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Quantum Time Evolution: Informal

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These lecture notes are an informal version of the lecture notes on the quantum time evolution, though perhaps more accessible as a first read. Be aware that the conventional notation slightly differs between the two lecture notes and that some important notions might lack deserved accenting.

1. Introduction

Last time, we saw that quantum states are merely vectors in a vector space. But last time, we only considered static states. None of our states had an element of time evolution in them. In other words, the states we considered were taken at a particular time. We would like to upgrade our states to contain the notion of time, if not motivated by the direct observation that we do, in fact, seem to live in a world governed by time.

Let us pour the whiskey and stuff the pipes, whilst we try not to butcher the mathematics as much. Consider a system that is at time some constant time $t = t_0$ represented by the state vector,

$$|\alpha\rangle \equiv |\alpha, t_0\rangle \, .$$

In the second line we specifically label that the state describes the system at time t_0. This is not too difficult to generalise to an arbitrary time, we could denote the state of the system after evolving it to an arbitrary time $t > t_0$ starting from the state at t_0 by

$$|\alpha, t\rangle \equiv |\alpha, t_0; t\rangle \, .$$

It is good to understand the initial time from where we transform the system, but we often let this be obvious from the context to avoid cluttering the equations. Secondly, the semi-colon is there to remind us that the t is not some sort of eigenvalue of a time operator $\hat{T}$, we are not ready for string theory yet. We are viewing the ket as a function of time, so the notation $|\alpha\rangle\,(t)$ would be more appropriate, though more confusing.

Having set the stage, we but need to relate the time-evolved state $|\alpha, t_0; t\rangle$ to the initial state $|\alpha, t_0\rangle$. How can we do this? If we, briefly, consider our system to be a not-so-very-free particle, then at some specific moment in time, the state of the particle will (among other quantum numbers) be determined by its momentum value. If we let the system go for a bit, then at a later time, the state of the particle will now be determined by a different momentum. Both of these states are described by vector in the vector space, but they will be different. So, in order to determine the relation between the initial and evolved state, we need to relate two vectors in the vector space. This is generally done by a linear map or a matrix, taking the first vector and outputting the second. Translating back to the quantum jargon, a linear map corresponds to an operator. In essence, we postulate that there exists a so-called time-evolution operator such that

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

taking a state at time t_0 to a different state at an arbitrary time t.

2. Properties of the time-evolution operator

Let's keep things trivial for now. What happens when we consider no time evolution at all? Mathematically, we mean

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

or a bit better mathematically,

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

What we are doing is taking the state – the vector – to itself. In terms of linear algebra, the linear map should be the identity, which translates to saying that the time evolution operator is given by

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

where $\hat{1}$ is the operator that takes a state to itself, i.e. the identity operator. When we represent the operator $\hat{1}$ using a matrix, it would, of course, be the identity matrix,

$$\hat{1} = \begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & \\ \vdots & \vdots & & \ddots \end{pmatrix}.$$

This is a property we require from our time-evolution operator.

Secondly, we could transform a state twice. Consider first a transformation from a state $|\alpha, t_0\rangle$ to the state $|\alpha, t_1\rangle$, explicitly given by

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

and we then transform the state $|\alpha, t_1\rangle$ to a state $|\alpha, t_2\rangle$, which is explicitly given by

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

Putting these transformations in sequence, we find

$$|\alpha, t_2\rangle = \hat{\mathcal{U}}(t_2, t_1)\, |\alpha, t_1\rangle = \hat{\mathcal{U}}(t_2, t_1)\hat{\mathcal{U}}(t_1, t_0)\, |\alpha, t_0\rangle\,. \tag{1}$$

Do notice that we are already very handwavy with the notation of the states by not writing down the initial time. This should be clear by looking at the time-evolution operator $\hat{\mathcal{U}}$.

But we could also consider the time evolution of the state $|\alpha, t_0\rangle$ immediately to the state $|\alpha, t_2\rangle$, which is given by

$$|\alpha, t_0\rangle = \hat{\mathcal{U}}(t_2, t_0) |\alpha, t_0\rangle . \tag{2}$$

By comparing Eqs. (1) and (2), we find that

$$\hat{\mathcal{U}}(t_2, t_0) = \hat{\mathcal{U}}(t_2, t_1)\hat{\mathcal{U}}(t_1, t_0)$$

In other words, we expect the time-evolution operator to decompose multiplicatively under intermediate time steps. This is a second property we require of the time-evolution operator.

3. Physiking the magik

We can exhaust the first property a bit better, if we are willing to evoke the anger of the mathematicians. We are willing. Let us consider an initial state at some arbitrary $|\alpha, t\rangle$ and evolve it through time with an infinitesimal time step $\mathrm{d}t$, giving the state $|\alpha, t + \mathrm{d}t\rangle$. We may write

$$|\alpha, t + \mathrm{d}t\rangle = \hat{\mathcal{U}}(t + \mathrm{d}t, t) |\alpha, t\rangle .$$

But from the first property we know that

$$\lim_{\mathrm{d}t \to 0} \hat{\mathcal{U}}(t + \mathrm{d}t, t) = \hat{\mathcal{U}}(t, t) = \hat{1}.$$

So, if we choose a value for $\mathrm{d}t$ that is really, really close to zero, then $\hat{\mathcal{U}}(t + \mathrm{d}t, t)$ is really, really close to $\hat{1}$. As any physicist can attest, this naturally calls for a Taylor expansion. We can write the time-evolution operator $\hat{\mathcal{U}}(t + \mathrm{d}t, t)$ as a polynomial in $\mathrm{d}t$ starting around $\hat{1}$. Note that if $\mathrm{d}t$ is really small, then $(\mathrm{d}t)^2 \equiv \mathrm{d}t^2$ is even really smaller, and its even smaller for higher powers of $\mathrm{d}t$. Formally, the Taylor expansion is given by

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

Here $\hat{\Omega}$ is an operator that, formally said, generates the time evolution; we return to this momentarily. The complex constant $(-i)$ is chosen for later convenience, but is merely a notational choice. Don't let it scare you off; you may ignore it or you may absorb it into the operator by defining $\hat{\omega} \equiv -i\hat{\Omega}$, in which case the Taylor expansion would read the more familiar,

$$\hat{\mathcal{U}}(t + \mathrm{d}t, t) = \hat{1} + \hat{\omega}\mathrm{d}t + \frac{1}{2}\hat{\omega}^2\mathrm{d}t^2 + \mathcal{O}\left(\mathrm{d}t^3\right).$$

We will proceed with the factor $(-i)$, but you are welcome to do the analysis without it.

To understand the Taylor expansion, we need to interpret the operator $\hat{\Omega}$. We do so the physics way: The first term in the Taylor expansion $\hat{1}$ has no associated units to it. The second term $-i\hat{\Omega}\mathrm{d}t$ should therefore be unitless. (It does not make sense to add metres to seconds; if one term is dimensionless, we can only add to it other dimensionless quantities.) Since dt has units of seconds s, the operator $\hat{\Omega}$ should have units of one over seconds $1/s$. Moreover, it should somehow contain the constant $\hbar$ since, after all, we are discussing quantum mechanical states. We could work out the units and see what we end up with, but we could be a bit smarter and recall that we have a familiar equation in physics relating the energy E of a photon to its frequency ν (with units $1/s$) by,

$$E = \hbar\nu \qquad \Longleftrightarrow \qquad \frac{E}{\hbar} = \nu$$

We could therefore postulate that $\hat{\Omega}$ is an operator related to energy divided by $\hbar$. But! We have an operator related to energy, namely the Hamiltonian! Therefore, we are going to make the humble guess that

$$\hat{\Omega} = \frac{\hat{H}}{\hbar}.$$

The Taylor expansion of the time-evolution operator then becomes to first order in dt,

$$\hat{\mathcal{U}}(t + \mathrm{d}t, t) = \hat{1} - i\frac{\hat{H}}{\hbar}\mathrm{d}t + \mathcal{O}\left(\mathrm{d}t^2\right).$$

We care only about first order, because we will soon send dt so close to zero that dt^2 becomes entirely negligible compared to dt.

Having extracted all this information, let us, for the sake of fun, choose an initial state $|\alpha, t_0\rangle$ and transform it for an arbitrary amount of time t to the time $|\alpha, t\rangle$ and then just transform a slightly more, $|\alpha, t + \mathrm{d}t\rangle$, where d$t$ is one such infinitesimal value. In terms of the time-evolution operators, this reads

$$\hat{\mathcal{U}}(t + \mathrm{d}t, t_0) = \hat{\mathcal{U}}(t + \mathrm{d}t, t)\hat{\mathcal{U}}(t, t_0).$$

The first term on the left-hand side looks familiar. We use the Taylor expansion and find,

$$\begin{aligned}\hat{\mathcal{U}}(t + \mathrm{d}t, t_0) &= \left(\hat{1} - \frac{i}{\hbar}\hat{H}\mathrm{d}t\right)\hat{\mathcal{U}}(t, t_0) \\ &= \hat{\mathcal{U}}(t, t_0) - \frac{i}{\hbar}\mathrm{d}t\hat{H}\hat{\mathcal{U}}(t, t_0).\end{aligned}$$

We subtract both sides with $\hat{\mathcal{U}}(t, t_0)$ to find,

$$\hat{\mathcal{U}}(t + \mathrm{d}t, t_0) - \hat{\mathcal{U}}(t, t_0) = -\frac{i}{\hbar}\mathrm{d}t\hat{H}\hat{\mathcal{U}}(t, t_0)$$

We now divide both sides with dt and formally take the d$t \to 0$ limit, so that

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

The first term looks familiar, this is the definition of the derivative with respect to time. Thus, finally,

$$\frac{\partial\hat{\mathcal{U}}(t, t_0)}{\partial t} = -\frac{i}{\hbar}\hat{H}\hat{\mathcal{U}}(t, t_0),$$

or upon yeeting the constants to the other side,

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

If we reinstate the states, we obtain

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

and we can evolve the states to obtain,

$$i\hbar \frac{\partial}{\partial t} |\alpha, t\rangle = \hat{H} |\alpha, t\rangle . \tag{3}$$

This is the ever-so-famous Schrödinger equation for the time-evolution operator. What this equation is saying to us is that, if such a time-evolution operator $\hat{\mathcal{U}}$ exists, then it must satisfy this Schrödinger equation.

4. Wavefunctions of sorts

We will investigate the existence of this time-evolution operator later, but perhaps it is useful to first consider an example familiar to us. Harmonic oscillator time:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}\omega^2 \hat{x}^2$$

We know that $\hat{p}$ acts on the position space $|x\rangle$ as a spatial derivative. What this means is that, though it might be difficult, we know how $\hat{H}$ acts on the position basis, $\hat{H}|x\rangle$. Upon daggering, this becomes

$$(\hat{H}|x\rangle)^\dagger = \langle x| \hat{H}^\dagger = \langle x| \hat{H}$$

since $\hat{H}$ is Hermitian or self-adjoint (since it needs to have real eigenvalues). If you need refreshing on this, you might do yourself a favour by reading the lecture notes on states in quantum mechanics (to be written and published).

In order to get information out of $\hat{H}|\alpha, t\rangle$, we could act with $\langle x|$. We assume that $|\alpha, t\rangle$ does not depend on x, so that we my write the Schrödinger equation Eq. (3) as,

$$i\hbar \frac{\partial}{\partial t} \langle x|\alpha, t\rangle = \hat{H} \langle x|\alpha, t\rangle$$

Mathematically, what we are doing is projecting the $|\alpha, t\rangle$ state onto the $|x\rangle$ basis, We will now make a definition, named the position wavefunction,

$$\psi_\alpha(x, t) \equiv \langle x|\alpha, t\rangle$$

where we often drop the subscript α. The Schrödinger equation then reads

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

called the Schrödinger (position) wave equation. The wave functions $\psi(x,t)$ are the coefficients of the state with respect to the position basis.

We could repeat this entire analysis exactly with the momentum states $|p\rangle$. We would then define the momentum wavefunction

$$\varphi(p,t) \equiv \langle p|\alpha,t\rangle\,,$$

so that we get the Schrödinger (momentum) wave equation,

$$i\hbar\frac{\partial}{\partial t}\varphi(p,t) = \hat{H}\varphi(p,t).$$

Since $|x\rangle$ and $|p\rangle$ are related by a Fourier transform, the position wave function $\psi(x,t)$ and the momentum wave function $\varphi(p,t)$ are also related by a Fourier transform. More on this later.

The wave equation formalism is useful when we want to express and calculate time evolution of states purely in terms of the known basis that is position basis.

5. Solving the Schrödinger equation explicitly

So far we have manifested a time-evolution operator and provided the properties it requires. Having manipulated these properties, we found the ultimate defining equation for the time-evolution operator: namely the Schrödinger equation. It remains to solve this Schrödinger equation to explicitly write the time-evolution in terms of the Hamiltonian.

This is easily done if the Hamiltonian does not explicitly depend on time. When observing the Schrödinger equation,

$$\frac{\partial}{\partial t}\hat{\mathcal{U}}(t,t_0) = -\frac{i}{\hbar}\hat{H}\hat{\mathcal{U}}(t,t_0)$$

If we so humble treat the operators as normal linear functions, then we see that the time-evolution operator is a function such that taking a time derivative of this function, we get back the exact same function with a pre-factor of $-\frac{i}{\hbar}\hat{H}$. This function is of course the exponential. Naively, we thus expect,

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

Unfortunately, we are dealing with operators, not functions. Fortunately, we can just define the exponential of an operator as

$$\exp\{A\} = \hat{1} + A + \frac{1}{2}A^2 + \frac{1}{3!}A^3 + \dots.$$

The reader can use this definition to use the exponential expression for the time-evolution operator and show it satisfies the Schrödinger equation for time-independent Hamiltonian.

What about time dependent Hamiltonians? Well, in the time independent case, we could smartly write the solution as

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

One can show that in the time dependent case, as long as the Hamiltonian commutes at different times, i.e. $H(t_1)H(t_2) = H(t_2)H(t_1)$, we find that the solution is given by

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

Once again, this is left as an exercise to the viewer.

For the general case, however, we cannot write the solution in terms of an exponential, unfortunately. The general solution is called the Dyson series and is explicitly given by an infitude of integrals,

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

As one may guess by now, this too is left as exercise to the reader.

Having solved the equations for the time-evolution operator, we see that the solution of it is explicitly given by some function of the Hamiltonian. It now makes sense when we say that the Hamiltonian governs the time evolution of states. The temporal dynamics of states is entirely determined by the Hamiltonian.