

4. Time and Change

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1 Classical Reminder

Knowing the state of a system is half the story. We also need a rule about how that state changes over time!

In Classical Mechanics, the evolution of states over time is deterministic and reversible. These requirements, are called the **Minus-First Law**, since it underlies everything else. It means that information is never lost!

If two identical isolated systems are in the same state at some point in time, then their histories and future must also be identical.

In Quantum Mechanics, this law is called **Unitarity**

2 Unitarity

From now on we will use the notation $|\Psi(t)\rangle$ for the representation of Quantum States.

Suppose that the state of a system at time t is $|\Psi\rangle$. To indicate it depends on time, we will write it as a function of it : $|\Psi(t)\rangle$. We can think of $|\Psi(t)\rangle$, as the history of the system.

Now the **Basic dynamical assumption** of Quantum Mechanics is :

If you know the state at one time, then the quantum equations of motion tell you what it will be later.

We take the initial time to be 0, and obviously denote time with t .

The state at time t is given by an operation called $U(t)$, acting on the initial state

In other words,

$$|\Psi(t)\rangle = U(t) |\Psi(0)\rangle \quad (1)$$

$U(t)$ is called the Time Development Operator.

3 Determinism in Quantum Mechanics

The time evolution of the state-vector is Deterministic But remember, that knowing the state, doesn't mean we can predict the result of a measurement! Knowing that the state of a spin is $|u\rangle$, doesn't tell us anything about σ_x and σ_y .

There is a difference between states and measurements in Quantum Mechanics as opposed to Classical Mechanics. As we will see later on, the relation between state and measurement is probabilistic and not absolute! A Quantum State is Deterministic, but a measurement isn't.

4 A better look at $U(t)$

$U(t)$ has its own requirements, just like the minus-First Law had its own.

1) $U(t)$ must be a linear operator

2) Distinctions must be conserved

We said in the principles of Quantum Mechanics, that 2 states must be distinguishable if they're orthogonal.

Suppose $|\Psi(0)\rangle$ and $|\Phi(0)\rangle$ are two distinguishable states. It follows that

$$\langle \Psi(0) | \Phi(0) \rangle = 0 \text{ Which implies, based on Unitarity, that } \langle \Psi(t) | \Phi(t) \rangle = 0$$

Using the requirements of the Time Development Operator and its properties, as well

as how Hermitian Conjugation works, it is easy to see why:

$$\langle \Psi(0) | U^\dagger(t) U(t) \Phi(0) \rangle = 0 \quad (2)$$

Now if we create another example and suppose that $\langle \Psi(0) | \Phi(0) \rangle = 1$, it is easy again to see how

$$\langle \Psi(0) | U^\dagger(t) U(t) \Phi(0) \rangle = 1 \quad (3)$$

(Exercise: Try to represent the above two equations in one equation! (Hint use the Kronecker delta symbol))

In other words, $U^\dagger(t)U(t)$ behaves like the unit operator I when it acts between any basis vectors.

That is also the very definition of Unitary:

An operator that satisfies $U^\dagger U = I$, is called Unitary

Time Evolution is Unitary!

We can now right our fifth principle of Quantum Mechanics:

5) The evolution of state vectors over time is unitary

5 The Hamiltonian

Just like we did in Classical Mechanics, we will build up finite time intervals by adding infinitesimal intervals. Later on we will use integrals, which do exactly that!

When addressing infinitesimal intervals, we will denote them with ϵ and not t !

There are 2 principles that go into the study of incremental changes:

1) $U^\dagger(\epsilon)U(\epsilon) = I$

2) Continuity: The state-vector changes smoothly over time.

It is obvious why when $\epsilon = 0$, the Time Development Operator is I !

(Exercise: Try to prove this claim!)

What Continuity tells us, is that when ϵ is very close to 0, $U(\epsilon)$ is very close to the unity Operator differing it from something of order ϵ .

Namely:

$U(\epsilon) = I - i\epsilon H$ Where i is the imaginary number and H the Hamiltonian, or Energy of the system. We will later on see what this is (both Hamiltonian and this evolution).

It follows that

$$U^\dagger(\epsilon) = I + i\epsilon H$$

We can now multiply $(I - i\epsilon H)(I + i\epsilon H)$, which results in I

Now if we carry the Calculations, we will see that the Hamiltonian is indeed a Hermitian Operator.

Knowing that the Hamiltonian is a Hermitian Operator means that H is an observable and has a complete set of eigenvalues and eigenvectors.

H is the notation for the Hamiltonian both in Classical Mechanics and Obviously in Quantum Mechanics.

As expected, when we measure the energy of a system, the result is an eigenvalue of the Hamiltonian.

Having showed all this, we can now calculate the Generalized Schrodinger Equation.

We said earlier that:

$$|\Psi(\epsilon)\rangle = U(t) |\Psi(0)\rangle \quad (4)$$

Now substituting with the new terms, we get:

$$|\Psi(\epsilon)\rangle = (I - i\epsilon H) |\Psi(0)\rangle \quad (5)$$

or simply

$$|\Psi(\epsilon)\rangle = |\Psi(0)\rangle - i\epsilon H |\Psi(0)\rangle \quad (6)$$

We now move the $|\Psi(0)\rangle$ term to the left side of the equation, and divide by ϵ , leaving us with ;

$$\frac{|\Psi(\epsilon)\rangle - |\Psi(0)\rangle}{\epsilon} = -iH |\Psi(0)\rangle \quad (7)$$

This should be pretty obvious by now, but the first term on the left-hand side, is nothing else than the definition of the derivative! Remember that ϵ is infinitesimal!

Since these kets are functions of time, we rewrite everything like:

$$\frac{\partial |\Psi\rangle}{\partial t} = -iH |\Psi\rangle \quad (8)$$

Which is the **Generalized Schrodinger Equation!**

6 The units

If you've ever seen the Schrodinger equation before, you are probably confused right now, because you cannot find the \hbar . \hbar is Planck's reduced constant, or $\frac{h}{2\pi}$
 $\hbar = 1.05457172... \cdot 10^{-34} \frac{Kgm^2}{s}$

If we take a look at

$$\frac{\partial |\Psi\rangle}{\partial t} = -iH |\Psi\rangle \quad (9)$$

, we see that there is a problem with units!

The Hamiltonian is the Energy of the system, so its units are Joules or $\frac{kgm^2}{s^2}$, and we see that the left hand side, isn't in Joules! That exactly is why we add \hbar , to balance out the units.

$$\hbar \frac{\partial |\Psi\rangle}{\partial t} = -iH |\Psi\rangle \quad (10)$$

\hbar is used a lot and in Biology and its size because it is a fundamental constant in our lives! In Quantum Mechanics, as we said, it's all about the micro-cosmos, and that's why, usually, you don't see \hbar , because we set it as our unit of measurement, or simply 1.

However, I will leave it in whenever we come across it, and trust me we will!

7 Expectation Values

Now let's take a break from Quantum Mechanics, and focus for a bit only on statistics!

In Quantum Mechanics, Average Values, are called **Expectation Values**

Suppose we have a probability function for the outcome of an experiment whose goal is to measure an observable L.

The outcome can only be an eigenvalue of L, λ_i , and its probability function is: $P(\lambda_i)$

In Quantum Mechanics, we will use the Dirac Notation for the expectation value, namely $\langle L \rangle$, instead of the classical notation with the line above the observable.

From the Point of View of mathematics, the expectation value is defined as:

$$\langle L \rangle = \sum_i \lambda_i P(\lambda_i) \quad (11)$$

Which in English, is a weighted sum, weighted with the probability function.
What are the physical meanings?
Suppose that we record the outcomes of many many identical experiments. $P(\lambda_i)$ is the fraction of λ_i observations.
The basic Hypothesis of statistics, is that if an experiment is repeated enough times, the experimental and mathematical results and notions of probability as well as the averages will agree.
Also, here is something to keep in mind, which is also very easy to prove:

$$\langle L \rangle = \langle A | L | A \rangle \quad (12)$$

That the average value of L can be found by sandwiching the observable between the bra and the ket of a state.

8 The Phase Factor

Generally, you can always multiply any state-vector by a factor $e^{i\theta}$, where $\theta \in R$. We can do that, because the physical meaning of the state vector doesn't change, since the term we multiply it by has a magnitude of 1. That is what I meant when I said we can ignore the phase factor.

9 Classical Mechanics and Expectation Values

The Expectation Values of Quantum Mechanics are the closest thing to a classical value.

The expectation values, change over time, because the whole state changes over time, or in other words, there is an expectation value for the state for each time t.
Lets now derive something very important, that you should remember because we will need it in chapters 8 and 9.

We said that

$$\langle L \rangle = \langle A | L | A \rangle \quad (13)$$

or in our case

$$\langle L \rangle = \langle \Psi(t) | L | \Psi(t) \rangle \quad (14)$$

We now use the Schrodinger Equation!

$$\frac{d}{dt} \langle \Psi(t) | L | \Psi(t) \rangle = \langle \dot{\Psi}(t) | L | \Psi(t) \rangle + \langle \Psi(t) | L | \dot{\Psi}(t) \rangle \quad (15)$$

(Note that there is a dot above some kets, indicating the time derivative of the quantity.
Now we can use

$$\hbar \frac{\partial |\Psi\rangle}{\partial t} = -iH |\Psi\rangle \quad (16)$$

, and with some easy algebra, we get:

$$\frac{d}{dt} \langle \Psi(t) | L | \Psi(t) \rangle = \frac{i}{\hbar} \langle \Psi(t) | HL | \Psi(t) \rangle - \frac{i}{\hbar} \langle \Psi(t) | LH | \Psi(t) \rangle \quad (17)$$

We can rewrite all this like:

$$\frac{d}{dt} \langle \Psi(t) | L | \Psi(t) \rangle = \frac{i}{\hbar} \langle \Psi(t) | [H, L] | \Psi(t) \rangle \quad (18)$$

You are probably confused right now! How can $HL=LH$ not be 0? Well that means that when H acts on $L|\Psi\rangle$ isn't the same as when L acts on $H|\Psi\rangle$. Now if you think about it, it makes sense that this can be true! For example if one is the Del operator and the other multiplies everything by a term y for example, the result is quite different. For example, suppose that L multiplies a function for example by y and the h operator takes its derivative with respect to y . (We will later see how functions can be vectors). Now consider a function $2y + 1$. If it first acts on L and then on H , we get $\frac{d}{dy} 2y^2 + y$, which is simply $4y + 1$, but if it first acts on H and then on L , we get $2 \cdot y$ which simply $2y$. See how they are different?

The term $HL-LH$ is called the **commutator** of H with L and is denoted by $[H, L]$. Generally, it is true that $[H, L] = -[L, H]$.

We can now rewrite the above, removing the sandwiches leaving us with a very important and interesting equation:

$$\frac{d}{dt} \langle L \rangle = -\frac{i}{\hbar} \langle [L, H] \rangle \quad (19)$$

If we assume that the probabilities are narrow, bell-shaped curves, then this equation tells us how the peaks of the curves move over time.

We can sometime write it like this:

$$\frac{d}{dt} L = -\frac{i}{\hbar} [L, H] \quad (20)$$

Keep in mind that $[L, H]$ is sandwiched by $\langle \Psi |$ and $|\Psi \rangle$

If you've read the Classical Mechanics chapters, then you might remember that we said, that $\dot{F} = \{F, H\}$, where F, H are Poisson Brackets

Later, Dirac Discovered a close connection between Poisson Brackets and Commutators, namely that:

$$[F, G] = i\hbar \{F, G\} \text{ or in our case } [LF, H] = i\hbar \{L, H\}$$

So we can rewrite

$$\frac{d}{dt} L = -\frac{i}{\hbar} [L, H] \quad (21)$$

as

$$\frac{d}{dt} L = -\frac{i}{\hbar} (i\hbar \{L, H\}) \quad (22)$$

or simply

$$\frac{d}{dt} L = \{L, H\} \quad (23)$$

10 Energy Conservation

In Quantum Mechanics, when we say that an observable Q is conserved, we mean that its expectation value doesn't change over time if the system isn't disturbed. or, an even stronger condition, that the expectation value of Q^2 doesn't change with time.

$$\frac{d}{dt} \langle Q^2 \rangle = 0$$

Of course, that is the same as saying that it commutes with the Hamiltonian or $[Q, H] = 0$. It is easy to see why $[Q^n, H] = 0$

Knowing this, we can now make an even stronger claim:

If Q commutes with the Hamiltonian, then the expectation values of all functions of Q are conserved!

This is what we mean by conservation in Quantum Mechanics.

Obviously, that means the Hamiltonian is conserved, since it commutes with itself, which tells us, that under very general conditions, Energy is Conserved in Quantum Mechanics.

11 Solving the Schrodinger Equation

$$i\hbar \frac{\partial \Psi(x)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + V(x)\Psi(x) \quad (24)$$

This is the iconic Schrodinger equation, which is a special case of the generalized equation we derived earlier.

$$\hbar \frac{\partial |\Psi\rangle}{\partial t} = -iH |\Psi\rangle \quad (25)$$

That is the time-dependent Schrodinger equation, and we will see more about it in chapters 8 and 9.

It says that the State-Vector changes continuously with time, in a unitary way, where H is the energy of the system.

Since H represents the Energy, all of its eigenstuff, are called energy eigenstuff, for example its eigenvalues can be also called energy eigenvalues, etc.

or, from the Mathematics point of view,

$$H |E_j\rangle = E_j |E_j\rangle \quad (26)$$

, which is the very definition of Eigenvalues and Eigenvectors.

However, we call this equation the **The Time-Independent Schrodinger Equation**

If we work in a particular basis, this equation determines the eigenvectors and values of H .

If the Hamiltonian is proportional to a specific spin component, it is very easy to find its eigenvalues, since we know the eigenvalues of the spin component because we have our Pauli Matrices.

Now Suppose we have found all the pairs of eigenvectors-values. We can now use that information to solve the Schrodinger Equation.

If we denote the state-vector with $|\Psi\rangle$, we define it as:

$$|\Psi\rangle = \sum_j a_j |E_j\rangle \quad (27)$$

Since the eigenvectors form the orthonormal basis, and $|\Psi\rangle$ changes with time, and the eigenvectors don't, it follows that the coefficients a_j must be time-dependent

$$|\Psi(t)\rangle = \sum_j a_j(t) |E_j\rangle \quad (28)$$

We can now use the time dependent Schrodinger Equation to get:

$$\sum_j \dot{a}_j(t) |E_j\rangle = -\frac{i}{\hbar} H \sum_j a_j(t) |E_j\rangle \quad (29)$$

We now use the Time-Independent Schrodinger Equation to rewrite the equation above as:

$$\sum_j \dot{a}_j(t) |E_j\rangle = -\frac{i}{\hbar} \sum_j E_j a_j(t) |E_j\rangle \quad (30)$$

Now, using simple algebra, we can move everything to one side and factor out the energy eigenvector to get:

$$\sum_j \dot{a}_j(t) + \frac{i}{\hbar} E_j a_j(t) |E_j\rangle = 0 \quad (31)$$

We can see here that in order for this to be true, we need $\dot{a}_j(t) + \frac{i}{\hbar} E_j a_j(t) |E_j\rangle = 0$, or simply

$$\frac{da_j(t)}{dt} = -\frac{i}{\hbar} E_j a_j(t) \quad (32)$$

Using some identities and differential calculus, we see that

$$a_j(t) = a_j(0) e^{-\frac{i}{\hbar} E_j t} \quad (33)$$

This is what tells us how a_j changes over time!

$a_j(0)$ are simply the values of the coefficients at time 0. If we start with a state-vector $|\Psi\rangle$ at time 0, then the coefficients are given by the projections of the state-vector on the basis eigenvectors.

$$a_j(0) = \langle E_j | \Psi(0) \rangle \quad (34)$$

We can now put everything together to write the full solution:

$$|\Psi(t)\rangle = \sum_j \langle E_j | \Psi(0) \rangle e^{-\frac{i}{\hbar} E_j t} |E_j\rangle \quad (35)$$

or, if we rearrange everything

$$|\Psi(t)\rangle = \sum_j |E_j\rangle \langle E_j | \Psi(0) \rangle e^{-\frac{i}{\hbar} E_j t} \quad (36)$$

You probably are confused on how we find the initial state, namely $|\Psi(0)\rangle$? The Answer is, that we assume that with the use of some Apparatus, we can prepare the system in a state that is known to us.

12 Solving Step by Step

1) Find the Hamiltonian

2) Prepare an initial state $|\Psi(0)\rangle$

3) Find the Eigenvalues and Eigenvectors by solving the Time-Independent Schrodinger Equation

$$H |E_j\rangle = E_j |E_j\rangle \quad (37)$$

4) Use the initial state-vector and the eigenvectors to find the initial coefficients

$$a_j(0) = \langle E_j | \Psi(0) \rangle \quad (38)$$

5) Rewrite $|\Psi(0)\rangle$ in terms of the Eigenvectors and its coefficients

$$|\Psi(0)\rangle = \sum_j a_j(0) |E_j\rangle \quad (39)$$

6) Capture time dependence by changing $a_j(0)$ with Equation 33

$$|\Psi(t)\rangle = \sum_j a_j(0) e^{-\frac{i}{\hbar} E_j t} |E_j\rangle \quad (40)$$

7) We can now find the Probability for each of the possible outcomes of an experiment. If we want to measure the observable L , that has eigenvalues λ_j and eigenvectors $|\lambda_j\rangle$ The Probability for the outcome λ_j is $P_{\lambda_j}(t) = |\langle \lambda_j | \Psi(t) \rangle|^2$

13 The Collapse

Up until now, we have seen the evolution of state-vectors over time and how they are deterministic. But, we don't want to measure the state-vector. That is not the point. What we want, is to **measure observables!**

We have seen, that knowing the state-vector doesn't mean that we know the result of any given measurement! Although it changes unitary over time, when we conduct a measurement, it jumps to an eigenstate of the observable. And that, as we've seen, happens unpredictably!

That phenomenon, the jump, is called the wave function collapse, in which **the entire superposition collapses to one single eigenstate** The system evolves differently between measurements and during measurements. That of course makes sense, since, in the first chapters we said that an action strong enough to measure one aspect of the system, also disrupts the system, and one of the ramifications of this disruptions is the difference in its evolution over time.