

Quantum dynamics....with the dynamics
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2-level system (oscillations forever) Part 1

In this section, we explore the dynamics of a two-level quantum system. Specifically, it consists of a system in which all other degrees of freedom are ignored, and we are only interested in the transition between two states of the system (e.g two electronic states, or two possible spin states, or two possible molecular configurations etc...). This consideration means that for our problem, we need two basis states, which will span the entire 2-dimensional complex space in which our system “exists”. Hence the wavefunction describing our system will be a linear combination of these two basis states.

We begin by describing our basis states:

- $\phi_1(r)$ and $\phi_2(r)$ are orthonormal states, that is:

$$\langle \phi_1 | \phi_1 \rangle = \langle \phi_2 | \phi_2 \rangle = 1 \quad (1.1)$$

$$\langle \phi_1 | \phi_2 \rangle = \langle \phi_2 | \phi_1 \rangle = 0 \quad (1.2)$$

(Recall that $\langle \phi_1 | \phi_1 \rangle = \int \phi_1^*(r) \phi_1(r) dr = 1$, with ϕ_1^* complex conjugate of ϕ_1)

The Hamiltonian:

- In addition, the states $|\phi_1\rangle$ and $|\phi_2\rangle$ are eigenstates of the Hamiltonian, that is:

$$H_0 |\phi_1\rangle = E_1 |\phi_1\rangle \text{ and } H_0 |\phi_2\rangle = E_2 |\phi_2\rangle \quad (1.3)$$

- From these considerations, we can see that the Hamiltonian will be a 2×2 diagonal Hermitian matrix.
- Indeed we can construct it as:

$$H_0 = E_1 |\phi_1\rangle \langle \phi_1| + E_2 |\phi_2\rangle \langle \phi_2| \quad (1.4)$$

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$$

- Now, we introduce a real, time-independent energy coupling term V which couples the two states to each other (but not to themselves). The new Hamiltonian can be written: $H = H_0 + V$. The two basis states are not eigenfunctions of H . We can find the eigenfunctions of H by diagonalizing the Hamiltonian. We will do this a bit later, as it is not necessary to visualize the oscillatory dynamics of the system.
- Since our basis states constitute a complete set, we can express the wavefunction of our system as linear combination of the basis states:

$$\Psi(r, t) = c_1(t)\phi_1(r) + c_2(t)\phi_2(r) \quad (1.5)$$

- Notice how the time-dependence of the wavefunction is contained in the coefficients. In addition, we know that the probability for our system to be in a given basis state $|\phi\rangle$ is given by $c(t)^*c(t) = |c|^2$. Hence, it will be informative to determine an expression for the coefficients.
- The time-dependent Schrödinger equation (TDSE) reads:

$$i\hbar \frac{\partial \Psi(r, t)}{\partial t} = H(r, t)\Psi(r, t) \quad (1.6)$$

$$i\hbar \frac{\partial [c_1(t)\phi_1 + c_2(t)\phi_2]}{\partial t} = H(r, t)[c_1(t)\phi_1 + c_2(t)\phi_2] \quad (1.7)$$

We can determine an expression for the time-evolution of each time-dependent coefficients, $c_1(t)$ or $c_2(t)$ by multiplying the TDSE by the complex conjugate of the corresponding stationary-state and integrating (in Dirac notation this amounts to multiplying by the bra $\langle \phi_1 |$ to obtain $c_1(t)$ for instance). Doing so for $\dot{c}_1(t)$ (recall any variable $\dot{q}(t) = \frac{dq}{dt}$) in Dirac notation we get:

$$i\hbar \left[\frac{\partial c_1(t)}{\partial t} \langle \phi_1 | \phi_1 \rangle + \frac{\partial c_2(t)}{\partial t} \langle \phi_2 | \phi_1 \rangle \right] = c_1(t) \langle \phi_1 | H(r, t) | \phi_1 \rangle + c_2(t) \langle \phi_1 | H(r, t) | \phi_2 \rangle \quad (1.8)$$

$$i\hbar \frac{\partial c_1(t)}{\partial t} = c_1(t) \langle \phi_1 | H(r, t) | \phi_1 \rangle + c_2(t) \langle \phi_1 | H(r, t) | \phi_2 \rangle \quad (1.9)$$

We do the same procedure with $\langle \phi_2 |$ to obtain an expression for $\dot{c}_2(t)$:

$$i\hbar \frac{\partial c_2(t)}{\partial t} = c_2(t) \langle \phi_2 | H(r, t) | \phi_2 \rangle + c_1(t) \langle \phi_2 | H(r, t) | \phi_1 \rangle \quad (1.10)$$

We can write this system of equations in matrix form:

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} E_1 & V_{12} \\ V_{21} & E_2 \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} \quad (1.11)$$

In our example, the Hamiltonian matrix is independent of time and we can write:

$$i\hbar \frac{\partial \mathbf{c}}{\partial t} = \mathbf{H} \mathbf{c} \text{ and } \mathbf{c}(t) = \exp \left(\frac{-i}{\hbar} \mathbf{H} t \right) \mathbf{c}(0) \quad (1.12)$$

where \mathbf{c} is a column vector and \mathbf{H} a matrix.

We can see if there is no interaction energy between states ($V_{21} = V_{12} = 0$), then the transition probability for a given state will be constant ($|c|^2 = cst$), the state remains in a stationary state and does not oscillate (which would give us the non-interacting two-state system we started with).

A brief note on the unitary evolution operator:

The wavefunction is a time-dependent quantity. We can define an evolution operator $\hat{U}(t, t_0)$ that propagates the wavefunction in time:

$$|\Psi(r, t)\rangle = \hat{U}(t, t_0) |\Psi(r, t_0)\rangle \quad (1.14)$$

This operator must satisfy certain properties, namely:

- **Unitarity:**

If the wavefunction is normalized at t_0 it must remain normalized at a later date t , hence, the operator \hat{U} should not change the norm of the wavefunction. As a result, we have:

$$\langle \Psi(r, t) | \Psi(r, t) \rangle = \langle \Psi(r, t_0) | \hat{U}^\dagger(t, t_0) \hat{U}(t, t_0) | \Psi(r, t_0) \rangle = 1 \quad (1.13)$$

For the above relation to hold, $\hat{U}^\dagger(t, t_0) \hat{U}(t, t_0) = \mathbf{1}$, where $\mathbf{1}$ is the identity operator. This implies that $\hat{U}^\dagger(t, t_0) = \hat{U}^{-1}(t, t_0)$.

- **Continuity**

$|\Psi(r, t)\rangle = \hat{U}(t, t) |\Psi(r, t)\rangle$, which implies that $\hat{U}(t, t) = \mathbf{1}$. The operator acting on the wavefunction at a time t , when the wavefunction is already at time t gives the wavefunction back again, hence the operator acts as an identity operator.

- **Composition**

We can propagate the wavefunction to two consecutive points in time, either by applying \hat{U} once or two times consecutively:

$$|\Psi(r, t_2)\rangle = \hat{U}(t_2, t_0) |\Psi(r, t_0)\rangle \quad (1.14)$$

or

$$|\Psi(r, t_2)\rangle = \hat{U}(t_2, t_1) \hat{U}(t_1, t_0) |\Psi(r, t_0)\rangle$$

Hence we have:

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

In order to obtain an expression for \hat{U} , we can insert it into the TDSE:

$$i\hbar \frac{\partial |\Psi(r, t)\rangle}{\partial t} = H(r, t) |\Psi(r, t)\rangle \quad (1.15)$$

with $t_0 = 0$

$$i\hbar \frac{\partial \hat{U}(t)}{\partial t} |\Psi(r, t=0)\rangle = H(r, t) \hat{U}(t) |\Psi(r, t=0)\rangle \quad (1.16)$$

$$i\hbar \frac{\partial \hat{U}(t)}{\partial t} = H(r, t) \hat{U}(t) \quad (1.17)$$

$$\hat{U}(t) = \exp\left(\frac{-i}{\hbar} \int_0^t H(r, t') dt'\right) \quad (1.18)$$

If $H(r, t)$ is time independent, it can be taken out of the integral, and the integral evaluates to t . Hence for a time-independent Hamiltonian, the unitary evolution operator is:

$$\hat{U}(t) = \exp\left(\frac{-i}{\hbar}Ht\right) \quad (1.19)$$

We thus see that the evolution operator is what we obtained in equation (1.12) above. We can thus use it to obtain an expression for the state $\Psi(r, t)$ at all times from the initial state $\Psi_0(r, t_0)$.

For creating the script and plots:

We define our basis vectors:

$$\phi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \phi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (1.20)$$

Constructing $\Psi_0(r, t_0)$ as a linear combination of the basis states:

$$\Psi_0(r, t_0) = \frac{1}{\sqrt{c_1^2 + c_2^2}} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad (1.21)$$

where $\frac{1}{\sqrt{c_1^2 + c_2^2}}$ is a normalizing constant.

Constructing $\Psi(r, t)$ from $\Psi_0(r, t_0)$, and our Hamiltonian defined in 1.11, we get:

$$\Psi(r, t) = \exp\left(\frac{-i}{\hbar}Ht\right) \Psi_0(r, t_0) \quad (1.22)$$

notice how 1.22 is the same as what we obtained from 1.14.

To evaluate $c_1(t)$, we only need to take the inner product of $\langle \phi_1 |$ with $|\Psi(r, t)\rangle$. Thus,

$$c_1(t) = \langle \phi_1 | \Psi(r, t) \rangle \quad (1.23)$$

$$\text{and } c_1(t)^* = \langle \Psi(r, t) | \phi_1 \rangle \quad (1.24)$$

this allows us to write:

$$|c_1|^2 = \langle \phi_1 | \Psi(r, t) \rangle \langle \Psi(r, t) | \phi_1 \rangle \quad (1.25)$$

and following a similar procedure for $|c_2|^2$, we obtain:

$$|c_2|^2 = \langle \phi_2 | \Psi(r, t) \rangle \langle \Psi(r, t) | \phi_2 \rangle \quad (1.26)$$

Using expressions [1.20](#) to [1.26](#) is all that is needed to write a script and make animated plots of the probability ($|c_1|^2$ and $|c_2|^2$) that the system would be found in state $|\phi_1\rangle$ or $|\phi_2\rangle$ upon measurement. This is the point at which the original authors of the mathematica notebook stop, and also where I stop in [my python script](#). When we make these plots, we see that the probability oscillates with time forever (see the graph below)

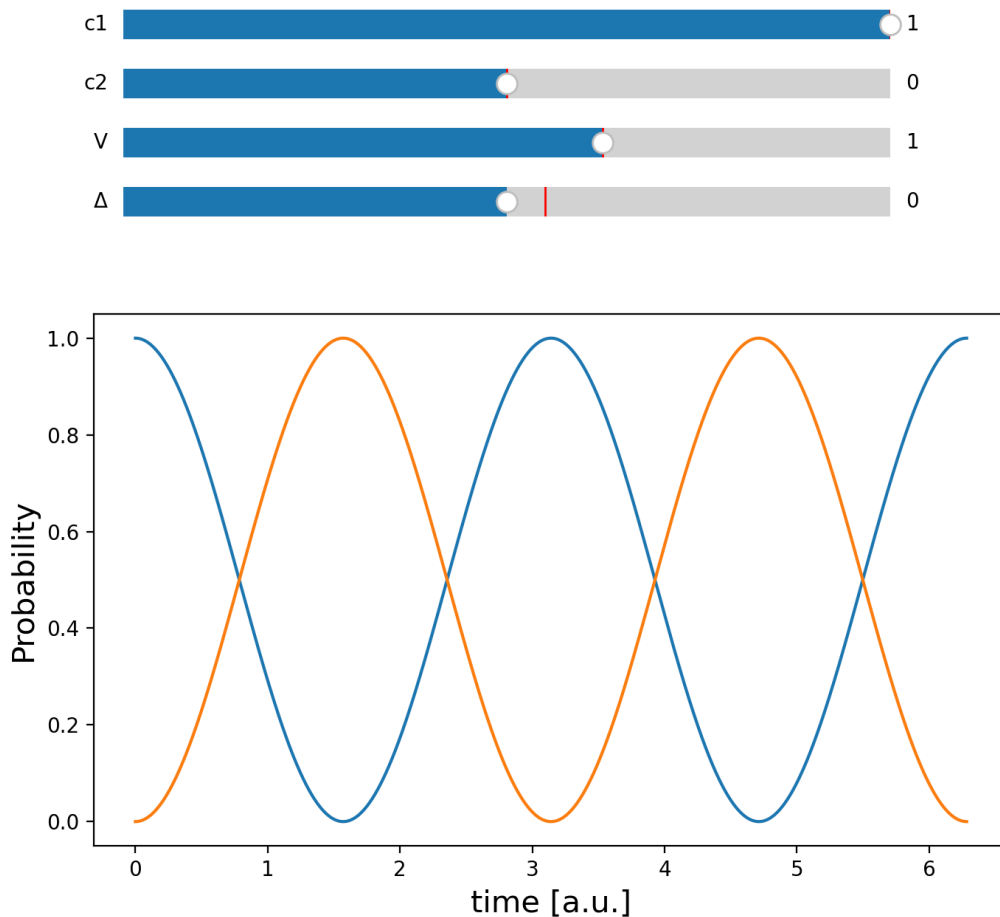


Figure 1. Oscillation of the probability of measuring the system in state 1 (blue) or 2 (orange) as a function of time

Although expressions [1.20](#) to [1.26](#) are sufficient to visualize the dynamics of such a system, I want to go further and go through diagonalizing the Hamiltonian in equation [1.11](#) and finding the corresponding eigenvectors, as this procedure teaches us a great deal about the physics of such a system. We will do this next.

2-level system with Eigenvectors and Eigenvalues (oscillations forever)

Part 2

We will consider a similar two-state system as above. But we will be interested first in the special case where the states are degenerate. This case means that:

$$H_0|\phi_1\rangle = E_0|\phi_1\rangle \text{ and } H_0|\phi_2\rangle = E_0|\phi_2\rangle \quad (2.1)$$

Now we introduce a real, time-independent coupling term $-V$ ($V > 0$), which as above couples the states to each other. The minus sign is chosen as a convention. The Hamiltonian for the system can thus be written as the Hermitian matrix:

$$H = \begin{pmatrix} E_0 & -V_{12} \\ -V_{21} & E_0 \end{pmatrix} \quad (2.2)$$

Note that for the hamiltonian to be Hermitian $V_{12} = V_{21}^*$ and since V is real, $V_{12} = V_{21}^* = V$. Diagonalizing this hamiltonian matrix, amounts to solving the equation:

$$(E_0 - \lambda)^2 = V^2 \quad (2.3)$$

$$\lambda_- = E_0 - V \text{ and } \lambda_+ = E_0 + V$$

setting $\lambda_- = E_-$ and $\lambda_+ = E_+$, we get:

$$E_- = E_0 - V \text{ and } E_+ = E_0 + V \quad (2.4)$$

Already from equation [2.4](#) we learn that the effect of the coupling term lifts the degeneracy of the system. Now, we obtain two states, that are indeed mixtures of the initial non-interacting states, that have energies below (E_-) and above (E_+) the energy of the non-interacting system. For a chemist, this picture is akin to constructing two new molecular orbitals from two initial atomic orbitals.

Now we ask, what combination of the basis states generates the state with energies E_- and E_+ . In order to answer this question, we need to find the eigenvectors and express them in the $\{|\phi\rangle\}$ basis.

Finding the $|\psi_-\rangle$ eigenvector:

$$H|\psi_-\rangle = E_-|\psi_-\rangle \quad (2.5)$$

since $|\psi_-\rangle$ can be written as a linear combination of $|\phi_1\rangle$ and $|\phi_2\rangle$, we can determine what the coefficients c_1 and c_2 need to be to satisfy eq. 2.5.

$$\begin{pmatrix} E_0 & -V \\ -V & E_0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = (E_0 - V) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad (2.6)$$

expanding gives:

$$c_1(E_0 - E_0 + V) - c_2V = 0 \quad (2.7)$$

$$c_1V = c_2V \Rightarrow c_1 = c_2 \quad (2.8)$$

if we choose $c_1 = 1 = c_2$, then we see that:

$$|\psi_-\rangle = \frac{1}{\sqrt{2}} (|\phi_1\rangle + |\phi_2\rangle) \quad (2.9)$$

where $\frac{1}{\sqrt{2}}$ is a normalization constant.

performing a similar procedure but with the other eigenvalue E_+ , we get:

$$|\psi_+\rangle = \frac{1}{\sqrt{2}} (|\phi_1\rangle - |\phi_2\rangle) \quad (2.10)$$

We see that the state $|\psi_-\rangle$ is the ground state of the system, and $|\psi_+\rangle$ the excited state, and that the energy needed to excite the system from the ground state to the excited state is given by:

$$\Delta E = 2V \quad (2.11)$$

Applications in Chemistry

Before looking at the analytical expression for time-evolution of this system, we should highlight that the concept discussed here is the one through which, the stabilization of certain chemical structures is understood. Indeed, in chemistry we usually speak of the

resonance stabilization of certain chemical structures like benzene for instance. In the figure 2 below, we show the two possible structures that one may draw on paper for benzene.

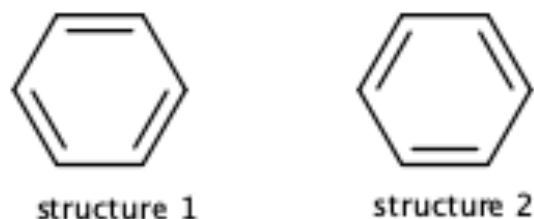


Figure 2. Structures that can be drawn for benzene molecule

These two structures correspond to two states, let's call them $|\phi_1\rangle$ and $|\phi_2\rangle$, for structures 1 and 2 respectively. Because of symmetry, the energies of the two states are the same, hence they are degenerate much like our example above. There exists a non-zero coupling energy between these two structures (off diagonal element V of the hamiltonian is different than zero). This coupling leads to a more stable structure of the benzene ground state, that is lower in energy (call it E_-) than that of the two isolated structure (E_0). To depict this stabilization, in chemistry, the two structures are usually drawn with two arrows pointing on opposite sides in between structures to signify that in the ground state, the molecule oscillates between structures 1 and 2, or simply by drawing one ring with dashed bonds or a circle in the center of the ring to depict that the electrons making up the bonds are moving around the ring (i.e. delocalization of electrons).

In the textbook by Cohen-Tannoudji, Diu and Laloë [1], they describe the benzene example, as well as that of molecule H_2^+ cation (and many other applications of this concept). Professor Barton Zwiebach from MIT also has a great explanation about this two-level system applied to the stabilization of the ammonia between it's two trigonal pyramidal shapes [2], as well as the application of the two-level system to electron spin states. These references are provided below.

Time Evolution of the Eigenstates

Now that we have obtained the eigenstates, we may want to understand how the system oscillates in time, and obtain expression for the probability of finding the system

in one of the non-interacting states. In order to achieve this, we will prepare the system in an initial state of our choice, and then apply the evolution operator onto the system.

Let us define our initial conditions, such that the system is in state $|\phi_1\rangle$ at $t = 0$. Thus we can write:

$$|\Psi_0\rangle = |\phi_1\rangle \quad (2.12)$$

from [2.9](#) and [2.10](#), we can write 2.12 as:

$$|\Psi_0\rangle = |\phi_1\rangle = \frac{1}{\sqrt{2}} (|\psi_+\rangle + |\psi_-\rangle) \quad (2.13)$$

Now we can apply our evolution operator onto the state $|\Psi_0\rangle$ to find $|\Psi_t\rangle$:

$$|\Psi_t\rangle = \frac{1}{\sqrt{2}} \left(\exp\left(\frac{-i(E_0 + V)t}{\hbar}\right) |\psi_+\rangle + \exp\left(\frac{-i(E_0 - V)t}{\hbar}\right) |\psi_-\rangle \right) \quad (2.14)$$

rewriting in the $\{\phi\}$ basis, we get:

$$|\Psi_t\rangle = \frac{1}{2} \exp\left(\frac{-iE_0t}{\hbar}\right) \left(\exp\left(\frac{-iVt}{\hbar}\right) (|\phi_1\rangle - |\phi_2\rangle) + \exp\left(\frac{iVt}{\hbar}\right) (|\phi_1\rangle + |\phi_2\rangle) \right) \quad (2.15)$$

We can simplify 2.15 using Euler's formula: $\exp(\pm i\theta) = \cos \theta \pm i \sin \theta$

hence:

$$|\Psi_t\rangle = \exp\left(\frac{-iE_0t}{\hbar}\right) \left(\cos\left(\frac{Vt}{\hbar}\right) |\phi_1\rangle + \sin\left(\frac{Vt}{\hbar}\right) |\phi_2\rangle \right) \quad (2.16)$$

2.16 gives us the time evolution of the wavefunction written in the $\{\phi\}$ basis. As we did above, we can determine the probability that the system would be found in state $|\phi_1\rangle$ upon measurement. We use the same method of shown in equation [1.25](#) and we obtain:

$$|c_1|^2 = \cos^2\left(\frac{Vt}{\hbar}\right) \quad (2.17)$$

and similarly:

$$|c_2|^2 = \sin^2 \left(\frac{Vt}{\hbar} \right) \quad (2.18)$$

We get, as we would have expected, that the probabilities of the system being found in state $|\phi_1\rangle$ or $|\phi_2\rangle$ oscillate with time. This result is identical to the one we obtain (seen in the [mathematica](#) or [python simulation](#)) without diagonalizing the hamiltonian. This fact should not be surprising as what we have done in parts 1 and 2 consists of two different ways of representing the same system, but the physics is the same. We do learn more about the system in part 2, however. For instance, we understand that the superposition of the stationary, non-interacting states give rise to two new states, in which, the lowest energy one help understand the increase in stability of certain species observed in nature. We also see that the oscillation of the probabilities depend on the strength of the coupling between the states.

We could have done these procedures for a non-degenerate system. In the non-degenerate case, we would have observed that $|c|^2$ depends on the coupling strength, and on the energy difference between the two non-interacting states. The procedures are the same, but the calculations are a bit more involved. The python script I have written, as well as the mathematica notebook from the original authors allow one to observe this effect by playing around with the values of the energy difference and the coupling strength. The references provided below (in particular that of Cohen-Tannoudji [1] and professor Tokmakoff [3]) provide an example. I will add a little bit of a mathematical background below, if the reader wishes to look at the references below and would like more help into understanding the mathematical manipulation done by the authors.

Mathematical Tools

Dirac Notation

Let \mathbf{v} be a 2-column vector with components a and b . It can be written as:

$$\mathbf{v} = \begin{pmatrix} a \\ b \end{pmatrix} \quad (3.1)$$

In Dirac notation, this vector is represented by a “ket” written:

$$|v\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \quad (3.2)$$

Let \mathbf{v}^\dagger be the conjugate transpose of \mathbf{v} , such that:

$$\mathbf{v}^\dagger = (a^* \ b^*) = \langle v| \quad (3.3)$$

a row vector, where $\langle v|$ in Dirac notation is known as a “bra”.

The inner product $\mathbf{v}^\dagger \mathbf{v}$ is define as:

$$(a^* \ b^*) \begin{pmatrix} a \\ b \end{pmatrix} = \langle v | v \rangle = a^2 + b^2 \quad (3.4)$$

where the inner product in Dirac notation, $\langle v | v \rangle$ is called a “braket”.

We can also write the outer product in Dirac notation. The outer product between two vectors \mathbf{v} and $\mathbf{w} = \begin{pmatrix} c \\ d \end{pmatrix}$ is a matrix and is defined as:

$$\mathbf{v} \otimes \mathbf{w} = \mathbf{v} \mathbf{w}^\dagger = |v\rangle \langle w|$$

$$\begin{pmatrix} a \\ b \end{pmatrix} (c^* \ d^*) = \begin{pmatrix} ac^* & ad^* \\ bc^* & bd^* \end{pmatrix} \quad (3.5)$$

Exponential of a Matrix

The matrix exponentials, such as the one we encountered in [1.12](#) can best be understood by using the Taylor expansion of the exponential function. The Taylor expansion of the exponential function is given by:

$$\exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \frac{x^5}{5!} + \dots \quad (3.6)$$

As a result, if the argument of the function is a matrix \mathbf{H} , then we can write:

$$\exp(\mathbf{H}) = 1 + \mathbf{H} + \frac{\mathbf{H}^2}{2!} + \frac{\mathbf{H}^3}{3!} + \frac{\mathbf{H}^4}{4!} + \frac{\mathbf{H}^5}{5!} + \dots \quad (3.7)$$

$$\exp(\mathbf{H}) = \sum_{n=0}^{\infty} \frac{\mathbf{H}^n}{n!}$$

Let us take the example of the unitary operator obtained in [1.19](#). Suppose that we have a wavefunction $|\psi_1\rangle$ that is an eigenfunction of a Hamiltonian H , such as $H|\psi_1\rangle = E_1|\psi_1\rangle$. Applying the evolution operator of [1.19](#) to this wavefunction gives:

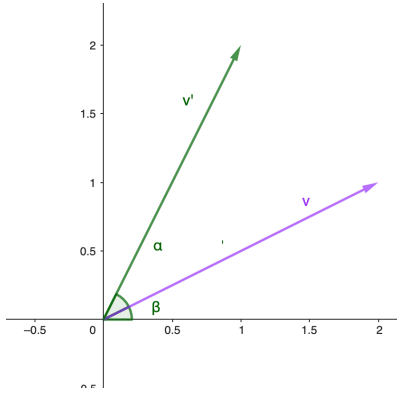
$$\hat{U}(t)|\psi_1\rangle = \exp\left(\frac{-i}{\hbar}Ht\right)|\psi_1\rangle \quad (3.8)$$

since $|\psi_1\rangle$ is an eigenstate of H , we can use equation 3.7 to show that the expansion in H applied to $|\psi_1\rangle$, is the same as an expansion in E_1 multiplied by $|\psi_1\rangle$, which is again the exponential function with E_1 instead of H . Hence, we can rewrite 3.8 as:

$$\hat{U}(t)|\psi_1\rangle = \exp\left(\frac{-i}{\hbar}E_1t\right)|\psi_1\rangle \quad (3.9)$$

What we have done in going from 3.8 to 3.9 is the same procedure that allowed us to obtain the expression in [2.14](#).

General Consideration of Orthogonal/Unitary Matrices



Suppose you have a vector $|v\rangle = \begin{pmatrix} v_x \\ v_y \end{pmatrix}$ in 2-D real space.

The norm squared of the vector is $\langle v | v \rangle = v_x^2 + v_y^2$. Suppose that we want to rotate the vector by an angle α , without parity inversion (i.e without rotating our coordinate axes, but only rotating the vector by α). We can call $|v'\rangle = \begin{pmatrix} v'_x \\ v'_y \end{pmatrix}$ our vector

after rotation, with norm equal to that of $|v\rangle$. Using trigonometry we could express the components of two vectors as:

$$\begin{aligned} v_x &= v \cos \beta \\ v_y &= v \sin \beta \end{aligned} \quad (3.10)$$

and,

$$\begin{aligned} v'_x &= v \cos (\beta + \alpha) \\ v'_y &= v \sin (\beta + \alpha) \end{aligned} \quad (3.11)$$

using trigonometric identities and 3.10, we find that we can rewrite 3.11 as:

$$\begin{aligned} v'_x &= v_x \cos \alpha - v_y \sin \alpha \\ v'_y &= v_y \sin \alpha + v_x \cos \alpha \end{aligned} \quad (3.12)$$

in matrix form, we obtain:

$$\begin{pmatrix} v'_x \\ v'_y \end{pmatrix} = \begin{bmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{bmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix} \quad (3.13)$$

the matrix in 3.13 is a rotation matrix, and acts on $|v\rangle$ to produce $|v'\rangle$, such that, if we denote the matrix by \mathbf{O} , we can write:

$$|v'\rangle = \mathbf{O} |v\rangle \quad (3.14)$$

Important properties of \mathbf{O}

Notice that the determinant of \mathbf{O} is equal to 1. The class of rotation matrices that have their determinant equal to 1, rotate vectors without parity inversion. This class of rotation matrix are usually qualified by the word *special*. In addition, notice how, when we multiply \mathbf{O} by its transpose \mathbf{O}^T , we obtain the identity matrix: $\mathbf{O}^T \mathbf{O} = \mathbf{O} \mathbf{O}^T = \mathbf{1}$. For this reason, \mathbf{O} is said to be an orthogonal matrix. The important consequence of the matrix being orthogonal is that it preserves the length of the vector upon rotation. Indeed:

$$\begin{aligned} |v'\rangle &= \mathbf{O} |v\rangle & (3.15) \\ \langle v' | v' \rangle &= \langle v | \mathbf{O}^T \mathbf{O} | v \rangle \\ \langle v' | v' \rangle &= \langle v | \mathbf{1} | v \rangle = \langle v | v \rangle \end{aligned}$$

The group of 2×2 orthogonal rotation matrices with unit determinant are called *special orthogonal 2×2 matrices* and form the group called $SO(2)$. Applying the same procedures to vectors in 3-D real space, allows us to obtain a 3×3 rotation matrix, that is part of the group $SO(3)$.

What good is this? Well, one thing the transformation in [3.14](#) allowed us to do, was to obtain a “different” vector $|v'\rangle$ from our initial vector $|v\rangle$ simply by rotating it. But if what we are ultimately interested in is the norm of the vector, then $|v'\rangle$ and $|v\rangle$ represent the same object (i.e. by symmetry), only expressed in different basis vectors (v_x, v_y) for $|v\rangle$ and (v'_x, v'_y) for $|v'\rangle$. In quantum mechanics, where the norm of the wavefunction is extremely important for describing the system, such a procedure as what we have just seen, can be important to obtain a wavefunction in different representations that, for instance may make computation more tractable, or help us gain insight into the physics of the system we seek to describe that would not have been obvious in a different representation (as we have seen for instance in [part 2](#)). The main consideration is that state vectors (wavefunctions) in quantum mechanics exist in a complex vector space known as Hilbert space. Hence the rotation matrices in that space are slightly different than what we obtained for \mathbf{O} .

Reference:

- 1) Cohen-Tannoudji, C.; Diu, B.; Lalöe, F., Quantum Mechanics. Wiley-Interscience: Paris, 1977; pp. 405-420
- 2) http://ocw2.mit.edu/courses/physics/8-05-quantum-physics-ii-fall-2013/lecture-notes/MIT8_05F13_Chap_07.pdf
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