

Chapter 2

Time Evolution in Closed Quantum Systems

Probably time evolution of physical systems is the main factor in order to understand their nature and properties. In classical systems time evolution is usually formulated in terms of differential equations (i.e. Euler–Lagrange’s equations, Hamilton’s equations, Liouville equation, etc.), which can present very different characteristics depending on which physical system they correspond to. From the beginning of the quantum theory, physicists have been often trying to translate the methods which were useful in the classical case to the quantum one, so was that Erwin Schrödinger obtained the first quantum evolution equation in 1926 [63].

This equation, called Schrödinger’s equation since then, describes the behavior of an *isolated* or *closed* quantum system, that is, by definition, a system which does not interchange information (i.e. energy and/or matter¹) with another system. So if our isolated system is in some pure state $|\psi(t)\rangle \in \mathcal{H}$ at time t , where \mathcal{H} denotes the Hilbert space of the system, the time evolution of this state (between two consecutive measurements) is according to

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}H(t)|\psi(t)\rangle, \quad (2.1)$$

where $H(t)$ is the Hamiltonian operator of the system. In the case of mixed states $\rho(t)$ the last equation naturally induces

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H(t), \rho(t)], \quad (2.2)$$

sometimes called von Neumann or Liouville-von Neumann equation, mainly in the context of statistical physics. From now on we consider units where $\hbar = 1$.

There are several ways to justify the Schrödinger equation, some of them related with heuristic approaches or variational principles, however in all of them it is necessary to make some extra assumptions apart from the postulates about states and

¹ One point to stress here is that a quantum system which interchanges information with a classical one in a known way (such as a pulse of a laser field on an atom) is also considered isolated.

observables; for that reason the Schrödinger equation can be taken as another postulate. Of course the ultimate reason for its validity is that the experimental tests are in accordance with it [64–66]. In that sense, the Schrödinger equation is for quantum mechanics as fundamental as the Maxwell's equations for electromagnetism or the Newton's Laws for classical mechanics.

An important property of Schrödinger equation is that it does not change the norm of the states, indeed

$$\begin{aligned} \frac{d}{dt} \langle \psi(t) | \psi(t) \rangle &= \left(\frac{d \langle \psi(t) |}{dt} \right) | \psi(t) \rangle + \langle \psi(t) | \left(\frac{d | \psi(t) \rangle}{dt} \right) \\ &= i \langle \psi(t) | H^\dagger(t) | \psi(t) \rangle - i \langle \psi(t) | H(t) | \psi(t) \rangle = 0, \end{aligned} \quad (2.3)$$

as the Hamiltonian is self-adjoint, $H(t) = H^\dagger(t)$. In view of the fact that the Schrödinger equation is linear, its solution is given by an evolution family $U(t, r)$,

$$| \psi(t) \rangle = U(t, t_0) | \psi(t_0) \rangle, \quad (2.4)$$

where $U(t_0, t_0) = \mathbb{1}$.

The Eq. (2.3) implies that the evolution operator is an isometry (i.e. norm-preserving map), which means it is a unitary operator in case of finite dimensional systems. In infinite dimensional systems one has to prove that $U(t, t_0)$ maps the whole \mathcal{H} onto \mathcal{H} in order to exclude partial isometries; this is easy to verify from the composition law of evolution families [67] and then for any general Hilbert space

$$U^\dagger(t, t_0) U(t, t_0) = U(t, t_0) U^\dagger(t, t_0) = \mathbb{1} \Rightarrow U^{-1} = U^\dagger. \quad (2.5)$$

On the other hand, according to these definitions for pure states, the evolution of some density matrix $\rho(t)$ is

$$\rho(t_1) = U(t_1, t_0) \rho(t_0) U^\dagger(t_1, t_0). \quad (2.6)$$

We can also rewrite this relation as

$$\rho(t_1) = \mathcal{U}_{(t_1, t_0)} [\rho(t_0)], \quad (2.7)$$

where $\mathcal{U}_{(t_1, t_0)}$ is a linear (unitary²) operator acting as

$$\mathcal{U}_{(t_1, t_0)} [\cdot] = U(t_1, t_0) [\cdot] U^\dagger(t_1, t_0). \quad (2.8)$$

Of course the specific form of the evolution operator in terms of the Hamiltonian depends on the properties of the Hamiltonian itself. In the simplest case in which H is time-independent (conservative system), the formal solution of the Schrödinger equation is straightforwardly obtained as

² It can be shown it is the only linear (isomorphic) isometry of trace-class operators. Actually the proof of theorem 3.4.1 is similar.

$$U(t, t_0) = e^{-i(t-t_0)H/\hbar}. \quad (2.9)$$

When H is time-dependent (non-conservative system) we can formally write the evolution as a Dyson expansion,

$$U(t, t_0) = \mathcal{T} e^{\int_{t_0}^t H(t') dt'}. \quad (2.10)$$

Note now that if $H(t)$ is self-adjoint, $-H(t)$ is also self-adjoint, so in this case we have physical inverses for every evolution. In fact when the Hamiltonian is time-independent, $U(t_1, t_0) = U(t_1 - t_0)$. So the evolution operator is not only a one-parameter semigroup, but a one-parameter group, with an inverse for every element $U^{-1}(\tau) = U(-\tau) = U^\dagger(\tau)$, such that $U^{-1}(\tau)U(\tau) = U(\tau)U^{-1}(\tau) = \mathbb{1}$. Of course in case of time-dependent Hamiltonians, every member of the evolution family $U(t, s)$ has the inverse $U^{-1}(t, s) = U(s, t) = U^\dagger(t, s)$, being this one also unitary.

If we look into the Eq. (2.7), we can identify ρ as a member of the Banach space of the set of trace-class self-adjoint operators, and $\mathcal{U}_{(t_1, t_0)}$ as some linear operator acting on this Banach space. Then everything considered for pure states concerning the form of the evolution operator is also applicable for general mixed states, actually the general solution to the Eq. (2.2) can be written as

$$\rho(t) = \mathcal{U}_{(t, t_0)} \rho(t_0) = \mathcal{T} e^{\int_{t_0}^t \mathcal{L}_{t'} dt'} \rho(t_0), \quad (2.11)$$

where the generator is given by the commutator $\mathcal{L}_t(\cdot) = -i[H(t), \cdot]$. This is sometimes called the, and by taking the derivative one immediately arrives to (2.2).



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