Time Evolution in Quantum Theory

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Abstract In quantum theory, time evolution (the way a physical system changes in time) is usually expressed in terms of an operator called the **hamiltonian**. In a model with time translation symmetry, the hamiltonian can also be regarded as an observable representing the system's total energy. This article introduces some basic principles and tools related to time evolution in quantum theory, with emphasis on the role of the hamiltonian and its conceptual relationship to the action principle.

Contents

1 The Heisenberg picture

Things that we could measure – or the mathematical entities that represent things we could measured – are called **observables**. In classical physics, all observables are compatible with each other, so we can treat them as having well-defined values. In any given model, we can specify those values at some initial time and then use the model's **equations of motion** to determine the values at other times.[1]

In quantum physics, most observables are not compatible with each other, so we cannot treat them all as having well-defined values (article 03431). Mathematically, observables are represented by operators on a Hilbert space,[2] and most operators do not commute with each other. In this case, describing time evolution of the *values* of the observables would not make sense. However, we can still describe time evolution using equations that relate *observables* at different times to each other. This is called the **Heisenberg picture**.

The **time slice principle** says that the algebra generated by the set of observables associated with any one time (any "time slice") should include the operators representing all observables – including those associated with other times.[3] Quantum theory does not usually predict the outcomes of individual measurements, but it does predict their statistics (article 03431). The time slice principle is important for *predicting* anything at all.

[1] A nonrelativistic model has a preferred time coordinate t. A relativistic model doesn't have a *preferred* time coordinate, but if the prescribed spacetime metric is **globally hyperbolic** (Witten (2021)), then we can *choose* a time coordinate t such that any hypersurface of constant t is a Cauchy surface. For the rest of this article, the prescribed spacetime metric is assumed to be globally hyperbolic, t denotes a chosen time coordinate, and the word **time** refers to this chosen coordinate. This way, the statements in this article apply to both nonrelativistic and relativistic models.

[2] More carefully: observables are represented by elements of an abstract algebra (which should at least have the structure of a C*-algebra, as defined in Murphy (1990)), and states are usually constructed by choosing a representation of the algebra in terms of operators on a Hilbert space (Witten (2021)).

[3] More carefully: the time slice principle says that the set of observables associated with any given *finite interval* of time should include the operators representing all observables (Schreiber (2008)).

2 Unitary time evolution operators

Let $\Omega(t)$ be the set of all observables associated with time t. Let s be a fixed reference time, and suppose that for each observable $A(s) \in \Omega(s)$ at the reference time, the corresponding observable $A(t) \in \Omega(t)$ at time t is given by

$$A(t) = U^{-1}(s,t)A(s)U(s,t), \tag{1}$$

where $U(s,t)$ is a unitary operator that depends on s, t but not on A. The unitary operators $U(s,t)$ are called **time evolution operators**. We can think of $A(t)$ and $A(s)$ as the "same" observable at different times, represented by different operators because we are using the Heisenberg picture. The time slice principle can be enforced by requiring that the time evolution operators belong to the algebra generated by the operators in $\Omega(s)$.

The statement that $U(s,t)$ is unitary means[4]

$$U^*(s,t) = U^{-1}(s,t). \tag{2}$$

The reference time s is arbitrary. To change it from s to a new reference time s', define $U(s',t)$ by the condition

$$U(s,s')U(s',t) = U(s,t) \tag{3}$$

so that (1) implies

$$A(t) = U^{-1}(s',t)A(s')U(s',t).$$

[4]In this article, A^* denotes the adjoint of an operator A, as in much of the math literature. In a matrix representation, the adjoint is usually denoted $A^\dagger$ instead. Article 74088 comments on the advantages of each notation.

3 The Schrödinger picture

When time evolution is implemented by a unitary transformation as in (1), we can use an alternate formulation in which all time-dependence is carried by the **state** (article 03431) instead of by the observables. This alternative formulation is called the **Schrödinger picture**.

To define the Schrödinger picture, choose a reference time s, and consider a state of the form[5]

$$\rho(\cdots) = \frac{\langle\psi|\cdots|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{4}$$

If we define

$$\big|\psi(t)\big\rangle \equiv U(s,t)|\psi\rangle \tag{5}$$

where $U(s,t)$ are the time evolution operators in equation (1), then

$$\begin{aligned}\langle\psi|A(t)|\psi\rangle &= \big\langle\psi(t)\big|A\big|\psi(t)\big\rangle \\ \langle\psi|\psi\rangle &= \big\langle\psi(t)\big|\psi(t)\big\rangle\end{aligned} \tag{6}$$

with $A \equiv A(s)$. Equation (6) is a trivial identity, but the left- and right-hand sides suggest two different ways of thinking. On the left-hand side, observables are time-dependent and states are not. That's the Heisenberg picture. On the right-hand side, the state is time-dependent and observables are not. That's the Schrödinger picture.

[5] In this case, the state can be represented by a single state-vector $|\psi\rangle$. Articles 77228 and 03431 introduce a more general perspective that motivates the notation $\rho(\cdots)$.

4 Which picture is better?

Observables may be time-dependent in a way that cannot be described by a unitary transform (1) alone, even though the time slice principle is still respected. In that case, we can still define a Schrödinger picture by moving *some* of the time-dependence to the state (the part that can be implemented by a unitary tranform (1)), but not all of it. In this case, the Heisenberg picture is conceptually simpler.

Even in a model where time evolution is described by a unitary transformation (1), different pictures have different advantages:

- The Heisenberg picture tends to make general principles easier to express, at least principles that relate directly to observables, like the causality principles in relativistic quantum field theory (article 21916).
- The Schrödinger picture can make some calculations easier to manage. It can also be useful conceptually: one definition of quantum field theory[6] uses an attractive generalization of the Schrödinger picture in which Hilbert spaces are associated with arbitrary hypersurfaces in arbitrary spacetimes.[7]
- An **interaction picture**, in which some time-dependence carried by observables and some by the state, is convenient in many practical calculations.

The rest of this article uses the Heisenberg picture, except in sections 7 and 10, where the Schrödinger picture is used instead.

[6] Monnier (2019)

[7] Article 21916 lists a few references about different definitions of quantum field theory.

5 Time translation symmetry

The rest of this article focuses on models with time translation symmetry. A model is said to have **time translation symmetry** if it satisfies (1) with time evolution operators $U(s,t)$ that depend only on the difference $t-s$, regardless of which reference time s we use. In this case, we can define

$$U(t-s) \equiv U(s,t). \tag{7}$$

Set $s'=0$ and $s=-t'$ in equation (3) to deduce that the time translation operators $U(t)$ satisfy

$$U(t')U(t) = U(t'+t) \qquad\qquad U(0)=1, \tag{8}$$

which implies

$$U^{-1}(t) = U(-t).$$

It also implies that all of the time translation operators commute with each other.[8] Equations (1) becomes[9]

$$A(t+s) = U^{-1}(t)A(s)U(t) \tag{9}$$

for any two times s,t.

To enforce the time slice principle, the time evolution operators $U(t)$ should themselves be expressible entirely in terms of the observables associated with any one time. The next section explains how this can be done efficiently, by writing the unitary operators $U(t)$ in terms of a single self-adjoint operator that can in turn be written in terms of observables.

[8]Proof: (8) holds for arbitrary t and t', so we can exchange t and t' to get $U(t)U(t') = U(t+t')$. Compare this to (8) and use the trivial identity $t'+t = t+t'$ to deduce $U(t')U(t) = U(t)U(t')$.

[9]To see this, use the identity $U(t+s-s) = U(t)$.

6 The hamiltonian

Let H be a self-adjoint operator: $H^* = H$. In some ways, such an operator can be manipulated as though it were an ordinary real variable. In particular, the family of operators

$$U(t) \equiv \exp(-iHt) \tag{10}$$

has the properties (8).[10] It also has the property

$$\frac{d}{dt}U(t) = -iHU(t). \tag{11}$$

According to **Stone's theorem**,[11] the converse is also true: any continuous family of unitary operators satisfying (8) can be written in the form (10) for some operator H.[12] Equation (9) can also be written in differential form:[13]

$$i\frac{d}{dt}A(t) = \big[A(t), H\big].$$

This is the **equation of motion** for the observables $A(t)$ in the Heisenberg picture.

The operator H is called the **hamiltonian**. Equations (9) and (10) say that the hamiltonian **generates** translations in time. A model is typically defined by specifying its observables at one time and then specifying the hamiltonian, because this implicitly specifies observables at all other times through equations (9) and (10). The time slice principle can be enforced by expressing the hamiltonian in terms of observables at a given reference time.

[10] The previous section used t for a point in time and s for a time shift, but that conceptual distinction is not important here.

[11] Riesz and Sz.-Nagy (1990), section 137, page 385

[12] Even though the unitary operators $U(t)$ are defined on the whole Hilbert space, their generator H may be **unbounded**, which means that it might not be defined on the whole Hilbert space, but it is defined on a dense subset of the Hilbert space. Where it is defined, the operator H is self-adjoint.

[13] The **commutator** of two operators A and B is defined by $[A, B] \equiv AB - BA$.

7 The Schrödinger equation

In the Schrödinger picture, using the notation (7) in equation (5) gives

$$\big|\psi(t)\big\rangle = U(t)|\psi\rangle. \tag{12}$$

Together with equation (11), this implies

$$i\frac{d}{dt}\big|\psi(t)\big\rangle = H\big|\psi(t)\big\rangle. \tag{13}$$

This is often called the **Schrödinger equation**.[14]

[14]Sometimes this name is used with a more narrow meaning, for the specific case of a strictly nonrelativistic single-particle model.

8 Energy

We can enforce the time slice principle by expressing the hamiltonian in terms of observables at a given reference time. This doesn't necessarily make H itself an observable (it would if all the constituent observables were compatible with each other), but the hamiltonian is typically considered to be an observable. We call this observable the system's **total energy**. Treating this as an observable can be mathematically convenient, even though we clearly cannot actually measure the *total* energy of a complex system of unlimited size. In any case, this defines the system's total energy only modulo an overall constant term, because if c is any constant, then replacing $H \to H + c$ doesn't affect equation (9):

$$e^{i(H+c)t} A e^{-i(H+c)t} = e^{iHt} A e^{-iHt} \tag{14}$$

for any operator A.

Time translation symmetry implies that the total energy is **conserved** (independent of time):

$$U^{-1}(t) H U(t) = H. \tag{15}$$

This is just the rule (9) applied to the observable H, using the fact that H commutes with itself. Equation (15) holds even if the hamiltonian is expressed in terms of other observables that are not individually invariant in time.

This article uses **natural units** in which **Planck's constant** $\hbar$ is equal to 1.[15] Its value in Standard International units is $\hbar \approx 1.05 \times 10^{-34}$ kg $\cdot$ m^2/s. If t is expressed in seconds and H (the energy observable) is expressed in Joules, then equation (10) becomes

$$U(t) = \exp(-iHt/\hbar). \tag{16}$$

[15]The quantity $h \equiv 2\pi\hbar$ is also called Planck's constant. The symbol $\hbar$ is pronounced "h-bar."

9 Stationary states

In a model with time translation symmetry, consider a state of the form (4) again, and now suppose that the state-vector $|\psi\rangle$ is an eigenvector of the hamiltonian H:

$$H|\psi\rangle \propto |\psi\rangle.$$

Such a state is called **stationary** because

$$\big\langle \psi \big| A(t) \big| \psi \big\rangle$$

is independent of t in this case. In a stationary state, nothing changes in time.

Since H is the observable describing the system's total energy, we can think of a stationary state as one that has a strictly well-defined total energy. In such a state, if we could measure the system's total energy, we would always get the same answer.[16]

At first, this might seem to contradict classical experience, where we often refer to *the* energy of a moving object. According to quantum theory, a moving object cannot have a strictly well-defined energy, even though it's energy may be well-defined for most practical purposes. The next section shows that even a tiny spread in energy can accommodate rapid macroscopic motion, so there is no conflict with everyday experience.

[16]This is an oxymoron, because in a model that is rich enough to describe the measurement itself as a time-dependent physical process, physical measurement processes *cannot occur* in a stationary state! A stationary state is one in which *nothing* changes in time. Most textbooks gloss over this, because – for legitimate practical reasons – most textbooks only consider what article 03431 calls the **artificial approach** to measurement, instead of using the (much more difficult) **natural approach** in which measurement is treated as a physical process within the model itself.

10 Energy, stationary states, and motion

This section shows that an everyday object can have an energy and velocity that are both sharply defined for all practical purposes.

Consider an object with mass m moving with constant velocity v, and suppose that at any given instant, its location is predictable as far as we can tell using measurements with resolution Δx, which may be much smaller than the size of the object. (As an example, we'll take $\Delta x \sim 1$ femtometer, which is comparable to the radius of a proton.) Suppose for simplicity that the object's state has the form (4), defined by a single state-vector. Use the Schrödinger picture, so that all time-dependence is carried by the state-vector: $\big|\psi(t)\big\rangle$. Any two state-vectors in which the object's location differs by more than Δx must be essentially orthogonal to each other, because we assumed that its location is predictable as far as we can tell using measurements with that resolution. The object is moving with constant velocity v, so we must have

$$\big\langle\psi(t_2)\big|\psi(t_1)\big\rangle \approx 0 \tag{17}$$

whenever $t_2 - t_1 \gtrsim \Delta x/v$.

Vaidman (1992) showed that if

$$\big\langle\psi(t_2)\big|\psi(t_1)\big\rangle = 0, \tag{18}$$

then the spread in energy (quantified by the standard deviation) must be at least

$$\Delta E \equiv \sqrt{\rho(H^2) - \rho(H)^2} \geq \frac{\pi\hbar}{2|t_2 - t_1|}, \tag{19}$$

where H is the hamiltonian and

$$\rho(\cdots) \equiv \frac{\langle\psi|\cdots|\psi\rangle}{\langle\psi|\psi\rangle}$$

is the state represented by the state-vector $\big|\psi(t)\big\rangle$ at any time t. (Thanks to equation (15), the value of t doesn't matter in $\rho(H^n)$.) For the scenario described above,

we need to achieve the condition (18) whenever $|t_2 - t_1| \sim (\Delta x)/v$, the time needed for the object to pass from one resolution cell to the next. This gives the bound

$$\Delta E \gtrsim \frac{\pi \hbar v}{2\,\Delta x}.$$

This is only a bound, so to determine how small ΔE can actually be, we need to consider an example. Consider an initial state-vector of the form

$$\big|\psi(0)\big\rangle = \sum_n z_n |n\rangle \tag{20}$$

where each unit vector $|n\rangle$ is a stationary state with energy E_n:

$$H|n\rangle = E_n|n\rangle \qquad\qquad \langle n|n\rangle = 1.$$

The Schrödinger equation (13) is satisfied by

$$\big|\psi(t)\big\rangle = \sum_n z_n(t)\,|n\rangle$$

with

$$z_n(t) \equiv z_n\, e^{-iE_n t}.$$

This implies

$$\big\langle\psi(t_2)\big|\psi(t_1)\big\rangle = \sum_n |z_n|^2 e^{iE_n(t_2-t_1)/\hbar}. \tag{21}$$

For simplicity, suppose that the magnitudes $|z_n|$ are all equal to 1 and that the energies E_n are equally spaced over an interval of width δE. For a macroscopic object, we can assume that the number N of terms in the sum is so large that $\delta E/N$ is negligible compared to δE, so the sum is well-approximated by an integral:

$$\big\langle\psi(t_2)\big|\psi(t_1)\big\rangle \propto \frac{1}{\delta E}\int_\epsilon^{\epsilon+\delta E} dE\; e^{iE(t_2-t_1)/\hbar} \propto \frac{\hbar}{(t_2-t_1)\,\delta E}\sin\left(\frac{(t_2-t_1)\,\delta E}{2\hbar}\right)$$

with proportionality factors that are independent of $t_2 - t_1$ and δE. The function on the right-hand side is exactly zero when $|t_2 - t_1| = 2\pi\hbar/\delta E$, and the standard deviation of the energy is

$$\Delta E = \frac{\delta E}{\sqrt{12}} = \frac{2\pi\hbar}{\sqrt{12}|t_2 - t_1|} > \frac{\pi\hbar}{2|t_2 - t_1|},$$

which is consistent with the bound (19). More importantly, the function on the right-hand side is negligible whenever $|t_2 - t_1| \gg \hbar/\delta E$ so if we take

$$\delta E \gg \frac{\hbar v}{\Delta x},$$

then we achieve the condition (17) whenever $t_2 - t_1 \gtrsim \Delta x/v$, as desired. Expressed as a fraction of the object's kinetic energy $E \approx mv^2/2$ (assuming that the object is moving slowly enough to use the nonrelativistic approximation), this inequality is

$$\frac{\Delta E}{E} \gg \frac{2\hbar}{(\Delta x)mv}. \tag{22}$$

For a quantitative example, suppose

$$\begin{aligned} \Delta x &= 1 \text{ femtometer} \\ m &= 1 \text{ gram} \\ v &= 2000 \text{ meter/second}. \end{aligned}$$

Then the required spread in energy, according to (22), is

$$\frac{\Delta E}{E} \gg 10^{-22}.$$

This says that for all practical purposes, the object can have a sharply defined kinetic energy, even if it is moving with a constant velocity with a sharply defined location at any given instant.

If the state had a *perfectly* well-defined energy, then nothing would change in time (section 9). The calculation in this section explains why that simple fact does not contradict everyday experience.

11 References

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