THE SCHRÖDINGER VERSUS THE HEISENBERG PICTURE

Unitary Operators

In the previous section we introduced the concept of time development by considering the time-evolution operator that affects state kets; that approach to quantum dynamics is known as the Schrodinger picture.

There is another formulation of quantum dynamics where observables, rather than state kets, vary with time; this second approach is known as the Heisenberg picture.

Before discussing the differences between the two approaches in detail, we digress to make some general comments on unitary operators.

Unitary operators are used for many different purposes in quantum mechanics.

In this book we introduced (Section 1.5) an operator satisfying the unitarity property.

In that section we were concerned with the question of how the base kets in one representation are related to those in some other representations.

The state kets themselves are assumed not to change as we switch to a different set of base kets even though the numerical values of the expansion coefficients for $|\alpha>$ are, of course, different in different representations.

Subsequently we introduced two unitary operators that actually change the state kets, the translation operator of Section 1.6 and the time-evolution operator of Section 2.1.

We have $|\alpha\rangle \rightarrow U|\alpha\rangle$ where U may stand for $\mathscr{T}(dx)$ or $\mathscr{U}(t, t_0)$.

Here U|α> is the state ket corresponding to a physical system that actually has undergone translation or time evolution.

It is important to keep in mind that under a unitary transformation that changes the state kets, the inner product of a state bra and a state ket remains unchanged:

$$\langle\beta|\alpha\rangle \Rightarrow \langle\beta|U^\dagger U|\alpha\rangle = \langle\beta|\alpha\rangle$$

Using the fact that these transformations affect the state kets but not operators, we can infer how <β|X|α> must change:

$$\langle\beta|X|\alpha\rangle \Rightarrow (\langle\beta|U^\dagger)\cdot X\cdot(U|\alpha\rangle) = \langle\beta|U^\dagger XU|\alpha\rangle$$

We now make a very simple mathematical observation that follows from the associative axiom of multiplication:

$$(\langle\beta|U^\dagger)\cdot X\cdot(U|\alpha\rangle)=\langle\beta|\cdot(U^\dagger XU)\cdot|\alpha\rangle$$

Is there any physics in this observation?

This mathematical identity suggests two approaches to unitary transformations:

Approach 1:

$$|\alpha\rangle\to U|\alpha\rangle$$

with operators unchanged

Approach 2:

$$X\to U^\dagger XU$$

with state kets unchanged

In classical physics we do not introduce state kets, yet we talk about translation, time evolution, and the like.

This is possible because these operations actually change quantities such as x and L, which are observables of classical mechanics.

We therefore conjecture that a closer connection with classical physics may be established if we follow approach 2.

A simple example may be helpful here.

We go back to the infinitesimal translation operator $\mathscr{T}(dx`)$.

The formalism presented in Section 1.6 is based on approach 1; $\mathscr{T}(dx`)$ affects the state kets, not the position operator:

$$|\alpha\rangle \rightarrow \left(1 - \frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)|\alpha\rangle$$

$$\mathbf{x} \rightarrow \mathbf{x}$$

In contrast, if we follow approach 2, we obtain

$$|\alpha\rangle \to |\alpha\rangle$$

$$\mathbf{x} \to \left(1+\frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)\mathbf{x}\left(1-\frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)$$

We can show that both approaches lead to the same result for the expectation value of x:

Approach 1:

$$|\alpha\rangle \to \left(1-\frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)|\alpha\rangle$$

$$\mathbf{x} \to \mathbf{x}$$

$$<\alpha|\left(1+\frac{\mathrm{ip.dx'}}{\hbar}\right)\mathbf{x}\left(1-\frac{\mathrm{ip.dx'}}{\hbar}\right)|\alpha>$$

$$\approx<\alpha|\mathbf{x}+\frac{\mathrm{i}}{\hbar}[\mathbf{p}.\mathrm{d}\mathbf{x}',\mathbf{x}]|\alpha>=<\alpha|\mathbf{x}|\alpha>+<\alpha|\mathrm{d}\mathbf{x}'|\alpha>$$

$$\langle\mathbf{x}\rangle \to \langle\mathbf{x}\rangle+\langle d\mathbf{x}'\rangle$$

$$[\mathbf{x}, \mathscr{T}(d\mathbf{x}')] = d\mathbf{x}'$$

Approach 2:

$$|\alpha\rangle \rightarrow |\alpha\rangle$$

$$\mathbf{x} \rightarrow \left(1+\frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)\mathbf{x}\left(1-\frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)$$

$$= \mathbf{x} + \left(\frac{i}{\hbar}\right)[\mathbf{p}\cdot d\mathbf{x}', \mathbf{x}]$$

$$= \mathbf{x} + d\mathbf{x}'$$

$$< \alpha | \mathbf{x} | \alpha > \rightarrow < \alpha | \mathbf{x} | \alpha > + < \alpha | \mathrm{dx}' | \alpha >$$

$$\langle \mathbf{x} \rangle \rightarrow \langle \mathbf{x} \rangle + \langle d\mathbf{x}' \rangle$$

Which is identical with the result obtained from approach 1.

State Kets and Observables in the Schrödinger and the Heisenberg Pictures

We now return to the time-evolution operator $\mathscr{U}(t, t_0)$.

In the previous section we examined how state kets evolve with time.

This means that we were following approach 1, known as the Schrödinger picture when applied to time evolution.

Alternatively we may follow approach 2, known as the Heisenberg picture when applied to time evolution.

In the Schrödinger picture the operators corresponding to observables like x, p_y, and S_z are fixed in time, while state kets vary with time, as indicated in the previous section.

In contrast, in the Heisenberg picture the operators corresponding to observables vary with time; the state kets are fixed, frozen so to speak, at what they were at t_0.

It is convenient to set t_0 in $\mathscr{U}(t, t_0)$ to zero for simplicity and work with $\mathscr{U}(t)$ which is defined by

$$\mathscr{U}(t, t_0 = 0) \equiv \mathscr{U}(t) = \exp\left(\frac{-iHt}{\hbar}\right)$$

Motivated by approach 2, we define the Heisenberg picture observable by

$$A^{(H)}(t) \equiv \mathscr{U}^{\dagger}(t) A^{(S)} \mathscr{U}(t)$$

At t = 0, the Heisenberg picture observable and the corresponding Schrödinger picture observable coincide:

$$A^{(H)}(0) = A^{(S)}$$

The state kets also coincide between the two pictures at t = 0; at later t the Heisenberg picture state ket is frozen to what it was at t = 0:

$$|\alpha, t_0 = 0; t\rangle_H = |\alpha, t_0 = 0\rangle$$

independent of t.

This is in dramatic contrast with the Schrödinger-picture state ket,

$$|\alpha, t_0 = 0; t\rangle_S = \mathscr{U}(t)|\alpha, t_0 = 0\rangle$$

The expectation value <A> is obviously the same in both pictures:

$${}_S\langle\alpha, t_0 = 0; t|A^{(S)}|\alpha, t_0 = 0; t\rangle_S = \langle\alpha, t_0 = 0|\mathscr{U}^\dagger A^{(S)}\mathscr{U}|\alpha, t_0 = 0\rangle$$

$$= {}_H\langle\alpha, t_0 = 0; t|A^{(H)}(t)|\alpha, t_0 = 0; t\rangle_H$$

The Heisenberg Equation of Motion

We now derive the fundamental equation of motion in the Heisenberg picture.

Assuming that $A^{(S)}$ does not depend explicitly on time, which is the case in most physical situations of interest, we obtain by differentiating:

$$\frac{dA^{(H)}}{dt} = \frac{\partial \mathcal{U}^\dagger}{\partial t} A^{(S)} \mathcal{U} + \mathcal{U}^\dagger A^{(S)} \frac{\partial \mathcal{U}}{\partial t}$$

We had:

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

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

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

Therefore, we can simplify the following equation

$$\frac{dA^{(H)}}{dt} = \frac{\partial \mathscr{U}^{\dagger}}{\partial t} A^{(S)} \mathscr{U} + \mathscr{U}^{\dagger} A^{(S)} \frac{\partial \mathscr{U}}{\partial t}$$

using

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

as follows:

$$= -\frac{1}{i\hbar} \mathscr{U}^{\dagger} H \mathscr{U} \mathscr{U}^{\dagger} A^{(S)} \mathscr{U} + \frac{1}{i\hbar} \mathscr{U}^{\dagger} A^{(S)} \mathscr{U} \mathscr{U}^{\dagger} H \mathscr{U}$$

$$= \frac{1}{i\hbar} [A^{(H)}, \mathscr{U}^{\dagger} H \mathscr{U}]$$

Because H was originally introduced in the Schrödinger picture, we may be tempted to define

$$H^{(H)} = \mathcal{U}^\dagger H \mathcal{U}$$

$$\mathcal{U}^\dagger H \mathcal{U} = H$$

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}[A^{(H)}, \mathcal{U}^\dagger H \mathcal{U}]$$

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}[A^{(H)}, H]$$

This equation is known as the Heisenberg equation of motion.

It is instructive to compare the Heisenberg equation with the classical equation of motion in Poisson bracket form.

In classical physics, for a function A of q 's and p's that does not involve time explicitly, we have

$$\frac{dA}{dt} = [A, H]_{\text{classical}}$$

Again, we see that Dirac's quantization rule leads to the correct equation in quantum mechanics.

Indeed, historically the Heisenberg equation was first written by P. A. M. Dirac, who—with his characteristic modesty—called it the Heisenberg equation of motion.

It is worth noting, however, that the Heisenberg equation makes sense whether or not $A^{(H)}$ has a classical analogue.

For example, the spin operator in the Heisenberg picture satisfies

$$\frac{dS_i^{(H)}}{dt} = \frac{1}{i\hbar}\left[S_i^{(H)}, H\right]$$

which can be used to discuss spin precession, but this equation has no classical counterpart because Sz cannot be written as a function of q 's and p's.

Rather than insisting on Dirac's rule, we may argue that for quantities possessing classical counterparts, the correct classical equation can be obtained from the corresponding quantum-mechanical equation via the ansatz,

$$\frac{[\ ,\ ]}{i\hbar} \rightarrow [\ ,\ ]_{\text{classical}}$$

Classical mechanics can be derived from quantum mechanics, but the opposite is not true.

Free Particles; Ehrenfesf s Theorem

We are now in a position to apply the Heisenberg equation of motion to a free particle of mass m.

The Hamiltonian is taken to be of the same form as in classical mechanics:

$$H = \frac{\mathbf{p}^2}{2m} = \frac{\left(p_x^2 + p_y^2 + p_z^2\right)}{2m}$$

Because p_i commutes with any function of p_j's, we have

$$\frac{dp_i}{dt} = \frac{1}{i\hbar}[p_i, H] = 0$$

Thus for a free particle, the momentum operator is a constant of the motion, which means that $p_i(t)$ is the same as $p_i(0)$ at all times.

Next

$$\frac{dx_i}{dt} = \frac{1}{i\hbar}[x_i, H] = \frac{1}{i\hbar}\frac{1}{2m}i\hbar\frac{\partial}{\partial p_i}\left(\sum_{j=1}^{3} p_j^2\right) = \frac{p_i}{m} = \frac{p_i(0)}{m}$$

$$x_i(t) = x_i(0) + \left(\frac{p_i(0)}{m}\right)t$$

which is reminiscent of the classical trajectory equation for a uniform rectilinear motion.

It is important to note that even though we have

$$\left[x_i(0), x_j(0)\right] = 0$$

at equal times, the commutator of the x_i's at different times does not vanish; specifically,

$$\left[x_i(t), x_i(0)\right] = \left[\frac{p_i(0)t}{m}, x_i(0)\right] = \frac{-i\hbar t}{m}$$

Applying the uncertainty relation to this commutator, we obtain

$$\langle(\Delta x_i)^2\rangle_t \langle(\Delta x_i)^2\rangle_{t=0} \geq \frac{\hbar^2 t^2}{4m^2}$$

Among other things, this relation implies that even if the particle is well localized at t = 0, its position becomes more and more uncertain with time, a conclusion which can also be obtained by studying the time-evolution behavior of free-particle wave packets in wave mechanics.

We now add a potential V(x) to our earlier free-particle Hamiltonian:

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

$$[p_i, G(\mathbf{x})] = -i\hbar \frac{\partial G}{\partial x_i}$$

$$\frac{dp_i}{dt} = \frac{1}{i\hbar}[p_i, V(\mathbf{x})] = -\frac{\partial}{\partial x_i} V(\mathbf{x})$$

$$\frac{d\mathbf{x}_i}{dt} = \frac{1}{i\hbar}[\mathbf{x}_i, \frac{p_i^2}{2m}] = \frac{1}{i\hbar}\frac{1}{2m}(-\frac{\hbar}{i}p_i - \frac{\hbar}{i}p_i) = \frac{p_i}{m}$$

$$[x_i, F(\mathbf{p})] = i\hbar \frac{\partial F}{\partial p_i}$$

$$\frac{dx_i}{dt} = \frac{p_i}{m}$$

We can use the Heisenberg equation of motion once again to deduce

$$\frac{d^2 x_i}{dt^2} = \frac{1}{i\hbar}\left[\frac{dx_i}{dt}, H\right] = \frac{1}{i\hbar}\left[\frac{p_i}{m}, H\right] = \frac{1}{m}\frac{dp_i}{dt}$$

By combining:

$$m\frac{d^2\mathbf{x}}{dt^2} = -\nabla V(\mathbf{x})$$

$$m\frac{d^2\mathbf{x}}{dt^2} = -\nabla V(\mathbf{x})$$

This is the quantum-mechanical analogue of Newton's second law.

By taking the expectation values of both sides with respect to a Heisenberg state ket that does not move with time, we obtain

$$m\frac{d^2}{dt^2}\langle\mathbf{x}\rangle = \frac{d\langle\mathbf{p}\rangle}{dt} = -\langle\nabla V(\mathbf{x})\rangle$$

This is known as the Ehrenfest theorem after P. Ehrenfest.

When written in this expectation form, its validity is independent of whether we are using the Heisenberg or the Schrödinger picture; after all, the expectation values are the same in the two pictures.

In contrast, the operator (first equation before taking the expectation values) form is meaningful only if we understand x and p to be Heisenberg-picture operators.

Base Kets and Transition Amplitudes

So far we have avoided asking how the base kets evolve in time.

A common misconception is that as time goes on, all kets move in the Schrödinger picture and are stationary in the Heisenberg picture.

This is not the case, as we will make clear shortly.

The important point is to distinguish the behavior of state kets from that of base kets.

We started our discussion of ket spaces in Section 1.2 by remarking that the eigenkets of observables are to be used as base kets.

What happens to the defining eigenvalue equation $A|a'\rangle = a'|a'\rangle$ with time?

In the Schrödinger picture, A does not change, so the base kets, obtained as the solutions to this eigenvalue equation at t = 0, for instance, must remain unchanged.

Therefore, unlike state kets, the base kets do not change in the Schrödinger picture.

The whole situation is very different in the Heisenberg picture, where the eigenvalue equation we must study is for the time-dependent operator

$$A^{(H)}(t) = \mathcal{U}^{\dagger} A(0) \mathcal{U}$$

$$A^{(H)}(\mathcal{U}^{\dagger}|a'\rangle) = a'(\mathcal{U}^{\dagger}|a'\rangle)$$

$$A|a'\rangle = a'|a'\rangle$$

$$\mathcal{U}^{\dagger} A(0) \mathcal{U} \mathcal{U}^{\dagger}|a'\rangle = a' \mathcal{U}^{\dagger}|a'\rangle$$

As time goes on, the Heisenberg-picture base kets, denoted by $|a',t\rangle_H$ move as follows:

$$|a',t\rangle_H = \mathscr{U}^\dagger |a'\rangle$$

Because of the appearance of $\mathscr{U}^+$ rather than $\mathscr{U}$ in the above equation, the Heisenberg-picture base kets are seen to rotate oppositely when compared with the Schrödinger-picture state kets; specifically, $|a`, t\rangle_H$ satisfies the " wrong-sign Schrödinger equation"

$$i\hbar\frac{\partial}{\partial t}|a',t\rangle_H = -H|a',t\rangle_H$$

Notice also the following expansion for $A^{(H)}(t)$ in terms of the base kets and bras of the Heisenberg picture:

$$A^{(H)}(t) = \sum_{a'} |a', t\rangle_H a'_H \langle a', t|$$

$$= \sum_{a'} \mathscr{U}^\dagger |a'\rangle a' \langle a'| \mathscr{U}$$

$$= \mathscr{U}^\dagger A^{(S)} \mathscr{U}$$

which shows that everything is quite consistent provided that the Heisenberg base kets change.

We see that the expansion coefficients of a state ket in terms of base kets are the same in both pictures:

$$c_{a'}(t) = \underbrace{\langle a'|}_{\text{base bra}} \cdot \underbrace{(\mathscr{U}|\alpha, t_0 = 0\rangle)}_{\text{state ket}} \quad \text{(the Schrödinger picture)}$$

$$c_{a'}(t) = \underbrace{(\langle a'|\mathscr{U})}_{\text{base bra}} \cdot \underbrace{|\alpha, t_0 = 0\rangle}_{\text{state ket}} \quad \text{(the Heisenberg picture)}$$

To illustrate further the equivalence between the two pictures, we study transition amplitudes, which will play a fundamental role in section 2.5, where we discuss PROPAGATORS AND FEYNMAN PATH INTEGRALS.

Suppose there is a physical system prepared at $t = 0$ to be in an eigenstate of observable A with eigenvalue a'.

At some later time t we may ask, What is the probability amplitude, known as the transition amplitude, for the system to be found in an eigenstate of observable B with eigenvalue b'?

Here A and B can be the same or different.

In the Schrödinger picture the state ket at t is given by $\mathscr{U}|a'\rangle$ while the base kets $|a'\rangle$ and $|b'\rangle$ do not vary with time; so we have:

$$\underbrace{\langle b'|}_{\text{base bra}} \cdot \underbrace{(\mathscr{U}|a'\rangle)}_{\text{state ket}}$$

In contrast, in the Heisenberg picture the state ket is stationary, that is, it remains as |a'> at all times, but the base kets evolve oppositely.

So the transition amplitude is

$$\underbrace{(\langle b'|\mathscr{U})}_{\text{base bra}} \cdot \underbrace{|a'\rangle}_{\text{state ket}}$$

Obviously the later two equations are the same.

They can both be written as

$$\langle b'|\mathscr{U}(t,0)|a'\rangle$$

In some loose sense this is the transition amplitude for "going" from state |a'> to state |b'>.

To conclude this section let us summarize the differences between the Schrodinger picture and the Heisenberg picture; see the following Table.

	Schrödinger picture	Heisenberg picture
State ket	Moving $\lvert\alpha, t_0; t\rangle = \mathscr{U}(t, t_0)\lvert\alpha, t_0\rangle$ $i\hbar\frac{\partial}{\partial t}\lvert\alpha, t_0; t\rangle = H\lvert\alpha, t_0; t\rangle$	Stationary
Observable	Stationary	Moving $A^{(H)}(t) \equiv \mathscr{U}^{\dagger}(t)A^{(S)}\mathscr{U}(t)$ $\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}[A^{(H)}, H]$
Base ket	Stationary	Moving oppositely $\lvert a', t\rangle_H = \mathscr{U}^{\dagger}\lvert a'\rangle$ $i\hbar\frac{\partial}{\partial t}\lvert a', t\rangle_H = -H\lvert a', t\rangle_H$