Time evolution operator

In quantum mechanics

- unlike position, time is *not* an observable.
- there is no Hermitean operator whose eigenvalues were the time of the system.
- time appears only as a parameter, not as a measurable quantity.

So, contradictory to teachings of the relativity theory, time and position are not on equal standing. In relativistic quantum field theories the equality is restored by degrading also the position down to the parameter level.
We consider a system which at the moment t_0 is in the state $|\alpha\rangle$. When time goes on there is no reason to expect it to remain in this state. We suppose that at a later moment t the system is described by the state

$$|\alpha, t_0; t\rangle, \quad (t > t_0),$$

where the parameter t_0 reminds us that exactly at that moment the system was in the state $|\alpha\rangle$. Since the time is a continuous parameter we obviously have

$$\lim_{t \to t_0} |\alpha, t_0; t\rangle = |\alpha\rangle,$$

and can use the shorter notation

$$|\alpha, t_0; t_0\rangle = |\alpha, t_0\rangle.$$

Let's see, how state vectors evolve when time goes on:

$$|\alpha, t_0\rangle \stackrel{\text{evolution}}{\longrightarrow} |\alpha, t_0; t\rangle.$$

We work like we did with translations. We define the *time evolution operator* $\mathcal{U}(t, t_0)$:

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

which must satisfy physically relevant conditions.

1. Conservation of probability

We expand the state at the moment t_0 with the help of the eigenstates of an observable A:

$$|\alpha, t_0\rangle = \sum_{a'} c_{a'}(t_0)|a'\rangle.$$

At a later moment we get the expansion

$$|\alpha, t_0; t\rangle = \sum_{a'} c_{a'}(t)|a'\rangle.$$

In general, we cannot expect the probability for the system being in a specific state $|a'\rangle$ to remain constant, i.e. in most cases

$$|c_{a'}(t)| \neq |c_{a'}(t_0)|.$$

For example, when a spin $\frac{1}{2}$ particle, which at the moment t_0 is in the state $|S_x;\uparrow\rangle$, is subjected to an external constant magnetic field parallel to the z-axis, it will precess in the xy-plane: the probability for the result $\hbar/2$ in the measurement $\boxed{\mathrm{SG}\hat{\boldsymbol{x}}}$ oscillates between 0 and 1 as a function of time. In any case, the probability for the result $\hbar/2$ *or* $-\hbar/2$ remains always as the constant 1. Generalizing, it is natural to require that

$$\sum_{a'} |c_{a'}(t_0)|^2 = \sum_{a'} |c_{a'}(t)|^2.$$

In other words, the normalization of the states does not depend on time:

$$\begin{aligned}\langle \alpha, t_0 | \alpha, t_0 \rangle &= \langle \alpha, t_0; t | \alpha, t_0; t\rangle \\ &= \langle \alpha, t_0 | \mathcal{U}^\dagger(t, t_0)\mathcal{U}(t, t_0) | \alpha, t_0\rangle.\end{aligned}$$

This is satisfied if we require $\mathcal{U}(t, t_0)$ to be unitary, i.e.

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

2. Composition property

The evolution from the time t_0 to a later time t_2 should be equivalent to the evolution from the initial time t_0 to an intermediate time t_1 followed by the evolution from t_1 to the final time t_2, i.e.

$$\mathcal{U}(t_2, t_0) = \mathcal{U}(t_2, t_1)\mathcal{U}(t_1, t_0), \quad (t_2 > t_1 > t_0).$$

Like in the case of the translation operator we will first look at the infinitesimal evolution

$$|\alpha, t_0; t_0 + dt\rangle = \mathcal{U}(t_0 + dt, t_0)|\alpha, t_0\rangle.$$

Due to the continuity condition

$$\lim_{t \to t_0} |\alpha, t_0; t\rangle = |\alpha\rangle$$

we have

$$\lim_{dt \to 0} \mathcal{U}(t_0 + dt, t_0) = 1.$$

So, we can assume the deviations of the operator $\mathcal{U}(t_0 + dt, t_0)$ from the identity operator to be of the order dt. When we now set

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

where Ω is a Hermitean operator, we see that it satisfies the composition condition

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

is unitary and deviates from the identity operator by the term $\mathcal{O}(dt)$.
The physical meaning of Ω will be revealed when we recall that in classical mechanics the Hamiltonian generates the time evolution. From the definition

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

we see that the dimension of Ω is frequency, so it must be multiplied by a factor before associating it with the Hamiltonian operator H:

$$H = \hbar\Omega,$$

or

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

The factor $\hbar$ here is not necessarily the same as the factor $\hbar$ in the case of translations. It turns out, however, that in order to recover Newton's equations of motion in the classical limit both coefficients must be equal.
Applying the composition property

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

we get

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

where the time difference $t - t_0$ does not need to be infinitesimal. This can be written as

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

Expanding the left hand side as the Taylor series we end up with the **Schrödinger equation of the time evolution operator**:

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

Multiplying both sides by the state vector $|\alpha, t_0\rangle$ we get

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

Since the state $|\alpha, t_0\rangle$ is independent on the time t we can write the Schrödinger equation of the state vectors in the form

$$i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle = H|\alpha, t_0; t\rangle.$$

In fact, in most cases the state vector Schrödinger equation is unnecessary because all information about the dynamics of the system is contained in the time evolution operator $\mathcal{U}(t, t_0)$. When this operator is known the state of the system at any moment is obtained by applying the definition

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

We consider three cases:
(**i**) The Hamiltonian does not depend on time. For example, a spin $\frac{1}{2}$ particle in a time independent magnetic field belongs to this category. The solution of the equation

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

is

$$\mathcal{U}(t, t_0) = \exp\left[-\frac{iH(t - t_0)}{\hbar}\right]$$

as can be shown by expanding the exponential function as the Taylor series and differentiating term by term with respect to the time. Another way to get the solution is to compose the finite evolution from the infinitesimal ones:

$$\lim_{N\to\infty}\left[1 - \frac{(iH/\hbar(t - t_0)}{N}\right]^N = \exp\left[-\frac{iH(t - t_0)}{\hbar}\right].$$

(**ii**) The Hamiltonian H depends on time but the operators H corresponding to different moments of time commute.
For example, a spin $\frac{1}{2}$ particle in the magnetic field whose strength varies but direction remains constant as a function of time.
A formal solution of the equation

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

is now

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

which, again, can be proved by expanding the exponential function as the series.
(**iii**) The operators H evaluated at different moments of time *do not* commute.
For example, a spin $\frac{1}{2}$ particle in a magnetic field whose direction changes in the course of time: H is proportional to the term $\boldsymbol{S}\cdot\boldsymbol{B}$ and if now, at the moment $t = t_1$ the magnetic field is parallel to the x-axis and, at the moment $t = t_2$ parallel to the y-axis, then $H(t_1) \propto BS_x$ and $H(t_2) \propto BS_y$, or $[H(t_1), H(t_2)] \propto B^2[S_x, S_y] \neq 0$. It can be shown that the formal solution of the Schrödinger equation is now

$$\mathcal{U}(t, t_0) =$$

$$1+\sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots$$
$$\int_{t_0}^{t_{n-1}}dt_n\,H(t_1)H(t_2)\cdots H(t_n).$$

This expansion is called the *Dyson series.* We will assume that our Hamiltonians are time independent until we start working with the so called interaction picture.
Suppose that A is an Hermitean operator and

$$[A,H]=0.$$

Then the eigenstates of A are also eigenstates of H, called *energy eigenstates.* Denoting corresponding eigenvalues of the Hamiltonian as $E_{a'}$ we have

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

The time evolution operator can now be written with the help of these eigenstates. Choosing $t_0=0$ we get

$$\begin{aligned}\exp\left(-\frac{iHt}{\hbar}\right) &= \sum_{a'}\sum_{a''}|a''\rangle\langle a''|\exp\left(-\frac{iHt}{\hbar}\right)|a'\rangle\langle a'| \\ &= \sum_{a'}\sum_{a''}|a''\rangle\langle a''|a'\rangle\exp\left(-\frac{iE_{a'}t}{\hbar}\right)\langle a'| \\ &= \sum_{a'}|a'\rangle\exp\left(-\frac{iE_{a'}t}{\hbar}\right)\langle a'|.\end{aligned}$$

Using this form for the time evolution operator we can solve every intial value problem provided that we can expand the initial state with the set $\{|a'\rangle\}$. If, for example, the initial state can be expanded as

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

we get

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

In other words, the expansion coefficients evolve in the course of time as

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

So, the absolute values of the coefficients remain constant. The relative phase between different components will, however, change in the course of time because the oscillation frequencies of different components differ from each other.
As a special case we consider an initial state consisting of a single eigenstate:

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

At some later moment this state has evolved to the state

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

Hence, if the system originally is in an eigenstate of the Hamiltonian H and the operator A it stays there forever. Only the phase factor $\exp(-iE_{a'}t/\hbar)$ can vary. In this sense the observables whose corresponding operators commute with the Hamiltonian, are *constants of motion.*
Observables (or operators) associated with mutually commuting operators are called *compatible.* As mentioned before, the treatment of a physical problem can in many cases be reduced to the search for a maximal set of compatible operators. If the operators $A, B, C, \ldots$ belong to this set, i.e.

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

and if, furthermore,

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

that is, also the Hamiltonian is compatible with other operators, then the time evolution operator can be written as

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

Here K' stands for the collective index:

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

Thus, the quantum dynamics is completely solved (when H does not depend on time) if we only can find *a maximal set of compatible operators commuting also with the Hamiltonian.*

Stationary states
Let's now look at the expectation value of an operator. We first assume, that at the moment $t = 0$ the system is in an eigenstate $|a'\rangle$ of an operator A commuting with the Hamiltonian H. Suppose, we are interested in the expectation value of an operator B which does not necessarily commute either with A or with H. At the moment t the system is in the state

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

In this special case we have

$$\begin{aligned}
\langle B\rangle &= \langle a'|\mathcal{U}^\dagger(t,0)B\mathcal{U}(t,0)|a'\rangle \\
&= \langle a'|\exp\left(\frac{iE_{a'}t}{\hbar}\right)B\exp\left(-\frac{iE_{a'}t}{\hbar}\right)|a'\rangle \\
&= \langle a'|B|a'\rangle,
\end{aligned}$$

that is, the expectation value *does not depend on time*. For this reason the energy eigenstates are usually called *stationary states*

Non-stationary states
We now look at the expectation value in a superposition of energy eigenstates, in a *non stationary state*

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

It is easy to see, that the expectation value of B is now

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

This time the expectation value consists of terms which oscillate with frequences determind by the Bohr frequency condition

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

As an application we look at how spin $\frac{1}{2}$ particles behave in a constant magnetic field. When we assume the magnetic moments of the particles to be $e\hbar/2m_ec$ (like electrons), the Hamiltonian is

$$H = -\left(\frac{e}{m_ec}\right)\boldsymbol{S}\cdot\boldsymbol{B}.$$

If we choose $\boldsymbol{B} \parallel \hat{\boldsymbol{z}}$, we have

$$H = -\left(\frac{eB}{m_ec}\right)S_z.$$

The operators H and S_z differ only by a constant factor, so they obviously commute and the eigenstates of S_z are also energy eigenstates with energies

$$\begin{aligned}
E_\uparrow &= -\frac{e\hbar B}{2m_ec} \quad \text{for state } |S_z;\uparrow\rangle \\
E_\downarrow &= +\frac{e\hbar B}{2m_ec} \quad \text{for state } |S_z;\downarrow\rangle.
\end{aligned}$$

We define the *cyclotron frequency* ω_c so that the energy difference between the states is $\hbar\omega_c$:

$$\omega_c \equiv \frac{|e|B}{m_e c}.$$

The Hamiltonian H can now be written as

$$H = \omega_c S_z,$$

when we assume that $e < 0$.
All information about the evolution of the system is contained in the operator

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

If at the moment $t = 0$ the system is in the state

$$|\alpha\rangle = c_\uparrow|S_z;\uparrow\rangle + c_\downarrow|S_z;\downarrow\rangle,$$

it is easy to see that at the moment t it is in the state

$$\begin{aligned}|\alpha, t_0 = 0; t\rangle &= c_\uparrow \exp\left(-\frac{i\omega_c t}{2}\right)|S_z;\uparrow\rangle \\ &\quad + c_\downarrow \exp\left(+\frac{i\omega_c t}{2}\right)|S_z;\downarrow\rangle.\end{aligned}$$

If the initial state happens to be $|S_z;\uparrow\rangle$, meaning that in the previous equation

$$c_\uparrow = 1, \quad c_\downarrow = 0,$$

we see that the system will stay in this state at all times. This was to be expected because the state is stationary.
We now assume that the initial state is $|S_x;\uparrow\rangle$. From the relation

$$|S_x;\uparrow\rangle = \frac{1}{\sqrt{2}}|S_z;\uparrow\rangle + \frac{1}{\sqrt{2}}|S_z;\downarrow\rangle$$

we see that

$$c_\uparrow = c_\downarrow = \frac{1}{\sqrt{2}}.$$

And so, $|S_x;\uparrow\rangle$
For the probabilities that at the moment t the system is in eigenstates of S_x we get

$$\begin{aligned}|\langle S_x;\uparrow|\alpha, t_0 = 0; t\rangle|^2 &= \cos^2\frac{\omega_c t}{2} \\ |\langle S_x;\downarrow|\alpha, t_0 = 0; t\rangle|^2 &= \sin^2\frac{\omega_c t}{2}.\end{aligned}$$

Even if the spin originally were parallel to the positive x-axis a magnetic field parallel to the z-axis makes the direction of the spin to rotate. There is a finite

probability for finding the system at some later moment in the state $|S_x;\downarrow\rangle$. The sum of probabilities corresponding to different orientations is 1.
It is easy to see that the expectation values of the operator $\boldsymbol{S}$ satisfy

$$\begin{aligned}
\langle S_x\rangle &= \left(\frac{\hbar}{2}\right)\cos\omega_c t\\
\langle S_y\rangle &= \left(\frac{\hbar}{2}\right)\sin\omega_c t\\
\langle S_z\rangle &= 0.
\end{aligned}$$

Physically this means that the spin *precesses* in the xy-plane.
Lastly we look at how the statevectors corresponding to different times are correlated. Suppose that at the moment $t=0$ the system is described by the state vector $|\alpha\rangle$, which in the course of time evolves to the state $|\alpha, t_0=0; t\rangle$. We define the *correlation amplitude* $C(t)$ as

$$\begin{aligned}
C(t) &= \langle\alpha|\alpha, t_0=0; t\rangle\\
&= \langle\alpha|\mathcal{U}(t,0)|\alpha\rangle.
\end{aligned}$$

The absolute value of the correlation amplitude tells us how much the states associated with different moments of time resemble each other.
In particular, if the initial state is an energy eigenstate $|a'\rangle$, then

$$C(t) = \exp\left(-\frac{iE_{a'}t}{\hbar}\right),$$

and the absolute value of the correlation amplitude is 1 at all times, i.e. the system is in stationary state. When the initial state is a superposition of energy eigenstates we get

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

When t is relatively large the terms in the sum oscillate rapidly with different frequencies and hence most probably cancel each other. Thus we expect the correlation amplitude decreasing rather rapidly from its initial value 1 at the moment $t=0$.
We can estimate the value of the expression

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

more concretely when we suppose that the statevectors of the system comprise so many, nearly degenerate, energy eigenvectors that we can think them almost to form a continuum. Then the summation can be replaced by the integration

$$\sum_{a'} \longrightarrow \int dE\,\rho(E), \quad c_{a'} \longrightarrow g(E)\Big|_{E\approx E_{a'}},$$

where $\rho(E)$ is the density of the energy eigenstates. The expression

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

can now be written as

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

which must satisfy the normalization condition

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

In many realistic physical cases $|g(E)|^2\rho(E)$ is concentrated into a small neighborhood (size ΔE) of a point $E = E_0$. Rewriting the integral representation as

$$\begin{aligned} C(t) &= \exp\left(-\frac{iE_0t}{\hbar}\right) \\ &\quad\times \int dE\, |g(E)|^2 \rho(E) \exp\left[-\frac{i(E-E_0)t}{\hbar}\right], \end{aligned}$$

we see that when t increases the integrand oscillates very rapidly except when the energy interval $|E - E_0|$ is small as compared with $\hbar/t$. If the interval, which satisfies $|E - E_0| \approx \hbar/t$, is much shorter than ΔE —the interval from which the integral picks up its contribution—, the correlation amplitudes practically vanishes. The characteristic time, after which the absolute value of the correlation amplitude deviates significantly from its initial value 1, is

$$t \approx \frac{\hbar}{\Delta E}.$$

Although this equation was derived for a quasi continuous energy spectrum it is also valid for the two state system in our spin precession example: the initial state $|S_x;\uparrow\rangle$ starts to lose its identity after the time $\approx 1/\omega_c = \hbar/(E_\uparrow - E_\downarrow)$ as we can see from the equation

$$|\langle S_x;\uparrow|\alpha, t_0 = 0; t\rangle|^2 = \cos^2\frac{\omega_c t}{2}.$$

As a summary we can say that due to the evolution the state vector describing the initial state of the system will not any more describe it after a time interval of order $\hbar/\Delta E$. This property is often called the *time and energy uncertainty relation*. Note, however, that this relation is of completely different character than the uncertainty relation concerning position and momentum because time is not a quantum mechanical observable.

We have formulated time-evolution of a quantum mechanical system in terms of time-evolution operator (i.e. H). However, the dynamics of the system can be carried out in 3 diferent ways:

Schrödinger picture

Time-evolution operator affects state kets and observables are left untouched ("our picture")

Heisenberg picture

Time-evolution operator affects observables (the corresponding operators) and state kets are left alone.

Interaction picture

State kets feel the effect of time-dependent potentials and the evolution of observables are carried out by time-independent Hamiltonian.

Obviously the resulting physics must be the same in every picture.

Hamiltonian

How do we construct appropriate Hamiltonian?

If the system has classical analogue:

- Assume Hamiltonian has the same form with classical observables replaced with operators. This way the quantum mechanics coincide with classical mechanics in the classical limit.
- If problems arise due to non-commuting operators, then let us demand Hamiltonian to be Hermitian (e.g. $xp \rightarrow \frac{1}{2}(x_{op}p_{op} + p_{op}x_{op})$

If there is no classical analogue for the system, we guess the form of Hamiltonian and compare with experimental data until our trial Hamiltonian reproduces the data.

Hand written transparencies related to the time-evolution operator can be found EXTRAS/time-evolution.pdf