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Quantum Time Evolution

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1. Introduction

This short paper will consider time evolution of states within the Hilbert space. As many have done before, we postulate that this evolution of time can be described by an operator – the time-evolution operator – that takes states from one moment in time to another. By physical arguments, we are able to restrict the freedom of this time-evolution operator. More importantly, we find that we can often express this operator in terms of the Hamiltonian. This is what it truly means when we say the recurring phrase that the Hamiltonian governs the time evolution of states.

Disclaimer: The hats on operators are left implied.

2. Time evolution of states

Suppose we have a quantum mechanical system with an associated Hilbert space $\mathcal{H}$ of physical states. Let the system initially be described by a state $|\alpha(t_0)\rangle \in \mathcal{H}$ at some constant time $t_0 \in \mathbb{R}$. At some later time $t \in \mathbb{R}$, with $t > t_0$, we expect to find the system in a state $|\alpha(t)\rangle \in \mathcal{H}$ that is not necessarily equal to the initial state $|\alpha(t_0)\rangle$. We wish to describe a relation between the two states under this temporal transformation.

To begin, we note that this transformation should be continuous; the path in the Hilbert space describing the time evolution of the states ought to be sufficiently nice (at least once differentiable) in that we do not expect discontinuous jumps or sudden directional changes of the path. This is motivated on physical grounds since we do not observe this discontinuous behaviour of state evolution. Mathematically, this assumed continuity means that our limit behaves properly,

$$\lim_{t \to t_0} |\alpha(t)\rangle = |\alpha(t_0)\rangle \,.$$

We *postulate* that there exists a family of double-parametrized operators $\mathcal{U} : \mathbb{R}^2 \to \mathcal{L}(\mathcal{H})$, the so-called **time-evolution operators** that describe the time evolution between the two states as,

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

We require some properties of the time evolution operator on both physical and mathematical grounds. Firstly, on the assumption of continuity, we find that

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

from which we can read that,

$$\lim_{t \to t_0} \mathcal{U}(t, t_0) = 1. \tag{1}$$

Secondly, probability densities should be conserved. More specifically, we require the probability of a state not to change over time; hence,

$$\langle \alpha(t_0) | \alpha(t_0) \rangle = \langle \alpha(t) | \alpha(t) \rangle = \langle \alpha(t_0) | \mathcal{U}^\dagger(t, t_0) \mathcal{U}(t, t_0) | \alpha(t_0) \rangle$$

From this, we see that

$$\mathcal{U}^\dagger(t, t_0) = \mathcal{U}^{-1}(t, t_0), \tag{2}$$

i.e., the time-evolution operator is unitary.

Thirdly, we require the composition rule

$$\mathcal{U}(t_2, t_0) = \mathcal{U}(t_2, t_1)\mathcal{U}(t_1, t_0). \tag{3}$$

This follows from evolving a state $|\alpha(t_0)\rangle \in \mathcal{H}$ to a state $|\alpha(t_1)\rangle \in \mathcal{H}$ as

$$|\alpha(t_1)\rangle = \mathcal{U}(t_1, t_0) |\alpha(t_0)\rangle$$

and consequently transform $|\alpha(t_1)\rangle$ to the state $|\alpha(t_2)\rangle \in \mathcal{H}$, from which

$$|\alpha(t_2)\rangle = \mathcal{U}(t_2, t_1) |\alpha(t_1)\rangle = \mathcal{U}(t_2, t_1)\mathcal{U}(t_1, t_0) |\alpha(t_0)\rangle .$$

We could also immediately transform the state from $|\alpha(t_0)\rangle$ to $|\alpha(t_2)\rangle$ as

$$|\alpha(t_2)\rangle = \mathcal{U}(t_2, t_0) |\alpha(t_0)\rangle ,$$

and the composition rule follows immediately by comparison.

We will take the properties Eqs. (1),(2), and (3) as assumptions for our time-evolution operator.

It turns out to be useful to consider the following time evolution,

$$\mathcal{U}(t + \mathrm{d}t, t_0) = \mathcal{U}(t + \mathrm{d}t, t)\mathcal{U}(t, t_0), \tag{4}$$

where we will consider $\mathrm{d}t \in \mathbb{R}$ to be infinitesimal. Using the continuity condition Eq.(1), we can Taylor expand the time-evolution operator around t to obtain,

$$\lim_{\mathrm{d}t \to 0} \mathcal{U}(t + \mathrm{d}t, t) = 1 - i\Omega \mathrm{d}t + \frac{(-i)^2}{2}\Omega^2 \mathrm{d}t^2 + \mathcal{O}\left(\mathrm{d}t^3\right).$$

The interested reader may find the justification for this Taylor expansion (in the case of a single-parameter operator) in the notes: "The Operator-valued Taylor expansion". The prefactor $-i$ ensures that the operator Ω is necessarily self-adjoint[1]. The operator Ω is called the **generator** of the time evolution, since the entire Taylor expansion is determined by only this operator Ω for any infinitesimal time evolution.[2]

[1] For the physicists: read self-adjoint as Hermitian.

[2] To consider a finite time t evolution, one could apply the infinitesimal time evolution a number of N times by splitting t into N parts, $\mathcal{U}^N = (1 - \frac{i\Omega t}{N})^N$. One could then formally take a $N \to \infty$ limit to obtain, $\lim_{N\to\infty} \mathcal{U}^N = \lim_{N\to\infty}(1 - \frac{i\Omega t}{N})^N = \exp\{-i\Omega t\}$.

We proceed from Eq. (4) to obtain up to the first order the expression,

$$\lim_{\mathrm{d}t\to 0} \mathcal{U}(t+\mathrm{d}t, t_0) = (1 - i\Omega \mathrm{d}t)\, \mathcal{U}(t, t_0).$$

We may recast this in a more intuitive way, namely

$$\lim_{\mathrm{d}t\to 0} \frac{\mathcal{U}(t+\mathrm{d}t, t_0) - \mathcal{U}(t, t_0)}{\mathrm{d}t} = -i\Omega \mathcal{U}(t, t_0).$$

We recognise the derivative and find a defining equation for the time-evolution operator in terms of the generator Ω, that is given by,

$$i\frac{\partial}{\partial t}\mathcal{U}(t, t_0) = \Omega \mathcal{U}(t, t_0). \tag{5}$$

To interpret this expression, we borrow some intuition from physics. Regardless of the overall physical dimension of the time evolution operator, each term in its Taylor expansion should be of the same dimension. In particular, this implies that Ω should be of unit $1/s$ where $\mathrm{d}t$ has time units s. The generator Ω is thus some sort of frequency. Upon demanding that $\hbar$ should make an appearance in the first order (quantum) correction, we find a valid combination to be $\Omega = \frac{H}{\hbar}$, where H is the Hamiltonian of the system. Eq. (5) then becomes the famously known Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t_0) = H\mathcal{U}(t, t_0). \tag{6}$$

When acting upon the state $|\alpha(t_0)\rangle$, we find the Schrödinger equation for states,

$$i\hbar\frac{\partial}{\partial t}\,|\alpha(t)\rangle = i\hbar\frac{\partial}{\partial t}\mathcal{U}(t, t_0)\,|\alpha(t_0)\rangle = H\mathcal{U}(t, t_0)\,|\alpha(t_0)\rangle = H\,|\alpha(t)\rangle\,. \tag{7}$$

Often, we know how to express the Hamiltonian H in terms of a position basis $|x\rangle$, or equivalently, a momentum basis $|p\rangle$. For the position basis, we can act with $\langle x|$ to find,

$$i\hbar\frac{\partial}{\partial t}\psi_\alpha(x,t) \equiv i\hbar\frac{\partial}{\partial t}\,\langle x|\alpha(t)\rangle = H\,\langle x|\alpha(t)\rangle \equiv H\psi_\alpha(x,t).$$

Here, $\psi_\alpha(x,t) = \langle \alpha(t)|x\rangle$ is called the **time dependent position wave function**. Similarly, we can act with $\langle p|$ to find,

$$i\hbar\frac{\partial}{\partial t}\phi_\alpha(p,t) \equiv i\hbar\frac{\partial}{\partial t}\,\langle p|\alpha(t)\rangle = H\,\langle p|\alpha(t)\rangle \equiv H\phi_\alpha(p,t),$$

where $\phi(p,t)$ is called the **time dependent momentum wave function**.

3. Solutions of the Schrödinger equation

The Schrödinger equation Eq. (6) is a first order partial differential equation of operators. The solution of this PDE cannot always be written algebraically, but it can always be expressed in terms of a multidimensional integral. The difficulty lies in the observation that the Hamiltonian itself may depend on time.

In case H does not explicitly depend on time, the solution is straightforward. We are inspired by the realisation that the time derivative of the time-evolution operator returns it with a time-independent prefactor. This is usually done with an exponential function, so we try the ansatz,

$$\mathcal{U}(t,t_0) = 1 + \frac{-i}{\hbar}H\cdot(t-t_0) + \frac{(-i)^2}{2\hbar^2}H^2\cdot(t-t_0)^2 + \frac{(-i)^3}{3!\hbar^3}H^3\cdot(t-t_0)^3 + \mathcal{O}\left((t-t_0)^4\right) \tag{8}$$

We differentiate with respect to time to find,

$$\begin{aligned}\frac{\partial}{\partial t}\mathcal{U}(t,t_0) &= \frac{-i}{\hbar}H + \frac{(-i)^2}{\hbar^2}H^2\cdot(t-t_0) + \frac{(-i)^3}{2\hbar^3}H^3\cdot(t-t_0)^2 + \mathcal{O}\left((t-t_0)^3\right)\\ &= -\frac{i}{\hbar}H\mathcal{U}(t,t_0).\end{aligned}$$

This proves that our ansatz Eq. (8) satisfies the Schrödinger equation Eq. (6) as long as the Hamiltonian is explicitly independent of time. We will introduce the short-hand notation

$$\exp\left\{-\frac{i}{\hbar}H\cdot(t-t_0)\right\} = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-iH\cdot(t-t_0)}{\hbar}\right)^n.$$

With this notation, we find that we can write the solution of $\mathcal{U}(t,t_0)$ in terms of H as,

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

The solution is still manageable when the Hamiltonian depends on time but commutes at different times,

$$[H(t_1),H(t_2)] \equiv H(t_1)H(t_2) - H(t_2)H(t_1) = 0.$$

We will state the solution here, where the reader is welcomed to show that the expression withstands the derivation,

$$\mathcal{U}(t,t_0) = \exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t}H(t')\mathrm{d}t'\right\}.$$

For an arbitrary Hamiltonian $H \in \mathcal{L}(\mathcal{H})$, we have the general solution

$$\hat{\mathcal{U}}(t,t_0) = \hat{1} + \frac{-i}{\hbar}\int_{t_0}^{t}\hat{H}(t')\mathrm{d}t' + \left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\, H(t_1)H(t_2) + \ldots.$$

The reader may verify this expression readily by differentiating with respect to time.

4. Schrödinger vs Heisenberg

Allow us to recap what we have seen so far. We started with a stationary state $|\alpha(t_0)\rangle$ that we fixed at some time t_0. We considered the time evolution of $|\alpha(t_0)\rangle$ to the state $|\alpha(t)\rangle$ and postulated that this transformation is given by the time-evolution operator

$\mathcal{U}(t, t_0) \in \mathcal{L}(\mathcal{H})$. We derived properties of this operator and found that we could express it in terms of the Hamiltonian $H \in \mathcal{L}(\mathcal{H})$; its exact form depending on the form of the Hamiltonian.

For this section, we will assume that the Hamiltonian H is independent of time, though the entire analysis can be done with arbitrary Hamiltonian. We will also take our initial time as $t_0 = 0$ for convenience. The time-evolution operator can then be expressed like,

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

There is, however, an ambiguity that we have not mentioned until now. We have considered time evolution of states, as

$$|\alpha(t)\rangle = \mathcal{U}(t)\,|\alpha(0)\rangle\,.$$

An arbitrary operator A then, will act on the transformed state as

$$A\,|\alpha(t)\rangle = A\mathcal{U}(t)\,|\alpha(0)\rangle\,.$$

However, in physics we cannot measure states or vectors but only scalar quantities. The physically relevant mathematical objects are inner products that represent measurable quantities. The latter can be immediately denoted,

$$\langle\alpha(t)|\,A\,|\alpha(t)\rangle = \langle\alpha(0)|\,\mathcal{U}^\dagger(t)A\mathcal{U}(t)\,|\alpha(0)\rangle = \langle\alpha|\,\mathcal{U}^\dagger(t,0)A(0)\mathcal{U}(t,0)\,|\alpha\rangle\,.$$

In the last equality we do not do anything other than change the notation slightly. This way of writing it down does seem indicate a change of perspective, where we can define the time evolved operator,

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

In this perspective, the operators are time dependent whereas the states are completely static. This is called the **Heisenberg interpretation**, in contrast to the **Schrödinger picture** where the states evolve with time and the operators are static. Both interpretations are entirely equivalent, distinguished only by mathematical preference.

5. Example

It is fruitful to consider an example, namely the quantum harmonic oscillator, and see how time affects the creation and annihilation operators. We work in the Heisenberg interpretation which will make the calculations more intuitive.[3] We recall the Hamiltonian in creation and annihilation form,

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).$$

[3] But remember, both interpretations are equally valid.

The Hamiltonian is independent of time, which means that we can immediately write down the time-evolution operator and its adjoint as,

$$\mathcal{U}(t) \equiv \mathcal{U}(t,0) = \exp\left\{-\frac{i}{\hbar}Ht\right\} = \exp\left\{-i\omega\left(a^\dagger a + \frac{1}{2}\right)t\right\},$$
$$\mathcal{U}^\dagger(t) \equiv \mathcal{U}^\dagger(t,0) = \exp\left\{\frac{i}{\hbar}Ht\right\} = \exp\left\{i\omega\left(a^\dagger a + \frac{1}{2}\right)t\right\}.$$

In the Heisenberg interpretation, we then find that our creation and annihilation operators evolve under time as,

$$a(t) = \mathcal{U}^\dagger(t)a\mathcal{U}(t) = e^{i\omega\left(a^\dagger a+\frac{1}{2}\right)t}ae^{-i\omega\left(a^\dagger a+\frac{1}{2}\right)t} = e^{i\omega t a^\dagger a}ae^{-i\omega t a^\dagger a},$$
$$a^\dagger(t) = \mathcal{U}^\dagger(t)a^\dagger\mathcal{U}(t) = e^{i\omega\left(a^\dagger a+\frac{1}{2}\right)t}a^\dagger e^{-i\omega\left(a^\dagger a+\frac{1}{2}\right)t} = e^{i\omega t a^\dagger a}a^\dagger e^{-i\omega t a^\dagger a}.$$

The right-most expressions for either equation require intensive labour to cast them into a useful form. We will forgo this effort and immediately state the relevant expressions,

$$e^{i\omega t a^\dagger a}ae^{-i\omega t a^\dagger a} = ae^{-i\omega t},$$
$$e^{i\omega t a^\dagger a}a^\dagger e^{-i\omega t a^\dagger a} = a^\dagger e^{i\omega t}.$$

The reader should feel welcome to derive these results and might find it useful to first calculate the commutator $\left[a, \exp\{-i\omega t a^\dagger a\}\right]$.

Putting everything together, we find the time dependent creation and annihilation operators,

$$a(t) = a(0)e^{-i\omega t}, \qquad a^\dagger(t) = a^\dagger(0)e^{i\omega t}.$$

This is the time evolution of the creation and annihilation operators. We see that a and $a^\dagger$ oscillate in opposite direction as an exponential with a frequency ω. Notice that the Hamiltonian remains constant in time,

$$\begin{aligned} H(t) = \mathcal{U}(t)^\dagger H\mathcal{U}(t) &= \hbar\omega\mathcal{U}^\dagger(t)\left(a^\dagger a + \frac{1}{2}\right)\mathcal{U}(t) = \hbar\omega\mathcal{U}^\dagger(t)a^\dagger a\mathcal{U}(t) + \frac{\hbar\omega}{2} \\ &= \hbar\omega\left(\mathcal{U}^\dagger(t)a^\dagger\mathcal{U}(t)\right)\left(\mathcal{U}^\dagger(t)a\mathcal{U}(t)\right) + \frac{\hbar\omega}{2} = \hbar\omega a^\dagger(t)a(t) + \frac{\hbar\omega}{2} \\ &= \hbar\omega a^\dagger(0)^{i\omega t}e^{-i\omega t}a(0) + \frac{\hbar\omega}{2} = \hbar\omega\left(a^\dagger(0)a(0) + \frac{1}{2}\right) = H(0). \end{aligned}$$

This reflects that energy is conserved in our quantum harmonic oscillator.

We can compare how our results fares against the well-known theory of the Hamiltonian formalism. We recall the original Hamiltonian of the quantum harmonic oscillator,

$$H = \frac{p^2}{2m} + \frac{m\omega^2x^2}{2}.$$

The Hamilton equations then read,

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial H}{\partial p} = \frac{p}{m}, \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial x} = -m\omega^2 x.$$

The creation and annihilation operator are expressed in terms of position and momentum as,

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right).$$

We can take the derivative with respect to time to find,

$$\begin{aligned}
\frac{\mathrm{d}a}{\mathrm{d}t} &= \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{i}{m\omega}\frac{\mathrm{d}p}{\mathrm{d}t}\right) = \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{p}{m} - i\omega x\right) \\
&= -i\omega\sqrt{\frac{m\omega}{2\hbar}}\left(\frac{ip}{m\omega} + x\right) = -i\omega a, \\
\frac{\mathrm{d}a^\dagger}{\mathrm{d}t} &= \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{\mathrm{d}x}{\mathrm{d}t} - \frac{i}{m\omega}\frac{\mathrm{d}p}{\mathrm{d}t}\right) = \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{p}{m} + i\omega x\right) \\
&= i\omega\sqrt{\frac{m\omega}{2\hbar}}\left(-\frac{ip}{m\omega} + x\right) = i\omega a^\dagger.
\end{aligned}$$

The differential equations $\dot{a} = -i\omega a$ and $\dot{a}^\dagger = i\omega a^\dagger$ have the immediate solutions,

$$a(t) = a(0)e^{-i\omega t}, \qquad a^\dagger(t) = a^\dagger(0)e^{i\omega t},$$

precisely as desired. Thus, we find that the time evolution of the creation and annihilation operators is described using an exponential.

This concludes the time evolution of the quantum harmonic oscillator.