QUANTUM MECHANICS: LECTURE 15

SALWA AL SALEH

Abstract

Matrix representation for spin states (spinors) and the geometric interpretation of spin . Finally we discuss a spin in a constant magnetic field.

CONTENTS

1 Matrix representation of spin states 1
2 Geometric representation 2
3 Spin in constant magnetic field 3
3.1 Stationary states 4
4 Electron paramagnetic resonance EPR 4

References 4

MATRIX REPRESENTATION OF SPIN STATES

In the last lecture, we have introduced the spin operators and their eigenstates. We discovered the algebra of spin operators, and derived the Pauli spin matrices. However, we only stated their properties abstractly without defining a particular representation for them, now we aim to realise the spin algebra in a simple representation.
Consider the eigenkets $|\chi_-\rangle$ and $|\chi_+\rangle$.They form a basis for a 2-D Hilbert space of the internal degree of freedom, we have called the ' spin' . It is natural to introduce a canonical representation for these kets as the column vectors :

$$|\chi_+\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{1}$$

$$|\chi_-\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2}$$

Now, the action of the spin operators $\hat{S}_1, \hat{S}_2, \hat{S}_3$ and the ladder spin operators $\hat{S}_+, \hat{S}_-$ on the kets is :

$$\begin{aligned} &\hat{S}_1|\chi_\pm\rangle = \frac{\hbar}{2}|\chi_\mp\rangle \qquad \hat{S}_2|\chi_\pm\rangle = \pm i\frac{\hbar}{2}|\chi_\mp\rangle \qquad \hat{S}_3|\chi_\pm\rangle = \pm\frac{\hbar}{2}|\chi_\pm\rangle \\ &\hat{S}_\pm|\chi_\mp\rangle = \hbar|\chi_\pm\rangle \qquad \hat{S}_\pm|\chi_\pm\rangle = 0 \end{aligned} \tag{3}$$

We can easily express the operators above as matrices, and with the help of the identity:

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma} \tag{4}$$

We may write the explicit expression of the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

And:

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$
$$\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

We shall only deal with the index-down matrices and drop the ket notion on the eigenstate, calling them. For convenience and consistency with quantum mechanics textbooks.
Sometimes, the states χ_+, χ_- are denoted by α and β, respectively. The spinor χ is defined as:

$$\chi = \begin{pmatrix} \chi_+ \\ \chi_- \end{pmatrix} \tag{5}$$

Moreover, we can define the Hermitian conjegate of the spinor:

$$\chi^\dagger = \begin{pmatrix} \chi_+^* & \chi_-^* \end{pmatrix} \tag{6}$$

That satisfies:

$$\chi^\dagger \chi = 1 \tag{7}$$

We can calculate the expected value for an operator $\hat{\Omega}$ acting on the spin Hilbert space by:

$$\langle \hat{\Omega} \rangle = \chi^\dagger \hat{\Omega} \, \chi \tag{8}$$

geometric representation

There is another representation for spin, connected to the ' spin vector ' pointing in the 3-D space. In spherical polar coordinates, one may write the spin states as:

$$\chi_+ = e^{i(\delta - \varphi/2)} \cos \frac{1}{2}\theta \qquad\qquad \chi_+ = e^{i(\delta + \varphi/2)} \sin \frac{1}{2}\theta \tag{9}$$

Where φ, θ are the polar and azimuthal angels, respectively and δ is an arbitrary phase.
In order to see why this representation is correct, we start by evaluating the probability of detecting the particle spinning up, w.r.t. the z direction:

$$|\chi_+|^2 = \cos^2 \frac{1}{2}\theta \tag{10}$$

Similarly for the down direction:

$$|\chi_-|^2 = 1 - \chi_+|^2 = 1 - \cos^2 \frac{1}{2}\theta = \sin^2 \frac{1}{2}\theta \tag{11}$$

It is clear now, what is the rôle of the magnitude of the spin states, in terms of θ. However, we need to discuss further the rôle that the phase plays.
Lets start by calculating the expected values of the spin operators:

$$\begin{aligned} \langle \hat{S}_x \rangle &= \frac{1}{2} \sin\theta \cos\varphi \\ \langle \hat{S}_y \rangle &= \frac{1}{2} \sin\theta \sin\varphi \\ \langle \hat{S}_z \rangle &= \frac{1}{2} \cos\theta \end{aligned} \tag{12}$$

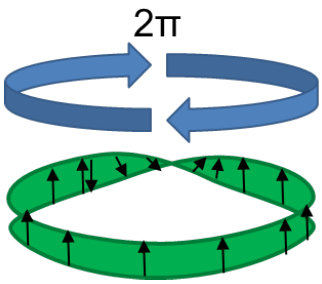

Figure 1: A spinor transformation can be thought of as a vector on a Möbius band.

Now, assume we wish to rotate the coordinates by an angle γ around z. We have the rotation matrix :

$$R(\gamma) = \begin{pmatrix} e^{i\gamma/2} & 0 \\ 0 & e^{-i\gamma/2} \end{pmatrix} \tag{13}$$

Applied to the spinor χ is equal to:

$$R(\gamma)\chi \ = \begin{pmatrix} e^{i(\delta-\frac{1}{2}(\varphi-\gamma))}\cos\frac{1}{2}\theta \\ e^{i(\delta+\frac{1}{2}(\varphi-\gamma))}\sin\frac{1}{2}\theta \end{pmatrix} \tag{14}$$

Notice that, in order for the spinor to return to its original state, before rotation, one needs not to make a 2ϕ rotation. Rather a rotation by 4π. This is the main characteristic of spinors, that makes them ' very' different from vectors, and manifesting itself in terms of the phase factor in the geometrical representation. Sometimes we denote this characteristic by saying that the ' group' of spin transformations **double covers** the 'group' of spatial transformations.

In order to picture this in a deeper way, one can think of the spinor's internal space as a Möbius band - illustrated in the figure 1. A vector on the Möbius band needs to be transported along the band twice, in order to return to its initial state.

SPIN IN CONSTANT MAGNETIC FIELD

A particle with a spin - an electron- for example is put in a constant magnetic filed, such that the direction of the field is parallel to the z-component of the spin. The Hamiltonian for such system is given by:

$$H = -\gamma\vec{B}\cdot\vec{S} \tag{15}$$

such that $\gamma = e/m$, the ratio between the electron's charge and its mass.And $\vec{B}\cdot\vec{S} = BS_z$.

It is clear that:

$$[H, S_z] = 0 \tag{16}$$

Implying that there exist eigenstates for H and S simultaneously. Since we already know the eigenstates for S_z, and represented by the spinor χ . We then write :

$$H\chi = E\chi \tag{17}$$

or:

$$-\gamma B\,S_z\chi = E\chi. \tag{18}$$

Since, $S_z\chi = \pm\frac{1}{2}\hbar\chi$ The eigenenergies are:

$$E_{\pm} = \mp\mu_B B \tag{19}$$

The constant $\mu_B = \frac{e\hbar}{2m_e}$ is Born magneton. It is necessary to add another constant g_s as we have seen earlier to this equation, known as the Landé g-factor, because the electron *precesses* in the magnetic field. We then have:

$$E_{\pm} = \mp g_s\mu_B B \tag{20}$$

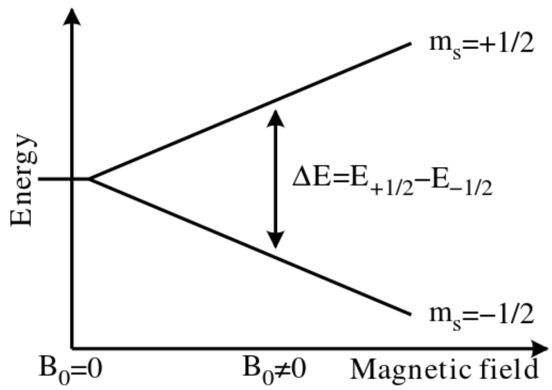

Figure 2: Energy states of electron in a magnetic field B.

Stationary states

Since we have found the energy spectrum for an electron in magnetic field, we may now write the time evolution of the state χ, using the equation:

$$\chi(t) = e^{-i\omega t}\chi(0) \tag{21}$$

We have then, for A and B are normilisation constants:

$$\chi(t) = Ae^{-i\omega t}\chi_+ + Be^{i\omega t}\chi_- \tag{22}$$

or:

$$\chi(t) = Ae^{i\frac{1}{2}\gamma Bt}\begin{pmatrix}1\\0\end{pmatrix} + Be^{-i\frac{1}{2}\gamma Bt}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}Ae^{i\frac{1}{2}\gamma Bt}\\Be^{-i\frac{1}{2}\gamma Bt}\end{pmatrix} \tag{23}$$

electron paramagnetic resonance epr

From the above analysis, we have learnt that an electron in a magnetic field could occupy one of two energy states, depending on m_s :

$$E_{m_s} = m_s g_s \mu_B B \tag{24}$$

A transition from one energy state to another, is obtained by absorption /

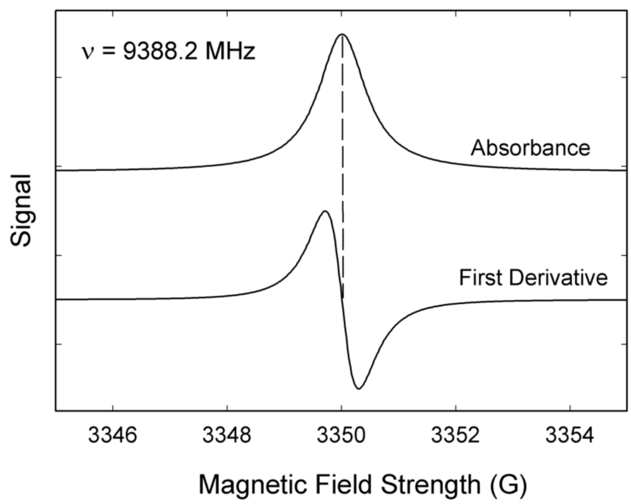

Figure 3: EPR absorbtion resonance for $\nu = 9388.3MHz$

emission of photon of energy equal to $\Delta E = g_s\mu_B B$:

$$h\nu_r = g_s\mu_B B \tag{25}$$

If an ensemble of electrons in the magnetic field is exposed to photons of frequency $\nu = nu_r$, then the electrons shall absorb them, otherwise no absorption will occur -only ellastic scattering-. This peak of absorption is known as **electron paramagnetic resonance** or EPR. Moreover, ν_r is kown as the resonance frequency.

This phenomena is very important in may areas , like measuring the value of the g factor, and detecting *free radicals* in biological systems.
In order to understand the reason for detecting absorption lines rather than the emission lines in EPR, we turn to calculating the population of electrons in the upper energy level n_{upper} and the lower level n_{lower}, using Maxwell-Blotzman statistics, under a thermodynamic termprature T :

$$\frac{n_{\text{upper}}}{n_{\text{lower}}} = \exp\left(-\frac{E_{\text{upper}} - E_{\text{lower}}}{kT}\right) = \exp\left(-\frac{\Delta E}{kT}\right) = \exp\left(-\frac{h\nu_r}{kT}\right) \tag{26}$$

Where k is Boltzmann constant .
We observe that at room temperature $T \sim 300K$ and typical microwave frequency $\nu_r \sim 9.7GHz$ the ratio is about $n_{upper}/n_{lower} \approx 0.998$. That means the upper population is slightly less than the lower one, implying transitions from the lower to upper energy states is more probable than the reverse transitions.