We turn to the problem of combining spatial and spin degrees of freedom. This is necessary for a particle like the electron, which not only has a charge but also a magnetic moment.

We have considered two cases already. In one (first row of table) we consider only the spatial degrees of freedom and ignore the spin. The particle has charge q. In an external electromagnetic field described by potentials $\Phi, \vec{A}$, its Hamiltonian is given in row 1.

As explained earlier in the course, the Hilbert space, which we call $\mathcal{E}_{orb}$ ("orbital") is determined by the CSCO, which in this case are the position observables $\vec{r} = (x, y, z)$. The basis states are $\{ |\vec{r}\rangle, \vec{r} \in \mathbb{R}^3 \}$, and $\mathcal{E}_{orb} = \text{span}\{ |\vec{r}\rangle, \vec{r} \in \mathbb{R}^3 \}$. Physically, $|\vec{r}\rangle$ represents the state of the system after a measurement has placed the particle in a small region of space around position $\vec{r}$.

Row	Hamiltonian	Hilbert Space	CSCO	Basis	State	Wave Function
1.	$H = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\Phi$	$\mathcal{E}_{orb}$	$\vec{r}$	$\{ \lvert\vec{r}\rangle, \vec{r} \in \mathbb{R}^3 \}$	$\lvert\phi\rangle$	$\phi(\vec{r}) = \langle \vec{r} \lvert \phi\rangle$
2.	$H = -\vec{\mu}\cdot\vec{B}(t)$	$\mathcal{E}_{spin}$	$(S^2), S_z$	$\{ \lvert sm\rangle, m = -s, \dots, +s \}$	$\lvert\chi\rangle$	$\chi(m) = \langle sm \lvert \chi\rangle$
3.	$H = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\Phi - \vec{\mu}\cdot\vec{B}$	$\mathcal{E}_{tot}$	$(\vec{r}, S_z)$	$\{ \lvert\vec{r} m\rangle, \vec{r} \in \mathbb{R}^3, m = -s, \dots, +s \}$	$\lvert\psi\rangle$	$\psi(\vec{r}, m) = \langle \vec{r} m \lvert \psi\rangle$

The *wave function* of a state $|\phi\rangle \in \mathcal{E}_{orb}$ is the expansion coefficients of $|\phi\rangle$ w.r.t. the basis states, that is,

$$\phi(\vec{r}) = \langle \vec{r}|\phi\rangle .$$

Operators such as $\vec{p}$, $\Phi(\vec{r},t)$, etc. that act on $\mathcal{E}_{orb}$ (that is, state vectors $|\phi\rangle$) have an associated action on the associated wave functions $\phi(\vec{r})$, for example $\vec{p}$ acting on $\phi(\vec{r})$ is $-i\hbar\nabla\phi(\vec{r})$, and $\Phi(\vec{r},t)$ acting on $\phi(\vec{r})$ is $\Phi(\vec{r},t)\,\phi(\vec{r})$.

Another case we have considered is when only the spin degrees of freedom are important, for example, when a spin interacts with a time-dependent magnetic field $\vec{B}(t)$, and the spatial dependence of $\vec{B}$ is not important. Then the Hamiltonian is

$$H = -\vec{\mu}\cdot\vec{B}$$

where

$$\vec{\mu} = g\,\frac{q}{2mc}\,\vec{S} .$$

In this case, the C.S.C.O. is (S^2, S_z). Actually, S^2 is superfluous, since it is a constant $s(s+1)\hbar^2$, where s (lower case) is the spin of the particle. We include S^2 or its quantum number s if we want to emphasize that the particle has spin s. The basis states are $\{|sm\rangle,\ m=-s,\dots,+s\}$, and the Hilbert space is

$$\mathcal{E}_{spin} = \mathrm{span}\,\{|sm\rangle,\ m=-s,\dots,+s\}.$$

If $|\chi\rangle$ is a state vector in $\mathcal{E}_{spin}$, then the wave function is

$$\chi(m) = \langle sm|\chi\rangle,$$

that is, it is the expansion coefficients of $|\chi\rangle$ with respect to the basis states. Physically the state $|sm\rangle$ represents the state of the spin after a measurement of S_z has yielded the value $m\hbar$ (for example, in a Stern-Gerlach apparatus).

At other times in this course we may write χ_m instead of $\chi(m)$ for the wave function, but we are attempting here to show the similarity between the spatial wave function $\phi(\vec{r}) = \langle\vec{r}|\phi\rangle$ and the spin wave function $\chi(m) = \langle sm|\chi\rangle$. We often arrange $\chi(m)$ or χ_m as a column vector,

$$\begin{pmatrix} \chi(s) \\ \chi(s-1) \\ \vdots \\ \chi(-s) \end{pmatrix} \qquad 2s+1 \text{ components}$$

which is called a "spinor". The spinor has $2s+1$ components that are complex numbers.

On the third row of the table we show what happens if both spatial and spin degrees of freedom are important. This happens, for example, inside a Stern-Gerlach apparatus, where the beam is split depending on the spin state (there is a coupling between spatial and spin degrees of freedom). The Hamiltonian on the third row is the sum of the two previous Hamiltonians, but now we allow $\vec{B}$ to be a function of both $\vec{r}, t$ (and similarly for $\vec{A}$ and Φ).

Now the CSCO consists of $(\vec{r}, S_z)$, where we omit the superfluous S^2. The basis states are simultaneous eigenstates of $\vec{r}$ and S_z, which we denote by $|\vec{r}m\rangle$. The basis is

$$\{\, |\vec{r},m\rangle \mid \vec{r}\in\mathbb{R}^3,\ m=-s,\dots,+s \,\}.$$

We call the Hilbert space $\mathcal{E}_{tot}$; it is the span of this basis,

$$\mathcal{E}_{tot} = \text{span}\,\{\, |\vec{r}m\rangle \mid \vec{r}\in\mathbb{R}^3,\ m=-s,\dots,+s \,\}.$$

If a state $|\psi\rangle \in \mathcal{E}_{tot}$, then its wave function is

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

It is the expansion coefficients of the state w.r.t. the basis.

In other places in this course or in the notes we may write $\psi_m(\vec{r})$ instead of $\psi(\vec{r},m)$, and we may arrange things in a $(2s+1)$-component spinor,

$$\begin{pmatrix} \psi_s(\vec{r}) \\ \psi_{s-1}(\vec{r}) \\ \vdots \\ \psi_{-s}(\vec{r}) \end{pmatrix}$$

where now the components are functions of position. But for now we stick with the notation $\psi(\vec{r},m)$, which emphasizes the similar role played by $\vec{r}$ and m (as labels of the basis states).

A special case of a wavefunction of a particle with spin is a product of a purely spatial times a purely spin wave function,

$$\psi(\vec{r}, m) = \phi(\vec{r})\,\chi(m) \qquad \text{(special case)}.$$

But a general wave function $\psi(\vec{r},m)$ cannot be represented as such a product.

It can, however, always be represented as a linear combination of such products. Let $\{\phi_a(\vec{r}),\ a=1,2,\dots\}$ be a basis of wave functions in $\mathcal{E}_{orb}$, and $\{\chi_b(m),\ b=1,2,\dots\}$ be a basis of wave functions in $\mathcal{E}_{spin}$. Then an arbitrary $\psi(\vec{r},m)$ can be written

$$\psi(\vec{r},m) = \sum_{ab} C_{ab}\ \phi_a(\vec{r})\,\chi_b(m)$$

where the expansion coefficients are given by

$$C_{ab} = \int d^3\vec{r} \sum_m \phi_a(\vec{r})^* \chi_b(m)^* \ \psi(\vec{r},m).$$

(We are assuming the bases $\{\phi_a\}$ and $\{\chi_b\}$ are orthonormal.)

In this example, the space $\mathcal{E}_{tot}$ is called the

<u>tensor product</u> of the spaces $\mathcal{E}_{orb}$ and $\mathcal{E}_{spin}$, and we write

$$\mathcal{E}_{tot} = \mathcal{E}_{orb} \otimes \mathcal{E}_{spin}.$$

We will not give the official mathematical definition of the tensor product, but the idea is that $\mathcal{E}_{tot}$ consists of wave functions that are all possible linear combinations of products of wave functions ~~of~~ taken from $\mathcal{E}_{orb}$ and $\mathcal{E}_{tot}$.

Likewise, when a wave function $\psi(\vec{r}, m)$ in $\mathcal{E}_{tot}$ can be written as a single product of wave functions in $\mathcal{E}_{orb}$ and $\mathcal{E}_{spin}$ (recall this is a special case),

$$\psi(\vec{r}, m) = \phi(\vec{r})\,\chi(m),$$

then we will write this in ket language as

$$|\psi\rangle = |\phi\rangle \otimes |\chi\rangle.$$

This defines the tensor product of <u>kets</u>, and it simply means, multiplication of the corresponding wave functions. Actually, in the physics literature it is common to omit the $\otimes$ and just write

$$|\psi\rangle = |\phi\rangle|\chi\rangle$$

for such a product. Although this is a special case, if we write $\{|\phi_a\rangle, a=1,\ldots\}$ and $\{|\chi_b\rangle, b=1,2,\ldots\}$ for bases in $\mathcal{E}_{orb}$ and $\mathcal{E}_{spin}$, then an arbitrary state

$|\psi\rangle \in \mathcal{E}_{tot}$ can be expanded as

$$|\psi\rangle = \sum_{ab} c_{ab}\, |\phi_a\rangle |\chi_b\rangle .$$

In fact, if we write

$$|ab\rangle = |\phi_a\rangle |\chi_b\rangle = |\phi_a\rangle \otimes |\chi_b\rangle ,$$

then $$c_{ab} = \langle ab|\psi\rangle .$$

Notice that we have been talking about two bases in $\mathcal{E}_{spin}$, $\{|sm\rangle\}$ and $\{|\chi_b\rangle\}$. These could be the same but the discussion is perhaps more clear if we don't require this. Similarly for the bases $\{|\vec{r}\rangle\}$ and $\{|\phi_a\rangle\}$ in $\mathcal{E}_{orb}$.

In the special case of the electron with $q=-e$, the Hamiltonian acting on $\mathcal{E}_{tot}$ is

$$H = \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2 - e\Phi - \vec{\mu}\cdot\vec{B} , \qquad (*)$$

where $$\vec{\mu} = -g\,\frac{e}{2mc}\,\vec{S} = -\frac{g}{2}\,\mu_B\,\vec{\sigma} ,$$

where $g \approx 2$ and $\mu_B = \dfrac{e\hbar}{2mc}$ $\left(\text{and } \vec{S} = \frac{\hbar}{2}\vec{\sigma} \right)$.

This is called the <u>Pauli Hamiltonian</u> (*), and $H|\psi\rangle = E\psi$ or $H|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$ is called the <u>Pauli equation</u>.