2+\hat{B}^2+\hat{A}\hat{B}+\hat{B}\hat{A})t^2}{2} + \cdots \end{aligned} \tag{3.29}$$

The most elementary Suzuki-Trotter approximation is the $n = 1$ case. In this case, there are two possible decompositions we could choose $e^{\hat{A}t}e^{\hat{B}t}$ or $e^{\hat{B}t}e^{\hat{A}t}$. If $\hat{A}$ and $\hat{B}$ do not commute, these different decompositions are not equal, but one can show that they both have the same accuracy. We shall study the first one, by first expanding each exponential as a power series,

$$e^{\hat{A}t}e^{\hat{B}t} = \sum_j \frac{\hat{A}^j t^j}{j!} \sum_k \frac{\hat{B}^k t^k}{k!} \tag{3.30}$$

and then expressing the full operator as a power series in t,

$$e^{\hat{A}t}e^{\hat{B}t} = \mathbb{1} + (\hat{A}+\hat{B})t + \left(\hat{A}^2/2 + \hat{B}^2/2 + \hat{A}\hat{B}\right) t^2 + \cdots \tag{3.31}$$

By comparing equations (3.29) and (3.31) we see that the $n = 1$ Trotter approximation has the correct t^0 and t^1 terms, but an error in the t^2 term. This means that the $n = 1$ approximation is accurate to first order in t and that the error is to order t^2. It can therefore be used as a good approximation if t is sufficiently small.

Now let us consider the $n = 2$ approximation. Here there are actually four possible decompositions we can consider. The reason for this is that the individual pairs of operators can applied in any order. Thus we have $e^{\hat{A}t/2}e^{\hat{B}t/2}e^{\hat{A}t/2}e^{\hat{B}t/2}$, $e^{\hat{B}t/2}e^{\hat{A}t/2}e^{\hat{B}t/2}e^{\hat{A}t/2}$, $e^{\hat{A}t/2}e^{\hat{B}t/2}e^{\hat{B}t/2}e^{\hat{A}t/2}$ and $e^{\hat{B}t/2}e^{\hat{A}t/2}e^{\hat{A}t/2}e^{\hat{B}t/2}$ possible choices. The latter two operators can be reduced to 3 operators in the product, since $e^{\hat{B}t/2}e^{\hat{B}t/2} = e^{\hat{B}t}$, so we shall study the third choice of operator here.

$$\begin{aligned} e^{\hat{A}t/2}e^{\hat{B}t}e^{\hat{A}t/2} &= \sum_j \frac{\hat{A}^j (t/2)^j}{j!} \sum_k \frac{\hat{B}^k t^k}{k!} \sum_l \frac{\hat{A}^l (t/2)^l}{l!} \\ &= \mathbb{1} + (\hat{A}+\hat{B})t + \frac{(\hat{A}^2+\hat{B}^2+\hat{A}\hat{B}+\hat{B}\hat{A})t^2}{2} + \cdots \end{aligned} \tag{3.32}$$

We see that this expression is exact to second order in t. If we wrote out further terms of the series we would see that the error here is of order t^3.

In general, one can show that for a given n, the approximation is valid to nth order in t and the error is of order t^{n+1}. Therefore, for many problems, a modest n suffices to provide a good approximation.

3.4 Schrödinger and Heisenberg Pictures

So far we have embodied the time-evolution of quantum systems in the time-dependence of their state-vector $|\psi(t)\rangle$

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle. \tag{3.33}$$

In quantum mechanics, the measurable quantities we can predict are statistical properties such as expectation values, and probabilities, all of which (as mentioned above) are described mathematically as an expectation value. For operator $\hat{O}$ the time-evolving expectation value can be written

$$\langle \hat{O}(t)\rangle = \langle \psi(t)|\hat{O}|\psi(t)\rangle \tag{3.34}$$

We can rewrite this expression

$$\langle \hat{O}(t)\rangle = \underbrace{\langle\psi(0)|U(t)^\dagger}_{\text{State evolves in time}}\ \hat{O}\ \underbrace{U(t)|\psi(0)\rangle}_{\text{State evolves in time}} \tag{3.35}$$

but now we see that there is another way of interpreting this

$$\langle \hat{O}(t)\rangle = \langle\psi(0)|\ \underbrace{U(t)^\dagger \hat{O} U(t)}_{\text{Operator evolves in time}}\ |\psi(0)\rangle. \tag{3.36}$$

Exactly the same expectation value is obtained when we leave the state fixed as $|\psi(0)\rangle$ and allow the observable to evolve in time as $U(t)^\dagger \hat{O} U(t)$.

The two *pictures* of quantum time evolution represented by equations (3.35) and (3.36) are called the **Schrödinger** and **Heisenberg** pictures respectively.

Schrödinger picture

The Schrödinger picture is the standard approach to quantum evolution, and the one which you have likely always encountered up to now. State vectors evolve

in time as $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ and observables remain constant in time.[1]. In this section, to avoid ambiguity, when I am expressing an operator or state in Schrödinger picture I will use an S subscript $|\psi(t)\rangle_S$ and $\hat{O}_S$. For the Heisenberg picture, I will use an H subscript.

Heisenberg Picture

At time $t = 0$, Schrödinger and Heisenberg pictures are equivalent. For all other times, in the Heisenberg picture, time-evolution is carried by the operators, which evolve as $O_H(t) = U(t)^\dagger \hat{O}(0) U(t)$, where $\hat{O}(0) = \hat{O}_S$, the operator in the Schrödinger picture. Expectation values are computed with respect to states which are constant in time $|\psi\rangle_H = |\psi(0)\rangle_H$.

You may wonder why we should introduce a new formalism for time- dependence. There are several reasons for using the Heisenberg picture. Firstly, it can simplify the calculations we make. Secondly, time-dependence in this picture is closer, in a sense, to classical physics, where observable quantities $x(t)$, $p(t)$ do vary in time. Thirdly, equations of motion in the Heisenberg picture are sometimes very reminiscent of the equivalent classical equations, allowing us to better pin-point similarities (and hence differences) between quantum and classical behaviour. Historically, the Heisenberg picture was developed (by Heisenberg) for his matrix mechanics formulation of quantum theory, developed in parallel to wave-function quantum mechanics.

An evolution equation in the Heisenberg picture

In the Schrödinger picture Schrödinger's equation allows us to compute $|\psi(t)\rangle_S$ given the Hamiltonian and the initial state $|\psi(0)\rangle$. The equivalent in the Heisenberg picture is, unsurprisingly, called the Heisenberg equation. This is a differential equation which allows us to compute $\hat{O}_H(t)$ given the Hamiltonian and the initial operator $\hat{O}_H(0)$.

We can derive this equation as follows. Consider the derivative

$$\frac{\partial}{\partial t}\hat{O}_H(t) = \frac{\partial}{\partial t}\left(U(t)^\dagger \hat{O}_H(0) U(t)\right) \tag{3.37}$$

[1] In certain cases, operators can vary in time in the Schrödinger picture also, for example if there is a time-varying magnetic field, however, here we shall ignore such cases.

We can compute this using the product rule

$$\frac{\partial}{\partial t}\hat{O}_H(t) = \frac{\partial}{\partial t}\left(U(t)^\dagger\right)\hat{O}_H(0)U(t) + U(t)^\dagger\frac{\partial}{\partial t}\left(\hat{O}_H(0)\right)U(t) + U(t)^\dagger\hat{O}_H(0)\frac{\partial}{\partial t}\left(U(t)\right) \tag{3.38}$$

The middle term is zero, since $\hat{O}_H(0)$ is constant. Earlier we saw that

$$\frac{\partial}{\partial t}\left(U(t)\right) = -\frac{i}{\hbar}H(t)U(t) \tag{3.39}$$

and

$$\frac{\partial}{\partial t}\left(U(t)^\dagger\right) = \frac{i}{\hbar}U(t)^\dagger H(t) \tag{3.40}$$

where $H(t)$ is the Schrödinger picture Hamiltonian (which may be time-varying). Hence,

$$\begin{aligned}
\frac{\partial}{\partial t}\hat{O}_H(t) &= \frac{i}{\hbar}\left(U(t)^\dagger H(t)\hat{O}_H(0)U(t) - U(t)^\dagger\hat{O}_H(0)H(t)U(t)\right) \\
&= \frac{i}{\hbar}\left(U(t)^\dagger H(t)U(t)U(t)^\dagger\hat{O}_H(0)U(t) - U(t)^\dagger\hat{O}_H(0)U(t)U(t)^\dagger H(t)U(t)\right) \\
&= \frac{i}{\hbar}\left(H_H(t)\hat{O}_H(t) - \hat{O}_H(t)H_H(t)\right) \\
&= \frac{i}{\hbar}[H_H(t), \hat{O}_H(t)]
\end{aligned} \tag{3.41}$$

where $H_H(t) = U(t)^\dagger H(t)U(t)$ is the Heisenberg picture Hamiltonian.

The final equation we come to is called the Heisenberg equation, which has a simple and compact form

$$\frac{\partial}{\partial t}\hat{O}_H(t) = \frac{i}{\hbar}[H_H(t), \hat{O}_H(t)] \tag{3.42}$$

.

Constants of Motion

It is clear from the Heisenberg equation that if $[H_H(t), \hat{O}_H(t)] = 0$ then $\hat{O}_H(t)$ is constant in time. This means that the expectation value of $\hat{O}_H(t)$ is a constant of motion. This well-known result is more self-apparent in the Heisenberg picture.

Interaction picture

In addition to the Heisenberg and Schrödinger pictures there is an intermediate picture of time-evolution called the Interaction picture. We shall study the Interaction picture in more detail at the end of chapter 4.