PHYS261 Atomic Physics and Physical Optics

Lectures

Thursday 4. September 2008
Tuesday 9. September 2008

Topics:

Helium; Antisymmetry of 2 electron wavefunction; Spin

Comment:

Thursday: One hour Only; Visiting a seminar;
Tuesday: Crashed the notes; Preliminary version; 2007 included
Preliminary version;

Parity homework

Decompose $f(r)$ into positive and negative parity parts
$p(r)$ is such that $p(r) = p(-r)$
$n(r)$ is such that $n(r) = -n(-r)$

$f(r)=p(r)+n(r)$
$f(-r)=p(-r)+n(-r)$ but this is also $f(-r)=p(r)-n(r)$ from above

Thus we obtain a set of equations

$$\begin{aligned} f(r) &= p(r)+n(r) \\ f(-r) &= p(r)-n(r) \quad \Rightarrow \quad 2\,p(r) = f(r) + f(-r) \\ & \qquad\qquad\qquad\quad\; 2\,n(r) = f(r) - f(-r) \end{aligned}$$

which gives us the answer
$p(r) = (\ f(r) + f(-r)\ )/2$
$n(r) = (\ f(r) - f(-r)\ )/2$

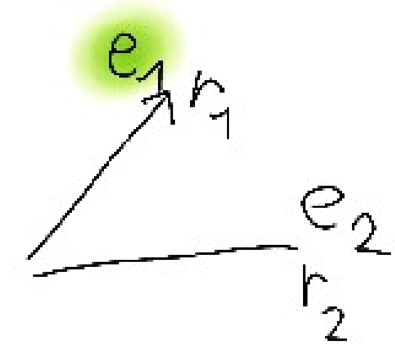
This simple property is somewhat anologous to the operations needed in constracting «symmetric» and «antisymmetric» functions for two electrons

Exchange symmetry $\rightleftarrows$ Pauli Principle

Indistinguishable particles / identical

$\underbrace{\Psi(r_1, r_2)}$ electron 1 in r_1

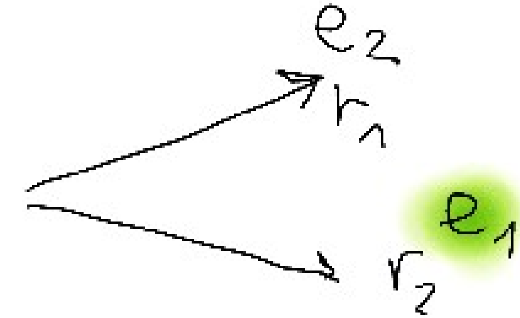
-"- 2 in r_2



$$\left|\Psi(r_1, r_2)\right|^2 \equiv \left|\Psi(r_2, r_1)\right|^2$$

indisting. —

Probability density



$$\varphi(r_1, r_2) + \varphi(r_2, r_1) = \Psi(r_1, r_2)$$

In analogy with the parity exercise

The "derivation" is more formal

$$|\psi(r_1, r_2)|^2 \equiv |\psi(r_2, r_1)|^2$$

$$\psi(r_1, r_2) \equiv \pm\psi(r_2, r_1)$$

$$\psi(r_1, r_2) \equiv e^{i\alpha}\psi(r_2, r_1)$$

We derive this through EXCHANGE Operation → <u>operator</u>

$$\mathbb{A}_{12}\,\psi(r_1, r_2) = \psi(r_2, r_1)$$

$$A_{12}\mathbb{A}_{12}\,\psi(r_1, r_2) = A_{12}\psi(r_2, r_1) = \psi(r_1, r_2)$$

$$A_{12} \cdot A_{12} = \mathbb{1}$$

$A_{12}^2 = 1$ $\qquad A_{12}\psi(1,2) = \psi(2,1) = e^{i\alpha}\psi(1,2)$

$\psi(1,2)$ satisfying the indistinguish.
must be an eigenfunction

$|e^{i\alpha}| = 1$ $\qquad$ only two possible eigenvalues

$$A_{12}^2 = 1 \Longrightarrow \left(e^{i\alpha}\right)^2 = 1 \qquad e^{2i\alpha} = 1$$

$$e^{i\alpha} \begin{cases} e^{i0} = 1 \Longrightarrow & \alpha = 0 \\ & \alpha = 2\pi + \dots \\ e^{i\pi} = -1 & \end{cases}$$

Operation of exchange $\begin{cases} + \\ - \end{cases}$ sign

Generalization to many particles

$$\psi(r_1, r_2) = \pm \psi(r_2, r_1)$$

$$\psi(r_1, r_2) \stackrel{?}{=} \varphi_1(r_1)\, \varphi_2(r_2) \;?$$

$$\psi_S(r_1, r_2) = \frac{1}{\sqrt{2}} \left[\varphi_1(r_1)\, \varphi_2(r_2) + \varphi_2(r_1)\, \varphi_1(r_2) \right]$$

$$\cancel{+ \varphi_1(r_2)\, \varphi_2(r_1)}$$

Normalization factor $\longrightarrow$ $\langle \varphi_1 | \varphi_2 \rangle = 0 \quad 1 \neq 2$

$$\psi_A(r_1, r_2) = \frac{1}{\sqrt{2}} \left[\varphi_1(r_1)\, \varphi_2(r_2) - \varphi_2(r_1)\, \varphi_1(r_2) \right]$$

S Symmetric

A Antisymmetric

$+$ $-$ (anti-) symmetric with respect to exchange

Spin — a "new" property
resembling angular momentum
(or magnetic dipole moment)
Why is angular momentum (normal)
related to magnetic moment ?

Spin "derived" from Dirac Equation
Relativistic Schrödinger Equation

Lecture

Tuesday 9. September 2008

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Spin $\longleftrightarrow$ Angular momentum (not really)

Orbital ang. mom $\vec{L}$ $\vec{l}$

Spin —"— $\vec{S}$ $\vec{s}$

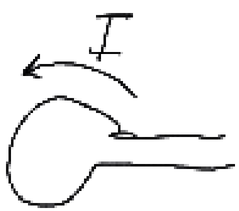
two systems $\longrightarrow$ total $\vec{L} = \vec{l}_1 + \vec{l}_2$

Generalize : $\vec{S} = \vec{s}_1 + \vec{s}_2$

Spin "more connected" with <u>Magnetic Moment</u>

Dipole $\rightarrow$ magnetic dipole .....

(Ferromagnets ....)



current loop ..... Magnetic moment

$\vec{\mu} = \vec{A} \cdot J \cdot \text{Const}$

area vector

$\vec{L}$ $\vec{\mu}$ .... simple connection

circular motion of charged particle
(orbital)

$\longrightarrow$ angula momentum

$\longrightarrow$ magnetic moment

Orbital angular M → Magnetic moment

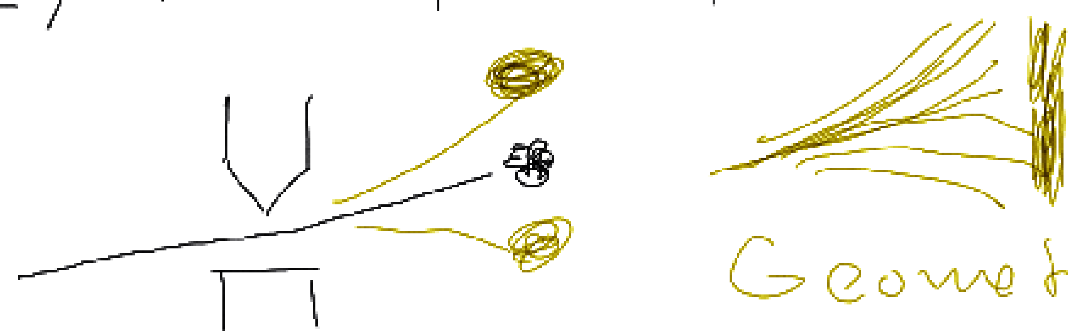
Spin magnetic moment $\xrightarrow[\text{associate}]{}$ spin angular moment

CAN BE "DERIVED" from DIRAC EQUATION

Pauli postulated

1) Spin $\vec{s}$ (Stern-Gerlach exp.)

2) Pauli principle (Aufbau → Build up)



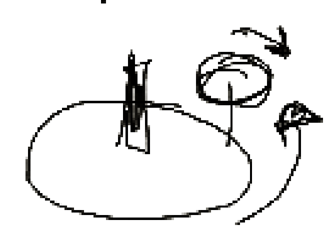
classical

Geometrical Quant.

Orbital, spatial motion

IF

Spin "motion" (internal) ((intrinsic))



→ MORE COMPLEX DESCRIPTION

we crashed on Lx, Ly, Lz
Wikipedia instead

Mathematical definition

[edit]

Angular momentum **L** is mathematically defined as the cross product of a wave function's position operator (**r**) and momentum operator (**p**):

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

In the special case of a single particle with no electric charge and no spin, the angular momentum operator can be written in the position basis as a single vector equation:

$$\mathbf{L} = -i\hbar(\mathbf{r} \times \nabla)$$

where ∇ is the gradient operator. This is a commonly encountered form of the angular momentum operator, though not the most general one.

We try the spin once more:

Eigenfunctions of $L^2 L_z \longrightarrow Y_{lm}(\vartheta, \varphi)$

— " — of $\sigma^2, \sigma_z \longrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$\sigma_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\sigma_y \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$\sigma_z \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\sigma^2 = 1 + 1 + 1$

$\sigma_x^2 = 1$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

etc. ...

Homework ....

Eigenvectors,
Eigenvalues

$$\vec{S} = \frac{\hbar}{2} \vec{\sigma} \qquad \left(\frac{\hbar}{2} \sigma_x, \frac{\hbar}{2} \sigma_y, \frac{\hbar}{2} \sigma_z \right)$$

$\begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdots \begin{pmatrix} f(x) \\ g(x) \end{pmatrix} \longrightarrow \chi$

represent the spin variable

spin and space function

$$\begin{pmatrix} f(\vec{r}) \\ g(\vec{r}) \end{pmatrix}$$

space and spin motion depend "on each other)

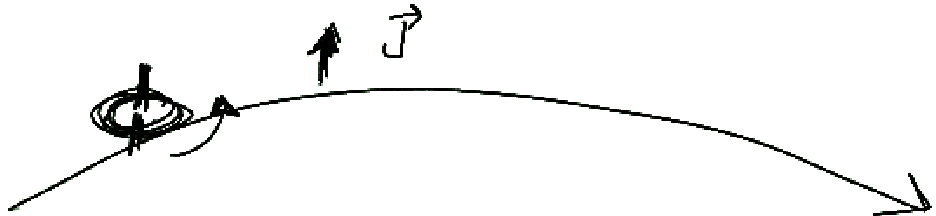
$$u(\vec{r}) \cdot \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

a_1, a_2 numbers

independent

Product

assumption



QM $\sqrt{L(L+1)}\,\hbar$ CM $|L|$

integer L

half integer for S

$\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix}$ described by Pauli Spinor

$\begin{pmatrix}b\\a\end{pmatrix}$ $\begin{bmatrix}a\\b\end{bmatrix}$ up dow $\left.\begin{matrix}|a|^2\\|b|^2\end{matrix}\right\}$ Probability

L_x L_y L_z ψ

σ_z $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ $-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)$ L_z

σ_x $\begin{pmatrix}0&1\\1&0\end{pmatrix}$ $-i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)$ L_x

σ_y $\begin{pmatrix}0&-i\\i&0\end{pmatrix}$ $\frac{1}{2}\hbar\,\sigma_x$ $\frac{1}{2}\hbar\,\sigma_y$ $\frac{1}{2}\hbar\,\sigma_z$ $\boxed{e^{i\alpha\sigma_x}}$

... When you throw a spinning object, its L keeps the direction. The Earth keeps its L and therefore we have springs, summers, winters ... Discuss that .. (J and L are both used for angular momentum)

Lecture Thursday 30 August 2007 (Revised Sept. 5^{th}, 2007)

$$e^{i\alpha\begin{pmatrix}0&1\\1&0\end{pmatrix}} = I\cos\alpha + i\sin\alpha\begin{pmatrix}0&1\\1&0\end{pmatrix}$$

$$\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix} = \begin{pmatrix}1&0\\0&1\end{pmatrix} \qquad I = 1 = \begin{pmatrix}1&0\\0&1\end{pmatrix}$$

Pauli Matrices

$$e^{i\alpha\begin{pmatrix}0&1\\1&0\end{pmatrix}} = I\cos\alpha + i\sin\alpha\begin{pmatrix}0&1\\1&0\end{pmatrix}$$

$$\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix} = \begin{pmatrix}1&0\\0&1\end{pmatrix} \qquad I = 1 = \begin{pmatrix}1&0\\ \dots\end{pmatrix}$$

Pauli Matrices

$\begin{bmatrix}1\\0\end{bmatrix}$ $\uparrow$ + $\qquad$ $\begin{bmatrix}0\\1\end{bmatrix}$ $\downarrow$ − $\qquad$ $\uparrow$ $\downarrow$

$\uparrow(1)\uparrow(2)$ sym.

$\downarrow(1)\downarrow(2)$ sym

$\frac{1}{\sqrt{2}}\left(\uparrow(1)\downarrow(2)+\downarrow(1)\uparrow(2)\right)$ SYM.

$\uparrow(1)\downarrow(2)$

$\downarrow(1)\uparrow(2)$ no symmetry

$\frac{1}{\sqrt{2}}\left(\uparrow(1)\downarrow(2)-\downarrow(1)\uparrow(2)\right)$ 0 — because $\frac{1}{2}+(-\frac{1}{2})$

Antisymmetric

4 possible $\longrightarrow$ 3 symmetric triplet $S=1$

1 antisymmetric singlet $S=0$

$(2S+1)$ 3

1

$\vec{S}_1 \wedge \vec{S}_2$ $\qquad$ $\vec{S}=\vec{S}_1+\vec{S}_2$ . . . .

Eigenvalues and vectors of $\vec{S}\cdot\vec{S}=S^2$

QUALITATIVE "PROOF"

space SYMMETRIC – Spin ANTISYMMETRIC (spin SINGLET)
space ANTISYMMETRIC – Spin SYMMETRIC (spin TRIPLET)

$$\Psi_A(1,2) = \phi_A(1,2)\,\Xi_S(1,2)$$

$$\Psi_A(1,2) = \phi_S(1,2)\,\Xi_A(1,2)$$

$$\left[\phi_a(r_1)\chi_a(1)\,\phi_b(r_2)\chi_b(2) - \phi_b(r_1)\chi_b(1)\,\phi_a(r_2)\chi_a(2)\right]$$

$$\left[\phi_a(r_1)\phi_b(r_2) \pm \phi_b(r_1)\phi_a(r_2)\right]\left[\chi_a(1)\chi_b(2) \mp \chi_b(1)\chi_a(2)\right]$$

SPACE symmetric	SPIN antisymmetric
SPACE antisymmetric	SPIN symmetric

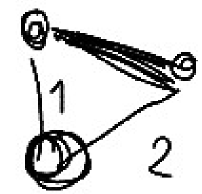
The reason is simple to see now: repulsion is reduced for space asymmetric function
Space asymmetric vanishes (-> 0) when r1 -> r2

Space symmetric → Spin singlet

Space antisymmetric → spin triplet

$$T_1+T_2+V_1+V_2+V_{12}$$

$$+\frac{e^2}{|\vec{r}_1-\vec{r}_2|}$$



space symmetric $\qquad \varphi_a(r_1)\,\varphi_b(r_2)$

$\vec{r}_1=\vec{r}_2 \qquad \varphi_a(r)\,\varphi_b(r)+\varphi_a(r)\,\varphi_b(r)$

BIG REPULSION

space antisymmetric $\qquad$ SMALL REPULSION

$\vec{r}_1=\vec{r}_2 \qquad \varphi_a(r)\,\varphi_b(r)-\varphi_a(r)\,\varphi_b(r)$ $\qquad$ 0 zero

The story you should learn to perform:

Here starting:
The two electron atoms have the spin symmetry feature. You can make the total wavefunction antisymmetric by taking symmetric spin and space function antisymmetric. Or you can take antisymmetric spin and then this aplies space function is symmetric. Symmetric spins are called triplet, because there are 3 of them, antisymmetric is a singlet.

Two electrons repel each other. The repulsion adds energy, positive potential.

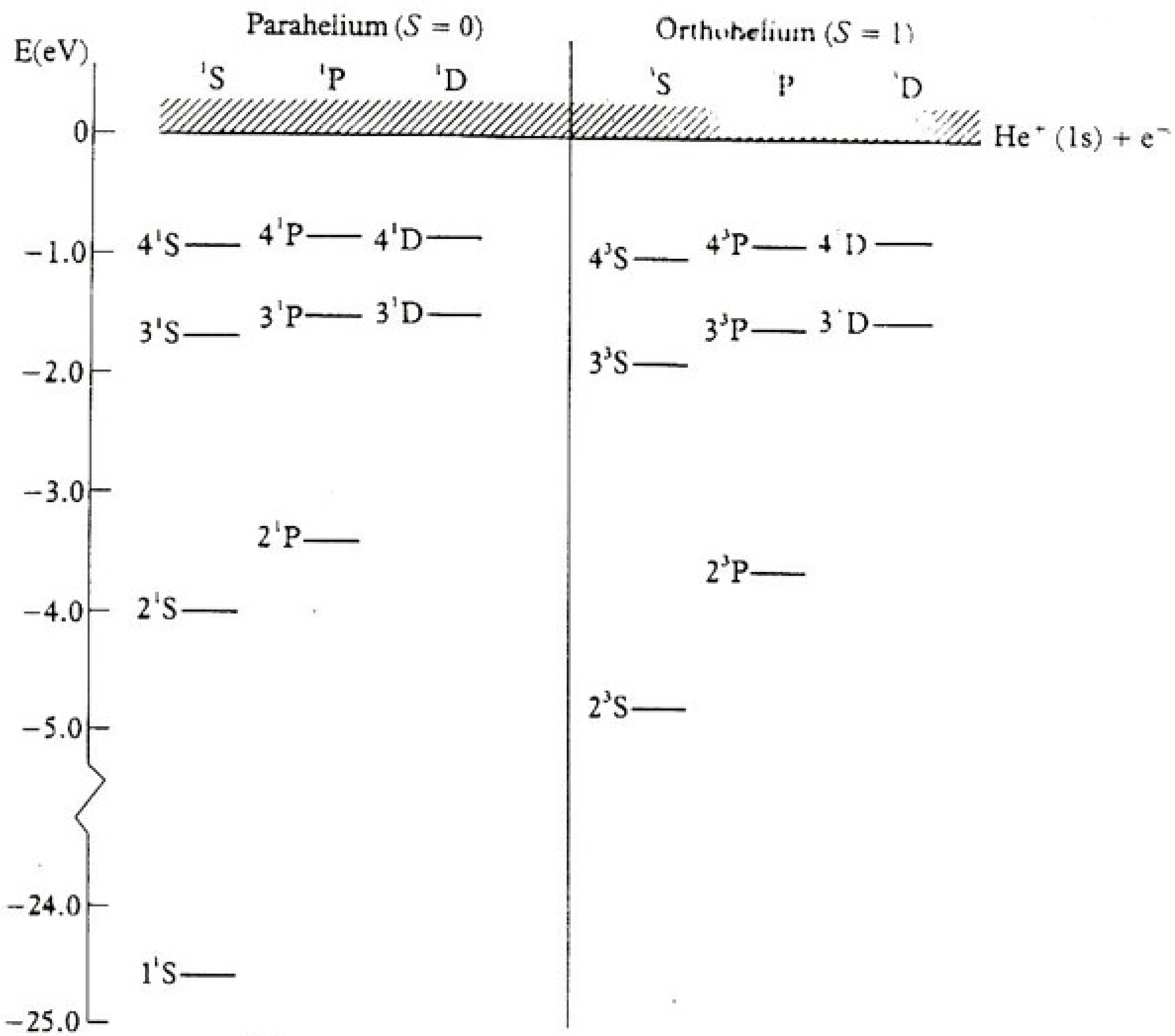
It is now possible to see that the repulsion is larger for singlets than for corresponding triplet. Think e.g. about 1s 2p orbitals, as states a and b. Then schematically

Psi(antisym) -> a(1) b(2) – b(1) a(2)   Psi(sym) -> a(1) b(2) + b(1) a(2)

when the repulsion is greatest? It is when r1->r2 - and then Psi(sym) is BIG,
Psi(antisym) is very small ...

So if you manage to follow:
triplet -> spin SYM -> space ASYM -> for r1->r2 Psi(antisym) is very small the repulsion is very small .
singlet -> spin ASYM -> space SYM -> for r1->r2 Psi(sym) is BIG, the repulsion is BIG,

Experiment – Level scheme for Helium



The experimental values of the lowest energy levels of helium.
$E = 0$ corresponds to the ionisation threshold.

Lecture Thursday 30 August 2007 (Revised Sept. 5th, 2007)

Spin degrees of freedom + Something on Dirac Equation

It might be useful to read about spin in textbooks on Quantum Theory, as well as many different entries on Wikipedia and **Hyperphysics**

(http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html to get there -just google it instead of copying this long link). Both of these sources should be taken as orientation, i.e. not too seriously – i.e. not as «authoritative».

Dirac equation: The story is fascinating. Originally intended to repair the inconsistencies of relativistic Schrödinger euation:

obtained by replacing T+V=E by $p^2 + m^2c^4 = E^2$

from Hyperphysics:

$$E = mc^2 = \sqrt{p^2c^2 + m_0^2c^4}$$

just according to the above. E was taken as in non-rel Schrödinger euation, but the square root was «linearized» using unknown objects, now known as Dirac Matrices:

$$E\, y = c(\, a_x\, p_x + a_y\, p_y + a_z\, p_z + b\, m\, c^2\,)\, y$$

(here E and p_i are the usual operators), but are new type of objects, Dirac spinors.

It lead later to explanation of antiparticles etc etc.

P.A.M. Dirac is one of the most important contributors to modern physics (read about him)

Explanation of Spectra – repeat your SELECTION RULES – then you can understand how the spectrum is related to the Level scheme