Quantum Dynamics

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As in classical mechanics, time is a parameter in quantum mechanics. It is distinct from space in the sense that, while we have Hermitian operators, $\hat{\mathbf{X}}$, for position and therefore expect a measurement of postion to yield any eigenvalue of $\hat{\mathbf{X}}$, there is no $\hat{T}$ operator for measurements of time. We cannot expect measurements to yield distributions of eigenvalues of time, perhaps because we are stuck in one particular time ourselves. In any case, while there are differences between time and space, there does still exists a unitary time translation operator, and its infinitesimal generator − energy − is an central observable.

In classical physics we make a distinction between *active* transformations which transform the physical position and other variables, and *passive* transformations which leave the physical particles fixed and transform the coordinates. The same distinction occurs in quantum mechanics. A given time-dependent wave function, $\psi(\mathbf{x}, t) = \langle \mathbf{x} \mid \psi \rangle (t)$, has the same two interpretations. We may describe the system by an explicitly time-dependent ket,

$$|\psi\rangle = |\psi, t\rangle$$

taking the basis kets, $|a\rangle$, (whatever they are) as fixed. The state is then a time varying vector in the space spanned by the fixed basis kets.

$$\psi(\mathbf{x}, t) = \langle \mathbf{x} \mid \psi, t\rangle$$

Alternatively, we may let the state be a fixed ket, while the basis kets evolve in time, $|a, t\rangle$,

$$\psi(\mathbf{x}, t) = \langle \mathbf{x}, t \mid \psi\rangle$$

The two descriptions are equivalent, though one or the other may be convenient for a given problem. In perturbation theory, it is even useful to mix the two pictures, giving part of the time dependence to the basis and the rest to the state. For the moment, we consider time-dependent states in a fixed basis.

In quantum mechanics, the terms active and passive are replaced, respectively by speaking of the *Schrödinger picture* and the *Heisenberg picture*. In the Schrödinger picture, the state vector becomes time dependent with the basis fixed, coresponding to an active transformation in classical physics. The Heisenberg picture begins by letting the *operators* become time dependent, with the consequence that their eigenstates and therefore the basis, becomes time dependent.

1 The time translation operator

We define the time translation operator to be the mapping that takes any time-dependent state from some initial time, t_0, to a later time, t,

$$\hat{\mathcal{U}}(t, t_0) |\psi, t_0\rangle = |\psi, t_0; t\rangle$$

In the limit as $t \to t_0$, this must be the identity,

$$\begin{aligned} \hat{\mathcal{U}}(t_0, t_0) |\psi, t_0\rangle &= |\psi, t_0; t_0\rangle \\ &= |\psi, t_0\rangle \end{aligned}$$

We require time evolution to preserve probabilities, so by Wigner's theorem it must be either unitary or antiunitary, and there is no conflict in taking it to be unitary,

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

In a fixed basis $|a\rangle$, we may expand any state as

$$|\psi, t\rangle = \sum_a c_a(t)\,|a\rangle$$

Notice that the time dependence allows the state to move from one eigenstate to another. Since the state is normalized at all times, we require

$$\begin{aligned}
1 &= \langle \psi, t_0; t \mid \psi, t_0; t\rangle \\
&= \left(\sum_{a'} c_a^*(t)\,\langle a'|\right)\left(\sum_a c_a(t)\,|a\rangle\right) \\
&= \sum_a \sum_{a'} c_a^*(t)\,c_a(t)\,\langle a' \mid a\rangle \\
&= \sum_a \sum_{a'} c_a^*(t)\,c_a(t)\,\delta_{aa'} \\
&= \sum_a |c_a(t)|^2
\end{aligned}$$

Unitarity of the time translation operator requires this to hold at every time t.

We may write $\hat{\mathcal{U}}(t, t_0)$ as an exponential,

$$\hat{\mathcal{U}}(t, t_0) = e^{-\frac{i}{\hbar}\hat{\Omega}(t)}$$

Then, for an infinitesimal time change, $t = t_0 + dt$,

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

where unitarity of $\hat{\mathcal{U}}(t, t_0)$ requires $\hat{\Omega}^{\dagger} = \hat{\Omega}$.

2 The Schrödinger equation

Consider three sequential times, $t_0 < t_1 < t_2$. It must be the case that acting with on an arbitrary state with $\hat{\mathcal{U}}(t_0, t_2)$ gives the same result as acting with $\hat{\mathcal{U}}(t_0, t_1)$ followed by $\hat{\mathcal{U}}(t_1, t_2)$:

$$\hat{\mathcal{U}}(t_0, t_2)\,|\psi, t_0\rangle = \hat{\mathcal{U}}(t_1, t_2)\,\hat{\mathcal{U}}(t_0, t_1)\,|\psi, t_0\rangle$$

since both of these must give $|\psi, t_0; t_2\rangle$. Since the times are arbitrary, this gives an operator equality,

$$\hat{\mathcal{U}}(t_0, t_2) = \hat{\mathcal{U}}(t_1, t_2)\,\hat{\mathcal{U}}(t_0, t_1)$$

Now examine the time evolution of the time translation operator, $\hat{\mathcal{U}}(t, t_0)$, at some time t. Translating the time t by an additional small amount Δt,

$$\begin{aligned}
\hat{\mathcal{U}}(t + \Delta t, t_0) &= \hat{\mathcal{U}}(\Delta t, t)\,\hat{\mathcal{U}}(t, t_0) \\
&= \left(\hat{1} - \frac{i}{\hbar}\hat{H}(t)\,\Delta t\right)\hat{\mathcal{U}}(t, t_0) \\
&= \hat{\mathcal{U}}(t, t) - \frac{i\Delta t}{\hbar}\hat{H}(t)\,\hat{\mathcal{U}}(t, t_0)
\end{aligned}$$

Rearranging,

$$\hat{H}(t)\hat{\mathcal{U}}(t,t_0) = i\hbar \frac{\hat{\mathcal{U}}(t+\Delta t,t_0)-\hat{\mathcal{U}}(t,t_0)}{\Delta t}$$

so taking the limit as $\Delta t \to 0$,

$$\hat{H}(t)\hat{\mathcal{U}}(t,t_0) = i\hbar\frac{\partial}{\partial t}\hat{\mathcal{U}}(t,t_0) \tag{1}$$

This is the Schrödinger equation for the time evolution operator. Finally, let this operator relation act on an initial state, $|\psi,t_0\rangle$, to give the time evolution equation for that state,

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

This gives the *time-dependent Schrödinger equation*,

$$\hat{H}(t)|\psi,t\rangle = i\hbar\frac{\partial}{\partial t}|\psi,t\rangle$$

This is basis independent form of the familiar Schrödinger equation.

Since the state is arbitrary, we recognize the generator of time translations as the Hamiltonian,

$$\hat{\Omega}(t) = i\hbar\frac{\partial}{\partial t} = \hat{H}$$

3 The full time evolution operator

As we did the the translation operator, we may recover the form for a finite time translation trom the infinitesimal solution. We distinguish three cases:

1. $\hat{H}$ independent of time
2. $\hat{H}$ depends on time, but $\left[\hat{H}(t),\hat{H}(t')\right]=0$ for any two times, t,t'.
3. $\left[\hat{H}(t),\hat{H}(t')\right]\neq 0$

The first case may be solved by direction integration of the Schrödinger equation for $\hat{\mathcal{U}}(t,t_0)$,

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

With $\hat{H}(t)=\hat{H}$ constant, this immediately gives

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

We may solve the second case by iterating the infinitesimal transformation. Dividing the time interval $t-t_0$ into n equal parts of length $\Delta t = \frac{t-t_0}{n}$, we take the product of n infinitesimal time translations, where the k^{th} time translation may be written to first order as

$$\hat{1} - \frac{i}{\hbar}\hat{H}(t_0+k\Delta t)\Delta t = e^{-\frac{i}{\hbar}\hat{H}(t_0+k\Delta t)\Delta t}$$

Then the finite transformation is

$$\begin{aligned}\hat{\mathcal{U}}(t,t_0) &= \lim_{n\to\infty}\left(\hat{1}-\frac{i}{\hbar}\hat{H}(t_0)\Delta t\right)\left(\hat{1}-\frac{i}{\hbar}\hat{H}(t_0+\Delta t)\Delta t\right)\left(\hat{1}-\frac{i}{\hbar}\hat{H}(t_0+2\Delta t)\Delta t\right)\ldots\left(\hat{1}-\frac{i}{\hbar}\hat{H}(t-\Delta t)\Delta t\right)\\ &= \lim_{n\to\infty}\prod_{k=0}^{n-1}e^{-\frac{i}{\hbar}\hat{H}(t_0+k\Delta t)\Delta t}\\ &= \lim_{n\to\infty}\exp\left(-\frac{i}{\hbar}\sum_{k=0}^{n-1}\hat{H}(t_0+k\Delta t)\Delta t\right)\\ &= \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,dt'\right)\end{aligned}$$

Notice that as $n\to\infty$ the linear approximation becomes exact and the sum becomes an integral. Because all of the $\hat{H}(t')$ commute, we see directly that this form of $\hat{\mathcal{U}}(t,t_0)$ satisfies the Schrödinger equation,

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

The general case is considerably more involved because we have to keep track of the order of the terms in the power series. The result, called the *Dyson series*, has the form

$$\begin{aligned}\hat{\mathcal{U}}(t,t_0) &= \lim_{n\to\infty}\left(\hat{1}-\frac{i}{\hbar}\hat{H}(t_0)\Delta t\right)\left(\hat{1}-\frac{i}{\hbar}\hat{H}(t_0+\Delta t)\Delta t\right)\left(\hat{1}-\frac{i}{\hbar}\hat{H}(t_0+2\Delta t)\Delta t\right)\ldots\\ &= \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n\int_{t_0}^{t}\hat{H}(t_1)\,dt_1\int_{t_0}^{t_1}\hat{H}(t_2)\,dt_2\ldots\int_{t_0}^{t_{n-1}}\hat{H}(t_n)\,dt_n\\ &\equiv \mathbb{T}\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,dt'\right)\end{aligned}$$

The crucial step occurs in noticing that the n^{th} term in the sum, may be extend each of the n integrals all the way from t_0 to the final time t and dividing by $n!$,

$$\left(-\frac{i}{\hbar}\right)^n\int_{t_0}^{t}\hat{H}(t_1)\,dt_1\int_{t_0}^{t_1}\hat{H}(t_2)\,dt_2\ldots\int_{t_0}^{t_{n-1}}\hat{H}(t_n)\,dt_n\to\frac{1}{n!}\left(-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,dt'\right)^n$$

with the caveat that in the resulting n^{th} power on the right must be *time ordered,*

$$\frac{1}{n!}\mathbb{T}\left(-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\,dt'\right)^n$$

meaning that the n factors of the Hamiltonian must be returned to the product form on the left with $t_1<t_2<\ldots<t_n$ in increasing order. This notational trick allows us to write the result as an exponential, but the final exponential is simply shorthand for the whole series

Almost all of the applications we consider will involve time-independent Hamiltonians.

4 Energy eigenkets

Suppose we choose as a basis the eigenkets of an operator $\hat{A}$ which commutes with the (time-independent) Hamiltonian,

$$\left[\hat{A},\hat{H}\right]=0$$

This operator could be the Hamiltonian itself, or another observable, but in either case, the eigenkets, $|a\rangle$, may be chosen to simultaneously be eigenkets of $\hat{H}$,

$$\hat{H}|a\rangle = E_a|a\rangle$$

Consider the time evolution of an arbitrary initial state, $|\psi, t_0\rangle$. In terms of the $\hat{A}$ basis,

$$\begin{aligned}|\psi, t_0\rangle &= \sum_a |a\rangle\langle a \mid \psi, t_0\rangle \\ &= \sum_a c_a|a\rangle\end{aligned}$$

where $c_a \equiv \langle a \mid \psi, t_0\rangle$. Then the time evolution is given by

$$\begin{aligned}|\psi, t_0; t\rangle &= \exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\psi, t_0\rangle \\ &= \sum_a c_a \exp\left(-\frac{i}{\hbar}\hat{H}t\right)|a\rangle \\ &= \sum_a c_a \exp\left(-\frac{i}{\hbar}E_n t\right)|a\rangle\end{aligned}$$

Defining time dependent expansion coefficients, $c_a(t) \equiv c_a e^{-\frac{i}{\hbar}E_a t}$, the state becomes

$$|\psi, t_0; t\rangle = \sum_a c_a(t)|a\rangle$$

In general, this means that the probabilities for measuring the system to be in different states varies with time. The only exceptions are the probatilities for measuring a fixed *energy* eigenstate. Concretely, the probability for measuring the state to have energy E_{a_0} at time t is

$$\begin{aligned}P(E_{a_0}) &= |\langle a_0 \mid \psi, t_0; t\rangle|^2 \\ &= |c_{a_0}(t)|^2 \\ &= \left|c_{a_0}e^{-\frac{i}{\hbar}E_{a_0}t}\right|^2 \\ &= |c_{a_0}|^2\end{aligned}$$

that is, the same as the original probability. However, the probability for finding a general superpostion changes. Let $|\chi\rangle = |E_1\rangle + |E_2\rangle$ be a superposition of eigenstates for energies E_1 and E_2. The probability of measuring the system to be in the state $|\chi\rangle$ is

$$\begin{aligned}P(\chi) &= |\langle \chi \mid \psi, t_0; t\rangle|^2 \\ &= |c_1(t) + c_2(t)|^2 \\ &= \left|c_1 e^{-\frac{i}{\hbar}E_1 t} + c_2 e^{-\frac{i}{\hbar}E_2 t}\right|^2\end{aligned}$$

We pull out a common phase and set $\Delta E = E_2 - E_1$. Then

$$\begin{aligned}P(\chi) &= \left|e^{-\frac{i}{2\hbar}E_1 t}e^{-\frac{i}{2\hbar}E_2 t}\left(c_1 e^{\frac{i}{2\hbar}\Delta E t} + c_2 e^{-\frac{i}{2\hbar}\Delta E t}\right)\right|^2 \\ &= \left(c_1 e^{\frac{i}{2\hbar}\Delta E t} + c_2 e^{-\frac{i}{2\hbar}\Delta E t}\right)\left(c_1^* e^{-\frac{i}{2\hbar}\Delta E t} + c_2^* e^{\frac{i}{2\hbar}\Delta E t}\right) \\ &= |c_1|^2 + |c_2|^2 + c_1 c_2^* e^{\frac{i}{\hbar}(E_2 - E_1)t} + c_1^* c_2 e^{-\frac{i}{\hbar}(E_2 - E_1)t} \\ &= |c_1|^2 + |c_2|^2 + 2\mathcal{R}e\left(c_1 c_2^* e^{\frac{i}{\hbar}(E_2 - E_1)t}\right)\end{aligned}$$

which is time dependent unless the energy is degenerate with $\Delta E = 0$.

The problem of quantum dynamics is now reduced to finding a maximal set of operators which commute with the Hamiltonian. We may then label states using these and study the time evolution of arbitrary initial states.

Exercise: Find the time evolution of a particle in an infinite square well,

$$V(x) = \begin{cases} \infty & x < -\frac{L}{2} \\ 0 & -\frac{L}{2} < x < \frac{L}{2} \\ \infty & x > \frac{L}{2} \end{cases}$$

when its state at time t_0 is:

1. $\langle x \mid \psi, t_0 \rangle = \sqrt{\frac{2}{L}} \cos \frac{\pi x}{L}$
2. $\langle x \mid \psi, t_0 \rangle = \sqrt{\frac{1}{L}} \cos \frac{\pi x}{L} + \sqrt{\frac{1}{L}} \cos \frac{3\pi x}{L}$

5 Expectation values of observables

Once we have the state of a system expanded in energy eigenkets, we can find the time dependence of the expectation values for any observable, $\hat{\mathcal{O}}$,

$$\begin{aligned} \langle \psi, t_0; t | \hat{\mathcal{O}} | \psi, t_0; t \rangle &= \sum_{a,a'} \langle \psi, t_0; t \mid a' \rangle \langle a' | \hat{\mathcal{O}} | a \rangle \langle a' \mid \psi, t_0; t \rangle \\ &= \sum_{a,a'} c^*_{a'}(t)\, c_a(t) \langle a' | \hat{\mathcal{O}} | a \rangle \\ &= \sum_{a,a'} c^*_{a'} c_a e^{-\frac{i}{\hbar}(E_a - E_{a'})t} \langle a' | \hat{\mathcal{O}} | a \rangle \end{aligned}$$

As an example, consider a 2-state system. The Hamiltonian for a spin-$\frac{1}{2}$ particle with magnetic moment $\boldsymbol{\mu} = \frac{e}{mc}\mathbf{S}$, in a magnetic field, $\mathbf{B}$, is

$$\begin{aligned} \hat{H} &= -\hat{\boldsymbol{\mu}} \cdot \mathbf{B} \\ &= -\frac{e}{mc} \hat{\mathbf{S}} \cdot \mathbf{B} \end{aligned}$$

Let $\mathbf{B} = -B\hat{\mathbf{k}}$ be constant, so the time-independent Hamiltonian is

$$\hat{H} = \frac{eB}{mc} \hat{S}_z$$

The energy eigenkets are then just the $|\pm\rangle$ eigenkets of $\hat{S}_z$ with energies

$$\begin{aligned} \hat{H} |\pm\rangle &= E_\pm |\pm\rangle \\ &= \pm \frac{e\hbar B}{2mc} |\pm\rangle \\ &= \pm \frac{\hbar \omega}{2} |\pm\rangle \end{aligned}$$

where $\omega \equiv \frac{eB}{mc}$. Setting $t_0 = 0$, the time evolution of a general normalized state,

$$|\chi\rangle = \cos\theta |+\rangle + e^{i\varphi} \sin\theta |-\rangle$$

is

$$\begin{aligned}
|\chi, t\rangle &= \hat{\mathcal{U}}(t,0)|\chi\rangle \\
&= e^{-\frac{i}{\hbar}\hat{H}t}|\chi\rangle \\
&= e^{-\frac{i}{\hbar}\hat{H}t}\left(\cos\theta|+\rangle + e^{i\varphi}\sin\theta|-\rangle\right) \\
&= e^{-\frac{i}{\hbar}E_+t}\cos\theta|+\rangle + e^{-\frac{i}{\hbar}E_-t}e^{i\varphi}\sin\theta|-\rangle \\
&= e^{-\frac{i\omega t}{2}}\cos\theta|+\rangle + e^{\frac{i\omega t}{2}}e^{i\varphi}\sin\theta|-\rangle \\
&= e^{-\frac{i\omega t}{2}}\left[\cos\theta|+\rangle + e^{i(\omega t+\varphi)}\sin\theta|-\rangle\right]
\end{aligned}$$

The probability for measuring the system to be in the spin-up state is then

$$\begin{aligned}
|\langle + \mid \chi, t\rangle|^2 &= \left|e^{-\frac{i\omega t}{2}}\left[\cos\theta\langle + \mid +\rangle + e^{i(\omega t+\varphi)}\sin\theta\langle + \mid -\rangle\right]\right|^2 \\
&= \cos^2\theta
\end{aligned}$$

which is the same as the initial probability. However, if we look at the probability that the x-component of spin is up, we find

$$\begin{aligned}
\left|\left\langle \hat{S}_x, + \mid \chi, t\right\rangle\right|^2 &= \left|\left(\frac{1}{\sqrt{2}}\langle+| + \frac{1}{\sqrt{2}}\langle-|\right)e^{-\frac{i\omega t}{2}}\left[\cos\theta|+\rangle + e^{i(\omega t+\varphi)}\sin\theta|-\rangle\right]\right|^2 \\
&= \frac{1}{2}\left|\left(\cos\theta + e^{i(\omega t+\varphi)}\sin\theta\right)\right|^2 \\
&= \frac{1}{2}\left(\cos\theta + e^{i(\omega t+\varphi)}\sin\theta\right)\left(\cos\theta + e^{-i(\omega t+\varphi)}\sin\theta\right) \\
&= \frac{1}{2}\left(\cos^2\theta + \sin^2\theta + \left(e^{-i(\omega t+\varphi)} + e^{i(\omega t+\varphi)}\right)\sin\theta\cos\theta\right) \\
&= \frac{1}{2}\left(1 + \sin 2\theta\cos(\omega t+\varphi)\right)
\end{aligned}$$

6 Time-energy uncertainty

Consider a system with a continuous energy spectrum and many particles. Let the state be expanded in energy eigenkets,

$$\begin{aligned}
|\psi, t_0; t\rangle &= \exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\psi, t_0\rangle \\
&= \int \rho(E)\,dE\,c(E)\exp\left(-\frac{i}{\hbar}\hat{H}t\right)|E\rangle \\
&= \int \rho(E)\,dE\,c(E)\,e^{-\frac{i}{\hbar}Et}|E\rangle
\end{aligned}$$

where $\rho(E)$ characterizes the distritubion of energy eigenstates and the orthonormality relation is

$$\rho(E')\langle E' \mid E\rangle = \delta(E - E')$$

Consider the correlation between the initial state, $|\psi, t_0\rangle$, and the state at time t,

$$\begin{aligned}
C(t) \equiv \langle \psi, t_0 \mid \psi, t_0; t\rangle &= \langle \psi, t_0 \exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\psi, t_0\rangle \\
&= \int \rho(E')\,dE'\,c^*(E')\langle E'|\int \rho(E)\,dE\,c(E)\,e^{-\frac{i}{\hbar}Et}|E\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \int\int \rho(E)\,\rho(E')\,dE dE'\;\; c^*(E')\,c(E)\,e^{-\frac{i}{\hbar}Et}\,\langle E' \mid E\rangle \\
&= \int dE' \int \rho(E)\,dE\;\; |c(E)|^2\,e^{-\frac{i}{\hbar}Et} \\
&= \int \rho(E)\,dE\;\; |c(E)|^2\,e^{-\frac{i}{\hbar}Et}
\end{aligned}
$$

Suppose the initial distribution is peaked around some energy E_0. Write $C(t)$ as

$$
\begin{aligned}
C(t) &= \int \rho(E)\,dE\;\; |c(E)|^2\,e^{-\frac{i}{\hbar}Et} \\
&= e^{-\frac{i}{\hbar}E_0 t}\int \rho(E)\,dE\;\; |c(E)|^2\,e^{-\frac{i}{\hbar}(E-E_0)t}
\end{aligned}
$$

For energies far from E_0, the exponential $e^{-\frac{i}{\hbar}(E-E_0)t}$ oscillates rapidly and the value of the integral is small as long as $\rho(E)$ and $c(E)$ vary slowly, and $(E-E_0)\,\Delta t \gg \hbar$. On the other hand, there will be coherent contributions for any time interval Δt such that

$$
\frac{(E-E_0)\,\Delta t}{\hbar} \gtrsim 1
$$

Therefore, times Δt and energies $E = E_0 + \Delta E$ contribute significantly, where

$$
\Delta E \Delta t \;\;\gtrsim\;\; \hbar
$$

This is a very different statement than the necessary relationship between the uncertainties in conjugate observables. In particular, recall that there is no Hermitian operator corresponding to a measurement of time, so the general result for noncommuting operators does not hold.

7 The Heisenberg picture

Heisenberg developed a different formulation of quantum mechanics, originally based on matrices, in which the dynamical equations of Hamiltonian mechanics take a very similar quantum form. Since the time-dependent dynamical variables of mechanics are replaced by operators in the quantum realm, those operators are time-dependent in the Heisenberg picture.

We take a different approach from the historical development. In keeping with the parallel between active and passive transformations, we begin by placing the time dependence in the basis kets. Start with the time-dependent wave function and let the basis carry the time dependence.

$$
\begin{aligned}
\psi(\mathbf{x},t) &= \langle \mathbf{x} \mid \psi\rangle(t) \\
&= \langle \mathbf{x}, t \mid \psi\rangle
\end{aligned}
$$

For this to agree with the Schrödinger picture result we set $|\psi, t_0\rangle = |\psi\rangle$ and require

$$
\begin{aligned}
\langle \mathbf{x}, t \mid \psi\rangle &= \langle \mathbf{x}|\hat{\mathcal{U}}(t,t_0)|\psi\rangle \\
&= \left(\langle \mathbf{x}|\hat{\mathcal{U}}(t,t_0)\right)|\psi\rangle
\end{aligned}
$$

Since $|\psi\rangle$ is arbitrary

$$
\langle \mathbf{x}|\hat{\mathcal{U}}(t,t_0) \;\;=\;\; \langle \mathbf{x}, t|
$$

and for the kets,

$$
|\mathbf{x}, t\rangle = \hat{\mathcal{U}}^\dagger(t,t_0)\,|\mathbf{x}, t_0\rangle
$$

Notice that while in the active Schrödinger picture states rotated with the action of $\hat{\mathcal{U}}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$, the basis transforms in the reverse sense with the adjoint, $\hat{\mathcal{U}}^\dagger(t,t_0) = e^{\frac{i}{\hbar}\hat{H}(t-t_0)}$.

7.1 Time dependent operators and the Heisenberg equation of motion

Next, consider how this affects the definition of the position operator through its eigenvalue equation. At the initial time, we have

$$\hat{\mathbf{X}}\left|\mathbf{x}\right\rangle = \mathbf{x}\left|\mathbf{x}\right\rangle$$

Multiplying on the left by $\hat{\mathcal{U}}^{\dagger}(t,t_0)$ and inserting the identity, $\hat{1} = \hat{\mathcal{U}}(t,t_0)\hat{\mathcal{U}}^{\dagger}(t,t_0)$ this becomes

$$\begin{aligned}\hat{\mathcal{U}}^{\dagger}\hat{\mathbf{X}}\hat{\mathcal{U}}\hat{\mathcal{U}}^{\dagger}\left|\mathbf{x}\right\rangle &= \mathbf{x}\hat{\mathcal{U}}^{\dagger}\left|\mathbf{x}\right\rangle \\ \hat{\mathcal{U}}^{\dagger}\hat{\mathbf{X}}\hat{\mathcal{U}}\left|\mathbf{x},t\right\rangle &= \mathbf{x}\left|\mathbf{x},t\right\rangle\end{aligned}$$

We see that the time-dependent basis kets are eigenkets of the time-dependent operator,

$$\hat{\mathbf{X}}(t) \equiv \hat{\mathcal{U}}^{\dagger}(t,t_0)\,\hat{\mathbf{X}}(t_0)\,\hat{\mathcal{U}}(t,t_0)$$

A similar argument holds for any Schrödinger picture observable, $\hat{A}_S$, and we let all operators change their time-dependence in this same way,

$$\hat{A}_H(t) \equiv \hat{\mathcal{U}}^{\dagger}(t,t_0)\,\hat{A}_S\hat{\mathcal{U}}(t,t_0)$$

Notice that $\hat{A}_S$ may or may not already have some additional explicit time dependence.

From the Schrödinger equation for the time translation operator, eq.(1), we immediately have

$$\begin{aligned}\frac{d\hat{A}_H(t)}{dt} &= \frac{\partial\hat{\mathcal{U}}^{\dagger}}{\partial t}\hat{A}_S\hat{\mathcal{U}} + \hat{\mathcal{U}}^{\dagger}\frac{\partial\hat{A}_S}{\partial t}\hat{\mathcal{U}} + \hat{\mathcal{U}}^{\dagger}\hat{A}_S\frac{\partial\hat{\mathcal{U}}}{\partial t} \\ &= \frac{i}{\hbar}\hat{\mathcal{U}}^{\dagger}\hat{H}(t)\,\hat{A}_S\hat{\mathcal{U}} + \hat{\mathcal{U}}^{\dagger}\frac{\partial\hat{A}_S}{\partial t}\hat{\mathcal{U}} - \frac{i}{\hbar}\hat{\mathcal{U}}^{\dagger}\hat{A}_S\hat{H}(t)\,\hat{\mathcal{U}} \\ &= \frac{i}{\hbar}\hat{\mathcal{U}}^{\dagger}\left[\hat{H}(t),\hat{A}_S\right]\hat{\mathcal{U}} + \hat{\mathcal{U}}^{\dagger}\frac{\partial\hat{A}_S}{\partial t}\hat{\mathcal{U}}\end{aligned}$$

Since $\hat{\mathcal{U}}$ commutes with the Hamiltonian,

$$\frac{i}{\hbar}\hat{\mathcal{U}}^{\dagger}\left[\hat{H}(t),\hat{A}_S\right]\hat{\mathcal{U}} = \frac{i}{\hbar}\left[\hat{H}(t),\hat{A}_H\right]$$

Writing the last term as $\hat{\mathcal{U}}^{\dagger}\left(\frac{\partial\hat{A}}{\partial t}\right)_S\hat{\mathcal{U}} = \left(\frac{\partial\hat{A}}{\partial t}\right)_H$ we have the *Heisenberg equation of motion*,

$$\frac{d\hat{A}_H(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}(t),\hat{A}_H(t)\right] + \left(\frac{\partial\hat{A}(t)}{\partial t}\right)_H \qquad (2)$$

This has exactly the form of the classical Hamiltonian equation of motion with the Poisson bracket $\{H,A\}$ replaced by $\frac{i}{\hbar}$ times the commutator, $\frac{i}{\hbar}\left[\hat{H},\hat{A}\right]$.

If a operator has no time dependence in the active picture $\frac{\partial\hat{A}_S(t)}{\partial t} = 0$, and commutes with the Hamiltonian $\left[\hat{H},\hat{A}_H\right] = 0$, then it is conserved

$$\frac{d\hat{A}_H(t)}{dt} = 0$$

again resembling the classical conservation result.

7.2 Ehrenfest's Theorem

In the Heisenberg picture, let the Hamiltonian be given by

$$\hat{H} = \frac{1}{2m}\hat{\mathbf{P}}^2 + V\left(\hat{\mathbf{X}}\right)$$

Then the rate of change of the momentum operator is given by

$$\begin{aligned}
\frac{d\hat{\mathbf{P}}}{dt} &= \frac{1}{i\hbar}\left[\hat{\mathbf{P}},\hat{H}\right] \\
&= \frac{1}{i\hbar}\left[\hat{\mathbf{P}},\frac{1}{2m}\hat{\mathbf{P}}^2+V\left(\hat{\mathbf{X}}\right)\right] \\
&= \frac{1}{i\hbar}\left[\hat{\mathbf{P}},V\left(\hat{\mathbf{X}}\right)\right]
\end{aligned}$$

and we show in the next section that

$$\left[\hat{\mathbf{P}},V\left(\hat{\mathbf{X}}\right)\right] = -i\hbar\boldsymbol{\nabla}V\left(\hat{\mathbf{X}}\right)$$

Therefore, we reproduce an operator form of the classical equation of motion,

$$\frac{d\hat{\mathbf{P}}}{dt} = -\boldsymbol{\nabla}V\left(\hat{\mathbf{X}}\right)$$

This holds only in the Heisenberg picture, but if we take expectation values, these are the same in both the Schrödinger and Heisenberg pictures, and we have the *Ehrenfest theorem*,

$$\frac{d\left\langle\hat{\mathbf{P}}\right\rangle}{dt} = -\left\langle\boldsymbol{\nabla}V\left(\hat{\mathbf{X}}\right)\right\rangle \tag{3}$$

In the special case of a free particle, $V=0$ and we may integrate,

$$\begin{aligned}
\frac{d\hat{\mathbf{P}}}{dt} &= 0 \\
\hat{\mathbf{P}}(t) &= \hat{\mathbf{P}}(0)
\end{aligned}$$

The position operator follows from

$$\begin{aligned}
\frac{d\hat{\mathbf{X}}}{dt} &= \frac{1}{i\hbar}\left[\hat{\mathbf{X}},\frac{1}{2m}\hat{\mathbf{P}}^2\right] \\
&= \frac{1}{m}\hat{\mathbf{P}}(t) \\
&= \frac{1}{m}\hat{\mathbf{P}}(0)
\end{aligned}$$

so integrating

$$\hat{\mathbf{X}}(t) = \hat{\mathbf{X}}(0)+\frac{1}{m}\hat{\mathbf{P}}(0)\,t$$

Notice that

$$\begin{aligned}
\left[\hat{X}_i(0),\hat{X}_j(t)\right] &= \frac{1}{m}\left[\hat{X}_i(0),\hat{P}_j(0)\right]t \\
&= \frac{i\hbar t}{m}\delta_{ij}
\end{aligned}$$

and there is an uncertainty relation

$$\left(\Delta\hat{X}(t)\right)^2\left(\Delta\hat{X}(0)\right)^2 \geq \frac{\hbar^2 t^2}{4m^2}$$

Any initial spread in the expectation of the position therefore grows in time.

8 Some useful commutation relations

First, consider the commutator of the position operator with a power of the momentum operator:

$$\hat{A}_k \equiv \left[\hat{X}, \hat{P}_x^k\right]$$

Using the identity

$$\begin{aligned}
\left[\hat{A}, \hat{B}\hat{C}\right] &= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} \\
&= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A} \\
&= \left[\hat{A}, \hat{B}\right]\hat{C} + \hat{B}\left[\hat{A}, \hat{C}\right]
\end{aligned}$$

and writing $\hat{P}_x^k$ as the product $\hat{P}_x^{k-1}\hat{P}_x$ this becomes

$$\begin{aligned}
\hat{A}_k &= \left[\hat{X}, \hat{P}_x^{k-1}\hat{P}_x\right] \\
&= \left[\hat{X}, \hat{P}_x^{k-1}\right]\hat{P}_x + \hat{P}_x^{k-1}\left[\hat{X}, \hat{P}_x\right] \\
&= \hat{A}_{k-1}\hat{P}_x + i\hbar\hat{P}_x^{k-1}
\end{aligned}$$

This gives a recursion relation $\hat{A}_k = \hat{A}_{k-1}\hat{P}_x + i\hbar\hat{P}_x^{k-1}$ for any $\hat{A}_k$ in terms of $\hat{A}_{k-1}$. iterating, we have

$$\begin{aligned}
\hat{A}_k &= \hat{A}_{k-1}\hat{P}_x + i\hbar\hat{P}_x^{k-1} \\
&= \left(\hat{A}_{k-2}\hat{P}_x + i\hbar\hat{P}_x^{k-2}\right)\hat{P}_x + i\hbar\hat{P}_x^{k-1} \\
&= \hat{A}_{k-2}\hat{P}_x^2 + 2i\hbar\hat{P}_x^{k-1} \\
&= \left(\hat{A}_{k-3}\hat{P}_x + i\hbar\hat{P}_x^{k-3}\right)\hat{P}_x^2 + 2i\hbar\hat{P}_x^{k-1} \\
&= \hat{A}_{k-3}\hat{P}_x^3 + 3i\hbar\hat{P}_x^{k-1}
\end{aligned}$$

and we suspect that continuing in this way will lead to

$$\hat{A}_k = i\hbar k\hat{P}_x^{k-1}$$

To prove this conjecture, notice that it works for $k = 1$ since $\hat{A}_1 = \left[\hat{X}, \hat{P}_x\right] = i\hbar$. Now suppose $\hat{A}_{n-1} = i\hbar\left(n-1\right)\hat{P}_x^{n-2}$. Then the recursion relation gives

$$\begin{aligned}
\hat{A}_n &= \hat{A}_{n-1}\hat{P}_x + i\hbar\hat{P}_x^{n-1} \\
&= i\hbar\left(n-1\right)\hat{P}_x^{n-2}\hat{P}_x + i\hbar\hat{P}_x^{n-1} \\
&= i\hbar n\hat{P}_x^{n-1}
\end{aligned}$$

completing the proof by induction.

Now, consider the commutator of the position operator with a function of the momentum operator:

$$\left[\hat{\mathbf{X}}, f\left(\hat{\mathbf{P}}\right)\right]$$

where we define a function of an operator to be the Taylor series for the function, with the variable replaced by the operator. First restricting our attention to the x-direction, we only need the Taylor series in the form

$$f\left(p_x, p_y, p_z\right) = \sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{\partial}{\partial p_x}\right)^k f\left(0, p_y, p_z\right)\left(p_x\right)^k$$

since $\hat{X}$ commutes with $\hat{P}_y$ and $\hat{P}_z$. Setting $\left(\frac{\partial}{\partial p_x}\right)^k f = f^{(k)}$, and replacing $p_x \to \hat{P}_x$,

$$f\left(\hat{\mathbf{P}}\right) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}\left(0, \hat{P}_y, \hat{P}_z\right)\left(\hat{P}_x\right)^k$$

Therefore,

$$\begin{aligned}
\left[\hat{X}, f\left(\hat{\mathbf{P}}\right)\right] &= \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}\left(0, \hat{P}_y, \hat{P}_z\right)\left[\hat{X}, \hat{P}_x^k\right] \\
&= \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}\left(0, \hat{P}_y, \hat{P}_z\right) i\hbar k \hat{P}_x^{k-1} \\
&= \sum_{k=0}^{\infty} \frac{1}{(k-1)!} f^{(k)}\left(0, \hat{P}_y, \hat{P}_z\right) i\hbar \hat{P}_x^{k-1}
\end{aligned}$$

Substituting back into our original commutation relation,

$$\begin{aligned}
\left[\hat{X}, f\left(\hat{\mathbf{P}}\right)\right] &= \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}\left(0, \hat{P}_y, \hat{P}_z\right)\left[\hat{X}, \hat{P}_x^k\right] \\
&= \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}\left(0, \hat{P}_y, \hat{P}_z\right) i\hbar k \hat{P}_x^{k-1} \\
&= i\hbar \sum_{k=0}^{\infty} \frac{1}{(k-1)!} f^{(k)}\left(0, \hat{P}_y, \hat{P}_z\right) \hat{P}_x^{k-1}
\end{aligned}$$

and we recognize the Taylor series for $\widehat{\left(\frac{\partial f}{\partial p_x}\right)}$. Therefore,

$$\left[\hat{X}, f\left(\hat{\mathbf{P}}\right)\right] = i\hbar \widehat{\left(\frac{\partial f}{\partial p_x}\right)}$$

The corresponding result holds for each component, so the derivative becomes a gradient,

$$\left[\hat{\mathbf{X}}, f\left(\hat{\mathbf{P}}\right)\right] = i\hbar \boldsymbol{\nabla}_{\hat{P}} f$$

Exercise:

Prove that

$$\left[\hat{\mathbf{P}}, f\left(\hat{\mathbf{X}}\right)\right] = -i\hbar \boldsymbol{\nabla}_{\hat{X}} f$$