

Notes of Quantum Mechanics

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Preface

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1.1 Introduction

We know the important role of angular momentum in classical mechanics; the total angular momentum of an isolated physical system is a **constant of motion**, even in some non-isolated systems. In other cases, when point particle is moving in a central potential (radial dependence only), the force on the particle is always directed towards the origin of the potential. Its moment with respect to this origin is zero, and the angular momentum theorem implies that:

$$\partial_t \mathcal{L} = 0.$$

The motion of the particle is therefore limited to a fixed plane, and satisfies the law of constant areas (Kepler's second law). All these properties have their equivalences in quantum mechanics.

With an angular momentum \mathcal{L} of a classical system is associated an observable \mathbf{L} , actually a set of three observables L_x, L_y, L_z , which correspond to the three components of \mathcal{L} in a Cartesian frame. We must also introduce typically quantum mechanical angular momenta, which have no classical equivalents.

We shall denote:

- **Orbital angular momentum** \mathbf{L} is any angular momentum that has a classical equivalent.
- **Spin angular momentum** \mathbf{S} is any intrinsic angular momentum of an elementary particle.
- **Total angular momentum** \mathbf{J} is the sum of \mathbf{L} and \mathbf{S} . We also used to refer to any angular momentum without specifying the type.

We will establish the general quantum mechanical properties associated with all AM, whatever their nature. These properties follow from the commutation relations satisfied by the three observables J_x, J_y, J_z , the components of an arbitrary AM \mathbf{J} . The origin of these commutation relations is the consequences of the quantization rules and the canonical relations.

1.2 Commutation relations characteristic of angular momentum

1.2.1 Orbital angular momentum

From the classical counterpart of a spinless particle with \mathcal{L} , we apply the quantization rules to get the equivalent relation in the observables in the quantum mechanics framework.

For instance,

$$\mathcal{L}_x = yp_z - zp_y \xrightarrow{\text{Quantization rules}} L_x = YP_z - ZP_y.$$

Then, in general we will have:

$$\mathbf{L} = \mathbf{R} \times \mathbf{P}. \quad (1.1)$$

Since we know the canonical relation for \mathbf{R}, \mathbf{P} , we can easily calculate the commutators of the operators L_x, L_y, L_z . For instance,

$$\begin{aligned} [L_x, L_y] &= [YP_z - ZP_y, ZP_x - XP_z] = [YP_z, ZP_x] + [ZP_y, XP_z] \\ &= Y[P_z, Z]P_x + X[Z, P_z]P_y = -i\hbar YP_x + i\hbar XP_y \\ [L_x, L_y] &= i\hbar L_z. \end{aligned}$$

Then, for the other cases we have the following commutation relations:

$$\text{Commutation relations for } \mathbf{L} \quad [L_x, L_y] = i\hbar L_z, [L_y, L_z] = i\hbar L_x, [L_z, L_x] = i\hbar L_y. \quad (1.2)$$

This result can be generalized to a system of N spinless particles. The total AM of such a system is, in quantum mechanics,

$$\text{AM in a system of } N \text{ spinless particles} \quad \mathbf{L} = \sum_{i=1}^N \mathbf{L}_i, \quad \mathbf{L}_i = \mathbf{R}_i \times \mathbf{P}_i. \quad (1.3)$$

Each of the individual AM \mathbf{L}_i satisfies the commutation relations (1.2) and commutes with \mathbf{L}_j when $j \neq i$ (state spaces of different particles).

1.2.2 Definition of angular momentum

The origin of these relations (1.2) lies in the geometric properties of rotations in three-dimensional space. This is why we shall adopt a more general point of view and define an angular momentum \mathbf{J} as any set of three observables J_x, J_y, J_z that satisfies

$$\text{Commutation relations for } \mathbf{J} \quad [J_x, J_y] = i\hbar J_z, [J_y, J_z] = i\hbar J_x, [J_z, J_x] = i\hbar J_y. \quad (1.4)$$

We then introduce the operator:

$$\text{Magnitude of } \mathbf{J} \quad \mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2 \quad (1.5)$$

the (scalar) square of the angular momentum \mathbf{J} . This operator is Hermitian, since the components are Hermitian. Moreover, \mathbf{J}^2 commutes with the these componentes:

$$[\mathbf{J}^2, \mathbf{J}] = \mathbf{0}. \quad (1.6)$$

For instance, for J_x :

$$\begin{aligned} [\mathbf{J}^2, J_x] &= [J_x^2 + J_y^2 + J_z^2, J_x] \\ &= [J_y^2, J_x] + [J_z^2, J_x] \\ &= J_y[J_y, J_x] + [J_y, J_x]J_y + J_z[J_z, J_x] + [J_z, J_x]J_z \\ &= -i\hbar J_y J_z - i\hbar J_z J_y + i\hbar J_z J_y + i\hbar J_y J_z \\ [\mathbf{J}^2, J_x] &= 0. \end{aligned}$$

AM theory in QM is founded **entirely** on the commutation relations (1.4). These relations imply that it is impossible to measure simultaneously the three components of an angular momentum; however, \mathbf{J}^2 and any component of \mathbf{J} are compatible.

1.2.3 Statement of the problem

In general, we must pick only a few of operators that forms the CSCO with the Hamiltonian as the components of an arbitrary AM \mathbf{J} do not commute; they are not simultaneously diagonalizable. We shall therefore seek the system of eigenvectors common to \mathbf{J}^2 and J_z .

1.3 General theory of angular momentum

We will determine the spectrum of \mathbf{J}^2 and J_z for the general case and study their common eigenvectors.

1.3.1 Definitions and notation

The J_+ and J_- operators

It is more convenient to introduce the ladder operators for J to use in favor of J_x and J_y :

$$\text{Ladder operators} \quad \begin{aligned} J_+ &= J_x + iJ_y \\ J_- &= J_x - iJ_y \end{aligned} \longleftrightarrow \begin{aligned} J_x &= \frac{1}{2}(J_+ + J_-) \\ J_y &= -\frac{i}{2}(J_+ - J_-) \end{aligned} . \quad (1.7)$$

They are not Hermitian; they are adjoints of each other. We will use the following operators: J_+ , J_- , J_z , \mathbf{J}^2 . These operators satisfy the commutation relation:

$$[J_z, J_+] = \hbar J_+, \quad [J_z, J_-] = -\hbar J_-, \quad [J_+, J_-] = 2\hbar J_z, \quad [\mathbf{J}^2, J_+] = [\mathbf{J}^2, J_-] = [\mathbf{J}^2, J_z] = 0. \quad (1.8)$$

Using (1.5) and the above relations, we can express \mathbf{J}^2 in the following form:

$$\mathbf{J}^2 = \frac{1}{2}(J_+ J_- + J_- J_+) + J_z^2.$$

Notation for the eigenvalues of \mathbf{J}^2 and J_z

According to (1.5), \mathbf{J}^2 is the sum of the squares of three Hermitian operators. Consequently, for any ket $|\psi\rangle$, the matrix element $\langle\psi|\mathbf{J}^2|\psi\rangle$ is positive or zero:

$$\langle\psi|\mathbf{J}^2|\psi\rangle = \langle\psi|J_x^2|\psi\rangle + \langle\psi|J_y^2|\psi\rangle + \langle\psi|J_z^2|\psi\rangle = \|J_x|\psi\rangle\|^2 + \|J_y|\psi\rangle\|^2 + \|J_z|\psi\rangle\|^2 \geq 0.$$

This implies that all the eigenvalues of \mathbf{J}^2 are positive or zero. We shall write the eigenvalues of \mathbf{J}^2 in the form $j(j+1)\hbar^2$, with $j \geq 0$, so that they have dimensions of \hbar^2 and the $j(j+1)$ is a dimensionless number. As for the eigenvalues of J_z , which have the same dimensions as \hbar , they are traditionally written as $m\hbar$, with m a dimensionless number.

Eigenequations for \mathbf{J}^2 and J_z

We shall label the eigenvector common to \mathbf{J}^2 and J_z by the indices j and m . However, as they don't constitute a CSCO, it is necessary to introduce a third index k in order to distinguish between the different eigenvectors corresponding to the same eigenvalues $j(j+1)\hbar^2$ and $m\hbar$ of \mathbf{J}^2 and J_z .

We shall therefore try to solve the simultaneously eigenequations:

$$\mathbf{J}^2|k, j, m\rangle = j(j+1)\hbar^2|k, j, m\rangle, \quad \text{and} \quad J_z|k, j, m\rangle = m\hbar|k, j, m\rangle. \quad (1.9)$$

1.3.2 Eigenvalues of \mathbf{J}^2 and J_z

We will prove three lemmas (as in the QHO) which will enable us to determine the spectrum of \mathbf{J}^2 and J_z .

Lemmas

a) **Properties of the eigenvalues of \mathbf{J}^2 and J_z**

If $j(j+1)\hbar^2$ and $m\hbar$ are the eigenvalues of \mathbf{J}^2 and J_z associated with the same eigenvector $|k, j, m\rangle$, then j and m satisfy the inequality:

$$-j \leq m \leq j. \quad (1.10)$$

b) **Properties of the vector $J_-|k, j, m\rangle$**

Let $|k, j, m\rangle$ be an eigenvector of \mathbf{J}^2 and J_z with the eigenvalues $j(j+1)\hbar^2$ and $m\hbar$.

i) $m = -j \implies J_-|k, j, -j\rangle = 0$.

ii) If $m > -j$, $J_-|k, j, m\rangle$ is a non-null eigenvector of \mathbf{J}^2 and J_z with the eigenvalues $j(j+1)\hbar^2$ and $(m-1)\hbar$.

c) **Properties of the vector $J_+|k, j, m\rangle$**

Let $|k, j, m\rangle$ be an eigenvector of \mathbf{J}^2 and J_z with the eigenvalues $j(j+1)\hbar^2$ and $m\hbar$.

i) $m = j \implies J_+|k, j, j\rangle = 0$.

ii) If $m < j$, $J_+|k, j, m\rangle$ is a non-null eigenvector of \mathbf{J}^2 and J_z with the eigenvalues $j(j+1)\hbar^2$ and $(m+1)\hbar$.

Determination of the spectrum of \mathbf{J}^2 and J_z

We shall show that the three lemmas above enable us to determine the possible values of j and m . The prove will be performed under iteration and is skipped.

Domain of the indices j, m

Let \mathbf{J} be an arbitrary AM, obeying the commutation relations (1.4). If $j(j+1)\hbar^2$ and $m\hbar$ denote the eigenvalues of \mathbf{J}^2 and J_z , then:

- The only possible values for j are positive integers or half-integers or zero: $0, 1/2, 1, 3/2, 2, 5/2, \dots$.
- For a fixed j , the only values possible for m are the $(2j+1)$ numbers: $-j, -j+1, \dots, j-1, j$.

Therefore, for a fixed j , the discretely indexed orthonormal basis $\{|j, m\rangle\}$ spans the $(2j+1)$ -dimensional state space \mathcal{E}_j .

1.3.3 Standard $\{|k, j, m\rangle\}$ representations

We shall now study the eigenvectors common to \mathbf{J}^2 and J_z .

The basis state

Given a pair of eigenvalues, $j(j+1)\hbar^2$ and $m\hbar$, the set of eigenvectors associated with this pair of eigenvalues forms a vector subspace of \mathcal{E} which we shall denote by $\mathcal{E}(j, m)$. We choose in $\mathcal{E}(j, m)$ an arbitrary orthonormal basis, $\{|k, j, m\rangle; k = 1, 2, \dots, g(j, m)\}$ with $g(j, m) \geq 1$ the dimension of this subspace.

The spaces $\mathcal{E}(k, j)$

Matrices representing the angular momentum operators

Let us give some examples of $(J_u)^{(j)}$ matrices:

i) $j = 0$

The subspaces $\mathcal{E}(k, j = 0)$ are one-dimensional, since zero is the only possible value for m . The $(J_u)^0$ matrices reduce to numbers, which according to C-51, are zero.

ii) $j = 1/2$

The subspaces $\mathcal{E}(k, j = 1/2)$ are two-dimensional $m \in \{1/2, -1/2\}$. If we choose the basis vector in this order, we find using C-51:

$$\begin{aligned} (J_z)^{(1/2)} &= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad (J_+)^{(1/2)} = \hbar \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad (J_-)^{(1/2)} = \hbar \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \\ (J_x)^{(1/2)} &= \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad (J_y)^{(1/2)} = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad (\mathbf{J}^2)^{(1/2)} = \frac{3}{4}\hbar^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \end{aligned}$$

iii) $j = 1$

The subspaces $\mathcal{E}(k, j = 1)$ are two-dimensional $m \in \{1, 0, -1\}$. Similarly,

$$\begin{aligned} (J_z)^{(1)} &= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad (J_+)^{(1)} = \hbar \begin{bmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix}, \quad (J_-)^{(1)} = \hbar \begin{bmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix}, \\ (J_x)^{(1)} &= \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad (J_y)^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad (\mathbf{J}^2)^{(1)} = 2\hbar^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \end{aligned}$$

iv) j arbitrary

The ladder operators can be written using C-51:

$$\begin{aligned} \langle k, j, m | J_x | k', j', m' \rangle &= \frac{\hbar}{2} \delta_{kk'} \delta_{jj'} [\sqrt{j(j+1) - m'(m'+1)} \delta_{m, m'+1} + \sqrt{j(j+1) - m'(m'-1)} \delta_{m, m'-1}] \\ \langle k, j, m | J_y | k', j', m' \rangle &= \frac{\hbar}{2i} \delta_{kk'} \delta_{jj'} [\sqrt{j(j+1) - m'(m'+1)} \delta_{m, m'+1} - \sqrt{j(j+1) - m'(m'-1)} \delta_{m, m'-1}]. \end{aligned}$$

$(J_x)^{(j)}$ is symmetrical and real, and $(J_y)^{(j)}$ is antisymmetrical and pure imaginary. Since the kets $|k, j, m\rangle$ are eigenvectors of \mathbf{J}^2 , we have:

$$\langle k, j, m | \mathbf{J}^2 | k', j', m' \rangle = j(j+1)\hbar^2 \delta_{kk'} \delta_{jj'} \delta_{mm'}.$$

The matrix $(\mathbf{J}^2)^{(j)}$ is therefore proportional to the $(2j+1) \times (2j+1)$ unit matrix: its diagonal elements are all equal to $j(j+1)\hbar^2$.

- The OZ axis chosen as the quantization axis is **entirely arbitrary**. All directions are physically equivalent, and we should expect the eigenvalues of J_x and J_y to be the same as those of J_z . In general, inside a given subspace $\mathcal{E}(k, j)$, the eigenvalues of J_x and J_y (like those of $J_u = \mathbf{J} \cdot \mathbf{u}$) are $j\hbar, (j-1)\hbar, \dots, (-j+1)\hbar, -j\hbar$. The corresponding eigenvectors $[(\mathbf{J}^2, J_x), (\mathbf{J}^2, J_y), \text{ or } (\mathbf{J}^2, J_z)]$ are linear combinations of the $|k, j, m\rangle$ with k and j fixed.

Eigenequations of J_{\pm}

An orthonormal basis $\{|k, j, m\rangle\}$ of the state space, composed of eigenvectors common to \mathbf{J}^2 and J_z :

$$\left. \begin{aligned} \mathbf{J}^2 |k, j, m\rangle &= j(j+1)\hbar^2 |k, j, m\rangle \\ J_z |k, j, m\rangle &= m\hbar |k, j, m\rangle \end{aligned} \right\} \quad (1.11)$$

is called a **standard basis** if the action of J_{\pm} on the basis vectors is given by:

$$\text{Eigenequation of } J_{\pm} \quad J_{\pm}|k, j, m\rangle = \hbar\sqrt{j(j+1) - m(m \pm 1)}|k, j, m \pm 1\rangle. \quad (1.12)$$

And,

$$J_-|k, j, -j\rangle = 0, \quad J_+|k, j, j\rangle = 0. \quad (1.13)$$

1.4 Application to orbital angular momentum

We return now to the orbital angular momentum \mathbf{L} of a spinless particle and see how the general theory developed applies to this particular case.

Using the $\{|\mathbf{r}\rangle\}$ representation, we shall show that the eigenvalues of the operator \mathbf{L}^2 are the numbers $l(l+1)\hbar^2$. Then, we shall indicate the eigenfunctions common to \mathbf{L}^2 and L_z and their principal properties.

1.4.1 Eigenvalues and eigenfunctions of \mathbf{L}^2 and L_z

Eigenequation in the $\{|\mathbf{r}\rangle\}$ representation

In the $\{|\mathbf{r}\rangle\}$ representation, the observables \mathbf{R} and \mathbf{P} correspond respectively to multiplication by \mathbf{r} and to the differential operator $(\hbar/i)\nabla$. The three components can therefore be written as

$$L_x = \frac{\hbar}{i}(y\partial_z - z\partial_y), \quad L_y = \frac{\hbar}{i}(z\partial_x - x\partial_z), \quad L_z = \frac{\hbar}{i}(x\partial_y - y\partial_x). \quad (1.14)$$

It is more convenient to work in spherical coordinates, since the various AM operators act only on the angular variables θ and ϕ , and not on r .

The conversion of a point M at $\mathbf{r} = (x, y, z)$ in the spherical coordinates $\mathbf{r} = (r, \theta, \phi)$ is therefore:

$$\begin{aligned} \text{Spherical coordinates} \quad & \begin{aligned} x &= r \sin \theta \cos \phi \\ y &= r \sin \theta \sin \phi \\ z &= r \cos \theta \end{aligned} \quad \text{with} \quad \begin{aligned} r &\geq 0 \\ 0 &\in [0, \pi] \\ \phi &\in [0, 2\pi] \\ d^3r &= r^2 \sin \theta dr d\theta d\phi \end{aligned} \end{aligned} \quad (1.15)$$

Using them in the AM operators yield

$$L_x = i\hbar \left(\sin \phi \partial_{\theta} + \frac{\cos \phi}{\tan \theta} \partial_{\phi} \right), \quad L_y = i\hbar \left(-\cos \phi \partial_{\theta} + \frac{\sin \phi}{\tan \theta} \partial_{\phi} \right), \quad L_z = \frac{\hbar}{i} \partial_{\phi} \quad (1.16)$$

$$\mathbf{L}^2 = -\hbar^2 \left(\partial_{\theta}^2 + \frac{1}{\tan \theta} \partial_{\theta} + \frac{1}{\sin^2 \theta} \partial_{\phi}^2 \right), \quad L_+ = \hbar e^{i\phi} (\partial_{\theta} + i \cot \theta \partial_{\phi}), \quad L_- = \hbar e^{-i\phi} (-\partial_{\theta} + i \cot \theta \partial_{\phi}). \quad (1.17)$$

In the $\{|\mathbf{r}\rangle\}$ representation, the eigenfunctions associated with the eigenvalues $l(l+1)\hbar^2$ of \mathbf{L}^2 and $m\hbar$ of L_z are the solutions of the following partial differential equations:

$$\begin{aligned} & \left[\partial_{\theta}^2 + \frac{1}{\tan \theta} \partial_{\theta} + \frac{1}{\sin^2 \theta} \partial_{\phi}^2 \right] \psi(r, \theta, \phi) = l(l+1)\psi(r, \theta, \phi) \\ & -i\partial_{\phi} \psi(r, \theta, \phi) = m\psi(r, \theta, \phi) \end{aligned} \quad (1.18)$$

We already know that l is integral or half-integral and that, for fixed l , m can take only the values $-l, \dots, l$. We also notice from the equations that r does not appear in any differential operator, so we can consider it to be a parameter and take into account only the θ - and ϕ -dependence of ψ .

Thus, we denote by $Y_l^m(\theta, \phi)$ a common eigenfunction of L^2 and L_z which corresponds to the eigenvalues $l(l+1)\hbar^2$ and $m\hbar$:

$$\begin{aligned} L^2 Y_l^m(\theta, \phi) &= l(l+1)\hbar^2 Y_l^m(\theta, \phi) \\ L_z Y_l^m(\theta, \phi) &= m\hbar Y_l^m(\theta, \phi) \end{aligned} \quad (1.19)$$

These equations have only one solution for each pair of allowed values of l and m , both indices are sufficient.

- Equation (1.19) gives the θ, ϕ -dependence of the eigenfunctions of L^2 and L_z , after which we construct the complete eigenfunction:

$$\phi_{l,m}(r, \theta, \phi) = f(r) Y_l^m(\theta, \phi). \quad (1.20)$$

The fact that $f(r)$ is arbitrary shows that L^2 and L_z do not form a CSCO in the space \mathcal{E}_r of functions of r .

- In order to normalize $\phi_{l,m}$ it is convenient to normalize Y_l^m and f **separately**:

$$\int_{r=0}^{\infty} \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} |\psi_{m,l}(r, \theta, \phi)|^2 r^2 \sin \theta dr d\theta d\phi = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} |Y_l^m(\theta, \phi)|^2 \sin \theta d\theta d\phi = \int_{r=0}^{\infty} r^2 |f(r)|^2 dr = 1. \quad (1.21)$$

Values of l and m

- **l and m must be integral**

Using $L_z = \frac{\hbar}{i} \partial_\phi$ in (1.19) we have:

$$\frac{\hbar}{i} \partial_\phi Y_l^m(\theta, \phi) = m\hbar Y_l^m(\theta, \phi) \longrightarrow Y_l^m(\theta, \phi) = F_l^m(\theta) e^{im\phi}. \quad (1.22)$$

We can cover all space by letting ϕ vary in $[0, 2\pi]$. We must have by continuity of the solution,

$$Y_l^m(\theta, \phi = 0) = Y_l^m(\theta, \phi = 2\pi) \implies e^{2im\pi} = 1. \quad (1.23)$$

Therefore, in an orbital AM l and m must be integer.

- **All integral values ≥ 0 of l can be found**

Given an integral value of l , we know from the previous section that:

$$L_+ Y_l^l(\theta, \phi) = 0.$$

Using (??) and (1.22) yields

$$[\partial_\theta - l \cot \theta] F_l^l(\theta) = 0.$$

This first-order ODE can be integrated noting that $\cos \theta d\theta = d(\sin \theta)/\sin \theta$. The solution is:

$$F_l^l(\theta) = c_l (\sin \theta)^l.$$

Thus, for each positive or zero integral value of l , there exists a function $Y_l^l(\theta, \phi)$ which is unique:

$$\text{Spherical harmonics} \quad Y_l^l = c_l (\sin \theta)^l e^{il\phi}. \quad (1.24)$$

Through repeated action of L_- , we construct $Y_l^{l-1}, \dots, Y_l^m, \dots, Y_l^{-l}$. We see then there corresponds to the pair of eigenvalues $l(l+1)\hbar^2$ and $m\hbar$ one and only one eigenfunction $Y_l^m(\theta, \phi)$, which can be computed from (1.24).

Fundamental properties of the spherical harmonics

We summarize some properties of spherical harmonics.

- **Recurrence relations**

$$\begin{aligned} e^{i\phi} [\partial_\theta - m \cot \theta] Y_l^m(\theta, \phi) &= \sqrt{l(l+1) - m(m+1)} Y_l^{m+1}(\theta, \phi) \\ e^{i\phi} [-\partial_\theta - m \cot \theta] Y_l^m(\theta, \phi) &= \sqrt{l(l+1) - m(m-1)} Y_l^{m-1}(\theta, \phi) \end{aligned} \quad (1.25)$$

- **Orthonormalization and closure relations**

Normalization imposed on the spherical harmonics yields

$$\int_0^{2\pi} \int_0^\pi \sin \theta Y_l^{m'*}(\theta, \phi) Y_l^m(\theta, \phi) \sin \theta d\theta d\phi = \delta_{l'l} \delta_{m'm}. \quad (1.26)$$

Furthermore, any function $f(\theta, \phi)$ can be expanded in terms of the spherical harmonics:

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{l,m} Y_l^m(\theta, \phi), \quad \text{with} \quad c_{l,m} = \int_0^{2\pi} \int_0^\pi f(\theta, \phi) Y_l^{m*}(\theta, \phi) d\theta d\phi. \quad (1.27)$$

The spherical harmonics therefore constitute an orthonormal basis in the space \mathcal{E}_Ω , which means the surface of a sphere with fixed value of r . This fact is expressed by the closure relation:

$$\sum_{l=0}^{\infty} \sum_{m=-l}^l Y_l^m(\theta, \phi) Y_l^{m*}(\theta', \phi') = \delta(\cos \theta - \cos \theta') \delta(\phi - \phi') = \frac{1}{\sin \theta} \delta(\theta - \theta') \delta(\phi - \phi'). \quad (1.28)$$

- **Parity and complex conjugation**

A reflection through the coordinate origin is expressed as $\mathbf{r} \rightarrow -\mathbf{r}$ in cartesian coordinates, and as

$$\begin{aligned} \text{Reflection} \quad r &\longrightarrow r \\ \theta &\longrightarrow \pi - \theta \\ \phi &\longrightarrow \pi + \phi \end{aligned} \quad (1.29)$$

in spherical coordinates. It is simple to show that a reflection in Y_l^m yields:

$$\text{Reflection in spherical harmonics} \quad Y_l^m(\pi - \theta, \pi + \phi) = (-1)^l Y_l^m(\theta, \phi). \quad (1.30)$$

Also, that a complex conjugation results in

$$\text{Complex conjugation of spherical harmonics} \quad [Y_l^m(\theta, \phi)]^* = (-1)^m Y_l^{-m}(\theta, \phi). \quad (1.31)$$

Standard bases of the wave function space of a spinless particle

We know that \mathbf{L}^2 and L_z do not constitute a CSCO in the wave function space of a spinless particle. We shall now indicate the form of the standard bases of this space. By repeated application of L_- on $\psi_{k,l,l}(\mathbf{r})$, we then construct the functions $\psi_{k,l,m}(\mathbf{r})$ which complete the standard basis for $m \neq l$. They satisfy the equations in and :

But we saw that all eigenfunctions common to \mathbf{L}^2 and L_z that correspond to given eigenvalues $l(l+1)\hbar^2$ and $m\hbar$ have the same angular dependence in $Y_l^m(\theta, \phi)$, and only the radial dependence differs. From

the same above equations we deduce that the functions $\psi_{k,l,m}(\mathbf{r})$ of a standard basis of the wave function space of a spinless particle have the form:

$$\psi_{k,l,m}(\mathbf{r}) = R_{k,l}(r)Y_l^m(\theta, \phi). \quad (1.32)$$

Notice the dependence indices for each term of the right-side. The orthonormalization relation for the radial function is:

$$\int_0^\infty R_{k,l}^*(r)R_{k',l}(r) r^2 dr = \delta_{kk'}. \quad (1.33)$$

Notice also the orthogonality is to respect to the k variable.

- If we want the basis function $\psi_{k,l,m}(\mathbf{r})$ to be continuous, only the radial functions corresponding to $l = 0$ can be non-zero at $r = 0$.

1.4.2 Physical considerations

Study of a $|k, l, m\rangle$ state

Calculations of the physical predictions concerning measurements of \mathbf{L}^2 and L_z

Chapter 2

Spin 1/2 and two-level systems

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2.1 Spin 1/2 particle: quantization of the angular momentum

We will study a fundamental experiment that revealed the quantization of a simple physical quantity, the angular momentum. We will see that the component along Oz of the AM can take only certain values ($\pm\hbar/2$), that is, is quantized.

A silver atom in the ground state is said to be a **spin 1/2 particle**. We shall also study the evolution of a spin 1/2 particle in a uniform magnetic field (Larmor precession).

2.1.1 Experimental demonstration

We are going to describe and analyze the Stern-Gerlach experiment, which demonstrated the quantization of the components of the angular momentum.

The Stern-Gerlach apparatus

The experiment consists of studying the deflection of a beam of neutral paramagnetic atoms (in this case silver atoms). The beam leaves a furnace E through a small opening and propagates in a straight line in the high vacuum existing inside the apparatus. Then, the atomic beam traverses the electromagnet A and thus being deflected before reaching the plate P .

This B-field has a plane of symmetry yOz that contains the initial direction Oy of the atomic beam. The B-field has no components along Oy , and its largest component is along Oz ; it varies strongly with z . Since the B-field has a conserved flux $\nabla \cdot \mathbf{B} = 0$, it must also have a component along Ox which varies with the distance x from the plane of symmetry.

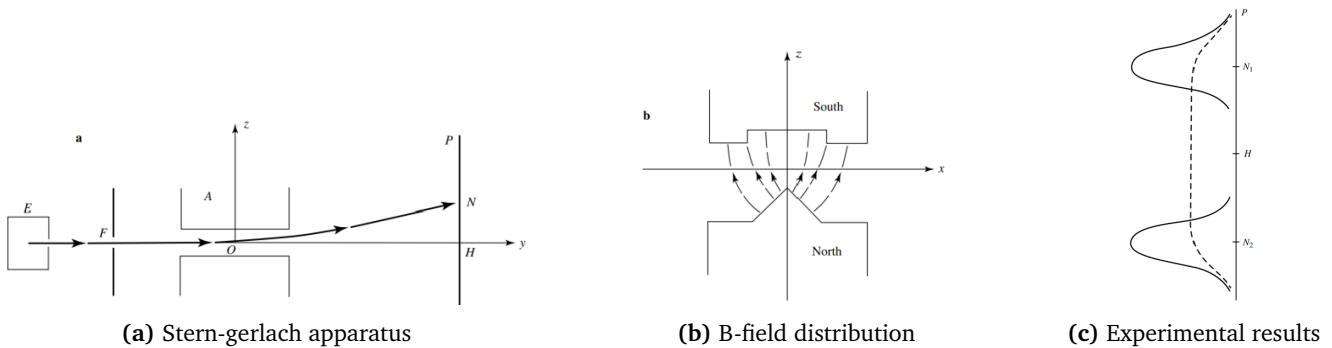


Figure 2.1 The Stern-Gerlach experiment.

Classical calculations of the deflection

The neutral silver atoms possess a permanent magnetic moment μ (they are paramagnetic atoms); the resulting forces are derived from the potential energy:

$$W_B = -\mu \cdot \mathbf{B}. \quad (2.1)$$

For a given atomic level, the magnetic moment μ and the angular momentum \mathbf{J} are proportional:

$$\mu = \gamma \mathbf{J}, \quad (2.2)$$

where γ is the **gyromagnetic ratio** of the level. Before the atoms traverse the electromagnet, the magnetic moments of the silver are oriented randomly (isotropically).

The resultant force exerted on the atom is:

$$\mathbf{F} = \nabla(\boldsymbol{\mu} \cdot \mathbf{B}). \quad (2.3)$$

The angular momentum theorem can be written:

$$\partial_t \mathbf{L} = \boldsymbol{\Gamma} = \gamma \mathbf{L} \times \mathbf{B}. \quad (2.4)$$

The atom thus behaves like a gyroscope: $\partial_t \mathbf{L}$ is perpendicular to \mathbf{L} , and the angular momentum turns about the magnetic field, the angle θ between $|\mathbf{L}|$ and \mathbf{B} remaining constant.

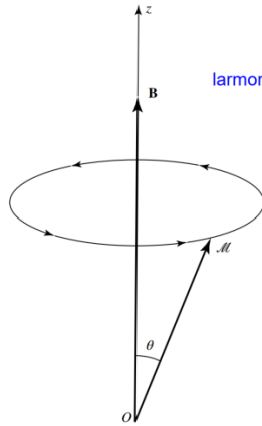


Figure 2.2 The effect of a uniform B-field \mathbf{B} is to cause $\boldsymbol{\mu}$ to turn about \mathbf{B} with a constant angular velocity (Larmor precession).

The rotational angular velocity is equal to the product of the gyromagnetic ratio γ and the modulus of the B-field.

To calculate the force \mathbf{F} , we can, to a very good approximation, neglect in the potential energy W the terms proportional to μ_x and μ_y and take μ_z to be constant. This is because the frequency of oscillation due to rotation of $\boldsymbol{\mu}$ is so great that only the time-average values of μ_x and μ_y can play a role in W , and these are both zero.

Consequently, it is as if the atom were submitted to the sole force:

$$\mathbf{F}' = \nabla(\mu_z B_z) = \mu_z \nabla B_z. \quad (2.5)$$

The force on the atom is therefore parallel to Oz and proportional to μ_z . Consequently, because this force produced the deflection HN, measuring HN is equivalent to measuring μ_z and L_z .

Results and conclusions

The results of the experiment (performed in 1922) are in complete contradiction with the preceding predictions. We do not observe a single spot centered at H, but two spots centered at N_1 and N_2 . The predictions of classical mechanics are therefore shown to be invalidated by the experiment.

It is possible, in order to describe the motion of the silver atoms, to construct wave packets whose width Δz and momentum dispersion Δp are negligible. They must satisfy the Heisenberg relation:

$$\Delta z \cdot \Delta p_z \geq \hbar.$$

Numerically, the mass M of a silver atom is $1.8 \times 10^{-25} \text{ kg}$. Δz and the velocity uncertainty $\Delta v_z = \Delta p_z / M$ must be such that:

$$\Delta z \cdot \Delta v_z \geq \frac{\hbar}{M} \approx 10^{-9}. \quad (2.6)$$

It is then easy to find uncertainties Δz and Δv_z which, while satisfying above, are negligible on the scale of the experiment being considered. It is possible to reason in terms of quasi-pointlike wave packets moving along classical trajectories. Therefore, it is correct to claim that measurement of the deflection HN constitutes a measurement of μ_z or L_z .

Conclusion of the experiment

If we measure the component L_z of the intrinsic angular momentum of a silver atom in its ground state, we can find only one or the other of two values corresponding to the deflections HN_1 and HN_2 . L_z is a **quantized** physical quantity whose discrete spectrum includes only two eigenvalues ($\pm \hbar/2$).

2.1.2 Theoretical description

We are now going to show how QM describes the degrees of freedom of a silver atom, that is, of a spin 1/2 particle. The idea is to give precise examples of kets and observables, to show how physical predictions can be extracted from them and how to distinguish clearly between the various stages of an experiment (preparation, evolution, measurement).

We must therefore define the state space and the observables corresponding to the components of \mathbf{L} : L_x, L_y, L_z , or more generally, $L_{\mathbf{u}} = \mathbf{L} \cdot \mathbf{u}$, where \mathbf{u} is an arbitrary unit vector.

The observable S_z and the spin state space

With L_z we must associate an observable S_z which has two eigenvalues $\pm \hbar/2$. We assume that these two eigenvalues are not degenerate, and we denote by $|\pm\rangle$ the respective orthonormal eigenvectors:

$$\text{Eigenequation of } S_z \quad S_z |\pm\rangle = \pm \frac{\hbar}{2} |\pm\rangle, \quad \text{with} \quad \begin{aligned} \langle + | + \rangle &= \langle - | - \rangle = 1 \\ \langle \pm | \mp \rangle &= 0 \end{aligned} \quad (2.7)$$

S_z alone forms a CSCO, and the spin state space is the two-dimensional space \mathcal{E}_s spanned by the eigenvectors $|\pm\rangle$. This is mathematically expressed by the closure relation:

$$\text{Closure relation of } \mathcal{E}_s \quad |+\rangle\langle +| + |-\rangle\langle -| = \mathbb{1}. \quad (2.8)$$

The very most general vector in \mathcal{E}_s is a linear superposition of these eigenvectors:

$$|\psi\rangle = \alpha |+\rangle + \beta |-\rangle, \quad \text{with} \quad |\alpha|^2 + |\beta|^2 = 1. \quad (2.9)$$

In the $\{|\pm\rangle\}$ basis, the matrix representing S_z is diagonal and is written as

$$S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (2.10)$$

The other spin observables

With the L_x and L_y components of \mathbf{L} will be associates the observables S_x and S_y . The three components of the angular momentum do not commute with each other but satisfy well-defined commutation relations. The matrices representing S_x and S_y in the basis of the eigenvectors $|\pm\rangle$ of S_z are the following:

$$S_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad S_y = \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}. \quad (2.11)$$

We see that they can be expressed in terms of the **Pauli matrices** $\sigma_x, \sigma_y, \sigma_z$.

As for the L_u component of \mathbf{L} along the unit vector \mathbf{u} , characterized by the angles (θ, ϕ) , it is written

$$L_u = \mathbf{L} \cdot \mathbf{u} = L_x \sin \theta \cos \phi + L_y \sin \theta \sin \phi + L_z \cos \theta. \quad (2.12)$$

Using the previous definitions of S_x, S_y, S_z , we easily find the matrix that represents the corresponding observable $S_u = \mathbf{S} \cdot \mathbf{u}$ in the $\{|\pm\rangle\}$ basis:

$$S_u = S_x \sin \theta \cos \phi + S_y \sin \theta \sin \phi + S_z \cos \theta = \frac{\hbar}{2} \begin{bmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{bmatrix}. \quad (2.13)$$

We now get the eigenvalues of each observable defined. The S_x, S_y, S_u operators have the **same eigenvalues**, $+\hbar/2$ and $-\hbar/2$, as S_z . This is equivalent to rotate the Stern-Gerlach device, as all directions of space have the same properties, it must be invariant under rotations. The measurements of L_x, L_y, L_u can therefore yield only one of two results: $+\hbar/2$ or $-\hbar/2$.

As for the eigenvectors of S_x, S_y, S_u , we shall denote them respectively by $|\pm\rangle_x, |\pm\rangle_y, |\pm\rangle_u$. The expansion of the eigenvectors of S_u in the $\{|\pm\rangle_z\}$ basis is:

$$\begin{aligned} \text{Eigenstates of } S_u \text{ in the } \{|\pm\rangle_z\} \text{ basis} \quad & \begin{aligned} |+\rangle_u &= \cos \frac{\theta}{2} e^{-i\phi/2} |+\rangle_z + \sin \frac{\theta}{2} e^{i\phi/2} |-\rangle_z \\ |-\rangle_u &= -\sin \frac{\theta}{2} e^{-i\phi/2} |+\rangle_z + \cos \frac{\theta}{2} e^{i\phi/2} |-\rangle_z \end{aligned} \end{aligned} \quad (2.14)$$

We see that S_x is obtained when $(\theta, \phi) = (\pi/2, 0)$ while for S_y through $(\theta, \phi) = (\pi/2, \pi)$.

2.2 Illustration of the postulates in the case of a spin 1/2

We are now to apply the postulates of QM to a certain number of experiments on silver atoms.

2.2.1 Actual preparation of the various spin states

In order to make predictions about the results of a measurement, we must know the state of the system immediately before the measurement.

Preparation of the states $|\pm\rangle$

Let assume we have the hole at N_1 . The atoms which are deflected downward continue to condense about N_2 , while some of those which are deflected upwards pass through N_1 of the plate.

Each of the atoms of the beam which propagates to the right of the plate is a physical system on which we have just performed a measurement of the observable S_z , the result being $+\hbar/2$: the atom is in the state $|+\rangle$.

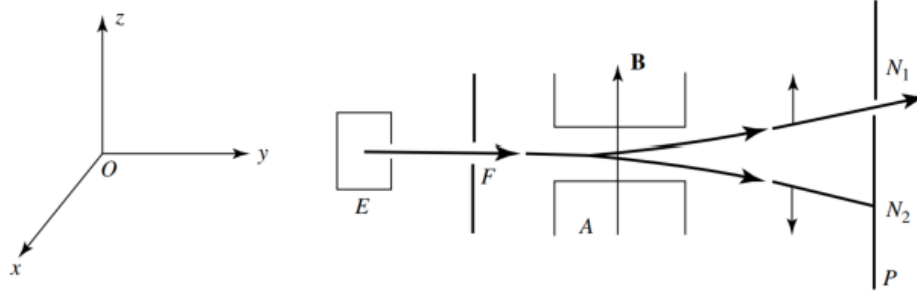


Figure 2.1 The atoms that pass through the hole made are all in the spin state $|+\rangle$. The Stern-Gerlach is then acting like a polarizer.

The device of the figure thus produces a beam of atoms which are all in the spin state $|+\rangle$, acting like a polarizer.

Preparation of the states $|\pm\rangle_x$, $|\pm\rangle_y$, $|\pm\rangle_z$

To prepare one of eigenstates of S_x (which is a CSCO), we must simply select, after a measurement of S_x , the atoms for which this measurement has yielded the corresponding eigenvalue. If we rotate the device through an angle of $+\pi/2$ about Oy , we obtain a beam of atoms whose spin state is $|+\rangle_x$.

By placing the Stern-Gerlach device so that the axis of the magnetic field is parallel to an arbitrary unit vector \mathbf{u} , and piercing the plate (at N_1 or N_2), we can prepare silver atoms in the spin state $|+\rangle_{\mathbf{u}}$ or $|-\rangle_{\mathbf{u}}$.

Preparation of the most general state

It is possible to prepare atoms whose spin state is described by the corresponding ket $|\psi\rangle$?

There exists, for all $|\psi\rangle$, a unit vector \mathbf{u} such that $|\psi\rangle$ is collinear with the ket $|+\rangle_{\mathbf{u}}$. We choose two complex numbers α, β that satisfy normalization equation in (2.9).

We find that there necessarily exists an angle θ such that

$$\cos \frac{\theta}{2} = |\alpha| \wedge \sin \frac{\theta}{2} = |\beta|, \quad \theta \in [0, \pi]. \quad (2.15)$$

Let us set

$$\begin{aligned} \varphi &= \arg \beta - \arg \alpha \\ \chi &= \arg \beta + \arg \alpha \end{aligned} \implies \begin{aligned} \arg \beta &= \frac{1}{2}\chi + \frac{1}{2}\varphi \\ \arg \alpha &= \frac{1}{2}\chi - \frac{1}{2}\varphi \end{aligned} \quad (2.16)$$

With this notation, the ket $|\psi\rangle$ is written as

$$|\psi\rangle = e^{i\chi/2} \left[\cos \frac{\theta}{2} e^{-i\varphi/2} |+\rangle + \sin \frac{\theta}{2} e^{i\varphi/2} |-\rangle \right]. \quad (2.17)$$

Consequently, to prepare silver atoms in the state $|\psi\rangle$, it suffices to place the Stern-Gerlach apparatus (with its plate pierced at N_1) so that its axis is directed along the vector \mathbf{u} .

2.2.2 Spin measurements

If we place two Stern-Gerlach magnets one after the other, we can verify experimentally the predictions of the postulates. The first acts like a polarizer, while the second is used to measure a specified component of the angular momentum L : the analyzer.

First experiment

Assuming the axes of the two devices parallel to Oz . The first one prepares the aomt in the state $|+\rangle$ and the second one measure L_z .

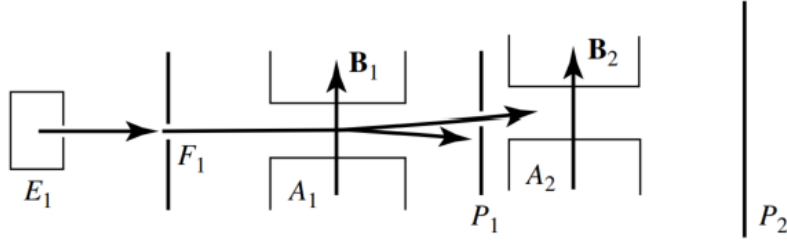


Figure 2.2 The result obtained is certain $+\hbar/2$.

Since the state of the system under study is an eigenstate of S_z which we want to measure, the measurement result is **certain**: we find, without fail, the corresponding eigenvalue $+\hbar/2$. This is indeed what is observed experimentally: all the atoms strike the second plate in the vicinity of N_1 , none hitting near N_2 .

Second experiment

Let us place the axis of the first device along the unit vector \mathbf{u} , with $\theta, \phi = \pi$. \mathbf{u} is therefore contained in the xOz plane. The axis of the second device remains parallel to Oz .

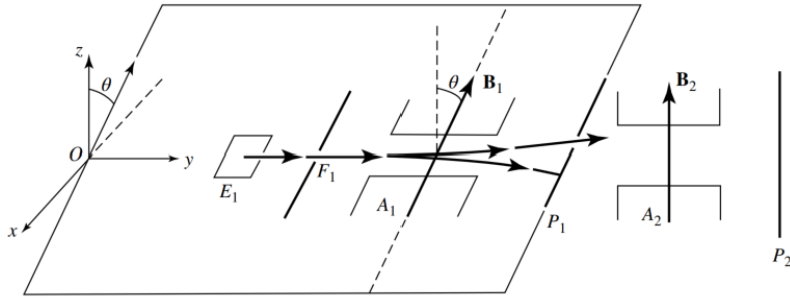


Figure 2.3 The possible results are $+\hbar/2$ with $\cos^2 \theta$ of change and $-\hbar/2$ with $\sin^2 \theta/2$.

According to (2.14), the spins state of the atoms when they leave the polarizer is:

$$|\psi\rangle = -\cos \frac{\theta}{2} |+\rangle + \sin \frac{\theta}{2} |-\rangle. \quad (2.18)$$

In this case, we find that certain atoms condense at N_1 , and others at N_2 . We can compute directly that the probabilities of the eigenstates are, respectively $\cos^2 \theta/2$ and $\sin^2 \theta/2$. We observe experimentally that the intensity of the spots corresponds to numbers of atoms which are proportional, to their respective probabilities.

The mean value of the results which would be obtained in a large number of identical experiments is $\langle S_z \rangle = \frac{\hbar}{2} \cos \theta$, which corresponds to the classical result.

Third experiment

Let us take the second experiment, but with the analyzer rotated until its axis is directed along Ox, so that it measures the L_x component of the AM.

We must expand the state $|\psi\rangle$ after the first device in terms of the eigenstates of S_x :

$$\begin{aligned} {}_x\langle +|\psi\rangle &= \frac{1}{\sqrt{2}}(\cos \frac{\theta}{2} + \sin \frac{\theta}{2}) = \cos(\frac{\pi}{4} - \frac{\theta}{2}) \\ {}_x\langle -|\psi\rangle &= \frac{1}{\sqrt{2}}(\cos \frac{\theta}{2} - \sin \frac{\theta}{2}) = \sin(\frac{\pi}{4} - \frac{\theta}{2}) \end{aligned} \quad (2.19)$$

The probability of find the eigenvalue $+\hbar/2$ of S_x is therefore $\cos^2(\frac{\pi}{4} - \frac{\theta}{2})$ and that of finding $-\hbar/2$, $\sin^2(\frac{\pi}{4} - \frac{\theta}{2})$.

It is possible to verify these predictions by measuring the intensity of the two spots on the plate situated at the exit of the second Stern-Gerlach device.

Mean values

If we calculate the mean value of the possible results in the second experiment, we obtain:

$$\langle S_z \rangle = \frac{1}{N} \left[\frac{\hbar}{2} N \cos^2 \frac{\theta}{2} - \frac{\hbar}{2} N \sin^2 \frac{\theta}{2} \right] = \frac{\hbar}{2} \cos \theta. \quad (2.20)$$

This is indeed the value of the matrix element $\langle \psi | S_z | \psi \rangle$. Similarly, the average of the measurement results in the third experiment is

$$\langle S_x \rangle = \frac{1}{N} \left[\frac{\hbar}{2} N \cos^2(\frac{\pi}{2} - \frac{\theta}{2}) - \frac{\hbar}{2} N \sin^2(\frac{\pi}{4} - \frac{\theta}{2}) \right] = \frac{\hbar}{2} \sin \theta. \quad (2.21)$$

The matrix element can be computed matricially:

$$\langle \psi | S_x | \psi \rangle = \frac{\hbar}{2} \begin{bmatrix} \cos \theta/2 & \sin \theta/2 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos \theta/2 \\ \sin \theta/2 \end{bmatrix} = \frac{\hbar}{2} \sin \theta. \quad (2.22)$$

The mean value of L_x is indeed equal to the matrix element, in the state $|\psi\rangle$, of the associated observable S_x .

There is an equivalence with the motion of classical mechanics. Using matrix computation, the mean values of S_x, S_y, S_z in the state $|+\rangle_u$ is:

$${}_u\langle + | S_x | + \rangle_u = \frac{\hbar}{2} \sin \theta \cos \phi, \quad {}_u\langle + | S_y | + \rangle_u = \frac{\hbar}{2} \sin \theta \sin \phi, \quad {}_u\langle + | S_z | + \rangle_u = \frac{\hbar}{2} \cos \theta. \quad (2.23)$$

These mean values are equal to the components of a classical angular momentum of modulus $\hbar/2$ oriented along the vector \mathbf{u} with angles (θ, ϕ) . However, recall that the only possible results of a measurements are $\pm\hbar/2$, not the above results of the mean values.

In the quantum sense, the motion of the atom is a linear superposition of the possible results, so both $\pm\hbar/2$ are traveling.

2.2.3 Evolution of a spin 1/2 particle in a uniform magnetic field

The interaction Hamiltonian and the Schrodinger equation

Consider a silver atom in a uniform magnetic field \mathbf{B}_0 , and choose the Oz axis along \mathbf{B}_0 . The classical potential energy of the magnetic moment $\boldsymbol{\mu} = \gamma \mathbf{J}$ of this atom is then:

$$W = -\boldsymbol{\mu} \cdot \mathbf{B}_0 = -\mu_z B_0 = \underbrace{-\gamma B_0}_{\omega_0} J_z, \quad (2.24)$$

where ω_0 is the **Larmor frequency**. Since we are quantizing only the internal degrees of freedom of the particle, J_z must be replaced by the operator S_z , and the classical energy above becomes an operator: it is the Hamiltonian H which describes the evolution of the spin of the atom in the field \mathbf{B}_0 :

$$H = \omega_0 S_z. \quad (2.25)$$

Since H is time-independent, we solve the respective eigenequation. We see that the eigenvectors of H are those of S_z :

$$H|\pm\rangle = \pm \frac{\hbar\omega_0}{2}|\pm\rangle = E_{\pm}|\pm\rangle. \quad (2.26)$$

There are therefore two energy levels, E_{\pm} . Their separation $\hbar\omega_0$ is proportional to the B-field; they define a single Bohr frequency:

$$\nu_{+-} = \frac{1}{\hbar}(E_+ - E_-) = \frac{\omega_0}{2\pi}. \quad (2.27)$$

- If \mathbf{B}_0 is parallel to the unit vector \mathbf{u} , the Hamiltonian (2.25) must be replaced by its general form:

$$\text{General form Hamiltonian} \quad H = \omega_0 \mathbf{S} \cdot \mathbf{u}. \quad (2.28)$$

- For silver atoms, $\gamma < 0$; ω_0 is therefore positive.

Larmor precession

Consider the spin at $t = 0$ in the state

$$|\psi(0)\rangle = \cos \frac{\theta}{2} e^{-i\phi/2} |+\rangle + \sin \frac{\theta}{2} e^{i\phi/2} |-\rangle. \quad (2.29)$$

We saw that any state can be put in this form. To calculate the state at $t > 0$, we apply the evolution operator:

$$|\psi(t)\rangle = \cos \frac{\theta}{2} e^{-i\phi/2} e^{-iE_+t/\hbar} |+\rangle + \sin \frac{\theta}{2} e^{i\phi/2} e^{-iE_-t/\hbar} |-\rangle = \cos \frac{\theta}{2} e^{-\frac{i(\phi+\omega_0 t)}{2}} |+\rangle + \sin \frac{\theta}{2} e^{\frac{i(\phi+\omega_0 t)}{2}} |-\rangle.$$

The presence of \mathbf{B}_0 therefore introduces a phase shift between $|+\rangle$ and $|-\rangle$. The direction of $\mathbf{u}(t)$ along which the spin component is $+\hbar/2$ with certainty is defined by the polar angles:

$$\begin{aligned} \theta(t) &= \theta \\ \phi(t) &= \phi + \omega_0 t \end{aligned} \quad (2.30)$$

The angle between $\mathbf{u}(t)$ and Oz therefore remains constant, but $\mathbf{u}(t)$ revolves about Oz at an angular velocity of ω_0 . This effect is called the **Larmor precession**.

It can be verified from $|\psi(t)\rangle$ that the probabilities of obtaining $+\hbar/2$ or $-\hbar/2$ in a measurement of this observable are time-independent. These probabilities are equal, respectively, to $\cos^2 \theta/2$ and $\sin^2 \theta/2$. The mean value of S_z is also time-independent:

$$\langle \psi(t) | S_z | \psi(t) \rangle = \frac{\hbar}{2} \cos \theta. \quad (2.31)$$

Because S_x and S_y do not commute with H , we have that

$$\langle \psi(t) | S_x | \psi(t) \rangle = \frac{\hbar}{2} \sin \theta \cos(\phi + \omega_0 t), \quad \langle \psi(t) | S_y | \psi(t) \rangle = \frac{\hbar}{2} \sin \theta \sin(\phi + \omega_0 t). \quad (2.32)$$

We again find the Bohr frequencies $\omega_0/2\pi$ of the system. Moreover, the mean values above behave like the components of a classical AM of modulus $\hbar/2$ undergoing Larmor precession.

2.3 Two-level systems

There exist numerous other cases in physics which, to a first approximation, can be treated as a two-level system.

Assume that we want to evaluate the effect of an external perturbation in two levels. Then the intensity of the perturbation is sufficiently weak, it can be shown that its effect on the two state can be computed, approximately, by ignoring all the other energy levels of the system. All the calculations can then be performed in a two-dimensional subspace of the state space. We will study certain general properties of two-level systems.

2.3.1 Outline of the problem

Notation

Consider a physical system whose state space is two-dimensional. For a basis, we choose the system of the two eigenstates $|\varphi_1\rangle$ and $|\varphi_2\rangle$ of the Hamiltonian H_0 whose eigenvalues are, respectively, E_1 and E_2 :

$$\begin{array}{l} \text{Eigen-equation in a two-level system} \\ H_0 |\varphi_1\rangle = E_1 |\varphi_1\rangle \\ H_0 |\varphi_2\rangle = E_2 |\varphi_2\rangle \end{array} \quad (2.33)$$

Assume we want to take into account an external perturbation, initially neglected in H_0 . The Hamiltonian, eigenstates and eigenvalues become:

$$H = H_0 + W \implies \begin{array}{l} H |\psi_+\rangle = E_+ |\psi_+\rangle \\ H |\psi_-\rangle = E_- |\psi_-\rangle \end{array}. \quad (2.34)$$

H_0 is called the unperturbed Hamiltonian and W , the perturbation or coupling. We also assume that W is time-independent. In the $\{|\varphi_1\rangle, |\varphi_2\rangle\}$ basis of H_0 , W is represented by a Hermitian matrix:

$$(W) = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}. \quad (2.35)$$

W_{11} and W_{22} are real, and $W_{12} = (W_{21})^*$. In the absence of coupling, E_1 and E_2 are the possible energies of the system, and the states $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are stationary states.

Consequences of the coupling

- E_1 and E_2 are no longer the possible energies of the system

An energy measurement will yield only one of the eigenvalues E_+ or E_- . We want to express these energies in terms of E_1, E_2 and the matrix elements W_{ij} .

- $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are no longer stationary states

Since $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are not generally eigenstates of the total Hamiltonian H , they are no longer stationary states. W therefore induces **transitions** between the two unperturbed states.

Reduction to a fictitious spin 1/2

With every two-level system, can be associated a **fictitious spin 1/2** placed in a static field B and described by a Hamiltonian whose form is identical to that of the initial two level system.

2.3.2 Static aspect: effect of coupling on the stationary states of the system

Expressions for the eigenstates and eigenvalues of H

In the $\{|\varphi_1\rangle, |\varphi_2\rangle\}$ basis, the matrix representing H is written

$$H = \begin{bmatrix} E_1 + W_{11} & W_{12} \\ W_{21} & E_2 + W_{22} \end{bmatrix}. \quad (2.36)$$

The eigenvalues (after diagonalization) are:

$$\text{Eigenvalues} \quad E_{\pm} = \frac{1}{2}(E_1 + W_{11} + E_2 + W_{22}) \pm \frac{1}{2}\sqrt{(E_1 + W_{11} - E_2 - W_{22})^2 + 4|W_{12}|^2}. \quad (2.37)$$

The eigenvectors associated are:

$$\begin{aligned} \text{Eigenstates} \quad |\psi_+\rangle &= \cos \frac{\theta}{2} e^{-i\phi/2} |\varphi_1\rangle + \sin \frac{\theta}{2} e^{i\phi/2} |\varphi_2\rangle \\ |\psi_-\rangle &= -\sin \frac{\theta}{2} e^{-i\phi/2} |\varphi_1\rangle + \cos \frac{\theta}{2} e^{i\phi/2} |\varphi_2\rangle \end{aligned} \quad (2.38)$$

The angles θ and ϕ are defined by:

$$\tan \theta = \frac{2|W_{12}|}{E_1 + W_{11} - E_2 - W_{22}}, \quad \theta \in [0, \pi], \quad \text{and} \quad W_{21} = |W_{12}| e^{i\phi}. \quad (2.39)$$

Discussion

- **Graphical representation of the effect of coupling**

We assume that $W_{11} = W_{22} = 0$, which reduces the eigenstates to:

$$E_{\pm} = \frac{1}{2}(E_1 + E_2) \pm \frac{1}{2}\sqrt{(E_1 - E_2)^2 + 4|W_{12}|^2}, \quad \text{and} \quad \tan \theta = \frac{2|W_{12}|}{E_1 - E_2}, \quad \theta \in [0, \pi].$$

We introduce two other parameters, the **detuning** Δ and **mean energy** E_m :

$$E_m = \frac{1}{2}(E_1 + E_2), \quad \text{and} \quad \Delta = \frac{1}{2}(E_1 - E_2). \quad (2.40)$$

We see that changing E_m reduces to shifting the origin along the energy axis. Also, the eigenvectors do not depend on E_m , and we then care only about the influence of Δ . Substituting these new parameters in the eigenvalues yield:

$$E_{\pm} = E_m \pm \sqrt{\Delta^2 + |W_{12}|^2} = E_c \pm \frac{\hbar\Omega}{2}, \quad \Omega = \sqrt{\Delta^2 + |\Omega_0|^2}. \quad (2.41)$$

By plotting the four energies $E_{1,2}, E_{\pm}$, we obtain for $E_{1,2}$ two straight lines of slope ± 1 . When Δ changes, E_{\pm} describe two branches of a hyperbola whose asymptotes are the two straight lines associated with the unperturbed levels. The minimum separation is $2|W_{12}|$.

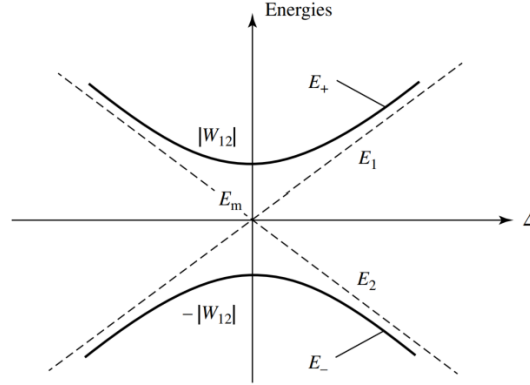


Figure 2.1 Variation of the energies E_{\pm} as a function of the energy difference Δ . In absence of coupling, the levels behaves as the dashed lines. Under the effect of non-diagonal coupling, the two perturbed levels gives the solid lines.

- **Effect of the coupling on the energy levels**

In the absence of coupling the energies $E_{1,2}$ cross at $\Delta = 0$. Under the effect of non-diagonal coupling, the two level repel each other. The diagram in solid lines is therefore called an **anti-crossing diagram**. Moreover, we see that, for any Δ , we always have:

$$|E_+ - E_-| > |E_1 - E_2|. \quad (2.42)$$

The coupling then separates the normal frequencies.

Near the asymptotes, $|\Delta| \gg |W_{12}|$, and the energies are written in power series expansion. On the other hand, at the center of the hyperbola, $\Delta = 0$, and the energies reduces to the following:

$$\begin{aligned} |\Delta| \gg |W_{12}| : \quad E_{\pm} &= E_m \pm \Delta \left(1 + \frac{1}{2} \left| \frac{W_{12}}{\Delta} \right|^2 + \dots \right) \\ \Delta = 0 : \quad E_{\pm} &= E_m \pm |W_{12}| \end{aligned}$$

Therefore, the effect of the coupling is much more important when the two unperturbed levels have the same energy.

- **Effect of coupling on the eigenstates**

Using the detuning and mean energy value, we have:

$$\tan \theta = \frac{|W_{12}|}{\Delta} = \frac{|\Omega_0|}{\Delta} \quad (2.43)$$

When $\Delta \ll |W_{12}|$ (strong coupling), $\theta \approx \pi/2$. On the other hand, when $\Delta \gg |W_{12}|$ (weak coupling), $\theta \approx 0$.

At the center of the hyperbola ($\Delta = 0$), and near the asymptotes ($\Delta \gg |W_{12}|$) we have:

$$\begin{aligned} \Delta = 0 : \quad |\psi_{\pm}\rangle &= \frac{1}{\sqrt{2}} \left[\pm e^{-i\phi/2} |\varphi_1\rangle + e^{i\phi/2} |\varphi_2\rangle \right] \\ \Delta \gg |W_{12}| : \quad |\psi_+\rangle &= e^{-i\phi/2} \left[|\varphi_1\rangle + e^{i\phi} \frac{|W_{12}|}{2\Delta} |\varphi_2\rangle + \dots \right] \\ |\psi_-\rangle &= e^{i\phi/2} \left[|\varphi_2\rangle - e^{-i\phi} \frac{|W_{12}|}{2\Delta} |\varphi_1\rangle + \dots \right] \end{aligned}$$

We see that for weak coupling, the perturbed states differ very slightly from the unperturbed states. For instance $|\psi_+\rangle$ is equal to the state $|\varphi_1\rangle$ slightly contaminated by a small contribution from the state $|\varphi_2\rangle$. On the other hand, for a strong coupling, the states $|\psi_{\pm}\rangle$ are very different from the state $|\varphi_{1,2}\rangle$.

2.3.3 Dynamical aspect: oscillation of the system between the two unperturbed states

Evolution of the state vector

Let the state vector of the system at t be:

$$|\psi(t)\rangle = a_1(t)|\varphi_1\rangle + a_2(t)|\varphi_2\rangle$$

The evolution of $|\psi(t)\rangle$ in the presence of coupling W is governed by the Schrodinger equation:

$$i\hbar\partial_t|\psi(t)\rangle = (H_0 + W)|\psi(t)\rangle \xrightarrow{\text{Projecting onto } \{|\varphi_{1,2}\rangle\}} \begin{cases} i\hbar\partial_t a_1(t) = E_1 a_1(t) + W_{12} a_2(t) \\ i\hbar\partial_t a_2(t) = W_{21} a_1(t) + E_2 a_2(t) \end{cases}$$

Is $|W_{12}| \neq 0$, these equations form a linear system of homogeneous coupled differential equations. The classical method involves looking the eigenpairs $(|\psi_{\pm}\rangle, E_{\pm})$ of the operator $H = H_0 + W$ and decompose $|\psi(0)\rangle$ in terms of $|\psi_{\pm}\rangle$:

$$|\psi(0)\rangle = \lambda|\psi_+\rangle + \mu|\psi_-\rangle \implies |\psi(t)\rangle = \lambda e^{-iE_+t/\hbar} |\psi_+\rangle + \mu e^{-iE_-t/\hbar} |\psi_-\rangle. \quad (2.44)$$

A system whose state vector is $|\psi(t)\rangle$ as above, oscillates between the two unperturbed states $|\varphi_1\rangle$ and $|\varphi_2\rangle$. To see this, we assume that at $t = 0$ the system is in $|\varphi_1\rangle$:

$$|\psi(0)\rangle = |\varphi_1\rangle \quad (2.45)$$

and compute the probability $P_{12}(t)$ of finding it in the state $|\varphi_2\rangle$ at time t .

Calculation of $P_{12}(t)$: Rabi's formula

Inverting (2.38) for $|\varphi_2\rangle$ yields:

$$|\psi(0)\rangle = |\varphi_1\rangle = e^{i\phi/2} \left[\cos \frac{\theta}{2} |\psi_+\rangle - \sin \frac{\theta}{2} |\psi_-\rangle \right] \longrightarrow |\psi(t)\rangle = e^{i\phi/2} \left[\cos \frac{\theta}{2} e^{-iE_+t/\hbar} |\psi_+\rangle - \sin \frac{\theta}{2} e^{-iE_-t/\hbar} |\psi_-\rangle \right] \quad (2.46)$$

The probability $P_{12}(t)$ is then, the projection of $|\psi(t)\rangle$ onto $|\varphi_2\rangle$:

$$\begin{aligned}
 P_{12}(t) &= |\langle\varphi_2|\psi(t)\rangle|^2 \\
 &= \left| e^{i\phi/2} \left[\cos \frac{\theta}{2} e^{-iE_+t/\hbar} \langle\varphi_2|\psi_+\rangle - \sin \frac{\theta}{2} e^{-iE_-t/\hbar} \langle\varphi_2|\psi_-\rangle \right] \right|^2 \\
 &= \left| e^{i\phi/2} \sin \frac{\theta}{2} \cos \frac{\theta}{2} [e^{-iE_+t/\hbar} - e^{-iE_-t/\hbar}] \right|^2 \\
 P_{12}(t) &= \sin^2 \theta \sin^2 \frac{(E_+ - E_-)t}{2\hbar}.
 \end{aligned}$$

Which can further expressed as

$$\text{Rabi's oscillation} \quad P_{12}(t) = \frac{4|W_{12}|^2}{4|W_{12}|^2 + (E_1 - E_2)^2} \sin^2 \left[\sqrt{4|W_{12}|^2 + (E_1 - E_2)^2} \frac{t}{2\hbar} \right]. \quad (2.47)$$

This expression is called **Rabi's formula**.

Discussion

We see from (2.47) that $P_{12}(t)$ oscillates over time with frequency $(E_+ - E_-)/\hbar$, which is the unique Bohr frequency of the system. The maximum value $\sin^2 \theta$ is achieved for all values of t such that

$$t = \frac{(2k+1)\hbar}{2(E_+ - E_-)}, \quad k = 0, 1, \dots \quad (2.48)$$

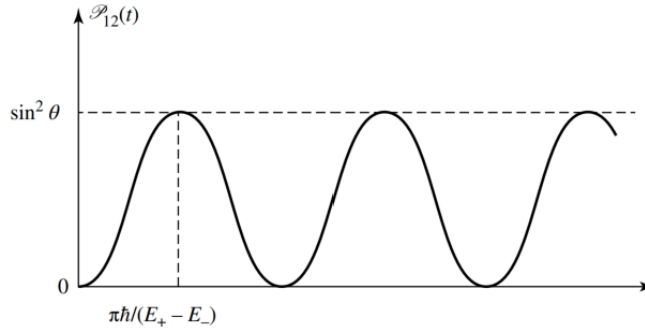


Figure 2.2 Evolution of $P_{12}(t)$ of finding the system in $|\varphi_2\rangle$ when initially was in $|\varphi_1\rangle$. When the states have the same unperturbed energy, the probability can attain the value 1.

- When $E_1 = E_2$, $(E_+ - E_-)/\hbar = 2|W_{12}|/\hbar$ and $\sin^2 \theta$ takes on its greatest possible value 1 at times $t = (2k+1)\pi\hbar/2|W_{12}|$. The frequency is proportional to the coupling.
- When $E_1 - E_2$ increases, so does $(E_+ - E_-)/\hbar$ while $\sin^2 \theta$ decreases. For weak coupling, $(E_+ - E_-) \approx (E_1 - E_2)$ and $\sin^2 \theta$ becomes very small. This is no surprising as the state $|\varphi_1\rangle$ is very close to the stationary state $|\psi_+\rangle$: the system, having started at $|\varphi_1\rangle$ evolves very little over time.

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