TUESDAY 8/2/2011

Spin. Necessity seen from experiments where level splittings are even.

Since $2j+1$ = even $\Rightarrow$ $j = \frac{1}{2}$-integer, we must have $\frac{1}{2}$-integer spins.

Since this cannot arise for orbital angular momentum, it must come from spin.

Insightful comment (Cohen-T): an electron, if it had orbital angular momentum, would need 3+3 coords (position + orientation). But instead it has just 3 positions.

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

Define the spin operator $\hat{\vec{S}}$ for a general particle as a set of 3 operators satisfying

$$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z \quad \& \text{ cyclic.}$$

The wave function of such a particle is valued in the product $\mathcal{H}_{\vec{r}} \otimes \mathcal{H}_s$ of position and spin space. The spin wave function $|s,m\rangle$ satisfies

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

$$S_z |s,m\rangle = m\hbar |s,m\rangle$$

We have shown that s can be integer or half-integer. The allowed values of m are $s, s-1, \ldots, -s$.

A given particle has a fixed value of s and all allowed values of m.

What is the meaning of $\mathcal{H}_{\vec{r}} \otimes \mathcal{H}_s$?

Wave functions in $\mathcal{H}_{\vec{r}}$ are of the form $\psi(\vec{r})$ (familiar).

The wave functions in $\mathcal{H}_s$ are of the form $\begin{pmatrix} a \\ b \end{pmatrix}$: two-component vectors ("spinors").

Now we assume that operators like $\vec{r}, \vec{p}, \vec{L}$ act only on $\mathcal{H}_{\vec{r}}$ while operators made of $\vec{S}$ act only on $\mathcal{H}_s$.

Thus the most general wave function in $\mathcal{H}_{\vec{r}} \times \mathcal{H}_s$ is obtained by:

(i) taking a basis $\psi_n(\vec{x})$ in $\mathcal{H}_{\vec{r}}$

(ii) taking a basis $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ in $\mathcal{H}_s$

So the most general wave fn is

$$\sum a_n \begin{pmatrix} \psi_n(x) \\ 0 \end{pmatrix} + \sum b_n \begin{pmatrix} 0 \\ \psi_n(x) \end{pmatrix} = \begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix}$$

For example in the position basis we know that the basis wave functions are

$$\psi(\vec r, \vec r_0) = \delta^3(\vec r - \vec r_0)$$

Because then $\hat{\vec r}\, \delta^3(\vec r - \vec r_0) = \vec r\, \delta^3(\vec r - \vec r_0)$

$$= \vec r_0\, \delta^3(\vec r - \vec r_0)$$

Orthonormality:

$$\int \psi^*(\vec r, \vec r_0)\, \psi^*(\vec r, \vec r_0{}')\, d^3\vec r$$
$$= \delta^3(\vec r_0 - \vec r_0{}')$$

Completeness:

$$\int \psi^*(\vec r, \vec r_0)\, \psi(\vec r', \vec r_0)\, \cancel{= 2\delta^3}\, d^3\vec r_0$$
$$= \delta^3(\vec r - \vec r').$$

(Analogues of: $\psi_n(\vec r)$ satisfying

$$\int d^3r\, \psi_n^*(\vec r)\, \psi_m(\vec r) = \delta_{nm}$$

$$\sum_n \psi_n^*(\vec r)\, \psi_n(\vec r') = \delta^3(\vec r - \vec r').$$

4

In a basis-independent language we write: the basis wave fns as

$$|\vec{r}_0\rangle$$

with $\hat{\vec{r}}\,|\vec{r}_0\rangle = \vec{r}_0\,|\vec{r}_0\rangle$ and $\langle\vec{r}_0{}'|\vec{r}_0\rangle = \delta^3(\vec{r}-\vec{r}_0)$.

$\downarrow$

$\int |\vec{r}_0\rangle\langle\vec{r}_0|\, d^3r_0 = \mathbb{1}$.

The position basis is obtained by defining

$$\psi(\vec{r},\vec{r}_0) = \langle\vec{r}\,|\vec{r}_0\rangle$$

$$= \delta^3(\vec{r}-\vec{r}_0) \quad \text{as expected.}$$

Now with spin we have instead the basis:

$|\vec{r}_0,+\rangle$ and $|\vec{r}_0,-\rangle$

with $\langle\vec{r}_0{}',+|\vec{r}_0,+\rangle = \langle\vec{r}_0{}',-|\vec{r}_0,-\rangle = \delta^3(\vec{r}_0-\vec{r}_0{}')$

and

$\langle\vec{r}_0{}',+|\vec{r}_0,-\rangle = \langle\vec{r}_0{}',-|\vec{r}_0,+\rangle = 0$.

~~with~~ satisfying:

$$\hat{S}_z\,|\vec{r}_0,\pm\rangle = \pm\frac{\hbar}{2}\,|\vec{r}_0,\pm\rangle$$

$$\hat{\vec{r}}\,|\vec{r}_0,\pm\rangle = \vec{r}_0\,|\vec{r}_0,\pm\rangle.$$

The general wave function is still abstractly written $|\psi\rangle$, but now ~~its~~ position-space components are:

$$\psi_+(\vec{r},\vec{r}_0) = \langle\vec{r}_0,+|\psi\rangle$$

$$\psi_-(\vec{r},\vec{r}_0) = \langle\vec{r}_0,-|\psi\rangle$$

~~Also $\int d^3r\,\langle\vec{r},+|\vec{r},+\rangle$~~

Also: $\int |\vec{r}_0,+\rangle\langle\vec{r}_0,+|\, d^3r_0 + \int |\vec{r}_0,-\rangle\langle\vec{r}_0,-|\, d^3r_0 = \mathbb{1}$

Note that just because we are in $\mathcal{H}_{\vec{r}} \times \mathcal{H}_s$ does not mean that every state is of the form $\psi(\vec{r}_0) \otimes \begin{matrix} |+\rangle \\ |-\rangle \end{matrix}$

~~Rather, ..~~ Such states are the special states

$$\begin{pmatrix} \psi_+(\vec{r}_0) \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ \psi_-(\vec{r}_0) \end{pmatrix}$$

But the most general ~~position~~ state ~~eigenstates~~ are linear combinations of these both in position and spin space:

$$\begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix}$$

where now $\psi_\pm(\vec{r})$ are not necessarily position eigenstates.

Normalisation: $\langle \psi | \psi \rangle = 1$

means:

$$\begin{pmatrix} \psi_+(\vec{r}) \\ \psi_-(\vec{r}) \end{pmatrix} \text{ satisfies}$$

$$\int d^3\vec{r} \left(|\psi_+|^2 + |\psi_-|^2 \right) = \underline{1}.$$

Now we can make operators out of the ingredients

$\hat{x}, \hat{p},$ $\hat{\vec{S}}$

where $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$

For example $\begin{pmatrix} \hat{x} & 0 \\ 0 & \hat{x} \end{pmatrix}$ is the position operator $\hat{x} \otimes \mathbb{1}$.

However the operators $\hat{x} \otimes \sigma_3$ is represented $\begin{pmatrix} \hat{x} & 0 \\ 0 & -\hat{x} \end{pmatrix}$

Schrodinger eqn.

Suppose we consider an electrically charged spin-$\frac{1}{2}$ particle of charge q in an electromagnetic field with scalar potential $\varphi(\vec{r}, t)$ and vector potential $\vec{A}(\vec{r}, t)$.

The free particle would have

$$H = \frac{\hat{\vec{p}}^{\,2}}{2m} = \frac{-\hbar^2}{2m} \vec{\nabla}^2$$

which in spin space is really

$$H \otimes \mathbb{1} = \begin{pmatrix} H & 0 \\ 0 & H \end{pmatrix}$$

In the presence of a field, the Hamiltonian proposed by Pauli is

$$H = \frac{1}{2m}\left(\vec{\sigma} \cdot (\hat{\vec{p}} - q\vec{A}(\vec{r}, t))\right)^2 + q\varphi(\vec{r}, t).$$

It is straightforward to check that in classical physics the corresponding Hamiltonian eqn of motion is $\ddot{\vec{r}} = q\vec{E} + q\dot{\vec{r}} \times \vec{B}$.

plus a magnetic moment

In fact,

$$\left[\sigma\cdot(\hat{\vec{p}}-q\vec{A})\right]^2$$

$$= \sigma^i\sigma^j\ (\hat{p}_i - qA_i)(\hat{p}_j - qA_j)$$

~~Now~~ $\cancel{\sigma^i\sigma^j = \frac{\hbar^2}{4}\delta^{ij} + \frac{i\hbar}{2}\epsilon^{ijk}\sigma^k}$

Now $\sigma^i\sigma^j = \delta^{ij} + i\,\epsilon^{ijk}\sigma^k$

So $\left[\vec{\sigma}\cdot(\hat{\vec{p}}-q\vec{A})\right]^2$

$$= (\hat{\vec{p}} - q\vec{A})^2 + i\,\epsilon^{ijk}\sigma^k\,(\hat{\vec{p}}_i - q\vec{A}_i)(\hat{\vec{p}}_j - q\vec{A}_j)$$

Now $\epsilon^{ijk}\,(\hat{\vec{p}}_i - q\vec{A}_i)(\hat{\vec{p}}_j - q\vec{A}_j)$

$$= \left[(\hat{\vec{p}}-q\vec{A}) \times (\hat{\vec{p}}-q\vec{A})\right]_k$$

$$= (\hat{\vec{p}}\times\hat{\vec{p}})_i + q^2(\vec{A}\times\vec{A})_k$$

$$-q(\hat{\vec{p}}\times\vec{A} + \vec{A}\times\hat{\vec{p}})_k$$

$$= -q\left(-i\hbar\,\vec{\nabla}\times\vec{A}\right) \cancel{+ i\hbar\,\vec{A}\times\vec{\nabla}\,)}$$

$$= i\hbar q B_i$$

Thus the extra term is $-\dfrac{q\hbar}{2m}\vec{\sigma}\cdot\vec{B}$

Hence

$$H = \frac{1}{2m}\left(\hat{\vec{p}} - q\vec{A}(\vec{r})\right)^2 + q\varphi(\vec{r})$$

$$- \frac{q\hbar}{2m}\left(\vec{\sigma}\cdot\vec{B}\right)$$

$$= H_0 - \frac{q\hbar}{2m}\,\vec{\sigma}\cdot\vec{B}$$

$$= \begin{pmatrix} H_0 & 0 \\ 0 & H_0 \end{pmatrix} - \frac{q\hbar}{2m}\begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}$$

$$= \begin{pmatrix} H_0 - \frac{q\hbar}{2m}B_z & -\frac{q\hbar}{2m}(B_x - iB_y) \\ -\frac{q\hbar}{2m}(B_x + iB_y) & H_0 + \frac{q\hbar}{2m}B_z \end{pmatrix}$$

The Hamiltonian is particularly simple if we choose the axes such that $\vec{B} = (0, 0, B_z)$:

$$\begin{pmatrix} H_0 - \frac{q\hbar}{2m}B_z & \\ & H_0 + \frac{q\hbar}{2m}B_z \end{pmatrix}$$

We see the classic effect of a magnetic field on a spin-$\frac{1}{2}$ particle: it <u>splits</u> the levels that we would have had in the absence of spin.

Cf Ex 4, pg 991 of Cohen-Tann. 2.

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~~Many par~~ Addition of angular momentum

Many particle system.

$\hat{\vec{L}}_i$: angular momentum op for each particle.

Central force : each angular mom. separately conserved.

Pairwise interactions among particles: each angular momentum not separately conserved. But, total angular mom is conserved.

eg: $H = H^{(1)} + H^{(2)}$

where $H^{(I)} = -\dfrac{\hbar^2}{2m^{(I)}} \vec{\nabla}^{(I)\,2} + V(\vec{r}^{(I)})$

then $[L^{(I)}, H^{(J)}] = 0$.

Now consider

$H = H^{(1)} + H^{(2)} + \tilde{V}(|\vec{r}^{(1)} - \vec{r}^{(2)}|)$

Since $[L^{(I)}, H^{J}] = 0$ we have

$$[L^{(I)}, H] = [L^{(I)}, \tilde{V}(|\vec{r}^{(1)} - \vec{r}^{(2)}|)]$$

For example:

$$[L^{(1)}_{z}, H] = -i\hbar\,(x_1^{(1)}\partial_2^{(1)} - x_2^{(1)}\partial_1^{(1)})\,V(|r^{(1)} - r^{(2)}|)$$

$$= -i\hbar\,(x^{(1)}\partial_y^{(1)} V - y^{(1)}\partial_x^{(1)} V)$$

We see explicitly that $\vec{L}^{(1)}$ fails to commute with H.

However, if we consider $\vec{L} = \vec{L}^{(1)} + \vec{L}^{(2)}$ then one easily sees that, due to the fact that V depends only on $|\vec{r}^{(1)} - \vec{r}^{(2)}|$, $[\vec{L}, V] = 0$ and hence

$$[\vec{L}, H] = 0.$$

(Do the exercise).

Now suppose we have a system with orbital angular momentum $\vec{L}$ and spin $\vec{S}$. The Hilbert space will be $\mathcal{H}_L \otimes \mathcal{H}_S$.

However the Hamiltonian might have a term $\vec{L}\cdot\vec{S}$. In this case $\vec{L}$ and $\vec{S}$ are not separately conserved: $[\vec{L}, H] \neq 0$ and even $[L_z, H] \neq 0$

However $\vec{J} = \vec{L} + \vec{S}$ does commute with this: $[\vec{L}+\vec{S}, \vec{L}\cdot\vec{S}] = 0$.

Generic problem:

$\vec{J}^{(1)}$, $\vec{J}^{(2)}$ are two separate non-conserved angular momenta (each could be spin or orbital or a combination). But $\vec{J} = \vec{J}^{(1)} + \vec{J}^{(2)}$ is conserved

One basis is given by $\vec{J}^{(1)2}$, $J_z^{(1)}$, $J^{(2)2}$, $J_z^{(2)}$. Another basis is given by $\vec{J}^2$, J_z. → better because $[\vec{J}, H] = 0$.

We are interested in converting from one basis to the other