Advanced Quantum Mechanics with Applications
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Lecture - 31
Quantum Dynamics: Two level system

So, many of the systems, they show two level structure which we have already seen and we are going to study Quantum Dynamics for these Two level systems.

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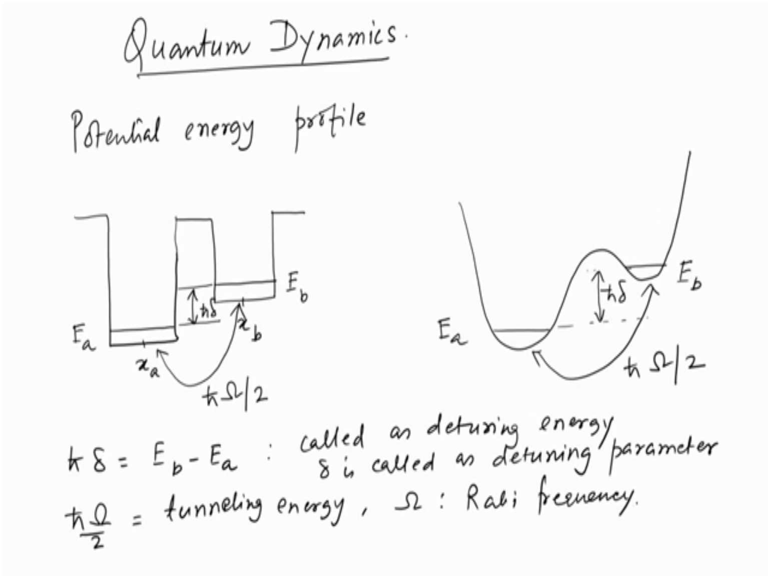

There are of course, more complicated systems such as three-level systems and higher-level systems; but of course, they are outside the ambit of this course and we will simply keep our discussion restricted to the two-level systems.

Many of the examples that we have seen in the past and they are say the spin half system which has two states basis states which are up and down or they could be you know the photons are also they have the polarization of the photons are there, left circularly polarized photons and right circularly polarized photons or there are other systems such as the ammonium molecule, where the 3 hydrogen atoms forms a planar triangle whereas, the nitrogen is at the top or it is at the bottom that forms a two level system as well.

So, these are the main focus of our study of quantum dynamics in these systems. So, the potential energy curve in this system. So, these are generic and can be applied to any of the two-level systems that we are talking about. So, the Potential energy profile or either one can talk about us rectangular barrier potential or one can talk about parabolic potential, where we are talking about 2 energy levels E a and E b. So, this corresponds to the a and this corresponds to b.

So, this is the E b and the difference between the energies is called as the detuning energy and we will write it as h cross delta; whereas, the coupling between the 2 wells will be written in terms of coupling or a tunnelling term which is will write it as h cross omega by 2. Similarly, in the parabolic we can define similar quantities which are again E a or and E b; whereas, the difference in energy which is called as the detuning energy which called as the h cross delta and as well as the tunnelling between them is again given by h cross omega by 2. This omega is called as a Rabi frequency and delta this delta is called as the detuning parameter.

So, we will write this h cross delta equal to E b minus E a and this is called as the detuning energy and this delta is called as a detuning parameter and h cross omega over 2 is the tunnelling energy and omega is called as the Rabi frequency.

So, we are going to study the dynamics of the wave function or the how the wave function evolves as a function of time with some given initial condition and we will write down the wave function in either of this potential the wave function is written as C a t and a plus C b t and b.

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$$|\psi(t)\rangle = C_a(t)|a\rangle + C_b(t)|b\rangle$$

$$|a\rangle = \begin{pmatrix}1\\0\end{pmatrix} \; ; \; |b\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

$$|\psi(t)\rangle = \begin{pmatrix}C_a(t)\\C_b(t)\end{pmatrix}$$

The Hamiltonian :

$$H = \hbar \begin{pmatrix}\delta & \Omega/2\\ \Omega/2 & 0\end{pmatrix}$$

Written in a symmetric fashion: $H = \frac{\hbar\delta}{2}\mathbb{1} + \frac{\hbar}{2}\begin{pmatrix}\delta & \Omega\\ \Omega & -\delta\end{pmatrix}$

Just to remind you that a s and b s are the basis states for these two-level problem and C a t and C b t are the coefficients that carry the time dependency, where while the basis states are time independent. So, the wave function is written as a linear combination of this.

And if we consider a spin half system which we are most familiar with, we can write down this as a spin up particle corresponding to an eigen value equal to 1 and this corresponding to a spin down particle corresponding to an eigen value minus 1 which we have seen. So, in this notation the psi of t can be written as C a of t and C b of t with a and b putting there and in which case the Hamiltonian of the system looks like.

Now, before we write down the Hamiltonian see there are 2 terms; one is the tunnelling energy which takes from barrier a 1 or barrier a to barrier b or the state a to state b. The same thing here in the other the parabolic well as well and there is also diagonal term which is the difference in energy between the 2 l s.

So, these 2 should be reflected there and of course, h cross is can be taken outside and then, it is omega by 2 and it is omega by 2 and it is 0. So, one of the energy level is a bigger than the other energy level by this detuning parameter delta and off diagonal elements, they talk about the tunnelling probability of a particle tunnelling or rather being able to make transitions between the 2 states of a two level system and.

So, this is the generic form the Hamiltonian. This is sometimes written in symmetric fashion as in which case, we simply take this detuning parameter and write it with a unit matrix and a plus h cross by 2 and delta omega minus omega sorry minus not minus omega; it is plus omega and minus delta omega and minus delta. So, that is the Hamiltonian and one can easily solve the eigenvalues for this.

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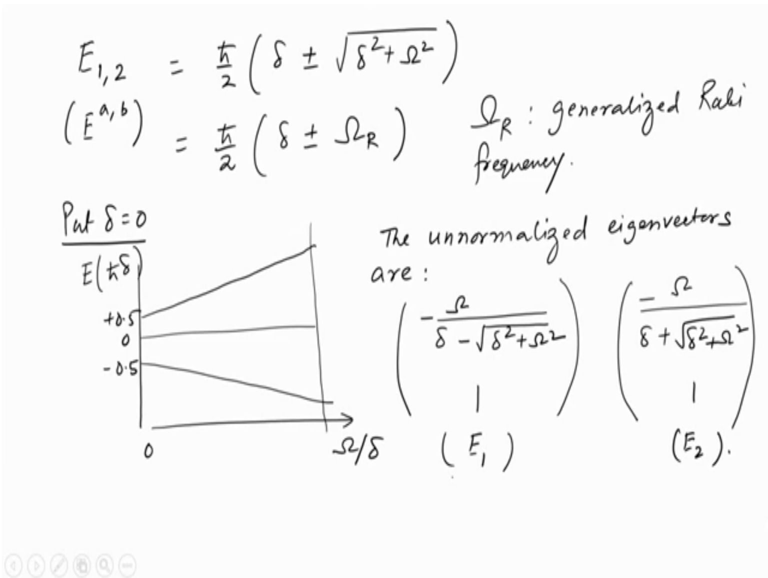

So, the eigenvalues are we can write it as 1 and 2 or you can simply write it as a and b. So, this is equal to h cross by 2 delta plus minus root over delta square plus omega square. And this is called as the; these are the energies of this two level system. One can see that this constant term that we have written here the first term, on the right hand side introduces a shift in the energy levels as compared to this to the energies this root over delta square plus omega square and this is written as h cross by 2 delta plus minus omega R, where omega R is called as the generalized Rabi frequency.

So, in the absence of detuning, the energy levels are simply minus h cross by 2 omega R and plus h cross by 2 omega R and so, this is if you put delta equal to 0; that is the detuning to be 0. At this moment of course, these delta omega time independent and then, these values can be plotted and they look like something like this ok.

So, this is E in terms of h cross delta and this is plotted as a function of omega over delta and so, it is something like minus 0.5 and this is plus 0.5 and this is 0 and so on and this maybe just brought it from, from 0 to some value. Now, corresponding to this plus and minus eigenvalues one can find out the eigenvectors. So, the unnormalized eigenvectors are minus omega divided by delta minus root over delta square plus omega square and 1; this corresponds to E 1 or E a whatever you want to call it.

So, this is for that and the other one is minus omega delta plus root over delta square plus omega square. Of course, here we have not put delta equal to 0 so, this is 1 again. So, this is corresponding to E 2. So, these are the unnormalized wave functions. This there is another way of writing down the Hamiltonian.

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Introducing the Pauli matrices

$$H = \frac{\hbar\delta}{2}\mathbb{1} + \hbar\left[\frac{\delta}{2}\sigma_z + \frac{\Omega}{2}\sigma_z\right]. \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The dynamics is governed by the time dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle.$$

H is time independent, $|\psi(t)\rangle$ can be written as,

$$|\psi(t)\rangle = U(t,0)\,|\psi(0)\rangle$$

$U(t,0)$ is a unitary operator.

$$UU^{\dagger} = \mathbb{1}$$

$$U(t_1,t_2)\,U(t_2,t_3) = U(t_1,t_3)$$

So, Introducing Pauli matrices; H, the Hamiltonian is written as the constant shift plus the h cross delta by 2 sigma z plus omega by 2 sigma x and so on. And so, this is where sigma z of course, what you are aware of, it is equal to 1 0 0 minus 1 and sigma x equal to 0 1 1 0. They are traceless and they all have eigenvalues equal to plus 1 or minus 1 and one can work out the eigenvectors as well.

So, the dynamics is a governed by the time dependent Schrodinger equation. Which is i h cross del del t of psi t equal to H psi t. The Hamiltonian is of course, is time independent and if that is so, psi t can be written as psi t equal to U t 0 and psi 0; that means, the wave function starting at t equal to 0 can be evolved to a wave function at t equal to t by using this operator U t 0 which is a time evolution operator.

And of course, some of the properties of the time evolution operators are that that the t 0 equal to is an unitary operator is a unitary operator and various other properties which are so, they can successively you know evolve in time. So, U U dagger equal to 1 and U or t 1 t 2 U t 2 t 3 equal to U t 1 t 3 and various other things which we will not discuss here. So, these are the time evolution operators that we will be using.

So, the form of the time evolution operator is the following.

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Here $U(t,0) = e^{-iHt/\hbar}$

$$= e^{-it/\hbar\left(\frac{\hbar\delta}{2}\mathbb{1} + \hbar\left[\frac{\delta}{2}\sigma_z + \frac{\Omega}{2}\sigma_x\right]\right)}.$$

$$e^{i\alpha(\hat{n}\cdot\vec{\sigma})} = \cos\alpha\,\mathbb{1} + i\,(\hat{n}\cdot\vec{\sigma})\sin\alpha$$

$$e^{i\hbar\frac{\delta}{2}\sigma_z}$$

So, U t 0, it is equal to exponential minus i H t by h cross and so this of course, means that if we take this Hamiltonian in the written in the form of rather written in terms of the Pauli matrices. So, this is t over h and there is a h cross delta by 2 and plus h cross delta by 2 sigma z plus omega by 2 sigma x and so on.

Now of course, you have in the exponential term or the argument of the exponential, there are matrices, there are 2 by 2 matrices including the Pauli matrices and Unit matrix. So, how to do that? One can go to so there are exponentials of the Pauli matrix. So, alpha is some constant say for example, and we have a n dot sigma. So, where sigma is Pauli matrices, then this is written as cos alpha unit matrix plus i n dot sigma sine alpha.

So, just to make things clear for at least for the one term that is written on top of here is sigma z. So, I am taking the term that is here; the term that is here. So, there is i t by h cross and into h cross delta by 2. So, this term I am writing in an exponential i. So, we will write it properly, but this is the term that we are talking about. So, there is a i t by h cross that is the factor that is outside.

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Here $U(t,0) = e^{-iHt/\hbar}$

$$= e^{-it/\hbar\left(\frac{\hbar\delta}{2}\mathbb{1} + \hbar\left[\frac{\delta}{2}\sigma_z + \frac{\Omega}{2}\sigma_x\right]\right)}.$$

$$e^{i\alpha(\hat{n}\cdot\vec{\sigma})} = \cos\alpha\,\mathbb{1} + i(\hat{n}\cdot\vec{\sigma})\sin\alpha$$

$$e^{-it/\hbar\cdot\hbar\frac{\delta}{2}\sigma_z} = e^{-it\frac{\delta}{2}\sigma_z} = e^{\alpha(\hat{n}\cdot\vec{\sigma})} \qquad \alpha = -\frac{it\delta}{2}$$

$$= \begin{pmatrix} \cos\frac{it\delta}{2} + i\sin\frac{it\delta}{2} & 0. \\ 0 & \cos\frac{it\delta}{2} - i\sin\frac{it\delta}{2} \end{pmatrix}$$

So, there is a exponential minus i t by h cross and then there is a h cross delta by 2 and then there is a sigma z. So, this can be written as exponential so, this h cross will cancel and we will have a exponential minus i t delta by 2 and a sigma z which is written as exponential alpha n dot sigma, where n cap is along the z direction and alpha is equal to minus i t delta by 2.

So, that can be written as cos of i t delta by 2 and plus i sine i t delta by 2 and there is a 0 and then, there is the there is a 0 and then, there is a cos i t delta by 2 and minus i sine i t by delta by 2 or there could be a sign change here. A rough it is only approximately that I am writing, you can see this later there could be a sign mistake here which is you should see this, you see this carefully and see this, but they could be written in this particular fashion.

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$$U(t,0) = \begin{pmatrix} \cos\frac{\Omega_R t}{2} + \frac{i\delta}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right) & \frac{i\Omega}{\Omega_R}\sin\frac{\Omega_R t}{2} \\ \frac{i\Omega}{\Omega_R}\sin\frac{\Omega_R t}{2} & \cos\frac{\Omega_R t}{2} - \frac{i\delta}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right) \end{pmatrix}$$

$\Omega_R = \sqrt{\Omega^2 + \delta^2}$: generalized Rabi frequency.

If $\delta = 0$

$$U(t,0) = \begin{pmatrix} \cos\frac{\Omega t}{2} & i\sin\Omega t/2 \\ i\sin\Omega t/2 & \cos\Omega t/2 \end{pmatrix}$$

So, if you do that then the U t 0 for this particular case is written as cos omega R t by 2 plus i delta by omega R sine of omega R t by 2 and i omega by omega R sin omega R t by 2 and i omega by omega R sin of omega R t by 2 cosine of omega R t by 2 minus i delta by omega R sin of omega R t by 2. So, that is the form of U t 0. It is little complicated, but it is still a 2 by 2 matrix which you should be able to handle.

And as we have said earlier that omega R is simply the generalized Rabi frequency if in addition to that, if we put the detuning equal to 0, then U t 0 of course, takes a slightly simpler and more tractable form and it is i sine omega t by 2 and this is i sine omega t by 2 cos omega t by 2 omega is called as the Rabi frequency, as opposed to the generalized Rabi frequency. So, this is the form of the time evolution operator for this two level system.

Now, let us take a particular case in order to evolve the system.

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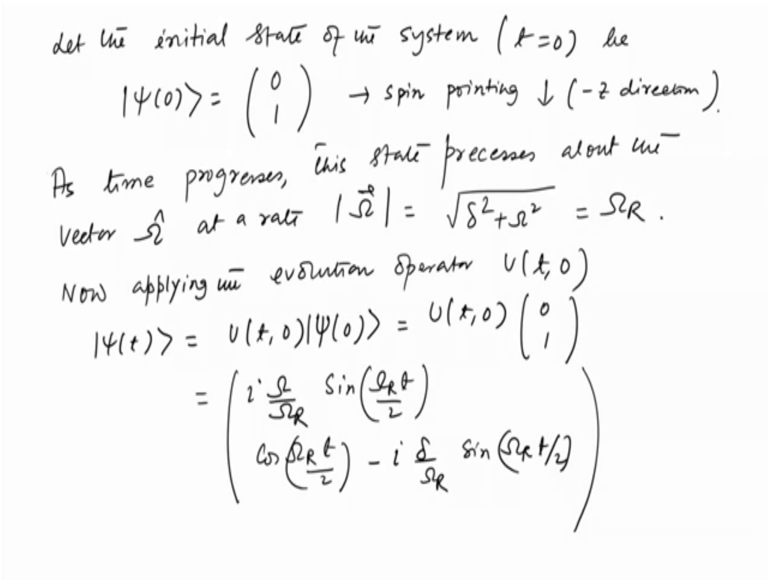

So, let the initial state of the system. So, by initial we mean t equal to 0 be psi 0 that is at t equal to 0 be this 0, 1 spinner which means that this corresponds to of course, the spin pointing in the negative z direction; spin pointing down or we can call it a negative z direction.

So, it precesses as time goes it precesses about a vector this omega cap at the rate will so, as time progresses, this state we will just call it a state precesses about the vector omega which is the at a rate which is omega equal to root over delta square plus omega square which is equal to omega R.

So, now applying the evolution operator U t 0, this notation of having 2 time indices is that the initial time is 0 and the final time is t. It could be t t prime also, where the initial time is t prime. So, I have psi of t which is equal to U t 0 psi of 0 and which is equal to U of t 0 and 0, 1. If you do this simplification, it becomes equal to i omega by omega R sine of omega R t by 2 and cosine of omega R by omega R t by 2 minus i delta by omega R sine omega R t by 2 and so on. So, that is the spinner which at time at a general time t equal to t some general time t that happens to this spinner 0, 1.

So, if we start from a spinner 0, 1; of course, this is what we are going to get by applying this U t 0 which has been written here. It is that applying on that. So, let us try to understand that what happens. So, one is that the top component; so, this is the top component here, this is the top component and this is the bottom component. This is how we will refer them to ok.

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(i) The top component starts off at $t=0$ with a value 0 and oscillates in time with angular frequency $(\Omega_R/2)$ and an amplitude $\left(\frac{\Omega}{\Omega_R}\right)$ ∴
Thus the probability for it to be in an excited state is $\left|\frac{\Omega}{\Omega_R}\right|^2$.

(ii) The bottom component has probability.
$$P(t) = 1 - |\text{top component}|^2.$$
Thus it starts from 1 at $t=0$ and oscillates, returning to a value 1 at $= \left(\frac{2\pi}{\Omega_R}\right) m$
m being an integer.

So, the top component starts off at t equal to 0 with a value 0, we know that there is a value 0 for that component and oscillates in time with angular frequency omega R by 2. So, that is omega R by 2 here and an amplitude which is a omega by omega R. So thus, the probability for it to be in an excited state is omega by omega R mod square. While the bottom component, it is not the components it is just component. The bottom component has probability P of t equal to 1 minus this top component square this entire let us just write top component mod square ok.

So, it of course, starts from 1 at t equal to 0 and oscillates returning to a value 1 at t equal to 2 pi by omega R into m; m being an integer. So, we have shown by a simple example that how the time evolution of a two level system occurs by writing down an unitary operator which is equal to nothing but the exponential i h t by h cross.

And then, of course, your the we have taken as a specific example of a spin down state and showed that how the components of a spin down state at t equal to 0, how that oscillates it. Of course, it does not stay always that in the spin down states and it sort of the oscillations as a function of time shows a sinusoidal variation and there is a finite probability for it to be in an excited state and so, is the other component that you know there is an oscillation of the kind that is shown in this by this expression which is the bottom part and so on.

In this particular way, all two level systems can be or this treatment can be generalized to all two level systems. It is just that we need to write it in write down the Hamiltonian and need to exponentiate the Hamiltonian. If the Hamiltonian is written in terms of the Pauli matrices, the exponentiation becomes simpler and one can simply do it by using this formula that we have given you here. This formula that is that you can see it here this formula and this formula is quite helpful; else if we do not have this form available, it still can be exponentiated.

However, the form can look a little intimidating, but it still remains a 2 by 2 matrix. It is a unitary 2 by 2 matrix and studying the evolution or the dynamics of the wave packet or the wave is not difficult task to do.