11/01/15

Review of quantum mechanics

Let us start this review with the most important Eq. in QM: the Schrödinger Eq (S-Eq for short)

$$\boxed{\frac{d|\alpha(t)\rangle}{dt} = -\frac{i}{\hbar}\hat{H}|\alpha(t)\rangle} \qquad (1)$$

this Eq. governs the time evolution of the state of the system, $|\alpha(t)\rangle$. This ket $|\alpha(t)\rangle$ tells you exactly where the system "is" at time t. At $t=0$ the state was $|\alpha(0)\rangle$. That is something we assume to know. Then at time t the state will have evolved to $|\alpha(t)\rangle$ according to Eq (1).

The ket $|\alpha(t)\rangle$ is an abstract vector which lives in a mathematical space called the Hilbert space. We will denote this mathematically as

$$|\alpha(t)\rangle \in \mathcal{H} \qquad (2)$$

[I use a calligraphic H to denote the Hilbert space. Please don't confuse with the Hamiltonian $\hat{H}$ appearing in (1)].

Each system has its own Hilbert space. For each space we can always find sets of vectors $|e_1\rangle, |e_2\rangle, \dots$ which are called a basis for this Hilbert space. By this we mean that $|\alpha(t)\rangle$ can be written as a linear combination of the $|e_i\rangle$:

$$|\alpha(t)\rangle = \alpha_1(t)|e_1\rangle + \alpha_2(t)|e_2\rangle + \dots \qquad (3)$$

The basis vectors do not depend on time, so the time dependence must be in the $\alpha_i(t)$. These are called the coefficients of $|\alpha(t)\rangle$ in the basis $|e_i\rangle$." We make this distinction because the choice of basis is not unique. Every Hilbert space has an infinite number of basis. The number of elements in a basis is called the dimension of the Hilbert space.

In QM we always choose the basis to be orthonormal:

$$\langle e_i | e_j \rangle = \delta_{ij} \tag{4}$$

By the way, recall that $\langle \alpha | \beta \rangle$ is the inner product between two vectors: $\langle \alpha |$ is the bra; $| \beta \rangle$ is the ket. Together they form the braket. There is a property about the inner product which is very important that you remember: changing the order is the same as taking the complex conjugate

$$\boxed{\langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle^*} \tag{5}$$

Now let us go back to Eq. (1). The quantity $\hat{H}$ is called the Hamiltonian or energy operator. This is the guy that changes from one problem to the other. For each system you must figure out the Hamiltonian. (which may turn out to be a difficult task).

The eigenvalue, eigenvector Eq. for the Hamiltonian is usually written as

$$\boxed{\hat{H}\,|n\rangle = E_n\,|n\rangle} \tag{4}$$

Like all observables, $\hat{H}$ is Hermitian: $\hat{H}^\dagger = \hat{H}$. This implies that its eigenvectors form an orthonormal basis

$$\langle n|m\rangle = \delta_{nm} \tag{5}$$

Moreover, its eigenvalues E_n must be real. They are called the energies of the system.

Since the $|n\rangle$ form a basis, we can decompose $|\alpha(t)\rangle$ in it:

$$|\alpha(t)\rangle = \sum_n c_n(t)\,|n\rangle \tag{6}$$

This is always possible, even though we don't know what the $c_n(t)$ are.

But we can try to plug this into Eq (3). The left-hand side is

$$\frac{d|\alpha(t)\rangle}{dt} = \frac{d}{dt}\sum_m c_m(t)|m\rangle = \sum_m \frac{dc_m}{dt}|m\rangle$$

The right-hand side, in turn, is

$$-\frac{i}{\hbar}\hat{H}|\alpha(t)\rangle = -\frac{i}{\hbar}\hat{H}\sum_m c_m(t)|m\rangle = -\frac{i}{\hbar}\sum_m c_m(t)\hat{H}|m\rangle$$

But according to (4), $\hat{H}|m\rangle = E_m|m\rangle$. Thus we conclude that

$$\sum_m \frac{dc_m}{dt}|m\rangle = \sum_m \left(-\frac{i}{\hbar}E_m c_m\right)|m\rangle$$

Since the $|m\rangle$ form a basis they must be linearly independent. Therefore each term in the sum on the left must be equal to each term on the right

$$\frac{dc_m}{dt} = -\frac{iE_m}{\hbar}c_m \qquad (7)$$

This is a very easy Eq. because it involves only numbers. If we call $c_m = x$ and $-iE_m/\hbar = a$ we get

$$\frac{dx}{dt} = ax \qquad (8)$$

This is the simplest differential Eq. there is. The solution is

$$x(t) = x(0)\, e^{at} \tag{9}$$

where $x(0)$ is the initial condition. Or, in terms of our original variables

$$\boxed{c_n(t) = c_n(0)\, e^{-i E_n t/\hbar}} \tag{10}$$

This is remarkable: we solved the S-Eq! I will write our result in a slightly different way by defining

$$\boxed{\omega_n = \frac{E_n}{\hbar}} \tag{11}$$

This way I don't have to worry about the $\hbar$ all the time. Then

$$\boxed{c_n(t) = c_n(0)\, e^{-i\omega_n t}} \tag{12}$$

[Note: some people write c_n instead of $c_n(0)$, just for simplicity. Here I am writting it as $c_n(0)$ just to emphasize that these coefficients are related to the initial conditions].

The complete solution is now given by Eq (6).

$$\boxed{|\alpha(t)\rangle = \sum_n c_n(0)\, e^{-i\omega_n t} |n\rangle} \tag{13}$$

The last thing we need to do is find the $c_n(0)$. This turns out to be very easy. First we write Eq (13) for $t=0$:

$$|\alpha(0)\rangle = \sum_n c_n(0)\,|n\rangle$$

Now we multiply on both sides by $\langle m|$ and use (5)

$$\langle m|\alpha(0)\rangle = \sum_n c_n \langle m|n\rangle = \sum_n c_n \delta_{mn} = c_m$$

Since this is true for any m, we go back to writing n:

$$\boxed{c_n(0) = \langle n|\alpha(0)\rangle} \qquad (14)$$

The coefficient is simply the projection of $|\alpha(0)\rangle$ onto $|n\rangle$.

This concludes the problem. To solve the S-Eq we just follow the steps

1) Find $|n\rangle$ and E_n
2) Compute $c_n(0)$ using (14)
3) Put everything together using (13)

The hardest step is always number 1.

Later I will come back to Eq (1) and show a different way to look at it.

Example: spin 1/2 particle

A spin 1/2 particle has only 2 states. We usually use as basis the vectors $|z+\rangle$ and $|z-\rangle$ which mean spin up and spin down in the z direction. We will also usually use the notation

$$|z+\rangle \equiv |+\rangle$$
$$|z-\rangle \equiv |-\rangle \tag{15}$$

Since there are only 2 states, we can represent them as vectors

$$|z+\rangle = |+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |z-\rangle = |-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{16}$$

An arbitrary vector in this Hilbert space may be represented as

$$|\alpha\rangle = \alpha_1 |z+\rangle + \alpha_2 |z-\rangle = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \tag{17}$$

The operators describing the spin in the x, y and z directions are called the Pauli matrices

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{18}$$

These are all written with respect to the basis $|\pm\rangle$.

Note that $\hat{\sigma}_z$ is diagonal therefore $|z\pm\rangle$ are eigenvectors of $\hat{\sigma}_z$

$$\hat{\sigma}_z \, |z\pm\rangle = \pm \, |z\pm\rangle \tag{19}$$

A typical Hamiltonian consists of a spin 1/2 in the presence of a magnetic field. If the field is in the z direction then

$$\hat{H} = \hbar\omega \, \hat{\sigma}_z \tag{20}$$

where $\omega \propto B$ [I don't want you to worry about this constant now. We will deal with it later].

This is quite a special case because the Hamiltonian is already diagonal. We can skip step 1.

$$\hat{H}|+\rangle = \hbar\omega\,|+\rangle \tag{21}$$
$$\hat{H}|-\rangle = -\hbar\omega\,|-\rangle$$

Step 2 is also very easy. Suppose

$$|\alpha(0)\rangle = \begin{bmatrix} a \\ b \end{bmatrix} = a|+\rangle + b|-\rangle \tag{22}$$

We already have the $c_n(0)$. There is no need to find them

$$c_+(0) = a$$

$$c_-(0) = b.$$

Hence our final solution is

$$\boxed{|\alpha(t)\rangle = a\, e^{-i\omega t}\,|+\rangle + b\, e^{i\omega t}|-\rangle} \qquad (23)$$

But suppose we applied the field in the x direction. then we would have

$$\hat{H} = \hbar\omega\,\hat{\sigma}_x \qquad (24)$$

This Hamiltonian is not diagonal, so we must perform step 1. But first please note that (24) is a bit stupid: there is nothing making the x direction special. We could've rotated our reference frame and redefined it as the z direction. But anyway, let us use (24), just for practice.

You can verify for yourself that the eigenvalues and eigenvectors of $\hat{\sigma}_x$ are

$$\lambda = 1 \qquad |x+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$$

$$\lambda = -1 \qquad |x-\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} \qquad (25)$$

ve can also write

$$|x\pm\rangle = \frac{1}{\sqrt{2}}\left[|z+\rangle \pm |z-\rangle\right] \qquad (26)$$

o emphasize that the $|x\pm\rangle$ are linear combinations of our asis kets.

When we multiply by a constant, the eigenvectors do not change. Thus we conclude that

$$\hat{H}|x_+\rangle = \hbar\omega|x_+\rangle \qquad (26)$$

$$\hat{H}|x_-\rangle = -\hbar\omega|x_-\rangle$$

Of course, the eigenvalues are the same as (21).

Next we proceed to step 2. Suppose $|\alpha(0)\rangle$ is the same as before

$$|\alpha(0)\rangle = \begin{bmatrix} a \\ b \end{bmatrix} = a|z_+\rangle + b|z_-\rangle$$

Now we can't skip step 2. We have

$$c_+(0) = \langle x_+|\alpha(0)\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \frac{a+b}{\sqrt{2}}$$

$$c_-(0) = \langle x_-|\alpha(0)\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \frac{a-b}{\sqrt{2}}$$

Hence the full solution is now

$$|\alpha(t)\rangle = \frac{(a+b)}{\sqrt{2}}e^{-i\omega t}|x_+\rangle + \frac{(a-b)}{\sqrt{2}}e^{i\omega t}|x_-\rangle \qquad (27)$$

This is the final answer. If you want you can write it in the $|\pm\rangle$ basis, but that is not necessary. This has all the information we need.

Back to reality

So far we have talked about things taking place in the Hilbert space. But that is just an abstract space. Now we need to recall how our results connect with reality; i.e, how we could measure these things in the lab.

There are 2 main quantities which we use: probabilities and the expectation value of operators. But as you may recall, the second is actually derived from the first.

The "connection to the real world" is a postulate; it cannot be proved, but is related to the way we construct the theory. It can be stated as follows:

The probability of finding the system in some state $|\beta\rangle$, given that it is in $|\alpha(t)\rangle$ is given by

$$\boxed{P(\beta|\alpha(t)) = |\langle\beta|\alpha(t)\rangle|^2} \tag{28}$$

For instance, if $|\alpha(t)\rangle$ is given by (23), then

$$\begin{aligned} \langle +|\alpha(t)\rangle &= a e^{-i\omega t} \quad \Rightarrow \quad P(+|\alpha(t)) = |a|^2 \\ \langle -|\alpha(t)\rangle &= b e^{i\omega t} \quad \Rightarrow \quad P(-|\alpha(t)) = |b|^2 \end{aligned} \tag{29}$$

Two things should be noted. First, these probabilities do not depend on time. This is not a coincidence. We will get back to it shortly

The second thing is that the state "must be somewhere", which means that a and b only make sense if

$$|a|^2 + |b|^2 = 1 \tag{30}$$

This is a particular case of a more general rule

$$P(\alpha|\alpha) = |\langle\alpha|\alpha\rangle|^2 = 1 \tag{31}$$

If you read this out loud it becomes obvious: the prob. of finding the system in $|\alpha\rangle$ given that it is in $|\alpha\rangle$ must be 1. We therefore <u>always</u> choose

$$\boxed{\langle\alpha|\alpha\rangle = 1} \tag{32}$$

In words: quantum states are always normalized. In terms of the general solution (13) this means that

$$\boxed{\sum_m |c_m(0)|^2 = 1} \tag{33}$$

In fact, now that we are talking about the c_n, note the following

$$\langle m|\alpha(t)\rangle = c_m(0)\,e^{-i\omega_m t} \tag{34}$$

which implies that

$$\boxed{P(m|\alpha(t)) = |c_m(0)|^2} \tag{35}$$

Please remember this formula. It has a very clear physical interpretation. The $c_m(0)$ are called the amplitud to find the system in the states $|m\rangle$. If you square the amplitudes you get the probabilities.

We have also just shown that the probability of finding the system in an energy eigenstate $|m\rangle$ is independent of time. This is a very special property of the energy eigenstates. For this reason we also call them stationary states.

Just to show you that this property is peculiar of the energy eigenstates, let us go back to (23) and compute

$$\langle x+|\alpha(t)\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix} a e^{-i\omega t} \\ b e^{i\omega t}\end{bmatrix} = \frac{a e^{-i\omega t} + b e^{i\omega t}}{\sqrt{2}}$$

For simplicity let us suppose a and b are real. This is not strictly necessary. Then

$$P(x+|\alpha(t)) = |\langle x+|\alpha(t)\rangle|^2$$

$$= \frac{(a e^{-i\omega t} + b e^{i\omega t})(a e^{i\omega t} + b e^{-i\omega t})}{2}$$

$$= \frac{a^2 + b^2 + 2ab\cos\omega t}{2}$$

$$= \frac{1 + 2ab\cos\omega t}{2}$$

So now we have something that depends explicitly on time.

The other thing we measure in the lab is the expectation value of observables. Let $\hat{A}$ be an observable. All observables are Hermitian, $\hat{A}^{\dagger} = \hat{A}$. Therefore, if we write

$$\hat{A} \, |a_i\rangle = a_i \, |a_i\rangle \tag{36}$$

we know that the eigenvalues a_i will always be real.

When we measure an observable, we always obtain one of its eigenvalues. For instance, if we measure the energy we may get E_1 or E_2 or E_{100}. But never $(E_1 + E_2)/2$ [unless there is some E_n which coincidentally has this exact value].

The probability of measuring $\hat{A}$ and getting a_i is, as before

$$P(a_i \,|\, \alpha(t)) = |\langle a_i | \alpha(t)\rangle|^2 \tag{37}$$

because "obtaining a_i" is the same as "finding the system in the state $|a_i\rangle$"

Suppose we now repeat the experiment many times: prepare the system in $|\alpha(t)\rangle$; measure $\hat{A}$; throw away the system and get a new one. Then we may ask "what is the average outcome of this experiment?"

Based on simple statistics, we write the answer as

$$\boxed{\langle \hat{A} \rangle = \sum_i a_i \, P(a_i \,|\, \alpha(t))} \qquad (38)$$

We call this "the expectation value of $\hat{A}$." The most important example is for the Hamiltonian. Since the probabilities are given by (35) we get

$$\boxed{\langle \hat{H} \rangle = \sum_n E_n \, P(n \,|\, \alpha(t)) = \sum_n E_n \, |c_n(0)|^2} \qquad (39)$$

This is <u>time</u> <u>independent</u>; it depends only on the original state of the system at time $t = 0$. This is how conservation of energy works in quantum mechanics.

There is another way to write $\langle \hat{A} \rangle$, which is usually more useful from a practical point of view. Since the $|a_i\rangle$ form a basis, they satisfy completeness: $\sum_i |a_i\rangle\langle a_i| = 1$. Then it can be shown that Eq (38) may be written as

$$\boxed{\langle \hat{A} \rangle = \langle \alpha(t) | \hat{A} | \alpha(t) \rangle} \qquad (40)$$

This is the most common and most usefull formula. If you want to find $\langle \hat{H} \rangle$, Eq (39) is almost always the best. For other operators, Eq (40) is usually preferred.

The wave-function

Position $\hat{x}$ and momentum $\hat{p}$ are both observables. We write their eigenvalue-eigenvector Eq as

$$\hat{x}|x\rangle = x|x\rangle$$
$$\hat{p}|k\rangle = \hbar k|k\rangle \qquad (41)$$

Since they are Hermitian, their eigenvalues are real and their eigenvectors form a basis. But there is one difference: $|x\rangle$ and $|k\rangle$ are <u>continuous</u> <u>kets</u>. The difference is that, instead of

$$\langle e_i|e_j\rangle = \delta_{ij}$$
$$\sum_i |e_i\rangle\langle e_i| = 1 \qquad (42)$$

hey satisfy

$$\boxed{\begin{aligned}\langle x|x'\rangle &= \delta(x-x')\\ \int dx\,|x\rangle\langle x| &= 1\end{aligned}} \qquad (43)$$

and similarly for $|k\rangle$]. It is easy to remember: for ontinuous kets replace sums by integrals and Kronecker eltas by Dirac deltas.

Position and momentum satisfy the canonical commutation relation

$$\boxed{[\hat{x}, \hat{p}] = i\hbar} \qquad (44)$$

A lot of things follow from this simple formula one of which is that

$$\boxed{\langle x | k \rangle := \phi_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}}} \qquad (45)$$

this formula says how to relate the $|x\rangle$ basis to the $|k\rangle$ basis.

Suppose we decompose a ket $|\alpha\rangle$ in a basis $|e_i\rangle$

$$|\alpha\rangle = \sum_i \alpha_i \, |e_i\rangle \tag{46a}$$

Then we know that

$$\alpha_i = \langle e_i | \alpha \rangle \tag{46b}$$

We could also have used the base $|x\rangle$. Then

$$|\alpha\rangle = \int \alpha_x \, |x\rangle \, dx \tag{47a}$$

the coefficients α_x are

$$\alpha_x = \langle x | \alpha \rangle \tag{47b}$$

They are a function of x in the sense that there is a different one for each x. Since they appear so oftenly we give them a new name and a special symbol. We call it a <u>wave-function</u> and write

$$\boxed{\psi_\alpha(x) = \langle x | \alpha \rangle} \tag{48}$$

Usually, there are several variations of this notation:

$\psi_m(x) = \langle x | m \rangle$ "ψ as a general wave-function symbol in the ket as subscript"

$\psi(x) = \langle x | \psi \rangle$ "Symbol in ket as wave-function"

$\Psi(x,t) = \langle x | \alpha(t) \rangle$ "Crazy, but I like it"

The wave function works in many aspects like a ket, in the sense that you can take linear combinations. For instance

$$\delta_{nm} = \langle n | m \rangle = \int dx \, \langle n | x \rangle \langle x | m \rangle = \int dx \, \psi_n^* \psi_m$$

thus, the inner product becomes an integral

$$\boxed{\int dx \, \psi_n^* \psi_m = \delta_{nm}} \qquad (49)$$

Just like $\quad \langle \alpha | \beta \rangle = \sum_i \alpha_i^* \beta_i$

The wave function is useful when dealing with Hamiltonians of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{50}$$

Suppose we want to find the eigenvalues and eigenvectors of this $\hat{H}$. Then

$$\hat{H}|n\rangle = \frac{\hat{p}^2}{2m}|n\rangle + V(\hat{x})|n\rangle = E_n|n\rangle$$

We have no idea what is $\hat{x}$ and $\hat{p}$ acting on $|n\rangle$, because $|n\rangle$ is an abstract vector. But we can make some progress if we move to the "coordinate representation". That is, we multiply by $\langle x|$ on both sides. The right-hand side (RHS) becomes

$$E_n\langle x|n\rangle = E_n\psi_n$$

In the LHS we have

$$\langle x|V(\hat{x})|n\rangle = V(x)\langle x|n\rangle = V(x)\psi_n$$

Moreover, it can be demonstrated from Eq (44) that

$$\boxed{\langle x|\hat{p}|n\rangle = -i\hbar\frac{\partial\psi_n}{\partial x}} \tag{51}$$

thus

$$\langle x|\frac{\hat{p}^2}{2m}|n\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2} \tag{52}$$

We then obtain

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2} + V(x)\psi_n = E\psi_n} \qquad (53)$$

This Eq is sometimes called the <u>time-independent</u> <u>S-Eq.</u> But please note that it is nothing more than the eigenvalue-eigenvector Eq. of $\hat{H}$ in the coordinate basis. The eigenvectors are now $\psi_n(x)$ (so we also call them eigenfunctions).

It is common to write

$$\boxed{\hat{p}\,\psi = -i\hbar\frac{\partial\psi}{\partial x}} \qquad (54)$$

But this is an abuse of notation the correct formula is given by (51). $\hat{p}$ is an abstract operator. It is not a derivative. But in the $|x\rangle$ basis, $\hat{p}$ acts like a derivative. So you can use (54) with impunity.

Similarly we also write

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)} \qquad (55)$$

This is again an abuse of notation. It is only correct in the $|x\rangle$ basis. The true formula is given by (50).

Example: The harmonic oscillator

The Hamiltonian of the harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 \qquad (56)$$

This is a very special problem that can be solved using only operator algebra. Define

$$\hat{x} = \frac{x_0}{\sqrt{2}} (\hat{a}^\dagger + \hat{a}) \qquad (57a)$$

$$\hat{p} = \frac{i p_0}{\sqrt{2}} (\hat{a}^\dagger - \hat{a}) \qquad (57b)$$

where

$$x_0 = \sqrt{\frac{\hbar}{m\omega}} , \qquad (57c)$$

$$p_0 = \frac{\hbar}{x_0} \qquad (57d)$$

Then (44) implies that

$$\boxed{[\hat{a}, \hat{a}^\dagger] = 1} \qquad (58)$$

and (56) becomes

$$\boxed{\hat{H} = \hbar\omega(\hat{a}^\dagger \hat{a} + 1/2)} \qquad (59)$$

The operator $\hat{a}^\dagger \hat{a}$ is Hermitian. Its eigenvalues and eigenvectors are

$$\boxed{\hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle} \qquad (60)$$

$$n = 0, 1, 2, 3, \ldots$$

thus the energies of the Harmonic oscillator are

$$\boxed{E_n = \hbar\omega(n+1/2)} \qquad (61)$$

We also have that

$$\boxed{\begin{aligned} \hat{a}|n\rangle &= \sqrt{n}\,|n-1\rangle \\ \hat{a}^{\dagger}|n\rangle &= \sqrt{n+1}\,|n+1\rangle \end{aligned}} \qquad (62)$$

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the solution of the time-dependent S-Eq is identical using wave-functions

$$\boxed{\Psi(x,t) = \sum_n c_n(0)\, e^{-i\omega_n t}\, \psi_n(x)} \qquad (63)$$

where

$$\boxed{c_n(0) = \langle n|\alpha(0)\rangle = \int dx\, \psi_n^*(x)\, \Psi(x,0)} \qquad (64)$$

More about the solution to the S-Eq

Let $\hat{A}$ be a Hermitian operator with

$$\hat{A}|a_i\rangle = a_i |a_i\rangle \tag{65}$$

Then, since it is Hermitian, the eigenvectors form a basis. Thus we may use 2 completeness relations to write

$$\hat{A} = \sum_{i,j} |a_i\rangle\langle a_i|\hat{A}|a_j\rangle\langle a_j|$$

But

$$\langle a_i|\hat{A}|a_j\rangle = a_j \langle a_i|a_j\rangle = a_j \delta_{ij}$$

So

$$\boxed{\hat{A} = \sum_i a_i |a_i\rangle\langle a_i|} \tag{66}$$

I really like this formula.

What about $\hat{A}^2$? Easy. From (65) we have that

$$\hat{A}^2|a_i\rangle = \hat{A}\hat{A}|a_i\rangle = a_i\hat{A}|a_i\rangle = a_i^2|a_i\rangle$$

Thus, $\hat{A}^2$ has the same eigenvectors of $\hat{A}$ and the eigenvalues are squared. Thus Eq (66) for $\hat{A}^2$ becomes

$$\hat{A}^2 = \sum_i a_i^2 |a_i\rangle\langle a_i| \tag{67}$$

This is readily extended to arbitrary powers of $\hat{A}$

$$\hat{A}^m = \sum_i a_i^m |a_i\rangle\langle a_i| \tag{68}$$

Now let $f(x)$ be some function described by means of a power series; i.e.

$$f(x) = \sum_{m=0}^{\infty} g_m x^m \tag{69}$$

we can construct $f(\hat{A})$ following the same recipe

$$f(\hat{A}) = \sum_{m=0}^{\infty} g_m \hat{A}^m \tag{70}$$

Functions of operators are <u>always</u> defined by means of a power series. Using (68) we get

$$f(\hat{A}) = \sum_{m=0}^{\infty} g_m \sum_i a_i^m |a_i\rangle\langle a_i| = \sum_i |a_i\rangle\langle a_i| \underbrace{\left[\sum_{m=0}^{\infty} g_m a_i^m\right]}_{f(a_i)}$$

$$\therefore \quad \boxed{f(\hat{A}) = \sum_i f(a_i) |a_i\rangle\langle a_i|} \tag{71}$$

So to get $f(\hat{A})$ you simply compute $f(a_i)$ for all eigenvalues.

The matrix exponential

The most important example is the exponential

$$\boxed{e^{\lambda\hat{A}} = \sum_{m=0}^{\infty} \frac{(\lambda\hat{A})^m}{m!} = 1 + \lambda\hat{A} + \frac{(\lambda\hat{A})^2}{2!} + \frac{(\lambda\hat{A})^3}{3!} + \dots} \qquad (72)$$

But please note that the matrix exponential does not satisfy the exponential property.

$$\boxed{e^{\hat{A}+\hat{B}} \neq e^{\hat{A}}\, e^{\hat{B}}} \qquad (73)$$

There are a series of formulas to deal with these situations, which generically go by the name of Baker-Campbell-Hausdorff formulas.

They are usually useful only when

$$[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0 \qquad (74)$$

which usually means that $[\hat{A}, \hat{B}]$ is a number (note that this is actually quite common). In this case we have

$$\boxed{e^{\lambda(\hat{A}+\hat{B})} = e^{\lambda\hat{A}}\, e^{\lambda\hat{B}}\, e^{-\frac{\lambda^2}{2}[\hat{A}, \hat{B}]}} \qquad (75)$$

So in this case you can separate $e^{\hat{A}+\hat{B}}$, but you gain an extra factor.

As a corollary we find that

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} \quad \text{iff} \quad [\hat{A}, \hat{B}] = 0 \tag{76}$$

(iff = if and only if)

If Eq (74) does not hold, Eq (75) must be replaced by a very complicated formula, which is almost always useless.

Another useful formula valid when (74) is true is

$$\boxed{e^{\hat{A}} e^{\hat{B}} = e^{\hat{B}} e^{\hat{A}} e^{[\hat{A}, \hat{B}]}} \tag{77}$$

Finally, there is a third formula also called the BCH formula which is <u>always true</u>. It reads

$$\boxed{e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}} = \hat{B} + \lambda [\hat{A}, \hat{B}] + \frac{\lambda^2}{2!} [\hat{A}, [\hat{A}, \hat{B}]] + \frac{\lambda^3}{3!} [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]] + \dots} \tag{78}$$

This formula turns out to be very useful because this sandwhich of an operator between $e^{\lambda \hat{A}}$ and $e^{-\lambda \hat{A}}$ appear very often.

Examples

An important example is $e^{i\phi\hat{\sigma}_3}$. This will appear later on when we talk about angular momentum. Now, using (71) and recalling that the eigenvalues of $\hat{\sigma}_3$ are ± 1 we obtain

$$e^{i\phi\hat{\sigma}_3} = e^{i\phi}|+\rangle\langle +| + e^{-i\phi}|-\rangle\langle -|$$

$$= e^{i\phi}\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} + e^{-i\phi}\begin{bmatrix}0\\1\end{bmatrix}\begin{bmatrix}0 & 1\end{bmatrix}$$

$$= e^{i\phi}\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + e^{-i\phi}\begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}$$

We thus conclude that

$$e^{i\phi\hat{\sigma}_3} = \begin{bmatrix}e^{i\phi} & 0\\0 & e^{-i\phi}\end{bmatrix} \qquad (79)$$

There is an important lesson to be learned here: when the matrix is diagonal, simply exponentiate the entries. But be careful: this is <u>only</u> true when the matrix is diagonal.

We can also do the same calculation using the definition of the exponential as a power series

$$e^{i\phi\hat{\sigma}_3} = 1 + i\phi\hat{\sigma}_3 + \frac{1}{2}(i\phi\hat{\sigma}_3)^2 + \frac{1}{3!}(i\phi\hat{\sigma}_3)^3 + \frac{1}{4!}(i\phi\hat{\sigma}_3)^4 + \ldots$$

But recall that $\sigma_3^2 = 1$ so $\sigma_3^3 = \sigma_3$, $\sigma_3^4 = \sigma_3^2 = 1$ and so on.

We thus have

$$e^{i\phi\hat{\sigma}_z} = 1 + i\phi\hat{\sigma}_z - \frac{\phi^2}{2} - i\frac{\phi^3}{3!}\hat{\sigma}_z + \frac{\phi^4}{4!} + i\frac{\phi^5}{5!}\hat{\sigma}_z - \frac{\phi^6}{6!} + \dots$$

$$= \left[1 - \frac{\phi^2}{2!} + \frac{\phi^4}{4!} - \frac{\phi^6}{6!} + \dots\right] + i\hat{\sigma}_z\left[\phi - \frac{\phi^3}{3!} + \frac{\phi^5}{5!} - \dots\right]$$

The two series that appear are those of $\cos\phi$ and $\sin\phi$

$$\cos\phi = 1 - \frac{\phi^2}{2} + \frac{\phi^4}{4!} - \frac{\phi^6}{6!} + \dots \qquad (80a)$$

$$\sin\phi = \phi - \frac{\phi^3}{3!} + \frac{\phi^5}{5!} - \frac{\phi^7}{7!} + \dots \qquad (80b)$$

Hence we conclude that

$$e^{i\phi\hat{\sigma}_z} = \cos\phi + i\hat{\sigma}_z\sin\phi \qquad (81)$$

If you open up this expression you may indeed verify that it is the same as (79). But this result is much nicer because if you go back to our derivation you will see that the only thing we used was the fact that $\hat{\sigma}_z^2 = 1$. Hence this is true for any operator with any dimension such that $\hat{A}^2 = 1$.

$$\boxed{e^{i\phi\hat{A}} = \cos\phi + i\hat{A}\sin\phi \qquad \text{if } \hat{A}^2 = 1} \qquad (82)$$

This includes all the other σ's. As an exercise, try to compute $\hat{\sigma}_x$ using (71) and see that it has the form (82).

Matrix exponential solution of the S-Eq

Let us now go all the way back to our formal solution of the S-Eq, Eq (13),

$$|\alpha(t)\rangle = \sum_m c_m(0)\, e^{-i\omega_m t}\, |m\rangle$$

If we substitute $c_m(0) = \langle m|\alpha(0)\rangle$ and $\omega_m = E_m/\hbar$ we get

$$|\alpha(t)\rangle = \sum_m e^{-iE_m t/\hbar}\, |m\rangle\langle m|\alpha(0)\rangle$$

$$= \left[\sum_m e^{-iE_m t/\hbar}\, |m\rangle\langle m|\right] |\alpha(0)\rangle$$

The whole thing under square brakets is one big operator. If we compare to Eq (71) we see that

$$\boxed{\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \sum_m e^{-iE_m t/\hbar}\, |m\rangle\langle m|} \qquad (83)$$

We call this the time-evolution operator or the time propagator

We then have

$$\boxed{|\alpha(t)\rangle = \hat{U}(t)\,|\alpha(0)\rangle} \qquad (84)$$

so the state $|\alpha(0)\rangle$ is propagated by means of $\hat{U}(t)$ to the state $|\alpha(t)\rangle$.

We can verify that $\hat{U}(t)$ is a unitary operator

$$\hat{U}(t)\hat{U}^{\dagger}(t) = e^{-i\hat{H}t/\hbar}\, e^{i\hat{H}t/\hbar} = 1 \qquad (85)$$

where I used the fact that, since $\hat{H}^{\dagger} = \hat{H}$, $\hat{U}^{\dagger} = e^{i\hat{H}t/\hbar}$. The fact that $\hat{U}$ is unitary is crucial because it ensures that the state $|\alpha(t)\rangle$ remains properly normalized

$$\langle\alpha(t)|\alpha(t)\rangle = \langle\alpha(0)|\hat{U}^{\dagger}(t)\,\hat{U}(t)|\alpha(0)\rangle$$

$$= \langle\alpha(0)|\alpha(0)\rangle$$

$$= 1$$

So if we start with a properly normalized state we end up with a properly normalized state.

If we differentiate (83) with respect to time we get

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

This is a remarkable fact: it shows that $\hat{U}(t)$ also satisfies the S-Eq

$$\boxed{\frac{d\hat{U}}{dt} = -\frac{i}{\hbar}\hat{H}\hat{U}} \qquad (86)$$

But this is an Eq. among operators. It is also subject to the initial condition

$$\hat{U}(0) = 1 \qquad (87)$$

We could also have inverted the argument. Start with the S-Eq

$$\frac{d}{dt}|\alpha(t)\rangle = -\frac{i}{\hbar}\hat{H}|\alpha(t)\rangle$$

Now change

$$|\alpha(t)\rangle \to x$$

$$-\frac{i\hat{H}}{\hbar} \to a$$

then we get the super easy differential equation

$$\frac{dx}{dt} = ax$$

whose solution is
$$x(t) = e^{at}x(0)$$

Going back to our original notation we arrive at

$$|\alpha(t)\rangle = e^{-i\hat{H}t/\hbar}|\alpha(0)\rangle$$

which shows why this is the solution of the S-Eq.

Note: all we are discussing assumes $\hat{H}$ is independent of time. Things get much much harder when we have $\hat{H}(t)$. We will treat these problems using an approximate technique called perturbation theory.

Finally, let us go back to the expectation value of an operator,

$$\langle \hat{A} \rangle = \langle \alpha(t) | \hat{A} | \alpha(t) \rangle$$

Using (84) we get

$$\langle \hat{A} \rangle = \langle \alpha(0) | e^{i\hat{H}t/\hbar} \hat{A} e^{-i\hat{H}t/\hbar} | \alpha(0) \rangle \tag{88}$$

This illustrates why the BCH expansion (78) is so useful. We can first use it to compute the product of the 3 operators and then take the sandwhich with $|\alpha(0)\rangle$.

The product that appears in (88) is very common and receives a special name. It is called the <u>Heisenberg representation</u> of the operator $\hat{A}$ (it was actually Dirac who invented this). We write it as

$$\boxed{\hat{A}_H(t) = e^{i\hat{H}t/\hbar} \hat{A} e^{-i\hat{H}t/\hbar}} \tag{89}$$