Quantum Dynamics

So far we have not discussed how physical systems change with time.

This chapter is devoted exclusively to the dynamic development of state kets and/or observables.

In other words, we are concerned here with the quantum mechanical analogue of Newton's (or Lagrange's or Hamilton's) equations of motion.

TIME EVOLUTION AND THE SCHRÖDINGER EQUATION

The first important point we should keep in mind is that time is just a parameter in quantum mechanics, not an operator.

In particular, time is not an observable in the language of the previous chapter.

Ironically, in the historical development of wave mechanics both L. de Broglie and E. Schrödinger were guided by a kind of covariant analogy between energy and time on the one hand and momentum and position (spatial coordinate) on the other.

Yet when we now look at quantum mechanics in its finished form, there is no trace of a symmetrical treatment between time and space.

The relativistic quantum theory of fields does treat the time and space coordinates on the same footing, but it does so only at the expense of demoting position from the status of being an observable to that of being just a parameter.

Time Evolution Operator

Our basic concern in this section is, How does a state ket change with time?

Suppose we have a physical system whose state ket at t_0 is represented by $|\alpha\rangle$.

At later times, we do not, in general, expect the system to remain in the same state $|\alpha\rangle$.

Let us denote the ket corresponding to the state at some later time by

$$|\alpha, t_0; t\rangle, \quad (t > t_0)$$

Because time is a continuous parameter, we expect

$$\lim_{t \to t_0} |\alpha, t_0; t\rangle = |\alpha\rangle$$

Or

$$|\alpha, t_0; t_0\rangle = |\alpha, t_0\rangle$$

Our basic task is to study the time evolution of a state ket:

$$|\alpha, t_0\rangle = |\alpha\rangle \xrightarrow{\text{time evolution}} |\alpha, t_0; t\rangle$$

Put in another way, we are interested in asking how the state ket changes under a time displacement t_0 -> t.

As in the case of translation, the two kets are related by an operator which we call the time-evolution operator $\mathscr{U}(t, t_0)$:

$$|\alpha, t_0; t\rangle = \mathscr{U}(t, t_0)|\alpha, t_0\rangle$$

What are some of the properties we would like to ascribe to the time-evolution operator?

The first important property is the unitary requirement for $\mathscr{U}(t, t_0)$ that follows from probability conservation.

Suppose that at t_0 the state ket is expanded in terms of the eigenkets of some observable A:

$$|\alpha, t_0\rangle = \sum_{a'} c_{a'}(t_0)|a'\rangle$$

Likewise, at some later time, we have

$$|\alpha, t_0; t\rangle = \sum_{a'} c_{a'}(t)|a'\rangle$$

In general, we do not expect the modulus of the individual expansion coefficient to remain the same:*

$$|c_{a'}(t)| \neq |c_{a'}(t_0)|$$

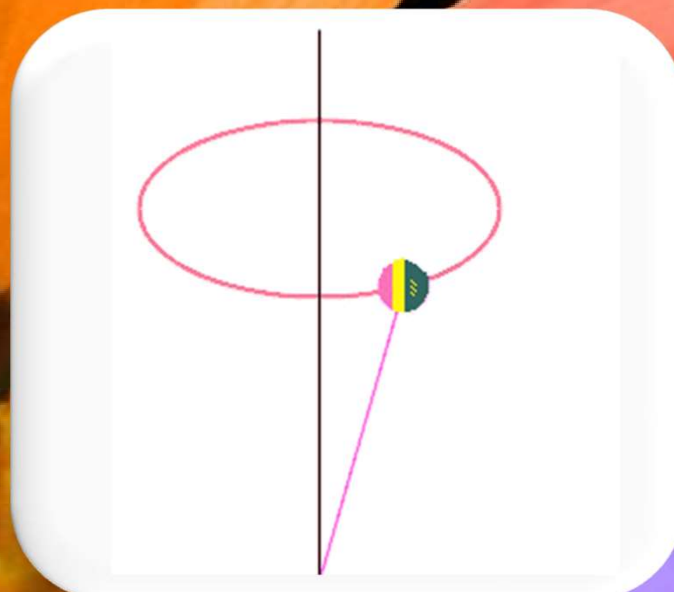
*We later show, however, that if the Hamiltonian commutes with A, then they are indeed equal.

For instance, consider a spin 1/2 system with its spin magnetic moment subjected to a uniform magnetic field in the z-direction.

To be specific, suppose that at t_0 the spin is in the positive x-direction; that is, the system is found in an eigenstate of Sx with eigenvalue ħ/2.

As time goes on, the spin precesses in the xy-plane, as will be quantitatively demonstrated later in this section.

This means that the probability for observing Sx + is no longer unity at $t > t_0$; there is a finite probability for observing Sx — as well.



Yet the sum of the probabilities for Sx+ and Sx- remains unity at all times.

Despite the individual expansion coefficients are not equal, generally we must have,.

$$\sum_{a'} |c_{a'}(t_0)|^2 = \sum_{a'} |c_{a'}(t)|^2$$

Stated another way, if the state ket is initially normalized to unity, it must remain normalized to unity at all later times:

$$\langle \alpha, t_0 | \alpha, t_0 \rangle = 1 \Rightarrow \langle \alpha, t_0; t | \alpha, t_0; t \rangle = 1$$

As in the translation case, this property is guaranteed if the time-evolution operator is taken to be unitary.

For this reason we take unitarity to be one of the fundamental properties of the $\mathscr{U}$ operator.

It is no coincidence that many authors regard unitarity as being synonymous with probability conservation.

$$\mathscr{U}^{\dagger}(t,t_0)\mathscr{U}(t,t_0)=1$$

1

Another feature is the composition property:

$$\mathscr{U}(t_2,t_0)=\mathscr{U}(t_2,t_1)\mathscr{U}(t_1,t_0), \quad (t_2>t_1>t_0)$$

2

This equation says that if we are interested in obtaining time evolution from t_0 to t_2, then we can obtain the same result by first considering time evolution from t_0 to t_1 then from t_1 to t_2—a reasonable requirement. Note that we read the equation from right to left!

$$|\alpha, t_0; t_0 + dt\rangle = \mathscr{U}(t_0 + dt, t_0)|\alpha, t_0\rangle$$

$$\lim_{dt \to 0} \mathscr{U}(t_0 + dt, t_0) = 1$$ 3

We assert that all these requirements are satisfied by

$$\mathscr{U}(t_0 + dt, t_0) = 1 - i\Omega\, dt \qquad \Omega^\dagger = \Omega$$

1

$$\mathscr{U}^\dagger(t_0 + dt, t_0)\mathscr{U}(t_0 + dt, t_0) = (1 + i\Omega^\dagger dt)(1 - i\Omega\, dt) \simeq 1$$

2

$$\mathscr{U}(t_0 + dt_1 + dt_2, t_0) = \mathscr{U}(t_0 + dt_1 + dt_2, t_0 + dt_1)\mathscr{U}(t_0 + dt_1, t_0)$$

$$(1 - i\Omega(dt_1 + dt_2)) = (1 - i\Omega dt_2)(1 - i\Omega dt_1) \cong (1 - i\Omega(dt_1 + dt_2))$$ ✓

The operator Ω has the dimension of frequency or inverse time.

Is there any familiar observable with the dimension of frequency?

We recall that in the old quantum theory, angular frequency ω is postulated to be related to energy by the Planck-Einstein relation

$$E = \hbar\omega$$

Let us now borrow from classical mechanics the idea that the Hamiltonian is the generator of time evolution (Goldstein 1980, 407-8). It is then natural to relate Ω to the Hamiltonian operator H:

$$\Omega = \frac{H}{\hbar}$$

To sum up, the infinitesimal time-evolution operator is written as

$$\mathcal{U}(t_0 + dt, t_0) = 1 - \frac{iH\,dt}{\hbar}$$

The Schrödinger Equation

We are now in a position to derive the fundamental differential equation for the time-evolution operator $\mathcal{U}(t, t_0)$.

$$\mathcal{U}(t + dt, t_0) = \mathcal{U}(t + dt, t)\,\mathcal{U}(t, t_0) = \left(1 - \frac{iH\,dt}{\hbar}\right)\mathcal{U}(t, t_0)$$

$$\mathcal{U}(t + dt, t_0) - \mathcal{U}(t, t_0) = -i\left(\frac{H}{\hbar}\right) dt\,\mathcal{U}(t, t_0)$$

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

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t_0)|\alpha, t_0\rangle = H\,\mathcal{U}(t, t_0)|\alpha, t_0\rangle$$

This is the Schrodinger equation for the time-evolution operator.

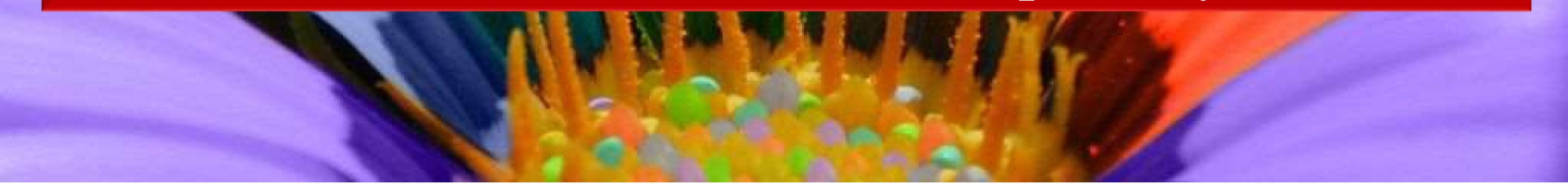
$$i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t\rangle = H |\alpha, t_0; t\rangle$$

If we are given $\mathscr{U}(t, t_0)$ and, in addition, know how $\mathscr{U}(t, t_0)$ acts on the initial state ket $|\alpha, t_0>$, it is not necessary to bother with the Schrodinger equation.

All we have to do is to apply $\mathscr{U}(t, t_0)$ to $|\alpha, t_0>$; in this manner we can obtain a state ket at any t.

Our first task is therefore to derive formal solutions to the Schrodinger equation for the time evolution operator.

There are three cases to be treated separately:



Case 1

The Hamiltonian operator is independent of time.

The Hamiltonian for a spin-magnetic moment interacting with a time-independent magnetic field is an example of this.

The solution in such a case is given by

$$i\hbar\frac{\partial}{\partial t}\mathscr{U}(t,t_0)=H\mathscr{U}(t,t_0) \quad \Rightarrow \quad \mathscr{U}(t,t_0)=\exp\left[\frac{-iH(t-t_0)}{\hbar}\right]$$

$$\exp\left[\frac{-iH(t-t_0)}{\hbar}\right]=1-\frac{iH(t-t_0)}{\hbar}+\left[\frac{(-i)^2}{2}\right]\left[\frac{H(t-t_0)}{\hbar}\right]^2+\cdots$$

$$U(t\rightarrow t_0,t_0)\rightarrow 1$$

$$\frac{\partial}{\partial t}\exp\left[\frac{-iH(t-t_0)}{\hbar}\right]=\frac{-iH}{\hbar}+\left[\frac{(-i)^2}{2}\right]2\left(\frac{H}{\hbar}\right)^2(t-t_0)+\cdots$$

Case 2

The Hamiltonian operator H is time-dependent but the H's at different times commute.

As an example, let us consider the spin-magnetic moment subjected to a magnetic field whose strength varies with time but whose direction is always unchanged.

The formal solution in this case is

$$\mathscr{U}(t, t_0) = \exp\left[-\left(\frac{i}{\hbar}\right)\int_{t_0}^{t} dt' H(t')\right]$$

This can be proved in a similar way. We simply replace $H(t-t_0)$ by integral$[dt'H(t')]^{t}_{t0}$.

Case 3. The H's at different times do not commute.

Continuing with the example involving spin-magnetic moment, we suppose, this time, that the magnetic field direction also changes with time: at $t=t_1$ in the x-direction, at $t=t_2$ in the y-direction, and so forth.

Because Sx and Sy do not commute, H(t1) and H(t2), which go like S*B, do not commute either.

The formal solution in such a situation is given by

$$\mathscr{U}(t,t_0)=1+\sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{n-1}}dt_n\,H(t_1)H(t_2)\cdots H(t_n)$$

which is sometimes known as the Dyson series.

In elementary applications, only case 1 is of practical interest. In the remaining part of this chapter we assume that the H operator is time-independent. We will encounter time-dependent Hamiltonians in Chapter 5.