SCPY 323: Quantum Mechanics II **2^{nd} Semester 2020-2021**

Lecture 3: Review of Schrödinger Equation

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3.1 Schrödinger Equation

We will now discuss Postulate IV. Suppose that we have already solved the eigenvalue problem and obtained eigenvalues E and the corresponding eigenvectors $|E\rangle$, that is,

$$H|E\rangle = E|E\rangle$$

Having solved the eigenvalue program, we can next solve the Schrödinger equation, which according to Postulate IV states that

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle .$$

In order to solve the Schrödinger Equation we first have to expand the wave function $\psi(t)$ in terms of eigenvectors of the Hamiltonian H:

$$|\psi(t)\rangle = \sum_E |E\rangle\langle E|\psi(t)\rangle = \sum_i a_E(t)|E\rangle ,$$

where $a_E(t) = \langle E|\psi(t)\rangle$. Therefore, we can rewrite the Schrödinger equation as

$$\begin{aligned} i\hbar\frac{d}{dt}\sum_E a_E(t)|E\rangle &= H\sum_E a_E(t)|E\rangle \\ &= \sum_E a_E(t)H|E\rangle \\ &= \sum_E a_E(t)E|E\rangle \\ \Rightarrow \quad \sum_E \left[i\hbar\frac{d\left[a_E(t)\right]}{dt} - a_E(t)E\right]|E\rangle &= 0 \\ \Rightarrow \quad i\hbar\frac{d\left[a_E(t)\right]}{dt} &= a_E(t)E \end{aligned}$$

This differential equation can be easily solved. The solution for $a_E(t)$ is:

$$a_E(t) = a_E(0)e^{-iEt/\hbar},$$

where $a_E(0)$ indicates the initial condition of the wave function, which can be calculated from

$$a_E(0) = \langle E|\psi(t=0)\rangle .$$

Since $|\psi(t=0)\rangle$ is given in a problem, $a_E(0)$ can be readily calculated. It basically indicates the overlap between the initial wave function and each eigenvector $|E\rangle$. Therefore, we have

$$|\psi(t)\rangle = \sum_E a_E(t)\,|E\rangle = \sum a_E(0)e^{-iEt/\hbar}\,|E\rangle = \sum_E \langle E|\psi(t=0)\rangle\, e^{-iEt/\hbar}\,|E\rangle\,.$$

That is, if we know $|\psi(t=0)\rangle$ and are able to solve the eigenvalue problem of the Hamiltonian H, then the state at time t can be determined. This way, the quantum mechanics theory is deterministic. We can rewrite $|\psi(t)\rangle$ as

$$|\psi(t)\rangle = \sum_E e^{-iEt/\hbar}\,|E\rangle\,\langle E|\psi(t=0)\rangle = U(t)\,|\psi(t=0)\rangle\,,$$

where

$$U(t) = \sum_E |E\rangle\,\langle E|\,e^{-iEt/\hbar}. \tag{3.1}$$

We call $U(t)$ a *time propagator*. You can prove for yourselves that $U(t)$ is a unitary operator. If the eigenstates are degenerate, then the equation above becomes

$$U(t) = \sum_\alpha \sum_E |E,\alpha\rangle\,\langle E,\alpha|\,e^{-iEt/\hbar},$$

where α indexes the degenerate states that have the same eigenvalue E. And if the E or α is continuous, the sum becomes an integral. Alternatively, we can write $U(t)$ as

$$U(t) = e^{-iHt/\hbar},$$

where H is the Hamiltonian. Since H is Hermitian, you can show that $U(t)$ is unitary. We can then expand $U(t)$ in terms of the eigenstate of H and obtain Eq. **??**. You can also prove that

$$|\psi(t)\rangle = e^{^{-iHt/\hbar}}\,|\psi(0)\rangle$$

satisfies the Schrödinger equation. Since $U(t)$ is a unitary operator, we can think of the time revolution of $|\psi(t)\rangle$ as a rotation of the vector $|\psi(t)\rangle$ in the Hilbert space. Therefore, the inner product $\langle\psi(t)\rangle\,|\psi(t)$ is invariant with time, that is,

$$\langle\psi(t)\rangle\,|\psi(t) = \langle\psi(0)\rangle\,|U^\dagger(t)U(t)\psi(0) = \langle\psi(0)\rangle\,|\psi(0).$$

As you can see, the propagator $U(t)$ indicates the time evolution of $|\psi(t)\rangle$ from time $t=0$ to time t. In general, we an define $U(t_2,t_1)$ to indicate the time evolution of the state from time t_1 to t_2, and we have

$$U(t_n,t_1) = U(t_n,t_{n-1})U(t_{n-1},t_{n-2})\ldots U(t_2,t_1).$$

The fact that we can divide $U(t)$ into an arbitrary small step is very useful in solving the time-dependent Schroödinger equation. However, that topic is beyond the scope of our class. In this class, we will only consider the time-independent Hamiltonian, that is, the Hamiltonian is not explicitly dependent on a variable t.

If $\psi(0)$ is equal to one of the eigenstate, we will have

$$|E(t)\rangle = |E\rangle\,e^{-iEt/\hbar}.$$

Since we can see that the norm $\langle E(t)\rangle\,|E(t)$ is invariant, we call this state *stationary state*. Therefore, the probability of finding the state in the state $|E(t)\rangle$ does not change with time, that is, if initially the state is in the eigenstate, then it will always be in the same eigenstate.

We can also find the expectation value of the measurable quantity associated with an operator Ω as a function of time by

$$\langle\psi(t)|\Omega|\psi(t)\rangle = \langle\psi(0)|U^\dagger(t)\Omega U(t)|\psi(0)\rangle\,.$$

As we discussed before in the section about the unitary operator. We can look at this expression from two different point of view. First, we can think of the state $|\psi(0)\rangle$ is *rotated* or "time-evoluted" by the propagator $U(t)$ and $\langle\psi(0)|$ by the propagator $U^\dagger$. This picture is called the active transformation as we have discussed or the *Schrödinger picture*. Alternatively, we can think of the state being fixed at $|\psi(0)\rangle$ and the operator Ω undergoes the time evolution through

$$\Omega \to U^\dagger(t)\Omega U(t).$$

This picture is called the passive transformation or the *Heisenberg picture*. However, no matter how you we at the time evolution of the state or the operator, at the end the expectation value are the same. Therefore, your description or your interpretation of quantum mechanics does not affect the outcome of the calculations, which are the most important here.

As an example, we will consider one of the exactly solvable problems in quantum mechanics, which is simple harmonic oscillators (SHO). I will assumer that you have already learned how to solve this problem using the differential equation method. Alternatively, in this class I will look at how to solve this problem using the operator method.

3.2 Propagator (time-evolution operator)

We learned from the previous section that if a state at time t_0 is $|\psi(t_0)\rangle$, the state at time t, $|\psi(t)\rangle$, is related to $|\psi(t_0)\rangle$ through the time-evolution operator or *propagator* $U(t;t_0)$, which is a unitary operator:

$$|\psi(t)\rangle = U(t;t_0)\,|\psi(t_0)\rangle$$

where for the time-independent Hamiltonian, we have

$$U(t;t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}.$$

We will next discuss the properties of the propagator.

Properties of $U(t;t_0)$

1. $U(t;t_0)$ is unitary and hence presevers probability and norm.

$$\begin{aligned} U^\dagger(t;t_0)U(t;t_0) &= \mathbb{1} \\ \Rightarrow \langle\psi(t)|\psi(t)\rangle &= \langle\psi,t_0|U^\dagger(t;t_0)U(t;t_0)|\psi,t_0\rangle \\ &= \langle\psi,t_0|\psi,t_0\rangle\,, \end{aligned}$$

   i.e. if $|\psi(t_0)\rangle$ is normalized, $|\psi(t)\rangle$ stays normalized. However, we note that each component of $|\psi(t)\rangle$ written in a basis can vary differently with time t, giving rise to the interference.

2. Composition Rule:

$$U(t;t_1)U(t_1;t_0) = U(t;t_0)$$

   When it acts on $|\psi,t_0\rangle$,

$$|\psi(t)\rangle = U(t;t_1)\,|\psi(t_1)\rangle = U(t;t_1)U(t_1;t_0)\,|\psi(t_0)\rangle = U(t;t_0)\,|\psi(t_0)\rangle\,.$$

   In general, we can divide a time interval between t_0 and t_N into N small intervals, and

$$U(t_N;t_0) = U(t_N;t_{N-1})U(t_{N-1};t_{N-2})\cdots U(t_2;t_1)U(t_1;t_0).$$

3. $U(t;t_0)$ becomes identity at $t = t_0$, that is,

$$\lim_{t\to t_0} U(t,;t_0) = \mathbb{1}.$$

All of the above properties can be satisfied if $U(t;t_0)$ has the following infinitesimal form

$$U(t_0+dt;t_0) = \mathbb{1} - \frac{i}{\hbar}H(t_0)dt + \mathcal{O}\left(dt^2\right)$$

Written in this form, $H(t_0)$ can be thought of as the generator of time-evolution similar to the momentum operator P, which is the generator of translation.

Schrödinger equation for $U(t;t_0)$

$$i\hbar\frac{d}{dt}U(t;t_0) = H(t)U(t;t_0) \tag{3.2}$$

We can use this equation to obtain the Schrödinger equation for $|\psi(t)\rangle$:

$$\begin{aligned} i\hbar\frac{d}{dt}|\psi(t)\rangle &= i\hbar\frac{\partial}{\partial t}U(t;t_0)|\psi(t_0)\rangle \\ &= H(t)U(t;t_0)|\psi(t_0)\rangle \\ \Rightarrow \quad i\hbar\frac{d}{dt}|\psi(t)\rangle &= H(t)|\psi(t)\rangle \end{aligned}$$

Our goal here is to solve Eq. **??** for $U(t;t_0)$. We can classify the solution into the following categories:

Case 1: Time-independent Hamiltonian where $H(t) = H(t_0) = H$. We can divide time between t_0 and t into N equal intervals. Each interval is $(t-t_0)/N$. We then take a limit where $N\to\infty$.

$$U(t;t_0) = \lim_{N\to\infty}\left(\mathbb{1} - \frac{i}{\hbar}H\left(\frac{t-t_0}{N}\right)\right)^N = e^{-\frac{i}{\hbar}H(t-t_0)}.$$

Case 2: Time-dependent Hamiltonian with $[H(t),H(t')] = 0$ for all time t and t', that is, the Hamiltonian remains compatible at all time. One example of this type of Hamiltonian is a spin in a magnetic field, which is constant in direction but varies in strength. The propagator in this case can be written as:

$$U(t;t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\ H(t')}.$$

We can verify that this expression for $U(t;t_0)$ satisfies Eq. **??**:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}U(t;t_0) &= \frac{\partial}{\partial t}\left[\int_{t_0}^{t} dt'\ H(t')\right]U(t;t_0) \\ &= H(t)U(t;t_0) \end{aligned}$$

Case 3: Time-dependent Hamiltonian with $[H(t),H(t')] \neq 0$. One example of this type of Hamiltonian is a spin in a magnetic field that is constantly changing its direction. Since, $H(t)$ and $H(t')$ are not compatible, we have to be careful with the order of the operators. From Eq. **??**, we can integrate both sides and obtain

$$\int_{t_0}^{t} dt'\ \frac{\partial}{\partial t'}U(t';t_0) = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\ H(t'U(t';t_0))$$

Since we have $U(t;t_0)$ on both sides of this equation, we cannot really solve for $U(t;t_0)$. However, we can approximate $U(t;t_0)$ using an iterative method:

- 0^{th} order: $U(t;t_0) = \mathbb{1}$.
- 1^{st} order: $U(t;t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H(t')$.
- 2^{nd} order: $U(t;t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\ H(t_1)H(t_2)$.
- 3^{rd} order: $U(t;t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\ H(t_1)H(t_2)$
  $+\left(\frac{-i}{\hbar}\right)^3 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3\ H(t_1)H(t_2)H(t_3)$.

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

  or we can rewrite it using the time ordering operator $\mathcal{T}$ in decreasing order of t,

  $$\boxed{U(t;t_0) = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \mathcal{T}\left[\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n\ H(t_1)H(t_2)\cdots H(t_n)\right]}.$$

  This expression is known as the **Dyson series**. Note that when using the time ordering operator, all upper limits in the integrals become t. This expression for $U(t;t_0)$can also be written as

  $$U(t;t_0) = \mathcal{T}\left[e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\ H(t')}\right]$$

For the majority of this class, we will only deal with Case 1. We will touch on Case 2 and probably Case 3 when we discuss time-dependent perturbation theory. Therefore, as of now, do not worry if you do not really know how to do calculations using these expressions for $U(t;t_0)$.

Propagator in the x-basis

We can write the propagator in the $x-$basis, which can be useful when we perform actual calculations. Basically, we want to write down the matrix element of $U(t;t_0)$ in the $x-$basis, which we will call $U(x,t;x',t_0)$.

$$\begin{aligned} U(x,t;x',t_0) &\equiv \langle x|U(t;t_0)|x'\rangle \\ &= \sum_{n'} e^{-\frac{i}{\hbar}E_{n'}(t-t_0)}\langle x|n'\rangle\langle n'|x'\rangle \\ &= \sum_{n'} e^{-\frac{i}{\hbar}E_{n'}(t-t_0)}\phi^*_{n'}(x)\phi_{n'}(x'). \end{aligned}$$

For a continuous case, we can replace the sum by an integral. For example, in the case of a free particle, the propagator in the $x-$basis is given by

$$\begin{aligned} U(x,t;x',t_0) &\equiv \langle x|U(t;t_0)|x'\rangle \\ &= \int_{-\infty}^{\infty} dp\ e^{-\frac{i}{\hbar}E_p(t-t_0)}\langle x|p\rangle\langle p|x'\rangle \\ &= \int_{-\infty}^{\infty} dp\ e^{-\frac{i}{\hbar}E_p(t-t_0)}\psi^*_p(x)\psi_p(x'), \end{aligned}$$

where $E_p = \dfrac{p^2}{2m}$ and $\psi_p(x) = \dfrac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$ is the eigenstate of the momentum operator in the $x-$basis. Once, we obtain $U(x,t;x',t_0)$, the wavefunction at time t can be calculated by

$$\begin{aligned}
\psi(x,t) &= \langle x|\psi(t)\rangle = \langle x|U(t;t_0=0)|\psi(0)\rangle \\
&= \int_{-\infty}^{\infty} dx' \; \langle x|U(t;t_0=0)|x'\rangle \langle x'|\psi(0)\rangle \\
&= \int_{-\infty}^{\infty} dx' \; U(x,t;x',0)\psi(x',0)
\end{aligned}$$

If we know $U(x,t;x',0)$ and the initial wavefunction $\psi(x,0)$, then we can caluclated $\psi(x,t)$. The difficulty here is to find $U(x,t;x',0)$, which for most systems is difficult to obtain.

Examples of Propagators

There are only few systems where we can write a propagator in an exact analytical form. Here, we will consider only two such systems. The first system is a system of free particle where $H = \dfrac{P^2}{2m}$, and the other is the simple harmonic oscillator that we just discussed in the previous lecture. For the free particle, the propagator is given by

$$U(x,t;x',0) \equiv \langle x|U(t)|x'\rangle = \sqrt{\frac{m}{2\pi\hbar i t}} e^{im\left(x-x'\right)^2/2\hbar t}.$$

I will let prove this expression in the homework. For the simple harmonic oscillator with

$$H = \frac{P^2}{2m} + \frac{m\omega^2 X^2}{2}$$

the propagator is given by

$$U(x,t;x',0) \equiv \langle x|U(t)|x'\rangle = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega t)}} \exp\left\{ \frac{im\omega}{2\hbar \sin(\omega t)} \left[\left(x^2 + x'^2\right)\cos(\omega t) - 2xx' \right] \right\}.$$

I took this expression from a paper by Barone et al. (*Am. J. Phys.* **71** (5), 483 (2003)) I will not try to prove it in this class but instead will give you the paper of Barone et al. to read (for fun!). All I need you to take away from this paper is to realize that the exact form of the propagator for the simple harmonic oscillator can be calculated.

Time-evolution of an arbitrary state

Now, we will consider the time-evolution of an arbitrary state $|\alpha, t_0\rangle$. At the initial time $t_0 = 0$, we can write this state in terms of the eigenstates $|n\rangle$ as

$$|\alpha, t_0 = 0\rangle = \sum_n |n\rangle \langle n|\alpha, 0\rangle \equiv \sum_n c_n(0)\,|n\rangle\,,$$

where $c_n(0) \equiv \langle n|\alpha, 0\rangle$ is a component of the initial state along the eigenstate $|n\rangle$. Next, let us consider the time evolution of $|\alpha, 0\rangle$. This is easy, since we know how the eigenstate, each component, evolves with time:

$$|\alpha(t)\rangle = U(t;0)\,|\alpha,0\rangle = \sum_{n,n'} c_n(0) e^{-\frac{i}{\hbar}E_{n'}t}\,|n'\rangle \langle n'|n\rangle = \sum_n c_n(0) e^{-\frac{i}{\hbar}E_n t}\,|n\rangle \equiv \sum_n c_n(t)\,|n\rangle\,,$$

where $c_n(t) \equiv e^{-\frac{i}{\hbar}E_n t}c_n(0)$ is the time-evolution of each coefficient of the eigenstate $|n\rangle$. We note that this phase change of each component of $|n\rangle$ depends on the eigenvalue E_n, which is normally different. Therefore, the relative phases of $|\alpha(t)\rangle$ changes with time, and hence $|\alpha(t)\rangle$ is different from the initial state $|\alpha, t_0\rangle$.

It is useful to find a complete set of commuting observables so that

$$[A_1, H] = [A_2, H] = \cdots = [A_n, H] = 0$$

and

$$[A_1, A_2] = [A_2, A_3] = \cdots = [A_{n-1}, A_n] = 0.$$

Therefore, we can find the orthonormal basis $|a_1, a_2, \cdots, a_n\rangle$ uniquely, and write $U(t; t_0)$ using this basis.

Expectation of observable as a function of t

Consider an observable A, which does not need to commute with H. We will calculate the expectation of A with respect to a time-evolving state $|n(t)\rangle$, where $|n\rangle$ is the eigenstate of H with the associated eigen-energy E_n.

$$\langle A\rangle_t = \langle n(t)\,|\,A\,|\,n(t)\rangle = \left\langle n\,\middle|\,U^\dagger(t;0)AU(t,0)\,\middle|\,n\right\rangle = \left\langle n\,\middle|\,e^{-iE_nt/\hbar}Ae^{iE_nt/\hbar}\,\middle|\,n\right\rangle = \langle n|A|n\rangle = \langle A\rangle_{t=0}\,.$$

Therefore, the expectation for the stationary state is time-independent.

Now, let us consider the expectation for an arbitrary state $|\alpha(t)\rangle$. The initial state is

$$|\alpha(0)\rangle = \sum_n c_n\,|n\rangle\,,$$

where $c_n = \langle n|\alpha\rangle$ and $|n\rangle$ is the eigenstate of H. The expectation of A with respect to the state $|\alpha(t)\rangle$ is:

$$\langle A\rangle_t = \left[\sum_{n'} c^*_{n'}\,\langle n'|\,e^{iE_{n'}t/\hbar}\right] A \left[\sum_{n''} c_{n''}e^{-iE_nt/\hbar}\,|n''\rangle\right] = \sum_{n',n''} c^*_{n'}c_{c''}\,\langle n'|A|n''\rangle\,e^{-i(E_{n''}-E_{n'})t/\hbar}.$$

The expectation of A with respect to an arbitrary state is time-dependent due to the oscillating terms with frequency $\omega = \dfrac{E_{n''}-E_{n'}}{\hbar}$

3.3 Schrödinger and Heisenberg Interaction Pictures

There are two interpretations how we can view the time evolution in quantum mechanics; one interpretation is called the *Schrödinger picture* and other called the *Heisenberg picture*.

Schrödinger picture

- $|\alpha(t)\rangle \in \mathcal{H}$ evolves with time.
- Operators are fixed.

Heisenberg picture

- $|\alpha\rangle \in \mathcal{H}$ is fixed.

- Operators evolves with time.

In order to understand these two pictures better, we will consider the expectation of an operator A with respect to an arbitrary state $|\alpha(t)\rangle$.

$$\langle A\rangle_t = \langle \alpha(t)\,|\,A\,|\,\alpha(t)\rangle = \left\langle \alpha(0)\,\middle|\,U^\dagger(t;0)AU(t;0)\,\middle|\,\alpha(0)\right\rangle$$

This expectation value must remain the same in both pictures. We can view it using either Schrödinger or Heisenberg picture.

Picture	"ket"	"bra"	Operator
Schroödinger	$\|\alpha(t)\rangle_S = U(t;0)\,\|\alpha(0)\rangle$	${}_S\langle\alpha(t)\| = \langle\alpha(0)\|\,U^\dagger(t;0)$	$A_S = A$
Heisenberg	$\|\alpha\rangle_H = \|\alpha(0)\rangle$	${}_H\langle\alpha\| = \langle\alpha(0)\|$	$A_H(t) = U^\dagger(t;0)AU(t;0)$

Therefore, we can rewrite the expectation as

$$\langle A\rangle_t = {}_S\langle \alpha(t)\,|\,A_S\,|\,\alpha(t)\rangle_S = {}_H\langle \alpha\,|\,A_H(t)\,|\,\alpha\rangle_H$$

Note that in the Schrödinger picture, the parameter t is with the state, while in the Heisenberg picture, t is a parameter for the operator. We can see that at $t = 0$,

$$|\alpha, 0\rangle_S = |\alpha\rangle_H \quad \text{and} \quad A_S = A_H(0),$$

at some later time t,

$$|\alpha(t)\rangle_S = U(t;0)\,|\alpha\rangle_H \quad \textit{and} \quad A_H(t) = U^\dagger(t;0)A_SU(t;0).$$

If the Hamiltonian is time-independent, then we can write

$$|\alpha(t)\rangle_S = e^{-\frac{i}{\hbar}Ht}\,|\alpha\rangle_H$$

and

$$A_H(t) = e^{\frac{i}{\hbar}Ht}A_Se^{-\frac{i}{\hbar}Ht}.$$

We note that in Heisenberg picture, since operators change with time, the eigenstates and hence a basis also change with time. So, we can ask how the basis changes in the Heisenberg picture. Let us suppose that in the Schrödinger picture, we can solve the following eigenvalue problem

$$A_S\,|a\rangle = a\,|a\rangle$$

for a and $|a\rangle$. In the Heisenberg picture, the operator becomes

$$A_H(t) = U^\dagger(t;0)AU(t;0).$$

So what are the eigenvalues and eigenstates for $A_H(t)$? Consider

$$A_H(t)\left(U^\dagger\,|a\rangle\right) = \left(U^\dagger A_SU\right)\left(U^\dagger\,|a\rangle\right) = U^\dagger A_S\,|a\rangle = U^\dagger a\,|a\rangle = a\left(U^\dagger\,|a\rangle\right).$$

Therefore, a is an eigenvalues and $U^\dagger\,|a\rangle$ is an eigenstate of $A_H(t)$. As a result, $U^\dagger\,|a\rangle$ form a basis in the Heisenberg picture. The new basis in the Heisenberg picture is

$$|a(t)\rangle_H = U^\dagger\,|a\rangle\,,$$

which means that the eigenstate or the basis in the Heisenberg picture "rotates" in an opposite sense from the rotation of state in the Schrödinger picture.

Transition Amplitude

We can look at the transition amplitude using either Schrödinger or Heisenberg picture. Suppose that at $t = 0$ a system is in an eigenstate $|a\rangle$ of A. Then at a later time t, B is measured and we want to know the probability that the system is in a state $|b\rangle$, which is an eigenstate of B. The transition amplitude in this case is equal to $\langle b|U|a\rangle$. In the Schrödinger picture, $|a\rangle$ evolves to $U(t;0)\,|a\rangle$ while B is fixed and hence the eigenstate $|b\rangle$ of B remains fixed. On the other hand, in the Heisenberg picture, $|a\rangle$ is fixed while B evolves with time and hence the eigenstate $|b\rangle$, which also acts as a basis, changes with time according to $U^\dagger\,|b\rangle$ for a "ket" or $\langle b|\,U$ for a "bra". We note that the probability P is hence equal to

$$P = |\langle b|U|a\rangle|^2\,,$$

in both Schrödinger and Heisenberg pictures.

3.3.1 Heisenberg Equation of Motion

If we want to make an analogy between classical and quantum mechanics, the Heisenberg interpretation provides a clearer picture. In classical physics, observables such as x and p evolves with time. Therefore, in quantum mechanics, one would expect observables X and P to evolve with time, which is what the Heisenberg picture provides, in order to be consistent with the classical mechanics. So, let us consider a time-derivative of an operator $A_H(t)$ in the Heisenberg picture.

$$\frac{dA_H(t)}{dt} = \frac{d}{dt}\left(U^\dagger A_S U\right) = \frac{\partial U^\dagger}{\partial t}A_S U + U^\dagger A_S\frac{\partial U}{\partial t} + U^\dagger\frac{\partial A_S}{\partial t}U,$$

but from the Schrödinger equation we have

$$\frac{\partial U}{\partial t} = \frac{1}{i\hbar}HU \quad \text{and} \quad \frac{\partial U^\dagger}{\partial t} = -\frac{1}{i\hbar}U^\dagger H.$$

Therefore, we can rewrite $\dfrac{dA_H(t)}{dt}$ as

$$\begin{aligned}
\frac{dA_H(t)}{dt} &= -\frac{1}{i\hbar}U^\dagger HA_S U + \frac{1}{i\hbar}U^\dagger A_S HU + U^\dagger\frac{\partial A_S}{\partial t}U \\
&= -\frac{1}{i\hbar}U^\dagger H\left(UU^\dagger\right)A_S U + \frac{1}{i\hbar}U^\dagger A_S\left(UU^\dagger\right)HU + \frac{\partial\left(U^\dagger A_S U\right)}{\partial t} \\
&= -\frac{1}{i\hbar}\left(U^\dagger HU\right)\left(U^\dagger A_S U\right) + \frac{1}{i\hbar}\left(U^\dagger A_S U\right)\left(U^\dagger HU\right) + \frac{\partial A_H}{\partial t} \\
&= -\frac{1}{i\hbar}HA_H + \frac{1}{i\hbar}A_H H + \dot{A}_H,
\end{aligned}$$

where $\left(U^\dagger HU\right) = H$, $\left(U^\dagger A_S U\right) = A_H$, and $\frac{\partial A_H}{\partial t} = \dot{A}_H$.

$$\Rightarrow \quad \frac{dA_H(t)}{dt} = \frac{1}{i\hbar}\left(A_H H - HA_H\right) + \dot{A}_H = \frac{1}{i\hbar}\left[A_H, H\right] + \dot{A}_H.$$

Therefore, the Heisenberg equation of motion is

$$\boxed{\frac{dA_H(t)}{dt} = \frac{1}{i\hbar}\left[A_H(t), H\right] + \dot{A}_H}$$

This equation is related to the Poisson bracket in classical mechanics, where

$$\frac{dA}{dt} = \{A, H\} ,$$

where A is an observable and H is a Hamiltonian in classical mechanics.

3.3.2 Time-energy uncertainty relation

Unlike observables X and P, t is not an operator in quantum mechanics. Hence, there is no direct analogue of the uncertainty relation of $\Delta X \Delta P$ for time and energy. However, we know that a state, which is not an eigenstate evolve or change with time. So, a question we can ask ourselves is that: *How rapidly does wave function change its form with t?* Let us define

$$c(t) = \langle \alpha | U(t; 0) | \alpha \rangle ,$$

which is the overlap of the initial state $|\alpha\rangle$ and the final state $U|\alpha\rangle$, to be the change of state at time t with respect to the state at $t = 0$. It is obvious that if $|\alpha\rangle$ is an eigenstate of H (a stationary state), then $|c(t)|^2 = 1$ for all time. However, in general for an arbitrary state, we have

$$|\alpha\rangle = \sum_n c_n |n\rangle ,$$

where $|n\rangle$ is an eigenstate of H, and

$$|\alpha(t)\rangle = U(t; 0) |\alpha\rangle = \sum_n c_n e^{-\frac{i}{\hbar} E_n t} |n\rangle .$$

Due to the oscillation and interference of the phase terms, the overlap decreases from 1, if $|\alpha\rangle$ is not an eigenstate of H. We note that for states whose energies are close together, it takes a long time for the states to spread out. On the other hand, if the states are far away from one another in terms of eigenenergies, then it does not take very long for them to spread out. Therefore, in this sense, a small uncertainty in energy gives rise to a large uncertainty in time and vice versa. We will derive this statement mathematically. Suppose that we measure an observable A with $[A, H] \neq 0$. We can then calculate a time derivative of the expectation value of A $\left(\frac{d\langle A\rangle}{dt}\right)$,

$$\frac{d\langle A\rangle}{dt} \sim \frac{\Delta A}{\Delta t} \quad \Rightarrow \quad \Delta t \sim \frac{\Delta A}{\frac{d\langle A\rangle}{dt}} .$$

But from the Heisenberg equation of motion, we know that

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar} \langle [A, H] \rangle .$$

From the Schmidt inequality, we have

$$\begin{aligned}
\langle \Delta A\rangle^2 \langle \Delta H\rangle^2 &\geq \frac{1}{4} |\langle [A, H]\rangle|^2 = \frac{\hbar^2}{4} \left| \frac{d\langle A\rangle}{dt} \right|^2 \\
\Rightarrow \quad \left[\frac{\langle \Delta A\rangle^2}{\left|\frac{d\langle A\rangle}{dt}\right|^2} \right] \langle \Delta H\rangle^2 &\geq \frac{\hbar^2}{4} \\
\Rightarrow \quad \langle \Delta t\rangle^2 \langle \Delta H\rangle^2 &\geq \frac{\hbar^2}{4} .
\end{aligned}$$

But we know that $\sqrt{\langle \Delta H \rangle^2} = \Delta E$ and $\sqrt{\langle \Delta t \rangle^2} = \Delta t$. Therefore, the time-energy uncertainty relation is equal to

$$\boxed{\Delta E \cdot \Delta t \geq \frac{\hbar}{2}}.$$

In other words, if a system has a small energy width (states are all close together), the shape of the wave-function change slowly.