Chapter 4

Time evolution of

In this chapter we study how a quantum mechanical system evolves with time. The state of a system due to interaction with another system that is subject to interaction, its state undergoes changes with time. These changes in state causes changes in the measurement of the different observables with time. In this we will learn how time dependent state vectors and the operators representing physical observables are governed in time.

1. The evolution operator, the quantum Hamiltonian, & the Schrödinger Equation

Suppose initially a system is described in a state \(| \Psi(0) \rangle \). Just like in the rotation operator \( \hat{R} \hat{O} \hat{R}^{-1} \) (that we saw in the previous chapters, meaning let's say here is an evolution operator that when this operator acts on \( \hat{O} \), any \( \hat{O}(t) \). When this operator acts on the initial state, it generates the state \(| \Psi(t) \rangle \), that means

\[ | \Psi(t) \rangle = U(t) | \Psi(0) \rangle \]  

---  Eq. (1)
And for corresponding bra-state vector
\[ \langle \Psi(t) | = \langle \Psi(0) | U^*(t) \]. \hspace{1cm} \text{Eq. (2)}

Whether stationary or evolving state, it is always normalized,
\[ \langle \Psi(t) | \Psi(t) \rangle = 1 \hspace{1cm} \text{Eq. (3)} \]
\[ \Rightarrow \langle \Psi(0) | U^*(t) U(t) | \Psi(0) \rangle = 1 \hspace{1cm} \text{Eq. (4)} \]

The fact that
\[ \langle \Psi(0) | \Psi(0) \rangle = 1 \hspace{1cm} \text{Eq. (5)} \]
requires the evolution operator must be unitary,
\[ U^*(t) U(t) = 1 \hspace{1cm} \text{Eq. (6)} \]

No if we do the time evolution process in an infinitesimal interval, \( dt \), we may write
\[ U(dt) = 1 - \frac{i \hat{H} dt}{\hbar} \hspace{1cm} \text{Eq. (7)} \]

where \( \hat{H} \) is the quantum Hamiltonian.

Using Eq. (6) & (7), we may write
\[ \hat{U}(t + at) = \hat{U}(t) \hat{U}(at) = \hat{U}(at) \hat{U}(t) \quad \text{Eq. (8)} \]

\[ \Rightarrow \hat{U}(t + at) = \left(1 - \frac{iH}{\hbar} at\right) \hat{U}(t) \]

\[ \Rightarrow \hat{U}(t + at) = \hat{U}(t) - \frac{iH}{\hbar} \hat{U}(t) at \]

or

\[ \frac{\hat{U}(t + at) - \hat{U}(t)}{at} = -\frac{iH}{\hbar} \hat{U}(t) \quad \text{Eq. (a)} \]

Note writing Eq. (8), we have used that the evolution in \( t + at \) can be subdivided into two steps (i.e., \( 0 \rightarrow at \) and then \( at \rightarrow t + at \)). Now writing noting that

\[ \lim_{\Delta t \to 0} \frac{d\hat{U}(t)}{dt} = \lim_{\Delta t \to 0} \left[ \frac{\hat{U}(t + at) - \hat{U}(t)}{\Delta t} \right] \]

we may write

\[ \frac{d\hat{U}}{dt} = -\frac{iH}{\hbar} \hat{U}(t) \quad \text{Eq. (8)} \]
The solution of which is given by

\[ U(t) = e^{\frac{-iHt}{\hbar}} \]  \hspace{1cm} \text{Eq. (9)}

using Eq. (1) and (8), we can also write

\[ i\hbar \frac{d}{dt} (\hat{\psi}(\psi_0)) = \hat{H} U(t) |\psi(0)\rangle \]

which leads to the Schrödinger equation given by

\[ i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \]  \hspace{1cm} \text{Eq. (9)}

**Energy eigenvalue equation and the state vector**

The energy eigenvalue equation is the eigenvalue equation for the quantum operator:

\[ \hat{A} |E\rangle = E |E\rangle \]

where \( E \) is the eigenvalue and \( |E\rangle \) is the eigenvector.
One solution to the Schrödinger equation in Eq. (4) can be expressed as

\[ |\Psi(t)\rangle = U(t)|\Psi(0)\rangle = e^{-\frac{i}{\hbar}Ht} |\Psi(0)\rangle \]

Suppose the initial state of the system is described by the energy eigenstate |E\rangle, then means

\[ |\Psi(0)\rangle = |E\rangle \] -- -- Eq. (6)

then

\[ |\Psi(t)\rangle = e^{-\frac{i}{\hbar}Ht} |E\rangle = e^{-\frac{i}{\hbar}Et} |E\rangle \] -- -- Eq. (7)

2. Schrödinger, Haüsgen, and Interaction pictures

Generally, the study of a quantum mechanical system essentially requires finding the expectation values of physical observables as a function of time. In quantum mechanics, these expectation values can be determined in three different ways, and in many combination thereof. They are
I. The Schrödinger picture. In this approach the time dependence is entirely carried by the state vectors $|\psi(t)\rangle$ and the operators is stationary. For example if $\hat{A}$ represent an observable the expectation value (time dependent)

$$\langle \hat{A}(t) \rangle = \langle \psi(t) | \hat{A}(0) | \psi(t) \rangle \quad \text{--- Eq. (8)}$$

Using the evolution operator, we have expressed the state vector

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle \quad \text{--- Eq. (9)}$$

which leads to

$$\langle \hat{A}(t) \rangle = \langle \psi(0) | \hat{U}^+(t) \hat{A}(0) \hat{U}(t) | \psi(0) \rangle \quad \text{--- Eq. (10)}$$

This gives

$$\hat{A}(t) = \hat{U}^+(t) \hat{A}(0) \hat{U}(t) \quad \text{--- Eq. (11)}$$

So what we need to solve is the Schrödinger equation

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{A} |\psi(t)\rangle \quad \text{--- Eq. (11)}$$

or

$$\frac{d\hat{U}}{dt} = -i \frac{\hat{A}}{\hbar} \hat{U}(t) \quad \text{--- Eq. (12)}$$
The Heisenberg Picture: it is possible to follow the time evolution of the quantum mechanical operators. It was shown first by Heisenberg. The equation of such operators can in fact be determined from Eq. (10)

$$\frac{d}{dt} \hat{A}(t) = \frac{1}{i} \left[ \hat{U}^+ (t) \hat{A} (0) \hat{U} (t) \right]$$

$$= \left[ \frac{d\hat{U}^+ (t)}{dt} \right] \hat{A} (0) \hat{U} (t) + \hat{U}^+ (t) \hat{A} (0) \frac{d\hat{U} (t)}{dt} \quad \text{--- Eq. (13)}$$

Recalling that

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

$$\Rightarrow \quad \frac{d\hat{U}^+ (t)}{dt} = -i \left( \hat{H} \hat{U} (t) \right)^+ = \frac{i \hat{U}^+ \hat{H}^+}{\hbar} = \frac{i}{\hbar} \hat{U}^+ \hat{H}$$

We can rewrite Eq. (13) as

$$\frac{d}{dt} \hat{A}(t) = \frac{i}{\hbar} \hat{U}^+ \hat{H} \hat{A} (0) \hat{U} (t) + \hat{U}^+ \hat{A} (0) \frac{d\hat{U} (t)}{dt}$$

Since \( \hat{A} \) commutes with \( \hat{U} \) and \( \hat{U}^+ \), we may write

$$\frac{d}{dt} \hat{A}(t) = \frac{i}{\hbar} \left[ \hat{A} \hat{U}^+ \hat{A} (0) \hat{U} (t) - \hat{U}^+ \hat{A} (0) \hat{U} \hat{H} \right]$$

$$+ \hat{U}^+ (t) \frac{d\hat{A}}{dt} \hat{U} (t)$$
Using
\[ \hat{A}(t) = \hat{U}^\dagger \hat{A}(0) \hat{U}, \quad \hat{U}^\dagger \frac{d\hat{A}}{dt} \hat{U} = \frac{d\hat{A}(t)}{dt} \]

we find
\[ \frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar} \left[ \hat{H}, \hat{A}(t) - \hat{A}(t) \hat{H} \right] \]

\[ \Rightarrow \quad \frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar} \left[ \hat{H}, \hat{A} \right] + \frac{d\hat{A}(t)}{dt} \quad \text{--- Eq. (14)} \]

The last term exists when the operator \( \hat{A} \) explicitly depends on time. If \( \hat{A} \) is not the case, we have
\[ \frac{d\hat{A}}{dt} = 0 \]

\[ \Rightarrow \quad \frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar} \left[ \hat{H}, \hat{A} \right] \]

In the Heisenberg picture, we have
\[ \langle \frac{d\hat{A}(t)}{dt} \rangle = \langle \Psi(0) | \frac{d\hat{A}(t)}{dt} | \Psi(0) \rangle \]

\[ = \frac{i}{\hbar} \langle \Psi(0) | [\hat{H}, \hat{A}] | \Psi(0) \rangle \]
\[
\begin{align*}
\frac{d}{dt} \left[ \langle \psi(t) | \hat{A}(t) | \psi(t) \rangle \right] &= \frac{i}{\hbar} \langle \psi(t) | [ \hat{E}, \hat{A} ] | \psi(t) \rangle \\
\Rightarrow \quad \frac{d}{dt} \langle \hat{A}(t) \rangle &= \frac{i}{\hbar} \langle \psi(t) | [ \hat{E}, \hat{A} ] | \psi(t) \rangle \\
\text{--- Eq. (15) ---}
\end{align*}
\]

**Interaction picture:**

Eq. (15) is the Heisenberg equation of motion. Since \( \langle \psi(t) \rangle \) contains all possible knowledge about the system, you have to solve the complete problem (the Schrödinger equation), which may be more than you need. In many cases, you only want to know one or a few observables of the system. The Heisenberg picture allows you to concentrate on precisely.

The **interaction picture** is useful when we often face situations where we already know the solutions of the problem in the absence of interaction. If we write the quantum Hamiltonian \( \hat{H} \) as

\[
\hat{H} = \hat{H}_f + \hat{H}_I \quad \text{--- Eq. (16) ---}
\]
The evolution operator

\[ \hat{U}(t) = e^{-i \frac{\hat{H} t}{\hbar}} \]

for the case where

\[ [\hat{H}_F, \hat{H}_I] = 0 \]

we can write

\[ \hat{U}(t) = e^{-i \frac{\hat{H}_F t}{\hbar}} e^{-i \frac{\hat{H}_I t}{\hbar}} \]

\[ \hat{U}(t) = e^{-i \frac{\hat{H}_F t}{\hbar}} e^{-i \frac{\hat{H}_I t}{\hbar}} \]

The state vector can then be expressed Eq. (19) as

\[ |\Psi(t)\rangle = \hat{U}(t) |\Psi(0)\rangle = e^{-i \frac{\hat{H}_F t}{\hbar}} e^{-i \frac{\hat{H}_I t}{\hbar}} |\Psi(0)\rangle \]

\[ \Rightarrow |\Psi(t)\rangle = e^{-i \frac{\hat{H}_F t}{\hbar}} |\Psi_I(t)\rangle \]

where

\[ |\Psi_I(t)\rangle = e^{-i \frac{\hat{H}_I t}{\hbar}} |\Psi_I(0)\rangle \]

Substituting Eq. (20) into the Schrödinger equation

\[ i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle \]

we find

\[ i\hbar \frac{d}{dt} \left[ e^{-i \frac{\hat{H}_F t}{\hbar}} |\Psi_I(t)\rangle \right] = [\hat{H}_F + \hat{H}_I] e^{-i \frac{\hat{H}_F t}{\hbar}} |\Psi_I(t)\rangle \]

\[ \Rightarrow \frac{i\hbar}{\hbar} \left[ \frac{-i \hat{H}_F}{\hbar} e^{-i \frac{\hat{H}_F t}{\hbar}} |\Psi_I(t)\rangle + \frac{i \hat{H}_F}{\hbar} e^{-i \frac{\hat{H}_F t}{\hbar}} \frac{d}{dt} |\Psi_I(t)\rangle \right] = \hat{H}_F e^{-i \frac{\hat{H}_F t}{\hbar}} |\Psi_I(t)\rangle + \hat{H}_I e^{-i \frac{\hat{H}_I t}{\hbar}} |\Psi_I(t)\rangle \]
\[ = \hat{H}_F \text{ e}^{\frac{-i\hat{H}_F t}{\hbar}} |\psi_I(t)\rangle + i\hbar \text{ e}^{\frac{i\hat{H}_F t}{\hbar}} \frac{d}{dt} |\psi_I(t)\rangle \]
\[ = \hat{H}_F \text{ e}^{\frac{-i\hat{H}_F t}{\hbar}} |\psi_I(t)\rangle + \hat{H}_I \text{ e}^{\frac{-i\hat{H}_F t}{\hbar}} |\psi_I(t)\rangle \]
\[ = i\hbar \text{ e}^{\frac{-i\hat{H}_F t}{\hbar}} \frac{d}{dt} |\psi_I(t)\rangle = \hat{H}_I \text{ e}^{\frac{-i\hat{H}_F t}{\hbar}} |\psi_I(t)\rangle \]
\[ \text{--- Eq. (21) ---} \]

Since \[ [\hat{H}_F, \hat{H}_I] = 0 \]

Since \( \hat{H}_F \) commutes with \( \hat{H}_I \) (i.e., \([\hat{H}_F, \hat{H}_I] = 0\)) we can easily show that
\[ [\hat{H}_I, \text{ e}^{\frac{i\hat{H}_F t}{\hbar}}] = 0 \]
so that Eq. (20) can be expressed as
\[ i\hbar \text{ e}^{\frac{-i\hat{H}_F t}{\hbar}} \frac{d}{dt} |\psi_I(t)\rangle = \hat{H}_I \text{ e}^{\frac{-i\hat{H}_F t}{\hbar}} |\psi_I(t)\rangle \]

Then follows that
\[ i\hbar \frac{d}{dt} |\psi_I(t)\rangle = \hat{H}_I |\psi_I(t)\rangle \]
where
\[ |\psi_I(t)\rangle = \text{ e}^{\frac{-i\hat{H}_I t}{\hbar}} |\psi(0)\rangle \]
Example 4.1 Precession of spin-\(\frac{1}{2}\) particle in a magnetic field. With an electron charge \(e\) and mass \(m\), an electron charge \(e\) and mass \(m\) can be considered to have magnetic dipole moment \(\vec{M}\).

(a) Write the expression for the classical Hamiltonian.

(b) Write the quantum Hamiltonian.

(c) Find the eigenstates and eigenvalues.

(d) Determine the state of the electron at a later time \(t\) when initially the electron is in the state

(i) \(|\psi(0)\rangle = |\pm z\rangle\)

(ii) \(|\psi(0)\rangle = |\pm x\rangle\)

(d) Using the state vector determine the probabilities

(i) \(P_{\pm z}, P_{-z}\)

(ii) \(P_{\pm x}, P_{-x}\)

and

(iii) The expectation values for \(\langle S^2 \rangle\), and \(\langle S_x \rangle\), \(\langle S_y \rangle\), \(\langle S_z \rangle\),
(f) Use the Heisenberg picture to find \langle S_x \rangle, \langle S_y \rangle, \text{ and } \langle S_z \rangle.

**Example 4.2**

The Hamiltonian for a spin-\( \frac{1}{2} \) particle in a magnetic field \( \mathbf{B} = B_0 \mathbf{\hat{z}} \) is given by

\[
\hat{H} = \omega_0 S_y
\]

where

\[
\omega_0 = \frac{g_0 B_0}{2mc}.
\]

Initially, the particle is in the state, \( |\Psi(0)\rangle = |\uparrow\rangle \)

(a) Find the state vector \( |\Psi(t)\rangle \)

(b) Find the expectation values for \( S_z \), \( S_x \) and \( S_y \) using the state vector.

(c) Find the expectation values using the Heisenberg picture.