

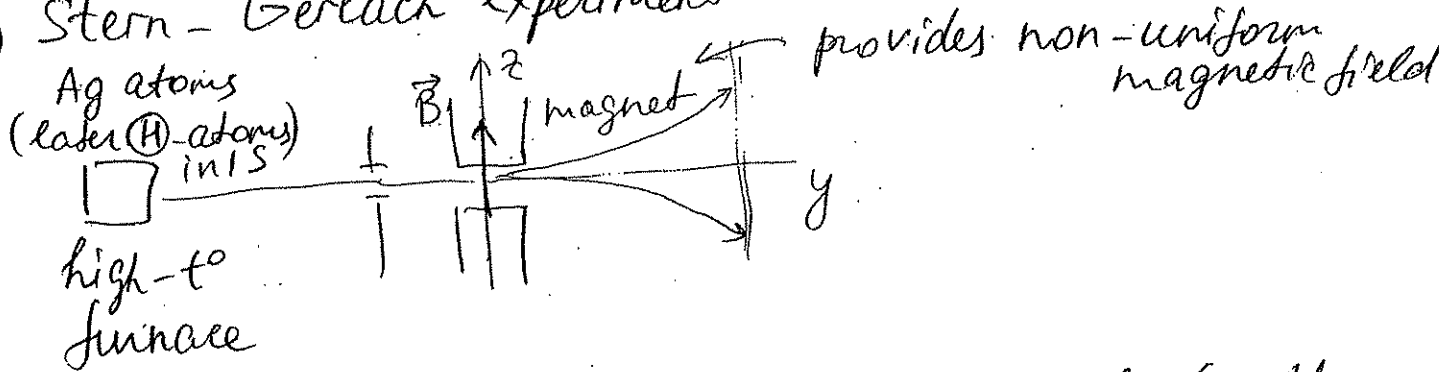
Spin

1925: Goudsmit & Uhlenbeck hypothesis

Every electron has an intrinsic angular momentum (spin) of $\frac{\hbar}{2}$, which corresponds to a magnetic moment of one Bohr magneton $\mu_B = \frac{q\hbar}{2m_e}$

This hypothesis was based on several experimental facts:

1) Stern - Gerlach experiment



(H)-atom in magnetic fields is described by (if the spin is not taken into account)

$$H = \underbrace{H_0}_{\frac{\vec{p}^2}{2m_e} = \frac{e^2}{r}} + \underbrace{H_1}_{-\vec{M} \cdot \vec{B}} + \underbrace{H_2}_{\frac{q^2 \vec{B}^2}{8m_e} (x^2 + y^2)}$$

$\vec{M} = \frac{q}{2m_e} \vec{L}$ ← orbital angular momentum

← diamagnetic term

← paramagnetic term

↓ typically much smaller than paramagnetic

The force acting on an atom in a non-uniform magnetic field is $\vec{F} = -\vec{\nabla}(-\vec{M} \cdot \vec{B}) = M_z \vec{\nabla} B_z$

Experimental result; beam splits into two components $\Rightarrow M_z$ can assume two values

If (H) -atoms are in 1s state $\Rightarrow l=0 \Rightarrow L_z=0 \Rightarrow M_z=0$ where from?
 \Downarrow must be something else (no splitting expected)

spin $\vec{S} \Rightarrow \vec{M}_s = \frac{q}{m_e} \vec{S}$

if $S_z |\psi\rangle = \hbar m_s |\psi\rangle$ (in general, $\vec{M} = g \left(\frac{q}{2m_e} \right) \vec{J}$)

$m_s = \pm \frac{1}{2} \Rightarrow S_z = \pm \frac{\hbar}{2}$

↑ gyromagnetic ratio

2) Anomalous Zeeman effect

Consider (H) -atom in a magnetic field (with no spin) \Rightarrow

$(H_0 + H_1) |n, l, m\rangle = ?$ Since $H_1 = -\vec{M} \cdot \vec{B} = -\frac{\mu_B}{\hbar} \vec{L} \cdot \vec{B} = -\frac{\mu_B}{\hbar} L_z B$ $\uparrow B \parallel O_z$
 $[H_0, H_1] = 0$ (because $[H_0, L_z] = 0$)
 then H_0 & H_1 share the same eigenstates \Rightarrow

$(H_0 - \frac{\mu_B}{\hbar} B L_z) |n, l, m\rangle = (E_n - \frac{\mu_B}{\hbar} B \cdot \hbar m) |n, l, m\rangle$

Energy in a B-field is $E_n - \mu_B B m$ ← degeneracy with respect to m is removed

This means that the n th level which is normally n^2 -degenerate

$$E_n = -\frac{E_1}{n^2} \quad \left\{ \begin{array}{l} m = -l \\ m = 0 \\ m = +l \end{array} \right. \quad E = E_n - \mu_B B m \quad (3)$$

splits into $(2l+1)$ -sublevels

Zeeman effect

Since l is an integer \Rightarrow supposed to get an odd number of levels

Experiment: even number \rightarrow "anomalous" Zeeman effect in (H) atom

introduce spin degrees of freedom

The system is described by a set $\{H, \vec{L}, L_z, \vec{S}, S_z\}$

Properties of spin operators

1) \vec{S} is an angular momentum

external (orbital) degrees of freedom \uparrow spin degrees of freedom \uparrow

general rules apply, e.g. $[S_i, S_j] = i\hbar \epsilon_{ijk} S_k$

2) Similar to the orbital angular momentum

$$\vec{L}^2 |l, m\rangle = \hbar^2 l(l+1) |l, m\rangle$$

$$\vec{S}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle$$

$$L_z |l, m\rangle = \hbar m |l, m\rangle$$

$$\Leftrightarrow S_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle$$

$$|m| \leq l$$

$$|m_s| \leq s$$

A given particle is characterized by a unique value of s

3) All spin observables commute with all orbital observables, e.g. $[\vec{L}^2, \vec{S}^2] = 0$, etc. (4)

4) In the case of the electron $s = \frac{1}{2} \Rightarrow$ there are $2s + 1 = 2$ spin degrees of freedom \Rightarrow

the spin states are $|+\rangle \equiv |\frac{1}{2}, \frac{1}{2}\rangle$

$|-\rangle \equiv |\frac{1}{2}, -\frac{1}{2}\rangle$

Then, $\vec{S}^2 |\pm\rangle = \hbar^2 \cdot \frac{3}{4} |\pm\rangle$ $\left\{ \begin{array}{l} s \\ m_s \end{array} \right. S_z |\pm\rangle = \pm \frac{\hbar}{2} |\pm\rangle$

• Orthogonality:

$$\langle + | - \rangle = \langle - | + \rangle = 0; \quad \langle + | + \rangle = \langle - | - \rangle = 1$$

• Closure:

$$|+\rangle \langle +| + |-\rangle \langle -| = 1$$

• Projection operators $P_+ = |+\rangle \langle +|$

$$P_- = |-\rangle \langle -|$$

• Raising & lowering operators

$$S_{\pm} = S_x \pm iS_y \quad \Rightarrow \quad S_{\pm} |\pm\rangle = 0$$

$$\text{Recall } \Rightarrow \begin{cases} S_- |+\rangle = \hbar |-\rangle \\ S_+ |-\rangle = \hbar |+\rangle \end{cases}$$

$$J_{\pm} |j, m\rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)} |j, m \pm 1\rangle$$

($j = \frac{1}{2}$, $m = m_s = \pm \frac{1}{2}$ for $|\pm\rangle$ in this case)

• Matrix representations

$$|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv \chi_+, \quad |-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \chi_-$$

Then, an arbitrary spin state would be described as

$$|\alpha\rangle = P_+ |\alpha\rangle + P_- |\alpha\rangle = |+\rangle \langle +|\alpha\rangle + |-\rangle \langle -|\alpha\rangle \doteq \begin{pmatrix} \langle +|\alpha\rangle \\ \langle -|\alpha\rangle \end{pmatrix} \equiv \begin{pmatrix} C_+ \\ C_- \end{pmatrix} \leftarrow \begin{matrix} \text{2-component} \\ \text{spinor} \end{matrix} = C_+ \chi_+ + C_- \chi_-$$

Similarly, $\langle \alpha| \doteq (\langle \alpha|+, \langle \alpha|-) = (C_+^*, C_-^*)$

Any operator in the $\{|+\rangle, |-\rangle\}$ basis can be represented by 2×2 matrix \Rightarrow

Ex. $S_z | \pm \rangle = \hbar \cdot (\pm \frac{1}{2}) | \pm \rangle$

$$S_z \doteq \begin{matrix} \begin{matrix} \downarrow \\ \begin{matrix} |+\rangle & |-\rangle \end{matrix} \end{matrix} \\ \begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix} \begin{matrix} \langle +| \\ \langle -| \end{matrix} \end{matrix} \quad \textcircled{=}$$

$$\begin{aligned} \langle +|S_z|+\rangle &= \frac{\hbar}{2} \\ \langle -|S_z|-\rangle &= -\frac{\hbar}{2} \\ \langle +|S_z|-\rangle &= 0 \end{aligned}$$

$$\textcircled{=} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Similarly, $S_+ \doteq \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad S_- \doteq \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

It is customary to introduce Pauli matrices

(6)

$$\hat{S} = \frac{\hbar}{2} \hat{\sigma}, \quad \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

↑
Pauli
matrices

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Properties of the Pauli matrices

- $\hat{\sigma}_x^2 = \hat{\sigma}_y^2 = \hat{\sigma}_z^2 = 1$ ← identity matrix
- $\hat{\sigma}_i \hat{\sigma}_j + \hat{\sigma}_j \hat{\sigma}_i = 0$ ($i \neq j$)
- $[\hat{\sigma}_i, \hat{\sigma}_j] = 2i \epsilon_{ijk} \hat{\sigma}_k$
- $\hat{\sigma}_i^\dagger = \hat{\sigma}_i$ ← Hermitian
- $\det \hat{\sigma}_i = -1$
- $\text{Tr} \hat{\sigma}_i = 0$

HW: prove that $(\hat{\sigma} \cdot \vec{a})(\hat{\sigma} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i \hat{\sigma} \cdot (\vec{a} \times \vec{b})$

Sakurai:

Reading: pp. 163-165
pp. 26-29

Examples of operations with Pauli matrices (7)

1) Express $(2I + \sigma_x)^{-1}$ as a linear combination of the Pauli matrices and I .

Solution ;

$$(2I + \sigma_x)^{-1} = \frac{1}{2} (I + \frac{\sigma_x}{2})^{-1} = \frac{1}{2} \left\{ I - \frac{\sigma_x}{2} + \left(\frac{\sigma_x}{2}\right)^2 - \left(\frac{\sigma_x}{2}\right)^3 + \dots \right\}$$

$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + \dots$$

$$= \frac{1}{2} \left\{ I - \frac{\sigma_x}{2} + \frac{I}{2^2} - \frac{1}{8} \sigma_x + \dots \right\} =$$

$\sigma_x^2 = I$

$$= \frac{1}{2} \left\{ I \left(1 + \frac{1}{2^2} + \frac{1}{2^4} + \dots \right) - \frac{\sigma_x}{2} \left(1 + \frac{1}{2^2} + \frac{1}{2^4} + \dots \right) \right\} =$$

$$= \frac{1}{2} \cdot \frac{4}{3} (I - \frac{\sigma_x}{2})$$

$\frac{1}{1 - \frac{1}{4}} = \frac{4}{3}$

$$= \boxed{\frac{2}{3} I - \frac{1}{3} \sigma_x}$$

geometric progression
 $\sum_{n=0}^{\infty} q^n = \frac{1}{1-q}$
 for $|q| < 1$

2) Expand σ_x^{-1} in terms of the Pauli matrices ⑧

Consider $\vec{n} = (1, 0, 0) \Rightarrow$

$$\underline{e^{-i\frac{\varphi}{2}\vec{\sigma}\cdot\vec{n}}} = \underline{e^{-i\frac{\varphi}{2}\sigma_x}} = \underline{\cos\frac{\varphi}{2} - i\sigma_x\sin\frac{\varphi}{2}}$$

Then, if $\varphi = \pi \Rightarrow e^{-i\frac{\pi}{2}\sigma_x} = 0 - i\sigma_x = -i\sigma_x$

so $\underline{\sigma_x = ie^{-i\frac{\pi}{2}\sigma_x}} \Rightarrow$

$$\sigma_x^{-1} = -ie^{i\frac{\pi}{2}\sigma_x} = -i \left(\underbrace{\cos\frac{\pi}{2}}_{0} + i \underbrace{\left(\sin\frac{\pi}{2}\right)\sigma_x}_{1} \right) \textcircled{=}$$

$\textcircled{=} \sigma_x \Rightarrow \boxed{\sigma_x^{-1} = \sigma_x}$

aka Direct products \rightarrow Tensor products

As we know, each quantum state of a particle is characterized by a state vector $|\psi\rangle \in \mathcal{E}$

If $|\psi\rangle$ describes a state of one particle in a 1D space $\Rightarrow |\psi\rangle \in \mathcal{E}_x$

Recall \Rightarrow Phys 657 \Rightarrow abstract space (sub-space of a Hilbert space) \uparrow called "state space"

If same in a 3D space $\Rightarrow |\psi\rangle \in \mathcal{E}_{\vec{r}}$

What is the relationship between \mathcal{E}_x and $\mathcal{E}_{\vec{r}}$?

Consider $\psi(\vec{r}) = \underbrace{\psi_x(x)}_{\in \mathcal{E}_x} \underbrace{\psi_y(y)}_{\in \mathcal{E}_y} \underbrace{\psi_z(z)}_{\in \mathcal{E}_z} \in \mathcal{E}_{\vec{r}}$

present this in terms of state vectors \Rightarrow

$|\psi\rangle = |\psi_x\rangle \otimes |\psi_y\rangle \otimes |\psi_z\rangle$
 $\in \mathcal{E}_{\vec{r}}$, where $\mathcal{E}_{\vec{r}} = \mathcal{E}_x \otimes \mathcal{E}_y \otimes \mathcal{E}_z$

\uparrow
 tensor product

The vector space \mathcal{E} is called the tensor product \otimes of \mathcal{E}_1 and \mathcal{E}_2 , i.e. $\mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_2$, if there is a vector $|\Psi_1\rangle \otimes |\chi_2\rangle \in \mathcal{E}$ associated with each pair of vectors $|\Psi_1\rangle \in \mathcal{E}_1$ and $|\chi_2\rangle \in \mathcal{E}_2$ satisfying the following conditions: ↑
belong to space \mathcal{E}_i

- It is linear with respect to multiplication by complex numbers.

$$(\lambda |\Psi_1\rangle) \otimes |\chi_2\rangle = \lambda (|\Psi_1\rangle \otimes |\chi_2\rangle)$$

$$|\Psi_1\rangle \otimes (\mu |\chi_2\rangle) = \mu (|\Psi_1\rangle \otimes |\chi_2\rangle)$$

- It is distributive with respect to vector addition.

$$|\Psi_1\rangle \otimes (|\chi_2\rangle + |\chi_2'\rangle) = |\Psi_1\rangle \otimes |\chi_2\rangle + |\Psi_1\rangle \otimes |\chi_2'\rangle$$

↑
another
vector
from space \mathcal{E}_2

←
from space \mathcal{E}_1

$$(|\Psi_1\rangle + |\xi_1\rangle) \otimes |\chi_2\rangle = |\Psi_1\rangle \otimes |\chi_2\rangle + |\xi_1\rangle \otimes |\chi_2\rangle$$

- When a basis has been chosen in each of the spaces \mathcal{E}_1 and \mathcal{E}_2 (e.g. $\{ |u_{i,1}\rangle \}$ in \mathcal{E}_1 and

$\{ |v_{j,2}\rangle \}$ in \mathcal{E}_2), the set of vectors

$\{ |u_{i,1}\rangle \otimes |v_{j,2}\rangle \}$ constitutes a basis in \mathcal{E}

If N_1 and N_2 are dimensions of E_1 and E_2 , the (11)
 dimension of $E = E_1 \otimes E_2$ is $N = N_1 N_2$

Note: the indexes 1 & 2 in E_1, E_2 may be referred to x and y , particles 1 and 2, etc.

Example Before we introduced spin, we described the (H) -atom states as $|n, l, m\rangle \in E_{\vec{r}}$

Introduction of spin requires spin variable ∞ -dimensional

$|S, m_s\rangle \in E_S \leftarrow$ for a given $(2s+1)$ -dimensional particle

Altogether $\Rightarrow |n, l, m; S, m_s\rangle = |n, l, m\rangle \otimes |S, m_s\rangle$

$$E = E_{\vec{r}} \otimes E_S$$

Theorem Operators acting in different spaces commute

Proof Consider arbitrary operators A_1 and B_2 acting in the spaces E_1 and E_2 , respectively.

Let's act on a state vector $|\Psi\rangle = |u_1\rangle \otimes |v_2\rangle$

To ensure proper dimensionality $E = E_1 \otimes E_2$

present A_1 and B_2 as $A_1 \otimes I_2$ and $I_1 \otimes B_2$

Then,

↑ identity in space E_2 ↑ in space E_1

$$[A_1 \otimes I_2, I_1 \otimes B_2] |\Psi\rangle = A_1 \otimes I_2 I_1 \otimes B_2 |\Psi\rangle -$$

$$- I_1 \otimes B_2 A_1 \otimes I_2 |\psi\rangle = A_1 \otimes I_2 I_1 |u_1\rangle \otimes B_2 |v_2\rangle \quad (2)$$

$$- I_1 \otimes B_2 A_1 |u_1\rangle \otimes I_2 |v_2\rangle = A_1 \otimes I_2 |u_1\rangle \otimes B_2 |v_2\rangle$$

$$- I_1 \otimes B_2 A_1 |u_1\rangle \otimes |v_2\rangle \stackrel{\text{see HW \# 8 (b)}}{=} A_1 |u_1\rangle \otimes B_2 |v_2\rangle -$$

$$- A_1 |u_1\rangle \otimes B_2 |v_2\rangle = 0 \Rightarrow [A_1 \otimes I_2, I_1 \otimes B_2] = 0$$

Examples of tensor product calculation

Consider basis vectors $|u_1\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|u_2\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

of the basis $\{|u_i\rangle\} \in \mathcal{E}_u \Leftrightarrow N_1 = 2 \leftarrow \text{dimensionality of the } \mathcal{E}_u$

and $|v_1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$; $|v_2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$; $|v_3\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

of the basis $\{|v_j\rangle\} \in \mathcal{E}_v$ with $N_2 = 3$

What is $|u_i\rangle \otimes |v_j\rangle \in \mathcal{E} = \mathcal{E}_u \otimes \mathcal{E}_v$?

$N = N_1 N_2 = 2 \cdot 3 = 6 \leftarrow \text{dimensionality of } \mathcal{E}$

The new basis vectors are $|u_1\rangle \otimes |v_1\rangle$, $|u_1\rangle \otimes |v_2\rangle$, $|u_1\rangle \otimes |v_3\rangle$, $|u_2\rangle \otimes |v_1\rangle$, $|u_2\rangle \otimes |v_2\rangle$, $|u_2\rangle \otimes |v_3\rangle$.

Let's write them out in terms of six-component vectors \Rightarrow
column

$$|u_1\rangle \otimes |v_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}; \quad |u_1\rangle \otimes |v_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad (3)$$

$$|u_1\rangle \otimes |v_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}; \quad |u_2\rangle \otimes |v_1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|u_2\rangle \otimes |v_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}; \quad |u_2\rangle \otimes |v_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Note: for arbitrary 2D vectors $|u\rangle$
and 3D $|v\rangle \Rightarrow$

$$|u\rangle \otimes |v\rangle = \begin{pmatrix} u_1 v_1 \\ u_1 v_2 \\ u_1 v_3 \\ \hline u_2 v_1 \\ u_2 v_2 \\ u_2 v_3 \end{pmatrix}$$

What if we take matrices instead of the vectors?

Consider $A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}; \quad I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

($N_1=2$) ($N_2=3$)

$$A \otimes I = \begin{pmatrix} a_{11} & 0 & 0 & a_{12} & 0 & 0 \\ 0 & a_{11} & 0 & 0 & a_{12} & 0 \\ 0 & 0 & a_{11} & 0 & 0 & a_{12} \\ \hline a_{21} & 0 & 0 & a_{22} & 0 & 0 \\ 0 & a_{21} & 0 & 0 & a_{22} & 0 \\ 0 & 0 & a_{21} & 0 & 0 & a_{22} \end{pmatrix} \Leftarrow 6 \times 6$$

In a general case of 2×2 matrix A & 3×3 matrix B (14)

\swarrow $(N_1=2)$ \nwarrow $(N_2=3)$

$$A \otimes B = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{11}b_{13} & a_{12}b_{11} & a_{12}b_{12} & a_{12}b_{13} \\ a_{11}b_{21} & a_{11}b_{22} & a_{11}b_{23} & a_{12}b_{21} & a_{12}b_{22} & a_{12}b_{23} \\ a_{11}b_{31} & a_{11}b_{32} & a_{11}b_{33} & a_{12}b_{31} & a_{12}b_{32} & a_{12}b_{33} \\ a_{21}b_{11} & a_{21}b_{12} & a_{21}b_{13} & a_{22}b_{11} & a_{22}b_{12} & a_{22}b_{13} \\ a_{21}b_{21} & a_{21}b_{22} & a_{21}b_{23} & a_{22}b_{21} & a_{22}b_{22} & a_{22}b_{23} \\ a_{21}b_{31} & a_{21}b_{32} & a_{21}b_{33} & a_{22}b_{31} & a_{22}b_{32} & a_{22}b_{33} \end{pmatrix}$$

Useful relations

$$\det(A \otimes B) = (\det A)^{N_2} (\det B)^{N_1}$$

(N_1 - dimensionality of A
 N_2 - - - - of B)

$$T_2(A \otimes B) = (T_2 A)(T_2 B)$$