4. Two-level systems

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4.1 Generalities

We have already seen some examples of systems described by two possible states. A neutron in an interferometer, taking either the upper or lower path. A photon linearly polarized either horizontally or vertically. A two level system (TLS) is the simplest system in quantum mechanics, but it already illustrates many characteristics of QM and it describes as well many physical systems. It is common to reduce or map quantum problems onto a TLS. We pick the most important states -the ones we care about– and then discard the remaining degrees of freedom, or incorporate them as a collection or continuum of other degrees of freedom termed a bath.

In a more abstract way, we can think of a TLS as carrying a binary information (the absence or presence of something, the information about a position, such as left or right, or up or down, etc.). Thus a TLS can be thought as containing a bit of information. By analogy with classical computers and information theory, TLS are thus called *qubits*. Their basis states are usually defined as $|0\rangle$ and $|1\rangle$ with a vector representation:

$$|0\rangle = \begin{bmatrix} 1\\0 \end{bmatrix}, \ |1\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$$

A general state is then $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$. If it is normalized we have $|\alpha|^2 + |\beta|^2 = 1$. Then, this state can also be written quite generally in terms of the two angles ϑ and φ :

$$|\psi\rangle = \cos(\vartheta/2)|0\rangle + e^{i\varphi}\sin(\vartheta/2)|1\rangle$$

For this state, the probability of finding the system in the 0[1] state is $\cos^2(\theta/2) [\sin^2(\theta/2)]$. Notice that I could have written the state also as

$$|\psi\rangle \equiv |\phi\rangle = e^{-i\phi/2}\cos(\vartheta/2)|0\rangle + e^{i\phi/2}\sin(\theta/2)|1\rangle$$

The two states are in fact equivalent up to a *global* phase factor. While relative phase factors (in a superposition) are very important, global phases are irrelevant, since they yield the same results in a measurement outcome.

? Question: Show that a global phase factor does not change measurement outcomes and measurement statistics.

1.(Measurement outcome) As the possible measurement outcomes are the eigenvalues of the measurement operators, the first is trivially true.

2.(Statistics) Let's consider an observable A with eigenvectors $|a\rangle = a_0|0\rangle + a_1|1\rangle$ corresponding to the eigenvalues a, then the probability of obtaining a from the measurement is $p(a) = ||\langle \psi | a \rangle||^2 = |a_0 \cos(\theta/2) + a_1 e^{i\phi} \sin(\theta/2)|^2 = ||\langle \varphi | a \rangle||^2 = |a_0 e^{-i\phi/2} \cos\theta/2 + a_1 e^{i\phi/2} \sin\theta/2|^2$.

Consider for example $|a\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. Then we obtain $p(a) = \frac{1}{2}(1 + \cos\varphi \sin\vartheta)$. Thus the *relative* phase of $|0\rangle$ w.r.t. $|1\rangle$ is important. But a global phase multiplying the state is not.



Image by MIT OpenCourseWare.

Fig. 2: Bloch sphere representation of a qubit (TLS) [From wikipedia]

Describing a TLS via the two angles θ and ϕ leads to a simple geometrical picture for the space occupied by this system. The angles define a point on a sphere of radius 1, which is called **Bloch sphere**. The TLS can then assume any of the points on the surface of the sphere via a unitary transformation (in the following, we will also interested in the points *inside* the sphere, as well as means to reach them). The unitary evolution for this particular system can then be described as *rotations* of the state vector in the sphere.

Using the example of a TLS we are thus going to introduce the concept of rotation and angular momentum, which can be generalized also to larger systems.

4.2 Rotations and angular momentum

4.2.1 Classical rotations

Let's review rotation in classical mechanics (geometry). The first property that we want to analyze is the fact that successive rotations about different axes do not commute. Consider for example to start with a vector aligned along the z axis and then effectuate two rotations, one about the y axis and one about the z axis. Depending on the order, we obtain a rotation or no rotation at all.

Rotation are represented in 3D by orthogonal 3×3 matrices. (an *orthogonal* matrix is such that $RR^T = R^T R = 1$. In particular, rotations about the 3 axes are as follow:

$$R_x(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\phi) & -\sin(\phi) \\ 0 & \sin(\phi) & \cos(\phi) \end{pmatrix}$$
$$R_y(\phi) = \begin{pmatrix} \cos(\phi) & 0 & \sin(\phi) \\ 0 & 1 & 0 \\ -\sin(\phi) & 0 & \cos(\phi) \end{pmatrix}$$
$$R_z(\phi) = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

It is easy then to show that $R_{\alpha}(\vartheta)R_{\beta}(\varphi) \neq R_{\beta}(\varphi)R_{\alpha}(\vartheta)$ unless $\alpha = \beta$. What about if the rotation angles are very small? We might expect then that the order matters less. We thus consider infinitesimal rotations, where $\phi = \epsilon \rightarrow 0$:

$$R_x(\epsilon) \approx \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 - \frac{\epsilon^2}{2} & -\epsilon \\ 0 & \epsilon & 1 - \frac{\epsilon^2}{2} \end{pmatrix}$$
$$R_y(\epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & 0 & \epsilon \\ 0 & 1 & 0 \\ -\epsilon & 0 & 1 - \frac{\epsilon^2}{2} \end{pmatrix}$$
$$R_z(\epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & -\epsilon & 0 \\ \epsilon & 1 - \frac{\epsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

If we then calculate for example $R_x(\epsilon)R_y(\epsilon) - R_y(\epsilon)R_x(\epsilon)$ we obtain:

$$R_x(\epsilon)R_y(\epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & 0 & \epsilon \\ \epsilon^2 & 1 - \frac{\epsilon^2}{2} & -\epsilon \left(1 - \frac{\epsilon^2}{2}\right) \\ -\epsilon \left(1 - \frac{\epsilon^2}{2}\right) & \epsilon & \left(1 - \frac{\epsilon^2}{2}\right)^2 \end{pmatrix}$$
$$R_y(\epsilon)R_x(\epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & \epsilon^2 & \epsilon - \frac{\epsilon^3}{2} \\ 0 & 1 - \frac{\epsilon^2}{2} & -\epsilon \\ -\epsilon & \epsilon - \frac{\epsilon^3}{2} & \left(1 - \frac{\epsilon^2}{2}\right)^2 \end{pmatrix}$$

and

$$R_x(\epsilon)R_y(\epsilon) - R_y(\epsilon)R_x(\epsilon) = \begin{pmatrix} 0 & -\epsilon^2 & \frac{\epsilon^3}{2} \\ \epsilon^2 & 0 & \frac{\epsilon^3}{2} \\ \frac{\epsilon^3}{2} & \frac{\epsilon^3}{2} & 0 \end{pmatrix}$$

Thus we see that

1. If we ignored terms $\propto \epsilon^2$ and higher, the rotations do commute.

2. At the second order in ϵ we can write the result as $R_x(\epsilon)R_y(\epsilon) - R_y(\epsilon)R_x(\epsilon) = R_z(\epsilon^2) - \mathbb{1}$. This result stands also for cyclic permutations of the subscripts. These commutation relationships are a guide in finding commutation relationships that the equivalent QM rotation operators should obey.

4.2.2 QM angular momentum as generator of rotations

In QM we can as well define rotations, as we already did for classical mechanics. Although we will first study examples for TLS, rotations can be defined for any system (even higher dimensional systems). Generally, a rotation will be represented by an operator $\mathcal{D}(R_{\alpha}(\phi))$ associated to a classical rotation $R_{\alpha}(\phi)$. We first define the action of an infinitesimal rotation. To do so we define the angular momentum operator **J** in terms of the infinitesimal rotation :

$$\mathcal{D}(R_{\mathbf{n}}(\delta\phi)) = \mathbb{1} - i\delta\phi\vec{J}\cdot\vec{n}$$

where \vec{n} is a unit vector. A finite rotation can be found by repeating many infinitesimal rotations. For example, for a rotation about z:

$$\mathcal{D}(R_z(\varphi)) = \lim_{N \to \infty} \left[\mathbb{1} - iJ_z \frac{\varphi}{N} \right]^N = \mathbb{1} - iJ_z \varphi - \frac{1}{2}J_z^2 \varphi^2 \dots = \exp\left(-iJ_z \varphi\right)$$

(Note that here again I took $\hbar = 1$.) The angular momentum can thus be considered as the generator of rotations.

A. Rotations properties

- Identity: $\exists 1 : 1\mathcal{D} = \mathcal{D}1 = \mathcal{D}$
- Closure: $\mathcal{D}_1\mathcal{D}_2$ is also a rotation \mathcal{D}_3 .
- Inverse: \exists and inverse such that $\mathcal{D}\mathcal{D}^{-1} = \mathbb{1}$
- Associativity $(\mathcal{D}_1\mathcal{D}_2)\mathcal{D}_3 = \mathcal{D}_1(\mathcal{D}_2\mathcal{D}_3)$

B. Commutation

In analogy with the classical case, we can write the commutation for the infinitesimal rotations:

$$\mathcal{D}_x(\epsilon)\mathcal{D}_y(\epsilon) - \mathcal{D}_y(\epsilon)\mathcal{D}_x(\epsilon)$$

$$=(\mathbb{1} - iJ_x\epsilon - \frac{1}{2}J_x^2\epsilon^2)(\mathbb{1} - iJ_y\epsilon - \frac{1}{2}J_y^2\epsilon^2) - (\mathbb{1} - iJ_y\epsilon - \frac{1}{2}J_y^2\epsilon^2)(\mathbb{1} - iJ_x\epsilon - \frac{1}{2}J_x^2\epsilon^2) = -(J_xJ_y - J_yJ_x)\epsilon^2 + O(\epsilon^3)$$

and equate this to $\mathcal{D}_z(\epsilon^2) - \mathbb{1} = -iJ_z\epsilon^2$. With this analogy we justify the definition of angular momentum operators as operators that generate the rotations and obey the commutation relationships:

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$$

C. Spin- $\frac{1}{2}$

Although angular momentum operators have some classical analogy, they are more general, as they describe for example physical properties that have no classical counterparts, such as the spin. In particular, the lowest dimension in which the commutation relationships above hold is 2. The angular momentum \mathbf{S} for a TLS is represented by the operators:

$$S_x = \frac{1}{2}\sigma_x = \frac{1}{2}(|0\rangle\langle 1| + |1\rangle\langle 0|)$$

$$S_y = \frac{1}{2}\sigma_y = \frac{i}{2}(|0\rangle\langle 1| - |1\rangle\langle 0|)$$

$$S_z = \frac{1}{2}\sigma_z = \frac{1}{2}(|0\rangle\langle 0| - |1\rangle\langle 1|)$$

where $\{\sigma_x, \sigma_y, \sigma_z\}$ are called Pauli operators or Pauli matrices. The Pauli matrices have the following properties:

- 1. $\sigma_{\alpha}^2 = 1$
- 2. $\sigma_i \sigma_j + \sigma_j \sigma_i = 0$, that is, they anticommute.
- 3. $\sigma_i \sigma_j = -\sigma_j \sigma_i = i\sigma_k$ (from the previous property)
- 4. Hermiticity: $\sigma_i^{\dagger} = \sigma_i$
- 5. Zero trace: $\operatorname{Tr} \{ \sigma_i \} = 0$
- 6. Determinant $det(\sigma_i) = -1$.

? Question: Show that S satisfies the commutation relationship.

1. Show it by multiplying the operators.

2. Write down the matrix form and perform matrix multiplications.

We can now check what is the action of the spin operators on the TLS state vector $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$:

$$\sigma_{x}|\psi\rangle = \alpha|1\rangle + \beta|0\rangle$$

$$\sigma_{y}|\psi\rangle = i\alpha|1\rangle - i\beta|0\rangle$$

$$\sigma_{z}|\psi\rangle = \alpha|0\rangle - \beta|1\rangle$$

in particular, σ_x swap the two components (spin flip) and σ_z invert the sign of the $|1\rangle$ component (phase shift), while σ_y does both.

D. Spin- $\frac{1}{2}$ rotations

We can now look at rotations of spin- $\frac{1}{2}$. In particular we want to calculate $\mathcal{D}_{\alpha}(\varphi) = e^{-iS_{\alpha}\varphi}$. For this we remember the property: $\sigma_{\alpha}^2 = \mathbb{1}$. With this, and using a Taylor expansion it is easy to show that we have

$$e^{-iS_{\alpha}\varphi} = \cos\left(\varphi/2\right)\mathbb{1} - i\sin\left(\varphi/2\right)S_{\alpha}$$

? Question: Calculate the exponential. From $(\sigma \cdot n)^2 = (\sigma_x n_x + \sigma_y n_y + \sigma_z n_z)^2 = \sigma_x^2 n_x^2 + n_x n_y (\sigma_x \sigma_y + \sigma_y \sigma_x) + \dots + n_y^2 \mathbb{1} + n_z^2 \mathbb{1} = \mathbb{1}$ and the Taylor expansion we obtain $e^{-i\varphi\sigma \cdot n} = \mathbb{1} \sum_{n \text{ even}} (-i\varphi)^n / n! + \sigma \cdot n \sum_{n \text{ odd}} (-i\varphi)^n / n! = \mathbb{1} \cos \varphi + \sigma \cdot n \sin \varphi.$

4.2.3 Example of Two-Level System: Neutron Interferometry

Now we can revisit the TLS examples we have seen earlier. In particular we notice that the polarization rotator is represented by rotation operators, in particular rotations around the x-axis $e^{-i\theta S_x}$.

Consider another very simple system, a neutron interferometer, such as the Mach-Zehnder interferometer.



Fig. 3: Neutron Interferometer

We send in a beam of neutrons. The first beamsplitter divides the neutron flux into two parts, that will go into the upper arm or the lower arm. Thus the state of the system is at this point in time

$$|\psi\rangle_1 = \alpha |U\rangle + \beta |L\rangle, \ \alpha^2 + \beta^2 = 1$$

We assume that the flux of neutrons is so low (neutrons can be very slow) so that only one neutron is present at any time inside the interferometer. The lower and upper beams are then reflected at the mirrors and recombined at the second beam splitter, after which the neutron flux is measured at one arm. If we assume that both beamsplitter works in the same way, delivering an equal flux to each arm (that is, the transmission and reflection are the same), then we have $|\psi\rangle_1 = (|U\rangle + |L\rangle)/\sqrt{2}$ and $|\psi\rangle_2 = |U\rangle$.

? Question: What is the propagator describing the action of the Beamsplitter? $U_{BS}|U\rangle = (|U\rangle + |L\rangle)/\sqrt{2}$ and we also know that $U_{BS}(|U\rangle + |L\rangle)/\sqrt{2} = |U\rangle$. We can verify that

$$U_{BS} = \frac{1}{\sqrt{2}} \left(\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right)$$

performs as we want. In particular, notice that $U_{BS}U_{BS} = 1$.

Thus, if our observable is the number of neutron in the upper arm, the measurement always returns 1 with certainty (probability =1).

Let's now consider the case in which we want to measure at point 1 how many neutrons are in the upper arm. The observable is just the projector onto the upper arm $Ob = P_U = |U\rangle \langle U|$ and we will detect one neutron (or zero neutrons) with probability $\frac{1}{2}$. In fact $p(U) = ||\langle \psi | U \rangle||^2 = \frac{1}{2}$. Also, the average value of the number of neutron in the upper arm is 1/2 as well, since

 $\langle Ob \rangle = |\langle \psi | P_U | \psi \rangle| = \frac{1}{2}$ After the measurement, the state is projected onto the upper arm, if we did detect a photon, or the lower arm, otherwise. We assume that the neutron is free to continue on its path after the measurement and we perform a second measurement after the second beamsplitter.

? Question: What is the probability of measuring 1 neutron in the upper part in this case? Now the state at 2 is $|\psi\rangle_2 = (|U\rangle \pm |L\rangle)/\sqrt{2}$, hence $p(U) = \langle \psi | U \rangle = \frac{1}{2}$.

4.2.4 Spinor behavior

By calculating $e^{-iS_{\alpha}\varphi}S_{\beta}e^{iS_{\alpha}\varphi}$ we see that the rotations of the operator give the following result:

$$S_x \xrightarrow{S_z} S_x \cos(\varphi) - S_y \sin(\varphi),$$
$$S_y \xrightarrow{S_z} S_y \cos(\varphi) + S_x \sin(\varphi),$$
$$S_z \xrightarrow{S_z} S_z$$

These are the same rotation rules we would have expected classically. In particular, taking the expectation values, we see that they correspond exactly to the rotations in 3D of a vector, with a periodicity of 2π . Things are a bit different (and more surprising) if we consider instead the state rotation. Consider the rotation of the state $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ with respect to S_z :

$$e^{-iJ_z\varphi}|\psi\rangle = e^{-i\varphi/2}\alpha|0\rangle + e^{i\varphi/2}\beta|1\rangle,$$

now the angle of rotation seems to be $\varphi/2$. This has an interesting consequence: if we rotate by $\varphi = 2\pi$ instead of returning to the initial state, as we would have expected, we obtain $e^{-iJ_z 2\pi}|\psi\rangle = -|\psi\rangle$. This is the so-called **spinor** behavior. Notice that from a simple measurement this minus sign (which is equivalent to a *global* phase) is irrelevant, hence we obtain the same expectation values for the angular momenta as before. We will see in P-Set on that experiments can be devised to show the spinor behavior (but they need to use more than one spin).

4.2.5 The SU(2) and SO(3) groups

A group G is a finite or infinite set of elements together with a binary operation (called the group operation) that together satisfy the four fundamental properties of closure, associativity, the identity property, and the inverse property. A rotation group is a group in which the elements are orthogonal matrices with determinant 1. In the case of three-dimensional space, the rotation group is known as the special orthogonal group or SO(3)⁹. The special unitary group SU(2) is the set of 2 by 2 unitary matrices with determinant +1 [it is a subgroup of the unitary group U(2)]. The two groups SO(3) and SU(2) both represent rotations, however there is a one-to-two correspondence for a given $R \in SO(3)$ there are 2 $U \in SU(2)$. This is because a 2π and 4π rotations are the same in SO(3) but they are 1 and -1 in SU(2).

⁹ For a more rigorous and extensive explanation see J.J. Sakurai "Modern Quantum Mechanics", Addison-Wesley (1994), page 168

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