

6.1: Time-dependent Schrödinger Equation

When we first introduced quantum mechanics, we saw that the fourth postulate of QM states that: *The evolution of a closed system is unitary (reversible). The evolution is given by the time-dependent Schrödinger equation*

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \mathcal{H}|\psi\rangle$$

where \mathcal{H} is the Hamiltonian of the system (the energy operator) and \hbar is the reduced Planck constant ($\hbar = h/2\pi$ with h the Planck constant, allowing conversion from energy to frequency units).

We will focus mainly on the Schrödinger equation to describe the evolution of a quantum-mechanical system. The statement that the evolution of a closed quantum system is unitary is however more general. It means that the state of a system at a later time t is given by $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, where $U(t)$ is a unitary operator. An operator is unitary if its adjoint U^\dagger (obtained by taking the transpose and the complex conjugate of the operator, $U^\dagger = (U^*)^T$) is equal to its inverse: $U^\dagger = U^{-1}$ and $UU^\dagger = 1$.

Note that the expression $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ is an integral equation relating the state at time zero with the state at time t . For example, classically we could write that $x(t) = x(0) + vt$ (where v is the speed, for constant speed). We can as well write a differential equation that provides the same information: the Schrödinger equation. Classically for example, (in the example above) the equivalent differential equation would be $\frac{dx}{dt} = v$ (more generally we would have Newton's equation linking the acceleration to the force). In QM we have a differential equation that control the evolution of closed systems. This is the Schrödinger equation:

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \mathcal{H}\psi(x, t)$$

where \mathcal{H} is the system's Hamiltonian. The solution to this partial differential equation gives the wavefunction $\psi(x, t)$ at any later time, when $\psi(x, 0)$ is known.

Solutions to the Schrödinger equation

We first try to find a solution in the case where the Hamiltonian $\mathcal{H} = \frac{\hat{p}^2}{2m} + V(x, t)$ is such that the potential $V(x, t)$ is time independent (we can then write $V(x)$). In this case we can use separation of variables to look for solutions. That is, we look for solutions that are a product of a function of position only and a function of time only:

$$\psi(x, t) = \varphi(x)f(t)$$

Then, when we take the partial derivatives we have that

$$\frac{\partial \psi(x, t)}{\partial t} = \frac{df(t)}{dt} \varphi(x), \quad \frac{\partial \psi(x, t)}{\partial x} = \frac{d\varphi(x)}{dx} f(t) \quad \text{and} \quad \frac{\partial^2 \psi(x, t)}{\partial x^2} = \frac{d^2 \varphi(x)}{dx^2} f(t)$$

The Schrödinger equation simplifies to

$$i\hbar \frac{df(t)}{dt} \varphi(x) = -\frac{\hbar^2}{2m} \frac{d^2 \varphi(x)}{dx^2} f(t) + V(x) \varphi(x) f(t)$$

Dividing by $\psi(x, t)$ we have:

$$i\hbar \frac{df(t)}{dt} \frac{1}{f(t)} = -\frac{\hbar^2}{2m} \frac{d^2 \varphi(x)}{dx^2} \frac{1}{\varphi(x)} + V(x)$$

Now the LHS is a function of time only, while the RHS is a function of position only. For the equation to hold, both sides have then to be equal to a constant (separation constant):

$$i\hbar \frac{df(t)}{dt} \frac{1}{f(t)} = E, \quad -\frac{\hbar^2}{2m} \frac{d^2 \varphi(x)}{dx^2} \frac{1}{\varphi(x)} + V(x) = E$$

The two equations we find are a simple equation in the time variable:

$$\frac{df(t)}{dt} = -\frac{i}{\hbar} E f(t), \quad \rightarrow f(t) = f(0) e^{-i \frac{Et}{\hbar}}$$

and

$$-\frac{\hbar^2}{2m} \frac{d^2 \varphi(x)}{dx^2} + V(x) \varphi(x) = E \varphi(x)$$

that we have already seen as the time-independent Schrödinger equation. We have extensively studied the solutions of the this last equation, as they are the eigenfunctions of the energy-eigenvalue problem, giving the stationary (equilibrium) states of quantum systems. Note that for these stationary solutions $\varphi(x)$ we can still find the corresponding total wavefunction, given as stated above by $\psi(x, t) = \varphi(x)f(t)$, which does describe also the time evolution of the system:

$$\boxed{\psi(x, t) = \varphi(x) e^{-i \frac{Et}{\hbar}}}$$

Does this mean that the states that up to now we called stationary are instead evolving in time?

The answer is yes, but with a caveat. Although the states themselves evolve as stated above, any measurable quantity (such as the probability density $|\psi(x, t)|^2$ or the expectation values of observable, $\langle A \rangle = \int \psi(x, t)^* A[\psi(x, t)]$) are still time-independent. (Check it!)

Thus we were correct in calling these states **stationary** and neglecting in practice their time-evolution when studying the properties of systems they describe.

Notice that the wavefunction built from one energy eigenfunction, $\psi(x, t) = \varphi(x)f(t)$, is only a particular solution of the Schrödinger equation, but many other are possible. These will be complicated functions of space and time, whose shape will depend on the particular form of the potential $V(x)$. How can we describe these general solutions? We know that in general we can write a basis given by the eigenfunction of the Hamiltonian. These are the functions $\{\varphi(x)\}$ (as defined above by the time-independent Schrödinger equation). The eigenstate of the Hamiltonian do not evolve. However we can write any wavefunction as

$$\psi(x, t) = \sum_k c_k(t) \varphi_k(x)$$

This just corresponds to express the wavefunction in the *basis* given by the energy eigenfunctions. As usual, the coefficients $c_k(t)$ can be obtained at any instant in time by taking the inner product: $\langle \varphi_k | \psi(x, t) \rangle$.

What is the evolution of such a function? Substituting in the Schrödinger equation we have

$$i\hbar \frac{\partial (\sum_k c_k(t) \varphi_k(x))}{\partial t} = \sum_k c_k(t) \mathcal{H} \varphi_k(x)$$

that becomes

$$i\hbar \sum_k \frac{\partial (c_k(t))}{\partial t} \varphi_k(x) = \sum_k c_k(t) E_k \varphi_k(x)$$

For each φ_k we then have the equation in the coefficients only

$$i\hbar \frac{dc_k}{dt} = E_k c_k(t) \rightarrow c_k(t) = c_k(0) e^{-i \frac{E_k t}{\hbar}}$$

A general solution of the Schrödinger equation is then

$$\psi(x, t) = \sum_k c_k(0) e^{-i \frac{E_k t}{\hbar}} \varphi_k(x)$$

Obs.

We can define the eigen-frequencies $\hbar \omega_k = E_k$ from the eigen-energies. Thus we see that the wavefunction is a superposition of waves φ_k propagating in time each with a different frequency ω_k .

The behavior of quantum systems –even particles– thus often is similar to the propagation of waves. One example is the diffraction pattern for electrons (and even heavier objects) when scattering from a slit. We saw an example in the electron diffraction video at the beginning of the class.

Obs.

What is the probability of measuring a certain energy E_k at a time t ? It is given by the coefficient of the φ_k eigenfunction, $|c_k(t)|^2 = \left| c_k(0) e^{-i \frac{E_k t}{\hbar}} \right|^2 = |c_k(0)|^2$. This means that the probability for the given energy is constant, does not change in time. Energy is then a so-called constant of the motion. This is true only for the energy eigenvalues, not for other observables'.

✓ Example 6.1.1

Consider instead the probability of finding the system at a certain position, $p(x) = |\psi(x, t)|^2$. This of course changes in time. For example, let

$$\psi(x, 0) = c_1(0)\varphi_1(x) + c_2(0)\varphi_2(x),$$

with

$$|c_1(0)|^2 + |c_2(0)|^2 = |c_1|^2 + |c_2|^2 = 1$$

and $\varphi_{1,2}$ normalized energy eigenfunctions. Then at a later time we have

$$\psi(x, t) = c_1(0)e^{-i\omega_1 t}\varphi_1(x) + c_2(0)e^{-i\omega_2 t}\varphi_2(x).$$

What is $p(x, t)$?

Solution

$$\begin{aligned} & |c_1(0)e^{-i\omega_1 t}\varphi_1(x) + c_2(0)e^{-i\omega_2 t}\varphi_2(x)|^2 \\ &= |c_1(0)|^2 |\varphi_1(x)|^2 + |c_2(0)|^2 |\varphi_2(x)|^2 + c_1^* c_2 \varphi_1^* \varphi_2 e^{-i(\omega_2 - \omega_1)t} + c_1 c_2^* \varphi_1 \varphi_2^* e^{i(\omega_2 - \omega_1)t} \\ &= |c_1|^2 + |c_2|^2 + 2 \operatorname{Re} [c_1^* c_2 \varphi_1^* \varphi_2 e^{-i(\omega_2 - \omega_1)t}] \end{aligned}$$

The last term describes a wave interference between different components of the initial wavefunction.

Obs.

The expressions found above for the time-dependent wavefunction are only valid if the potential is itself time-independent. If this is not the case, the solutions are even more difficult to obtain.

Unitary Evolution

We saw two equivalent formulation of the quantum mechanical evolution, the Schrödinger equation and the Heisenberg equation. We now present a third possible formulation: following the 4th postulate we express the evolution of a state in terms of a unitary operator, called the **propagator**:

$$\psi(x, t) = \hat{U}(t)\psi(x, 0)$$

with $\hat{U}^\dagger \hat{U} = 1$. (Notice that a priori the unitary operator \hat{U} could also be a function of space). We can show that this is equivalent to the Schrödinger equation, by verifying that $\psi(x, t)$ above is a solution:

$$i\hbar \frac{\partial \hat{U}\psi(x, 0)}{\partial t} = \mathcal{H}\hat{U}\psi(x, 0) \quad \rightarrow \quad i\hbar \frac{\partial \hat{U}}{\partial t} = \mathcal{H}\hat{U}$$

where in the second step we used the fact that since the equation holds for any wavefunction ψ it must hold for the operator themselves. If the Hamiltonian is time independent, the second equation can be solved easily, obtaining:

$$i\hbar \frac{\partial \hat{U}}{\partial t} = \mathcal{H}\hat{U} \quad \rightarrow \quad \hat{U}(t) = e^{-i\mathcal{H}t/\hbar}$$

where we set $\hat{U}(t=0) = 1$. Notice that as desired \hat{U} is unitary, $\hat{U}^\dagger \hat{U} = e^{i\mathcal{H}t/\hbar} e^{-i\mathcal{H}t/\hbar} = 1$.

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