

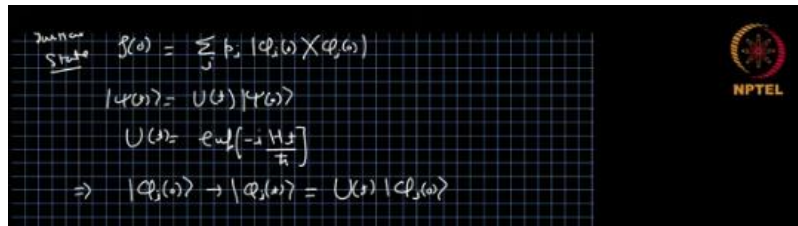
FOUNDATIONS OF QUANTUM THEORY: NON-RELATIVISTIC APPROACH

Dr. Sandeep K. Goyal
Department of Physical Sciences
IISER Mohali
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Lecture-10

Qubits: Unitary Transformation

We will be talking about the unitary transformation in qubits in general. So, first we talk about the time evolution. In mixed states, when our system is in a mixed state represented by a density matrix ρ , then how does the time evolution look like and what is the, how does the Schrodinger equation transforms? So, let us say in the beginning, the initial state we have, we represent it by a ρ of 0, where 0 stands for the time here. And it can be written as sum over i p_i and $|\phi_i\rangle_0$. So, we are choosing a preparation method for the initial state in such a way the probabilities are time independent and only the states are time dependent.

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Handwritten equations on a grid background with an NPTEL logo in the top right corner:

$$\rho(t) = \sum_j p_j |\phi_j(t)\rangle\langle\phi_j(t)|$$
$$|\psi(t)\rangle = U(t) |\psi(0)\rangle$$
$$U(t) = e^{-i \frac{Ht}{\hbar}}$$
$$\Rightarrow |\phi_j(0)\rangle \rightarrow |\phi_j(t)\rangle = U(t) |\phi_j(0)\rangle$$

From the pure states we know that ψ of t is given by unitary which depends on time, ψ of 0, where the unitary U of t is given by exponential of minus i times the Hamiltonian times the time over \hbar . This is the solution of the Schrodinger equation for pure states and time independent Hamiltonians. So, from here we can say that every individual state ϕ_i will go to ϕ_i of t given by U of t acting on ϕ_i of 0. So, every pure state in the ensemble will satisfy this time evolution. So, we can substitute it and get ρ of 0 goes to ρ of t which is given by sum over i p_i $|\phi_i(t)\rangle\langle\phi_i(t)|$ or we can say that this is equal to sum over i p_i $U |\phi_i(0)\rangle\langle\phi_i(0)| U^\dagger$ or $U \rho(0) U^\dagger$ where U is time dependent.

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$$\begin{aligned} \Rightarrow |\phi_j(t)\rangle &\rightarrow |\phi_j(t)\rangle = U(t) |\phi_j(0)\rangle \\ \rho(t) &\rightarrow \rho(t) = \sum_j p_j |\phi_j(t)\rangle \langle \phi_j(t)| \\ &= \sum_j p_j U |\phi_j(0)\rangle \langle \phi_j(0)| U^\dagger \\ &= U \rho(0) U^\dagger \end{aligned}$$

So, this is how the time evolution of a state of a mixed state of an ensemble looks like. If we take the derivative of the density matrix as a function of time with respect to time, then we get $\frac{dU}{dt} \rho(0) U^\dagger$. $\rho(0)$ is time independent, so we get $\frac{dU}{dt} U^\dagger$. $\frac{dU}{dt}$ is $\frac{d}{dt}$ of exponential of $-\frac{iHt}{\hbar}$ which can be written as $-\frac{iH}{\hbar}$ exponential of $-\frac{iHt}{\hbar}$ or we can write it as $-\frac{iH}{\hbar}$. Similarly, $\frac{dU^\dagger}{dt}$ will be $\frac{iH}{\hbar} U^\dagger$.

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$$\frac{d\rho(t)}{dt} = \frac{dU}{dt} \rho(0) U^\dagger + U \rho(0) \frac{dU^\dagger}{dt}$$

$$\begin{aligned} \frac{dU}{dt} &= \frac{d}{dt} e^{-\frac{iHt}{\hbar}} = -\frac{iH}{\hbar} e^{-\frac{iHt}{\hbar}} \\ &= -\frac{iH}{\hbar} U \\ \frac{dU^\dagger}{dt} &= \frac{iH}{\hbar} U^\dagger \end{aligned}$$

In fact, we can just take the Hermitian conjugate of this equation and we will get but when we take the Hermitian conjugate it will be $\frac{i}{\hbar} U^\dagger H$ not $\frac{i}{\hbar} H U^\dagger$ over \hbar but U is a function of H , solely a function of H , there is no other operator here, so U and H commute, so this is equal to, we can write it in any order $H U^\dagger$ or $U^\dagger H$ doesn't matter. So, with this we get $\frac{d\rho}{dt}$ to be $-\frac{i}{\hbar} H U \rho(0) U^\dagger$ over \hbar plus $\frac{i}{\hbar} H U \rho(0) U^\dagger$ over \hbar . H does not commute with ρ so it has to be here or we can write it outside doesn't matter because $H U^\dagger$ and H commute so we can write it in this way $U^\dagger H$ which is $-\frac{i}{\hbar} H \rho(t)$ minus $\rho(t) H$ and that is $-\frac{i}{\hbar} [H, \rho(t)]$. So, we started with the time evolution of pure state given by Schrodinger equation. And we derived the equation, dynamical equation of a density matrix.

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$$\frac{d\rho}{dt} = -\frac{j}{\hbar} [H\rho - \rho H]$$

$$\frac{d\rho}{dt} = -\frac{j}{\hbar} [H, \rho]$$

This has a name, it's called von Neumann equation or Liouville equation or Von Neumann-Liouville equation. So, the Schrodinger equation has been replaced by this even if you call it Schrodinger equation, I will not mind but then it has a name it is called Von Neumann or Liouville equation or Von Neumann-Liouville equation. So, this is the equation which determines the time evolution dynamics of a quantum system where the state is represented by a density operator. Of course, if the density operator itself represents a pure state, then we should retrieve the the Schrodinger equation back and that can be an interesting exercise for anyone who wants to try. Next will be the general unitary operations operators for qubits or sometimes they are called gates also.

So, for a qubit, a unitary operator U will be a 2 by 2 matrix. Let us write the most general 2 by 2 matrix, complex matrix a, b, b and d, where a, b, c and d all are complex numbers. Now, U need to satisfy certain equation, maybe U dagger U should be identity for it to be a unitary operator. So, that will put some restrictions on a, b, c and d. And this is what we want to find out. So, there is a similar way of doing it.

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$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix}; a, b, c, d \in \mathbb{C}$$

$$UU^\dagger = U^\dagger U = I$$

We can just multiply this U U dagger U dagger U and substitute to identity and there will be some n number of equations on a b c d, which can be solved to find the coefficient a b c d or at least the restrictions on them. But we can say U is U1, U2. U is a collection of two vectors where u1 is a two-dimensional vector given by a c and u2 is a two-dimensional vector given by b and d. Now, one of the conditions is U dagger U is identity. This implies that U dagger is u1 u2 and u1 u2 which will give a matrix in terms

of the inner product so u_1 and u_2 , so $u_1 u_1$, $u_1 u_2$, $u_2 u_1$ and $u_2 u_2$ and this is equal to the identity matrix, one zero zero one. If we compare element by element then we get $u_1 u_1$ to be one $u_2 u_2$ to be one these are the diagonals. What does it mean so $u_1 u_1$ inner product is a mod square b mod square equals 1 c and b mod square plus d mod square is 1.

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Handwritten mathematical derivation on a grid background showing the calculation of $U^\dagger U = I$ for a 2x2 unitary matrix $U = [u_1, u_2]$. The derivation shows that the inner products of the columns must satisfy $\langle u_1, u_1 \rangle = 1$, $\langle u_2, u_2 \rangle = 1$, and $\langle u_1, u_2 \rangle = 0$. This leads to the conditions $a^2 + c^2 = 1$ and $b^2 + d^2 = 1$.

$$U U^\dagger = U^\dagger U = I$$

$$U = [u_1, u_2]; \quad u_1 = \begin{bmatrix} a \\ c \end{bmatrix} \quad u_2 = \begin{bmatrix} b \\ d \end{bmatrix}$$

$$U^\dagger U = I = \begin{bmatrix} \langle u_1, u_1 \rangle & \langle u_1, u_2 \rangle \\ \langle u_2, u_1 \rangle & \langle u_2, u_2 \rangle \end{bmatrix} = \begin{bmatrix} \langle u_1, u_1 \rangle & \langle u_1, u_2 \rangle \\ \langle u_2, u_1 \rangle & \langle u_2, u_2 \rangle \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \begin{cases} \langle u_1, u_1 \rangle = 1 & a^2 + c^2 = 1 \\ \langle u_2, u_2 \rangle = 1 & b^2 + d^2 = 1 \end{cases}$$

So, it means each of the vectors u_1 and u_2 are normalized. So, a mod square plus c mod square is 1, b mod square plus d mod square is 1. Next is u_1, u_2 is 0, same as u_2, u_1 . So, it means u_1 and u_2 are orthogonal. One can easily see if we choose u_1 to be a c, then there is a unique orthogonal vector up to a phase.

So, that orthogonal vector will be minus c star, c star and with a phase exponential of i theta. So, this does not matter if we choose this form of u_1 and u_2 , then they are always orthogonal. This yields the matrix U to be a c minus c star exponential of i theta and a star exponential of i theta. So, this becomes the most general form of a 2 by 2 unitary.

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Handwritten mathematical derivation on a grid background showing the general form of a 2x2 unitary matrix U . It shows that $u_1 = \begin{bmatrix} a \\ c \end{bmatrix}$ and $u_2 = \frac{1}{e^{i\theta}} \begin{bmatrix} -c^* \\ a \end{bmatrix}$, leading to the matrix $U = \begin{bmatrix} a & -c^* e^{i\theta} \\ c & a e^{i\theta} \end{bmatrix}$.

$$\langle u_1, u_2 \rangle = 0 = \langle u_2, u_1 \rangle$$

$$\rightarrow u_1 = \begin{bmatrix} a \\ c \end{bmatrix} \quad u_2 = \frac{1}{e^{i\theta}} \begin{bmatrix} -c^* \\ a \end{bmatrix}$$

$$U = \begin{bmatrix} a & -c^* e^{i\theta} \\ c & a e^{i\theta} \end{bmatrix}$$

So, the set of all the unitaries, 2 by 2 unitaries, they form a group. Group is not just a group, it is a mathematical structure with certain rules defined over it. It is more like linear vector space, but slightly more number of rules on it. So, unitary, this 2 by 2

unitaries form a group called U2. Now, we can see that this U can be, can also be written as exponential of i theta over 2 a exponential of minus i theta over 2 b exponential of minus i theta over 2 minus minus c exponential of i theta over 2 and a star exponential of i theta over 2.

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Now, if we define alpha to be a exponential of minus i theta over 2 and beta to be c exponential of minus i theta over 2, then we get U to be exponential of i theta over 2 alpha beta minus beta star alpha star. It is a phase times a matrix. And what is this matrix? Let us call it W. So, we get exponential of i theta over 2 times W. We can check W is also unitary, with one additional property that determinant of W is 1. Such unitary operators with determinant 1, 2 by 2 unitaries with the determinant 1, they form a group.

Another group, which is called SU2, special unitary 2 by 2, special unitary and 2 by 2. So, special unitary 2 by 2 group is the group of all the unitary 2 by 2 unitaries with determinant 1. So, the difference between U2 and SU2 is the phase exponential of i theta. So, any U2 element can be written as some phase times SU2. So, we will be using U2 and SU2 interchangeably unless specified explicitly.

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So, that is the most general set of unitaries we have. Now, let us recall that any unitary operator can be written as an exponential of i times a Hermitian operator. We have covered it in the mathematical prerequisite that any arbitrary unitary can be written as an

exponential of Hermitian. So, of course, two-dimensional unitary can also be written as exponential of i times two-dimensional Hermitian operator. H being two-dimensional Hermitian can be written as sum over $\mu = 0$ to 3 , $h_\mu \sigma_\mu$, where σ_μ 's are σ_0 , σ_1 , σ_2 , σ_3 , which are identity, σ_x , σ_y and σ_z . They are the Pauli operators. And h_μ are the real numbers. Now, identity σ_0 commutes with all the others. So, we can write as exponential of $i h_0$ times exponential of $i \sum_{j=1}^3 h_j \sigma_j$.

Or we can write it as exponential of $i h$, not \hbar , it is just h . Exponential of i times h vector dot sigma vector. h dot sigma vector is just $h_j \sigma_j$ sum over j . And this is an exercise, will be equal to exponential of $i h_0 \cos$ of h bar magnitude times identity plus $i \sin$ of h bar magnitude times h direction h cap dot sigma vector, where h cap is h vector divided by h magnitude is a unit vector. So, in that way we can write a unitary 2×2 unitary in terms of the Hermitian operator.

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$$\begin{aligned} \rightarrow \text{Unitary} &= \exp(i \text{Hermitian}) \\ U &= \exp(iH); \quad H = \sum_{\mu=0}^3 h_\mu \sigma_\mu \\ &= e^{i h_0} \exp\left(i \sum_{j=1}^3 h_j \sigma_j\right) = e^{i h_0} \exp(i \hat{h} \cdot \sigma) \end{aligned}$$

Hermitian operator can be decomposed in the sigma matrices and then we can find this simple form of a unitary operator in terms of sigma matrices. Another exercise is, prove that W equals exponential of $i h$ vector dot sigma vector. There is no identity here. It belongs to $SU(2)$. That is prove that this is unitary and prove that it has determinant 1.

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$$\begin{aligned} \text{Exercise } U &= \exp(i \hat{h} \cdot \sigma) \\ \hat{h} &= \frac{\mathbf{h}}{|\mathbf{h}|} \text{ Unit vector.} \\ \text{Exercise: prove that } W &= \exp(i \hat{h} \cdot \sigma) \in SU(2) \end{aligned}$$

Now, we will discuss the action of a unitary operator U on pure states. So, for that, let us take very simple examples. Let us take it to be exponential of $i \theta \sigma_z$ where we have just one Pauli operator σ_z and not y and x and since why we have chosen this

thing because sigma z is a diagonal matrix so exponential of a diagonal matrix is also a diagonal matrix and we get exponential of i theta and it is actually conventionally we take a minus sign here the minus theta 0 or theta by 2 0 exponential of i theta over 2. Now, what will be the action of this?

Let me call it alpha because we already have theta somewhere else. So, if our state psi is written in terms of cos theta over 2, sine theta over 2, exponential of i phi. This is a canonical form of the state, pure state psi. Now, what is the action of U on psi? That will be cos of theta over 2, exponential of minus i alpha over 2 and sine of theta over 2, exponential of i phi plus alpha over 2.

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$$U = e^{-i\left(\frac{\alpha}{2}\sigma_z\right)} = \begin{pmatrix} e^{-i\frac{\alpha}{2}} & 0 \\ 0 & e^{i\frac{\alpha}{2}} \end{pmatrix}$$

$$|\psi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

We can take exponential of minus i alpha over 2 common so that first element is real cos of theta over 2 sine of theta over 2 exponential of i phi plus alpha. So, the action of U which was exponential of i alpha over 2 minus i sigma z is to perform the following transformation, theta goes to theta and phi goes to phi plus alpha. Later on, it will be revealed that this is equivalent to rotation about z axis by an angle alpha. Similarly, we can choose a unitary U, let us put a subscript y, which is exponential of minus i theta sigma y.

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$$U|\psi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} e^{-i\frac{\alpha}{2}} \\ \sin\frac{\theta}{2} e^{i(\phi+\alpha)} \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i(\phi+\alpha)} \end{pmatrix}$$

- Action of $U = e^{-i\left(\frac{\alpha}{2}\sigma_z\right)} \rightarrow \phi \rightarrow \phi + \alpha$

By using the expression we used earlier, we can get by using this expression, we can calculate that it will be cos of theta times identity minus i sine of theta times sigma y which will be cos theta, minus sine theta, sine theta and cos theta. If we take a state with phi zero then we get, so i am taking theta here should be alpha, so that we do not be confused this theta with the theta of the state alpha alpha alpha alpha, cos of theta over

two sine of theta over two we are choosing a state with phi zero then U y acting on psi will result in cos of, conventionally we should put two here reasons will be clear soon cos of theta over two cos of alpha over two, minus sine of theta over two, sine of alpha over two, cos of theta over two, sine of alpha over two and sine of theta over two, cos of alpha over 2 which is nothing but cos of theta plus alpha over 2 and sin of theta plus alpha over 2. So, the action of U y is to take theta to theta plus alpha phi we do not know because we have put phi to be zero so this will later on it will be revealed that this will be a rotation about y axis by an angle alpha. Similarly, U n cap which can be written as exponential of minus i theta over 2, n cap dot sigma, where n cap is unit vector.

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$$\begin{aligned}
 U_y &= \exp\left[-i\frac{\alpha}{2}\sigma_y\right] = \begin{bmatrix} \cos\frac{\alpha}{2} & -i\sin\frac{\alpha}{2} \\ i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{bmatrix} \\
 |+\rangle &= \begin{bmatrix} \cos\frac{\alpha}{2} \\ \sin\frac{\alpha}{2} \end{bmatrix} \quad \phi=0 \\
 U_y|+\rangle &= \begin{bmatrix} \cos\frac{\alpha}{2}\cos\frac{\alpha}{2} - \sin\frac{\alpha}{2}\sin\frac{\alpha}{2} \\ \cos\frac{\alpha}{2}\sin\frac{\alpha}{2} + \sin\frac{\alpha}{2}\cos\frac{\alpha}{2} \end{bmatrix} = \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix}
 \end{aligned}$$

This unitary will be equivalent to rotation about n cap by an angle alpha. We will know what is the meaning of this rotation, what is this space we are talking about when we talk about the blocks here. But for the time being, we can think of it as some kind of rotations happening in the Hilbert space, which is equivalent to rotations in the three-dimensional real space. And that correspondence will be established later on. One very useful decomposition in terms of unitaries of, 2 by 2 unitaries is the Euler angle of decomposition.

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$$\begin{aligned}
 U_n &\rightarrow \sigma \rightarrow \sigma + \alpha \quad \text{Rotation about } \hat{n} \text{ by an angle } \alpha \\
 U_{\hat{n}} &= \exp\left[-i\frac{\alpha}{2}\hat{n}\cdot\sigma\right] \quad \hat{n} \rightarrow \text{unit vector} \\
 &\text{Rotation about } \hat{n} \text{ by an angle } \alpha.
 \end{aligned}$$

So, here we start with a unitary, an arbitrary unitary, which I recall as alpha beta minus beta star alpha star. This is the SU 2 . We take only SU 2 . We have seen that U is just a phase times SU 2 . So, once we know the decomposition of SU 2 , the decomposition for U 2 should not be very difficult to find.

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Euler-angle decomposition

$$U = \begin{bmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{bmatrix} \in SU(2)$$

$$U = U_z(\theta_1) U_y(\theta_2) U_z(\theta_3)$$

So, this unitary can be decomposed as unitary about z of with some angle alpha or delta, unitary about y, with angle eta gamma, let me call it theta 1 theta 2 and unitary about z, theta 3. Let me repeat that an arbitrary unitary SU 2, can be decomposed as a unitary, which is rotation about z, rotation about y and rotation about z with some angles theta 1, theta 2 and theta 3. This is not a mistake or a typo that the first and the third unitary are about z and second one is about y. It can also be y, z, y, of course, the theta will change or y, x, y or any two sigma matrix or the directions we can choose out of three. So, we take U to be alpha, which is a exponential of i theta and beta, which is b exponential of i gamma, minus beta star and alpha star. U about z, U of z at delta will be exponential of minus i delta sigma z, which is exponential of minus i delta 0 0 exponential of i delta. So, U z delta U U z eta, let us calculate this and it will be exponential of minus i delta, 0, 0 exponential of i delta. a exponential of i theta, b exponential of i gamma, minus b exponential of minus i gamma and a exponential of minus i theta. e exponential of minus i eta, 0, 0, e exponential of i eta. When we take the product, it will be a exponential of i theta minus delta minus eta, minus b exponential of minus i gamma plus delta minus eta, b exponential of i gamma plus delta minus eta and a exponential of minus i theta minus delta minus eta.

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Proof:

$$U = \begin{bmatrix} a e^{i\alpha} & -b e^{i\gamma} \\ b e^{i\gamma} & a e^{i\alpha} \end{bmatrix}$$

$$U_z(\delta) = e^{i\delta \sigma_z} = \begin{bmatrix} e^{i\delta} & 0 \\ 0 & e^{-i\delta} \end{bmatrix}$$

$$U_z(\theta) U U_z(\eta) = \begin{bmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{bmatrix} \begin{bmatrix} a e^{i\alpha} & -b e^{i\gamma} \\ b e^{i\gamma} & a e^{i\alpha} \end{bmatrix} \begin{bmatrix} e^{-i\eta} & 0 \\ 0 & e^{i\eta} \end{bmatrix}$$

Our aim is to show that for some choice of delta and eta, this whole matrix can be made real. And why do we want to do that? Because we have seen earlier that the rotation about y is a real matrix. That is the real matrix. So, for whatever value of alpha we want, it will always be a real matrix.

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$$\begin{aligned}
 U_z(r) U U_z(\eta) &= \begin{bmatrix} e^{-i\sigma} & 0 \\ 0 & e^{i\sigma} \end{bmatrix} \begin{bmatrix} a e^{-i\gamma} & -b e^{i\gamma} \\ b e^{-i\gamma} & a e^{i\gamma} \end{bmatrix} \begin{bmatrix} e^{-i\eta} & 0 \\ 0 & e^{i\eta} \end{bmatrix} \\
 &= \begin{bmatrix} a e^{i(\sigma-\delta-\eta)} & -b e^{-i(\gamma-\eta)} \\ b e^{i(\eta-\gamma)} & a e^{-i(\sigma-\delta+\eta)} \end{bmatrix}
 \end{aligned}$$

So, we want to choose delta and eta in such a way this product of three matrices is real. To make it real, the phases should vanish. We can see that this is one phase and it is the negative of that phase. This is one phase and it is the negative of that phase. So, it means we need to make only two phases zero which is theta minus delta minus eta is zero and gamma plus delta minus eta is zero. Theta and gamma are from the given U and delta and eta are something we need to choose.

So, if we add the two, we get theta plus gamma minus two eta is zero. This implies that eta is theta plus gamma over two. And if we subtract the two, we get theta minus gamma minus two delta is zero or delta to be theta minus gamma over two. This means that unitary about z of theta minus gamma over two, unitary and unitary about z of theta plus gamma over two is a real matrix which is rotation about y, rotation about y in terms of a and b. So, if a square plus b square is one that is the normalization condition of the first vector, then a can be thought of as cos of zeta and b can be thought of as sine of zeta.

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$$\begin{aligned}
 \rightarrow \sigma - \delta - \eta &= 0 & \gamma + \delta - \eta &= 0 \\
 \sigma + \gamma - 2\eta &= 0 & \Rightarrow \eta &= \frac{\sigma + \gamma}{2} \\
 \sigma - \gamma - 2\delta &= 0 & \Rightarrow \delta &= \frac{\sigma - \gamma}{2}
 \end{aligned}$$

So, this becomes a unitary about theta and then we can write U as U z of, U z dagger of theta minus gamma over 2, U y of zeta, U z of theta plus gamma over 2 dagger. One thing is interesting, U z of theta minus gamma over 2 dagger is same as U z of minus theta minus gamma over 2. So, from there we can see that U can be written as U z of gamma minus theta over 2, U y of theta, U dagger z of U z of minus theta minus gamma over 2. Hence, we can decompose any unitary, any 2 by 2 unitary in terms of the rotation about z, rotation about y and rotation about z. And the corresponding magnitude of the rotations are called the Euler angles. This is the Euler angle representation, decomposition.

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$$\Rightarrow U_z(\frac{\sigma_y}{\tau}) U_z(\frac{\sigma_x}{\tau}) = U_y(\epsilon)$$

$$U = U_z^\dagger(\frac{\sigma_x}{\tau}) U_y(\epsilon) U_z(\frac{\sigma_x}{\tau})$$

$$U_z^\dagger(\frac{\sigma_x}{\tau}) = U_z(-\frac{\sigma_x}{\tau})$$

$$U = U_z(\frac{\sigma_x}{\tau}) U_y(\epsilon) U_z(-\frac{\sigma_x}{\tau}) \quad \text{Gor}$$