Quantum Mechanics: Time Dependence

May 20, 2025

1 Motivation

Quantum dynamics is central to the understanding how quantum systems evolve in time and provides a direct link between a system's energy structure and its temporal behavior. By studying the time-dependent Schrödinger equation and its equivalent formulations, you'll see how interference, tunneling, and entanglement naturally arise, generating insights that range from interpreting atomic spectra and modeling molecular reactions to enabling coherent control in quantum technologies. In summary, quantum dynamics provides an essential foundation for both fundamental research and transformative applications.

2 Time Dependent Schroedinger Equation

Consider a quantum system described by a state vector $\mid \psi(t)\rangle$. In the position representation, the wavefunction is

$$\psi(x,t) = \langle x \mid \psi(t)\rangle.$$

We define an operator, $\hat{U}$, that describes the evolution of the system as it evolves from t to Δt

$$|\psi(x, t+\Delta t) >= \hat{U}\left(\Delta t\right)|\psi(t)>$$

We also require that the wavefunction remains normalized as the system evolves

$$\begin{aligned} 1 &=< \psi(t+\Delta t)|\psi(t+\Delta t)> \\ &=< \psi(t)|\hat{U}^{+}\hat{U}|\psi(t)> \end{aligned}$$

and we conclude that the time evolution operator, U, is unitary

$$\hat{U}^{+}\hat{U} = 1$$

we define the time evolution operator as

$$\hat{U}\left(\Delta t\right) = 1 - \frac{i}{\hbar}\hat{H}\Delta t$$

and we write

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

we rearrange this equation and obtain:

$$\begin{aligned}&i\hbar\frac{d}{dt}\hat{U}\\ &= \lim_{\Delta t\to 0}\frac{\hat{U}(t+\Delta t)-\hat{U}(t)}{\Delta t}\\ &= \hat{H}\hat{U}\end{aligned}$$

similarly, we can obtain an equation for the time evolution of the initial state

$$\begin{aligned}&i\hbar\frac{d}{dt}|\psi(t)>\\ &= \lim_{\Delta t\to 0}\frac{|\psi(t+\Delta t)> -|\psi(t)>}{\Delta t}\\ &= \lim_{\Delta t\to 0}\frac{\hat{U}(t+\Delta t)-\hat{U}(t)}{\Delta t}|\psi(t_0)>\\ &= \hat{H}\hat{U}|\psi(t_0)>\\ &= \hat{H}|\psi(t)>\end{aligned}$$

and combining the first and last equation, we obtain the time-dependent Schroedinger equation

$$i\hbar\frac{d}{dt}|\psi(t)>= \hat{H}|\psi(t)>$$

or after projecting into position space, we obtain the more familiar looking time-dependent Schroedinger equation

$$i\hbar\frac{d}{dt}\psi(x,t) = H(x,t)\psi(x,t)$$

we can provide a closed form for the time evolution operator

$$\begin{aligned}i\hbar\frac{d}{dt}\hat{U} &= \hat{H}\hat{U}\\ \hat{U}\left(t\right) &= exp\left(-\frac{i}{\hbar}\int^{t}\hat{H}\left(t\right)dt\right)\end{aligned}$$

in other words, time evolution has the form of a time-dependent phase factor. However, note, that time evolution may lead to emerging relative phases (unlike a global phase, that is immaterial in quantum mechanics). The time evolution operator simplifies significantly if the operator, $\hat{H}$, is time independent, as will see in the next section.

3 Time Independent Schroedinger Equation

If the operator, $\hat{H}$, is time independent the form of the time evolution operator simplifies to

$$\hat{U}\left(t\right) = exp\left(-\frac{i}{\hbar}\hat{H}t\right)$$

an alternative to derive this same formula is to realize that we apply the time evolution operator N times such that

$$\Delta t = \frac{t}{N}$$

$$\begin{aligned} \hat{U}\left(t\right) = \hat{U}\left(\Delta t\right)\hat{U}\left(\Delta t\right)\cdots\hat{U}\left(\Delta t\right) \\ = U\left(\Delta t\right)^{N} \\ = \left(1 - \frac{i}{\hbar}\hat{H}\frac{t}{N}\right)^{N} \\ = exp\left(-\frac{i}{\hbar}\hat{H}t\right) \end{aligned}$$

exactly the same result as before, and again highlighting that time evolution in quantum mechanics is expressed as a change in relative phases

$$|\psi(t)>= exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\psi(t=0)>$$

We still need to clarify what the operator $\hat{H}$ represents in the context of quantum evolution. Since the exponent has to be dimensionless, and the units of $\hbar$ are $[energy{*}s]$, it follows that $\hat{H}$ itself my have the unites of $[energy]$. Expanding on this results from dimensional analysis, we clarify the significance of $\hat{H}$further, by computing how the expectation value of this operator changes with time. Consider the case that $\hat{H}$is time independent

$$\begin{aligned} < \psi(t)|\hat{H}|\psi(t)> \\ =< \psi(t=0)|\hat{U}^{+}\hat{H}\hat{U}|\psi(t=0)> \\ =< \psi(t=0)|\hat{H}|\psi(t=0)> \end{aligned}$$

since $\left[\hat{H},\hat{U}\right]=0$. We find that in this case the time average does not change. In summary, all of these lines of evidence suggests that $\hat{H}$can be identified with the Hamiltonian of the system, and for the average energy, corresponding to the average Hamiltonian we have

$$< E >=< \psi|\hat{H}|\psi >$$

Let's follow this identification somewhat further, and consider the (energy) eigenstates of the system Hamiltonian

$$\hat{H}|E>= E|E>$$

for which we find

$$exp\left(-\frac{i}{\hbar}\hat{H}t\right) = exp\left(-\frac{i}{\hbar}Et\right)$$

and

$$|\psi(t)>= exp\left(-\frac{i}{\hbar}\hat{H}t\right)|E>= exp\left(-\frac{i}{\hbar}Et\right)|E>$$

and as argued above, the state simply picks up a phase as the system evolves. However, this does not preclude a rich and varied quantum dynamics. Compare the single state dynamics with superposition state dynamics. If we have a system initialized in a single energy eigenstate, we find

$$|\psi(t)>= exp\left(-\frac{i}{\hbar}Et\right)|E>$$

and the state only picks up an overall phase and remains equivalent to the original state. Now consider a system prepared in a superposition of energy states

$$|\psi(t=0)>= a_1|E_1> +a_2|E_2>$$

and the state evolves following

$$\begin{aligned} |\psi(t)>= exp\left(-\frac{i}{\hbar}\hat{H}t\right)|\psi(t=0)> \\ = exp\left(-\frac{i}{\hbar}\hat{H}t\right)(a_1|E_1> +a_2|E_2>) \\ = exp\left(-\frac{i}{\hbar}\hat{H}t\right)a_1|E_1> +exp\left(-\frac{i}{\hbar}\hat{H}t\right)a_2|E_2> \\ = exp\left(-\frac{i}{\hbar}E_1t\right)a_1|E_1> +exp\left(-\frac{i}{\hbar}E_2t\right)a_2|E_2> \end{aligned}$$

and the relative phases do not cancel (unless the energies of the two states are the same, $E_1 = E_2$), leading to non-trivial quantum dynamics.

4 Quantum Dynamics - Frameworks

In quantum mechanics time evolution can be described in three equivalent but complementary frameworks: in the Schrödinger picture, state vectors evolve in time; in the Heisenberg picture, all time-dependence is carried by the operators, making symmetries and conservation laws especially transparent; and in the Interaction picture, one splits the Hamiltonian into a "free" part—whose evolution defines a rotating reference frame—and an "interaction" part, which is treated against that background. Understanding these three pictures encompasses everything from direct wavefunction dynamics to operator algebra to systematic perturbation theory in quantum field theory.

4.1 Schroedinger Picture

Core Idea. The quantum state carries all time dependence, while operators representing observables remain fixed (unless they have explicit time dependence). A state vector, $|\psi_S(t)>$, evolves according to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi_S(t)>=\hat{H}|\psi_S(t)>$$

The formal solution is

$$|\psi_S(t)>=U(t,t_0)\,|\psi_S(t)>$$
$$U(t,t_0)=exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(t)\,dt\right)$$

If the Hamiltonian does not explicitly depend on time the equation for the for evolution operator simplifies to

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

Operator Behavior. Any operator (with no explicit time dependence) is constant

$$\hat{A}_S(t)=\hat{A}_S(t_0)=\hat{A}_S$$

Pros & Cons:

- Advantage: Directly connects to wavefunction dynamics; intuitive when solving simple time-dependent potentials.
- Limitation: For many-body or field theories, tracking the evolution of a high-dimensional wavefunction becomes increasingly challenging.

4.2 Heisenberg Picture

Core Idea. Operators evolve in time, absorbing the full dynamics, while state vectors remain constant (often taken at the initial time). State Definition. Choose

$$|\psi_H>=|\psi_S(t_0)>$$

independent of time, t. We recognize that operator averages depend on the system we are describing, not how we are describing the system. We start from the evolution of an operator average in the Schroedinger picture using this expectation

$$\begin{aligned} < A >_H =& < A >_S \\ =& < \psi_S(t)|\hat{A}_S|\psi_S(t) > \\ =& < \psi_S(t_0)|\hat{U}^+\hat{A}_S\hat{U}|\psi_S(t_0) > \\ =& < \psi_H|\hat{A}_H|\psi_H > \end{aligned}$$

and we identify

$$A_H = \hat{U}^+\hat{A}_S\hat{U}$$

Differentiating yields the Heisenberg equation of motion for operators:

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

Expectation Values. Identical to Schrödinger picture (as expected):

$$< A > (t) = < \psi_H|\hat{A}_H|\psi_H > = < \psi_S(t)|\hat{A}_S|\psi_S(t) >$$

Pros & Cons:

- Advantage: Particularly well-suited for quantum field theory and many-body physics, where mode operators (creation/annihilation) evolve and states (e.g., vacuum) stay fixed.
- Limitation: Less intuitive if one thinks in terms of wavefunction evolution; interaction with explicitly time-dependent Hamiltonians can complicate operator equations.

4.3 Interaction Picture

Core Idea. A hybrid approach splitting the Hamiltonian, $\hat{H} = \hat{H}_0 + \hat{V}(t)$. $\hat{H}_0$ is time independent and drives the operator evolution, while the "interaction", $\hat{V}(t)$, drives the state evolution. This picture underpins time-dependent perturbation theory and quantum field theory. Define the free evolution operator

$$U(t, t_0) = exp\left(-\frac{i}{\hbar}\hat{H}_0(t - t_0)\right)$$

and interaction-picture operators:

$$\hat{A}_H = \hat{U}^+ \hat{A}_S \hat{U}$$

They satisfy

$$i\hbar \frac{\partial}{\partial t} \hat{A}_I(t) = \left[\hat{A}_I(t), \hat{H}_0\right]$$

Interaction-picture state:

$$|\psi_I(t)>= U^+(t, t_0)\,|\psi_S(t)>$$

It evolves according to

$$i\hbar \frac{\partial}{\partial t} |\psi_I(t)>= \hat{V}_I(t)\,|\psi_I(t)>$$

$$\hat{V}_I = \hat{U_0}^+ \hat{V}(t)\,\hat{U}_0$$

The formal solution for the state-evolution operator is given by the Dyson series:

$$|\psi_I(t)>= \mathcal{T}exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t)\,dt\right]|\psi_I(t_0)>$$

where T is time-ordering. Pros & Cons.:

- Advantage: Enables perturbative expansions in $\hat{V}$; central to scattering theory (S-matrix) and quantum electrodynamics.
- Limitation: Requires a clear separation of "free" vs. "interaction" parts; less straightforward if no natural splitting exists.

Comparison of the Three Pictures

Feature	Schroedinger	Heisenberg	Interaction
State time-dependence	Yes	No	Yes, $\hat{V}_I$
Operator time-dependence	No	Yes	Partial, $\hat{H}_0$
Utility	Wave-packet dynamics, foundational quantum mechanics	Field theory; many-body theory	Perturbation theory; scattering
Choose	Exact or numerical solution of time-dependent Schroedinger equation	Operator algebra; high-dimensional problems	Time-dependent perturbation; Feynman diagrams

5 Conclusion

Although physically equivalent, each picture offers unique insights:

1. Schrödinger picture appeals to our classical intuition of evolving wave-functions and is often used in quantum-mechanics courses and numerical simulations.

2. Heisenberg picture shifts focus to operator dynamics, streamlining treatments in quantum field theory and many-body physics.
3. Interaction picture is an elegant hybrid of both approaches, providing a natural framework for perturbation theory and scattering processes.

In summary, a conceptual understanding of quantum dynamics provides you with a versatile tool for treating advanced topics in modern physics, encompassing physics, chemistry, quantum technologies as well as many other current and emerging fields in science and engineering.

6 Exercises

Not yet, for a collection of problems in quantum dynamics check quantum mechanics textbooks.