Energy Eigenkets

To be able to evaluate the effect of the time-evolution operator on a general initial ket |α> we must first know how it acts on the base kets used in expanding |α>.

This is particularly straightforward if the base kets used are eigenkets of A such that

$$[A, H] = 0$$

then the eigenkets of A are also eigenkets of H, called energy eigenkets, whose eigenvalues are denoted by $E_{a'}$

$$H|a'\rangle = E_{a'}|a'\rangle$$

$$\exp\left(\frac{-iHt}{\hbar}\right)=\sum_{a'}\sum_{a''}|a''\rangle\langle a''|\exp\left(\frac{-iHt}{\hbar}\right)|a'\rangle\langle a'|$$

$$=\sum_{a'}|a'\rangle\exp\left(\frac{-iE_{a'}t}{\hbar}\right)\langle a'|$$

As an example, suppose that the initial ket expansion reads

$$|\alpha,t_0=0\rangle=\sum_{a'}|a'\rangle\langle a'|\alpha\rangle=\sum_{a'}c_{a'}|a'\rangle$$

$$|\alpha,t_0=0;t\rangle=\exp\left(\frac{-iHt}{\hbar}\right)|\alpha,t_0=0\rangle=\sum_{a'}|a'\rangle\langle a'|\alpha\rangle\exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$

Therefore, the expansion coefficient changes with time as

$$c_{a'}(t=0)\rightarrow c_{a'}(t)=c_{a'}(t=0)\exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$

which its modulus unchanged.

Notice that the relative phases among various components do vary with time because the oscillation frequencies are different.

A special case of interest is where the initial state happens to be one of {|a`>} itself.

$$|\alpha, t_0 = 0\rangle = |a'\rangle$$

$$|\alpha, t_0 = 0; t\rangle = |a'\rangle \exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$

so if the system is initially a simultaneous eigenstate of A and H, it remains so at all times.

The most that can happen is the phase modulation, exp(-$iE_{a`}t/h$).

It is in this sense that an observable compatible with H is a constant of the motion.

We will encounter this connection once again in a different form when we discuss the Heisenberg equation of motion.

In summery:

In the foregoing discussion the basic task in quantum dynamics is reduced to finding an observable that commutes with H and evaluating its eigenvalues.

Once that is done, we expand the initial ket in terms of the eigenkets of that observable and just apply the time-evolution operator.

This last step merely amounts to changing the phase of each expansion coefficient.

Even though we worked out the case where there is just one observable A that commutes with H, our considerations can easily be generalized when there are several mutually compatible observables all also commuting with H:

$$[A, B] = [B, C] = [A, C] = \cdots = 0$$

$$[A, H] = [B, H] = [C, H] = \cdots = 0$$

$$\exp\left(\frac{-iHt}{\hbar}\right) = \sum_{K'} |K'\rangle \exp\left(\frac{-iE_{K'}t}{\hbar}\right) \langle K'|$$

$$|K'\rangle = |a', b', c', \ldots\rangle$$

It is therefore of fundamental importance to find a complete set of mutually compatible observables that also commute with H.

Once such a set is found, we express the initial ket as a superposition of the simultaneous eigenkets of A, B, C,... and H.

The final step is just to apply the time-evolution operator. In this manner we can solve the most general initial-value problem with a time-independent H.

Time Dependence of Expectation Values

It is instructive to study how the expectation value of an observable changes as a function of time.

Suppose that at t = 0 the initial state is one of the eigenstates of an observable A that commutes with H.

We now look at the expectation value of some other observable B, which need not commute with A nor with H.

$$|a', t_0 = 0; t\rangle = \mathscr{U}(t, 0)|a'\rangle$$

$$\langle B \rangle = \left(\langle a' | \mathscr{U}^{\dagger}(t,0) \right) \cdot B \cdot \left(\mathscr{U}(t,0) | a' \rangle \right)$$

$$= \langle a' | \exp\left(\frac{iE_{a'}t}{\hbar} \right) B \exp\left(\frac{-iE_{a'}t}{\hbar} \right) | a' \rangle$$

$$= \langle a' | B | a' \rangle$$

which is independent of t.

So the expectation value of an observable taken with respect to an energy eigenstate does not change with time.

For this reason an energy eigenstate is often referred to as a stationary state.

The situation is more interesting when the expectation value is taken with respect to a superposition of energy eigenstates, or a nonstationary state.

Suppose that initially we have

$$|\alpha, t_0 = 0\rangle = \sum_{a'} c_{a'} |a'\rangle$$

$$\langle B \rangle = \left[\sum_{a'} c_{a'}^* \langle a'| \exp\left(\frac{iE_{a'}t}{\hbar}\right)\right] \cdot B \cdot \left[\sum_{a''} c_{a''} \exp\left(\frac{-iE_{a''}t}{\hbar}\right)|a''\rangle\right]$$

$$= \sum_{a'}\sum_{a''} c_{a'}^* c_{a''} \langle a'|B|a''\rangle \exp\left[\frac{-i(E_{a''} - E_{a'})t}{\hbar}\right]$$

So this time the expectation value consists of oscillating terms whose angular frequencies are determined by N. Bohr's frequency condition

$$\omega_{a''a'} = \frac{(E_{a''} - E_{a'})}{\hbar}$$

Spin Precession

It is appropriate to treat an example here.

We consider an extremely simple system which, however, illustrates the basic formalism we have developed.

We start with a Hamiltonian of a spin 1/2 system with magnetic moment $e\hbar/2m_ec$ subjected to an external magnetic field **B**:

$$H = -\left(\frac{e}{m_e c}\right)\mathbf{S}\cdot\mathbf{B}$$

$$H = -\left(\frac{eB}{m_e c}\right)S_z$$

Because Sz and H differ just by a multiplicative constant, they obviously commute.

The Sz eigenstates are also energy eigenstates, and the corresponding energy eigenvalues are

$$E_{\pm} = \mp \frac{e\hbar B}{2m_e c}, \quad \text{for } S_z \pm$$

$$\omega \equiv \frac{|e|B}{m_e c}$$

$$H = \omega S_z$$

$$\mathcal{U}(t,0) = \exp\left(\frac{-i\omega S_z t}{\hbar}\right)$$

Suppose that at t = 0 the system is characterized by

$$|\alpha\rangle = c_+|+\rangle + c_-|-\rangle$$

We apply this to the initial state.

The base kets for expanding the initial ket are obviously the S_z eigenkets, |+> and |->, which are also energy eigenkets.

$$|\alpha, t_0 = 0; t\rangle = c_+ \exp\left(\frac{-i\omega t}{2}\right)|+\rangle + c_- \exp\left(\frac{+i\omega t}{2}\right)|-\rangle$$

$$H|\pm\rangle = \left(\frac{\pm\hbar\omega}{2}\right)|\pm\rangle$$

Specifically, let us suppose that the initial ket |a> represents the spin-up (or, more precisely, Sz +) state |+ >, which means that

$$c_+ = 1, \qquad c_- = 0$$

At a later time, it is still in the spin-up state, which is no surprise because this is a stationary state.

Next, let us suppose that initially the system is in the Sx + state.

$$c_+ = c_- = \frac{1}{\sqrt{2}}$$

It is straightforward to work out the probabilities for the system to be found in the Sx ± state at some later time t:

$$|\langle S_x \pm|\alpha, t_0=0; t\rangle|^2 = \left|\left[\left(\frac{1}{\sqrt{2}}\right)\langle +| \pm \left(\frac{1}{\sqrt{2}}\right)\langle -|\right]\cdot\left[\left(\frac{1}{\sqrt{2}}\right)\exp\left(\frac{-i\omega t}{2}\right)|+\rangle + \left(\frac{1}{\sqrt{2}}\right)\exp\left(\frac{+i\omega t}{2}\right)|-\rangle\right]\right|^2$$

$$= \left|\frac{1}{2}\exp\left(\frac{-i\omega t}{2}\right) \pm \frac{1}{2}\exp\left(\frac{+i\omega t}{2}\right)\right|^2 = \begin{cases} \cos^2\dfrac{\omega t}{2}, & \text{for } S_x+, \\ \sin^2\dfrac{\omega t}{2}, & \text{for } S_x-. \end{cases}$$

Even though the spin is initially in the positive x-direction, the magnetic field in the z-direction causes it to rotate; as a result, we obtain a finite probability for finding Sx - at some later time.

The sum of the two probabilities is seen to be unity at all times, in agreement with the unitarity property of the time-evolution operator.

$$\langle S_x \rangle = \left(\frac{\hbar}{2}\right)\cos^2\left(\frac{\omega t}{2}\right) + \left(\frac{-\hbar}{2}\right)\sin^2\left(\frac{\omega t}{2}\right) = \left(\frac{\hbar}{2}\right)\cos \omega t$$

Why? **Because we had that**

$$\langle A \rangle \equiv \langle \alpha | A | \alpha \rangle$$

$$\langle A \rangle = \sum_{a'} \sum_{a''} \langle \alpha | a'' \rangle \langle a'' | A | a' \rangle \langle a' | \alpha \rangle$$

$$= \sum_{a'} \underset{\substack{\uparrow \\ \text{measured value } a'}}{a'} \underbrace{|\langle a' | \alpha \rangle|^2}_{\text{probability for obtaining } a'}$$

Or in another way you can also as an exercise directly find the expectation value of S_x at time t as follows:

$$\langle S_x \rangle = \langle \alpha, t_0 = 0; t | S_x | \alpha, t_0 = 0; t \rangle$$

Where, we have:

$$|\alpha, t_0 = 0; t\rangle = c_+ \exp\left(\frac{-i\omega t}{2}\right)|+\rangle + c_- \exp\left(\frac{+i\omega t}{2}\right)|-\rangle$$

$$c_+ = c_- = \frac{1}{\sqrt{2}}$$

$$S_x = \frac{\hbar}{2}\left[(|+\rangle\langle -|) + (|-\rangle\langle +|)\right]$$

Anyway, we have:

$$\langle S_x \rangle = \left(\frac{\hbar}{2}\right)\cos\omega t$$

so this quantity oscillates with an angular frequency corresponding to the difference of the two energy eigenvalues divided by ħ.

This is in agreement with our following general formula:

$$\langle B \rangle = \left[\sum_{a'} c_{a'}^{*}\langle a'|\exp\left(\frac{iE_{a'}t}{\hbar}\right)\right]\cdot B\cdot\left[\sum_{a''} c_{a''}\exp\left(\frac{-iE_{a''}t}{\hbar}\right)|a''\rangle\right]$$

$$= \sum_{a'}\sum_{a''} c_{a'}^{*}c_{a''}\langle a'|B|a''\rangle\exp\left[\frac{-i(E_{a''}-E_{a'})t}{\hbar}\right]$$

Similar exercises with S_y and S_z show that

$$\langle S_y \rangle = \left(\frac{\hbar}{2}\right) \sin \omega t$$

$$\langle S_z \rangle = 0$$

Physically this means that the spin precesses in the xy-plane.

We will comment further on spin precession when we discuss rotation operators in Chapter 3.

Correlation Amplitude and the Energy-Time Uncertainty Relation

We conclude this section by asking how state kets at different times are correlated with each other.

Suppose the initial state ket at $t = 0$ of a physical system is given by $|\alpha>$.

With time it changes into $|\alpha, t_0 = 0;t>$, which we obtain by applying the time-evolution operator.

We are concerned with the extent to which the state ket at a later time t is similar to the state ket at $t = 0$.

We therefore construct the inner product between the two state kets at different times:

$$C(t) \equiv \langle \alpha | \alpha, t_0 = 0; t \rangle$$

$$= \langle \alpha | \mathscr{U}(t, 0) | \alpha \rangle$$

which is known as the **correlation amplitude**.

The modulus of C(t) provides a quantitative measure of the "resemblance" between the state kets at different times.

As an extreme example, consider the very special case where the initial ket |α> is an eigenket of H; we then have

$$C(t) = \langle a' | a', t_0 = 0; t \rangle = \exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$

so the modulus of the correlation amplitude is unity at all times—which is not surprising for a stationary state.

In the more general situation where the initial ket is represented by a superposition of {|a'>}, we have

$$C(t) = \left(\sum_{a'} c_{a'}^{*} \langle a'|\right)\left[\sum_{a''} c_{a''} \exp\left(\frac{-iE_{a''}t}{\hbar}\right)|a''\rangle\right]$$

$$= \sum_{a'} |c_{a'}|^{2} \exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$

As we sum over many terms with oscillating time dependence of different frequencies, a strong cancellation is possible for moderately large values of t.

We expect the correlation amplitude that starts with unity at t = 0 to decrease in magnitude with time.

To estimate in a more concrete manner, let us suppose that the state ket can be regarded as a superposition of so many energy eigenkets with similar energies that we can regard them as exhibiting essentially a quasi-continuous spectrum.

It is then legitimate to replace the sum by the integral

$$\sum_{a'} \rightarrow \int dE \, \rho(E)$$

$$c_{a'} \rightarrow g(E)\Big|_{E \simeq E_{a'}}$$

$$C(t) = \int dE \, |g(E)|^2 \rho(E) \exp\left(\frac{-iEt}{\hbar} \right)$$

$$\int dE \, |g(E)|^2 \rho(E) = 1$$

In a realistic physical situation $|g(E)|^2\rho(E)$ may be peaked around $E = E_0$ with width A.

$$C(t) = \exp\left(\frac{-iE_0 t}{\hbar}\right)\int dE|g(E)|^2\rho(E)\exp\left[\frac{-i(E-E_0)t}{\hbar}\right]$$

We see that as t becomes large, the integrand oscillates very rapidly unless the energy interval $|E — E_0|$ is small compared with $\hbar/t$.

If the interval for which $|E — E_0| \sim \hbar/t$ holds is much narrower than ΔE—the width of $|g(E)|^2\rho(E)$—we get essentially no contribution to C(t) because of strong cancellations.

The characteristic time at which the modulus of the correlation amplitude starts becoming appreciably different from 1 is given by

$$t \simeq \frac{\hbar}{\Delta E}$$

Even though this equation is obtained for a superposition state with a quasi-continuous energy spectrum, it also makes sense for a two-level system; in the spin-precession problem considered earlier, the state ket, which is initially $|S_X +>$, starts losing its identity after $\sim 1/\omega = \hbar/(E_+ - E_-)$, as is evident from:

$$|\langle S_x \pm | \alpha, t_0 = 0; t\rangle|^2 = \begin{cases} \cos^2 \dfrac{\omega t}{2}, & \text{for } S_x + , \\ \sin^2 \dfrac{\omega t}{2}, & \text{for } S_x - . \end{cases}$$

To summarize, as a result of time evolution the state ket of a physical system ceases to retain its original form after a time interval of order ħ/ΔE.

In the literature this point is often said to illustrate the time-energy uncertainty relation

$$\Delta t \, \Delta E \simeq \hbar$$

However, it is to be clearly understood that this time-energy uncertainty relation is of a very different nature from the uncertainty relation between two incompatible observables discussed in Section 1.4. In Chapter 5 we will come back to the above equation in connection with time-dependent perturbation theory.