

To completely describe an electron in an atom, four quantum numbers are needed: energy (n), angular momentum (ℓ), magnetic moment (m_ℓ), and spin (m_s).

The Principal Quantum Number

This quantum number describes the electron shell or energy level of an atom. The value of n ranges from 1 to the shell containing the outermost electron of that atom. For example, in caesium (Cs), the outermost valence electron is in the shell with energy level 6, so an electron in caesium can have an n value from 1 to 6. For particles in a time-independent potential, as per the Schrödinger equation, it also labels the n th eigen value of Hamiltonian (H). This number has a dependence only on the distance between the electron and the nucleus (i.e. the radial coordinate r). The average distance increases with n , thus quantum states with different principal quantum numbers are said to belong to different shells.

The Azimuthal Quantum Number

The angular or orbital quantum number, describes the sub-shell and gives the magnitude of the orbital angular momentum through the relation. $\ell = 0$ is called an s orbital, $\ell = 1$ a p orbital, $\ell = 2$ a d orbital, and $\ell = 3$ an f orbital. The value of ℓ ranges from 0 to $n - 1$ because the first p orbital ($\ell = 1$) appears in the second electron shell ($n = 2$), the first d orbital ($\ell = 2$) appears in the third shell ($n = 3$), and so on. This quantum number specifies the shape of an atomic orbital and strongly influences chemical bonds and bond angles.

The Magnetic Quantum Number

The value of the m_ℓ quantum number is associated with the orbital orientation. The magnetic quantum number describes the energy levels available within a sub-shell and yields the projection of the orbital angular momentum along a specified axis. The values of m_ℓ range from $-\ell$ to $+\ell$, with integer steps between them. The s sub-shell ($\ell=0$) contains one orbital, and therefore the m_ℓ of an electron in an s sub-shell will always be 0. The p sub-shell ($\ell=1$) contains three, so the m_ℓ of an electron in a p sub-shell will be -1 , 0, or 1. The d sub-shell ($\ell=2$) contains five orbitals, with m_ℓ values of -2 , -1 , 0, 1, and 2.

The Spin Projection Quantum Number

This spin quantum number describes the intrinsic angular momentum of the electron within that orbital and gives the projection of the spin angular momentum (s) along the specified axis. The values of

m_s range from $-s$ to $+s$. An electron has spin $s = \frac{1}{2}$, consequently m_s will be $\pm\frac{1}{2}$, corresponding to spin and opposite spin. Each electron in any individual orbital must have different spins because of the Pauli Exclusion Principle. Thus an orbital can never contain more than two electrons.

Quantum Numbers	Symbol	Possible Values
Principal Quantum Number	n	1, 2, 3, 4
Angular Momentum Quantum Number	ℓ	0, 1, 2, 3, $n-1$
Magnetic Quantum Number	m_ℓ	$-\ell \dots -1, 0, 1, \dots \ell$
Spin Quantum Number	s	$+\frac{1}{2}, -\frac{1}{2}$

Quantization of Angular Momentum

In addition to quantized energy (specified by principle quantum number n), the solutions subject to physical boundary conditions also have quantized orbital angular momentum L . The magnitude of the vector L is required to obey

$$L = [\ell(\ell+1)]^{1/2} \hbar$$

where ℓ is the orbital quantum number.

Bohr model of the hydrogen atom also had quantized angular moment $L = n\hbar$, but the lowest energy state $n=1$ would have $L=\hbar$. In contrast, the Schrödinger equation shows that the lowest state has $L=0$. This lowest energy-state wave function is a perfectly symmetric sphere. For higher energy states, the vector L has in addition only certain allowed directions, such that the z -component is quantized as

$$L_z = m_\ell \hbar \qquad m_\ell = \pm 0, \pm 1, \pm 2, \pm 3, \dots, \pm \ell$$

Table summarizes the quantum states of the hydrogen atom. For each value of the quantum number n , there are n possible values of the quantum number ℓ . For each value of ℓ , there are $2\ell+1$ values of the quantum number m_ℓ .

n	ℓ	m_ℓ	Spectroscopic Notation	Shell
1	0	0	1s	K
2	0	0	2s	L
2	1	-1, 0, 1	2p	
3	0	0	3s	M
3	1	-1, 0, 1	3p	
3	2	-2, -1, 0, 1, 2	3d	
4	0	0	4s	N
...

How many distinct states of the hydrogen atom (n, ℓ, m_ℓ) are there for the $n = 3$ state? What are their energies?

The $n = 3$ state has possible ℓ values 0, 1, or 2. Each ℓ value has m_ℓ possible values of (0), (-1, 0, 1), or (-2, -1, 0, 1, 2). The total number of states is then $1 + 3 + 5 = 9$. There is another quantum number s , for electron spin ($\pm 1/2$), so there are actually 18 possible states for $n = 3$. Each of these states have the same n , so they all have the same energy.