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Paper No. : Lasers, Atomic and Molecular Spectroscopy

Module: Pauli Exclusion Principle

Development Team

Principal Investigator: Dr. VinayGupta , Professor

Department Of Physics and Astrophysics, University Of Delhi, New Delhi-110007

Paper coordinator: Dr. Devendra Mohan, Professor
Department of Applied Physics
Guru Jambheshwar University of Science And Technology, Hisar-125001

Content Writer: Dr. Devendra Mohan, Professor
Department of Applied Physics
Guru Jambheshwar University of Science And Technology, Hisar-125001

Content Reviewer: Ms. KirtiKapoor
Department of Applied Physics
Guru Jambheshwar University of Science And Technology, Hisar-125001

Description of Module	
Subject Name	Physics
Paper Name	Lasers, Atomic and Molecular Spectroscopy
Module Name/Title	Pauli Exclusion Principle
Module Id	

Contents:

The students will be able to learn about the Quantum states of electrons and Pauli exclusion principle role in different fields, particularly the building block for atomic spectra

Pauli Exclusion Principle:

The **Pauli exclusion principle** is the quantum mechanical principle that states that two or more identical fermions (particles with half-integer spin) cannot occupy the same quantum state within a quantum system simultaneously.

In case of electrons in atoms, the statement can be read as: it is impossible for two electrons of a poly-electron atom to have the same values of the four quantum numbers:

n, the principal quantum number,

ℓ, the angular momentum quantum number,

m_ℓ, the magnetic quantum number, and

m_s, the spin quantum number.

If two electrons are lying in the same orbital, and their n, ℓ and m_ℓ values are the same, then their m_s must be different, that infers the electrons must have opposite half-integer spins of 1/2 and −1/2. This principle was formulated by **Austrian physicist Wolfgang Pauli in 1925** for electrons, and later extended to all fermions with his spin-statistics theorem.

In other words, the total wave function for two identical fermions is anti-symmetric with respect to exchange of the particles. That simply means that the wave function changes its sign in case the space and spin co-ordinates of any two particles are interchanged.

However, Particles with an integer spin (bosons), donot obey Pauli Exclusion Principle because any number of identical bosons can occupy the same quantum state.

Conclusively, the Pauli Exclusion Principle dictates the behavior of all fermions (quarks, electrons and neutrinos i.e. half-integer spin :1/2, 3/2, 5/2, etc. particles), while bosons (particles with integer spin) will follow other principles. Noteworthy, atoms can have different overall "spin" that determines whether they are fermions or bosons ,e.g. Helium-3 has spin 1/2 and is therefore is considered as fermion, while Helium-4 that has 0 spin and therefore is a boson.

The Pauli Exclusion Principle determines many properties of the matter, from its large-scale stability to the chemical behavior of atoms.

The theory of quantum mechanics describes the fermions by anti-symmetric states. In contrast, particles with integer spin (bosons) have symmetric wave functions; unlike fermions these share the same quantum states. Fermions take their name from the Fermi–Dirac statistical distribution while bosons from Bose–Einstein distribution.

Pauli's Exclusion Principle states that

No two electrons in an atom can have identical quantum numbers, $\mathbf{n, l, m_l}$ **&** $\mathbf{m_s}$**.**

as the energy states are designated with these four quantum numbers, the statement can be re written as: **an energy state can't accommodate more than one electron with a given set of four quantum numbers**.

Alternatively,

No two Fermions can exist in identical quantum energy states.

The establishment of the principle has made us to understand the concepts of band theory of solids, modeling of the atomic shell structure and building of the periodic table. However, the understanding of shell structure of atom facilitates the analysis of the atomic spectra.

Each electron is associated with n, l, m_l and m_s; four quantum numbers. Where the significance of each is

n (principal quantum number) --any integer >0; determines energy to first approximation & forms shell

L (orbital quantum number) --integer up to $(n-1)$; n & l form a sub shell

m_l (magnetic quantum number)-- integer from $-l$ to $+l$; gives orientation of the orbital

m_s (spin quantum number)-- $\pm\frac{1}{2}$; gives the orientation of the spin

On the basis of Pauli's principle, number of electrons in a shell and the net angular moments associated with them can be found.

Pauli Exclusion Principle through Quantum mechanics:

The Pauli Exclusion Principle with a single-valued many-particle wave function is equivalent to requiring the wave function to be anti- symmetric. An anti-symmetric two-particle state is represented as a sum of states in which one particle is in one state and the other in other state , and is given by:

Anti-symmetry (when the particles are exchanged) means that A(r,s) = −A(s,r). This means A(r,s) = 0 when r = s that is , Pauli exclusion.

Quantum mechanically, Pauli's Exclusion Principle dictates that the '**total eigen function of a system of several electrons must be antisymmetric with respect to exchange of the coordinates (position and spin) of two electrons**'.

Considering a system of two non-interacting electrons, one with potential energy, V_1 & the eigenfunction $\psi(1)$ and the second with values V_2 & $\psi(2)$. As the electrons are non-interacting, total potential energy of the system is V_1+V_2. Now,if it is assumed that the electron '1' is in spin quantum state α and '2' in spin quantum state β, total eigenfunction of the system is $\Psi_T=\psi_\alpha(1)\psi_\beta(2)$ and on exchange of the particles

$\Psi'_T=\psi_\beta(1)\psi_\alpha(2)$

Though the eigenvalues corresponding to Ψ_T and Ψ'_T are same yet these functions are not same due to doubly degenerate states, but the probability density functions $\Psi_T * \Psi_T$ and $\Psi'^*_T \Psi'_T$ change on the exchange of indistinguishable electrons '1' & '2'. On the other hand, it must not change on exchange of indistinguishable particles.

The total eigenfunction can be constructed by taking the linear combination of Ψ_T and Ψ'_T. This satisfies time-independent Schrödinger equation and also, the probability density does not change on exchange of particles.

$\Psi_S=\frac{1}{\sqrt{2}}\left[\psi_\alpha(1)\psi_\beta(2)+\psi_\beta(1)\,\psi_\alpha(2)\right]$ Symmetric wave function

$\Psi_A=\frac{1}{\sqrt{2}}\left[\psi_\alpha(1)\,\psi_\beta(2)-\psi_\beta(1)\,\psi_\alpha(2)\right]$ Anti-symmetric wave function

Any measurable quantity that can be obtained from Ψ_S and/ or Ψ_A will not be affected by the exchange of particles.If the two electrons are in the same space and spin states, Ψ_A is identically equal to zero. It implies that when the two particles are in a state with the same space & spin quantum numbers, the system can't be described by Ψ_A.

In other words two particles must have different sets of four quantum numbers. For a system of several electrons, the principle is expressed as:

A system consisting of several electrons (Fermions) must be described by an Anti-symmetric total eigenfunction.

Atoms and the Pauli principle

One of the important consequences of the principle is the elaboration of electron shell structure of atoms and the way atoms share electrons therby explaining the variety of chemical elements and their combinations. It is known that an electrically neutral atom contains bound electrons equal in number to the protons in the nucleus. Electrons, being fermions, cannot occupy the same quantum state as other electrons, so electrons have different spins (within an atom) at the same electron orbital.

Considering the case of neutral helium atom that has two bound electrons, both can occupy the lowest-energy (1s) states by acquiring opposite spin; as spin is part of the quantum state of the electron, the two electrons are in different quantum states and do not violate the Pauli principle.

But the spin can take only two different values (eigenvalues). Further extending the concept to lithium atom, with three bound electrons, the third electron cannot reside in 1s state, and therefore must occupy one of the higher-energy 2s states. The number of electrons in the outermost shell decides the chemical properties.The idea can be extended to successively larger elements where shells of successively higher energy are occupied.

Solid state properties and the Pauli principle

In conductors and semiconductors, there are very large numbers of orbital that effectively form a continuous band structure of energy levels. In metal conductors, electrons lie in degenerate states that they cannot contribute much to the thermal capacity of a metal. All most all types of mechanical, electrical, magnetic, optical and chemical properties of solids are the direct consequences of Pauli exclusion principle

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Stability of matter with Pauli Exclusion Principle

The stability of the electrons in an atom is not directly related to the exclusion principle, but the quantum theory of the atom describes it very well. The Heisenberg uncertainty principle explains the idea that close approach of an electron to the nucleus of the atom necessarily increases its kinetic energy. The stability of large systems with many electrons and many nucleons is also explained by the Pauli Exclusion Principle.

The Pauli Exclusion Principle suggest that the bulk matter is stable and occupies volume, as Paul Ehrenfest (1931) has pointed out that the electrons of each atom cannot all fall into the lowest-energy orbital and hence must occupy successively larger shells. Atoms cannot be squeezed too closely together and therefore occupy a volume.

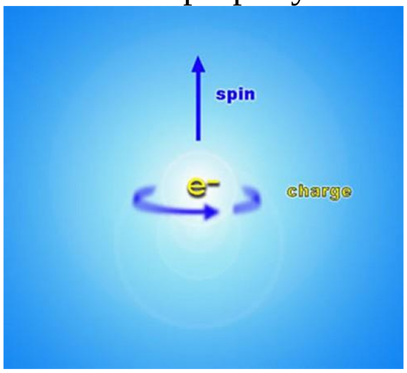
Freeman Dyson and Andrew Lenard (1967), considered the balance of attractive; electron–nuclear and repulsive such as electron–electron and nuclear–nuclear forces and showed that ordinary matter would collapse and occupy a much smaller volume without the Pauli principle.

In conclusion, the electrons of the same spin are kept apart by a repulsive exchange interaction that is a short-range effect, acting simultaneously with the long-range electrostatic or Coulombic force. This effect is partly observed in the macroscopic world that two solid objects cannot be in the same place at the same time.

SPIN AND THE PAULI EXCLUSION PRINCIPLE

Spin is considered as a rotation of particles around their
own axis. The question is whether something as small as an electron is spinning at all. In general, though, spin obeys the same mathematical laws of angular momentum as objects do spinning in classical physics (such as the Earth revolving around its own axis), and there are two important aspects: the speed of rotation and the direction of the axis it rotates about (‘up’ and ‘down’).

The concept of spin was first discovered in 1922 by Otto Stern and Walther Gerlach, and they inferred from the experiments that the intrinsic angular momentum, or spin, of a particle such as an electron is quantized which implies that it could only take certain discrete values. The spin of composite particles like protons, neutrons and atomic nuclei, is the sum of the spins and orbital angular momentum of the constituent particles, and is therefore follow the same quantization conditions. Spin is therefore a completely quantum mechanical property of a particle.



Now the difference between bosons and fermions is understood as: bosons have symmetric wave functions while fermions have anti-symmetric wave functions. Just to understand the concept of spin with half-integer spin that an electron has to spin around TWICE before it presents the same face as earlier. While the probability waves of bosons “flip” or invert before they interfere with each other, Fermions, however, do not flip their probability waves. Therefore, the spins of particles need to be added together using special rules for addition of angular momentum.

Another way of stating the principle is that **no two fermions in a quantum system can have the same values of all four quantum numbers at any given time**. A very high density white dwarf stars, is explained and also the very existence of different types of atoms in the universe and the large-scale stability and bulk of matter.

By recognizing is the Pauli Exclusion Principle that no two electrons can occupy the same quantum state simultaneously, it effectively stops electrons from "piling up" on top of each other. This explains why matter occupies space exclusively for itself and does not allow other material objects to pass through it and at the same time allows radiations to pass.

The existence of the different atoms in the periodic table of elements and the sheer variety of the universe around us is also understood by this principle. In case an atom gains a new electron, it always goes into the lowest energy state available of course, the outermost shell. Two atoms with ‘closed’ shells cannot form a chemical bond with each other as the electrons in one atom does not find available quantum states in the other that it can occupy. In this way, the arrangement of electrons in the outermost shell affects the chemical properties of an element and how atoms are able to bond and combine with other atoms. Same way, the molecules interact to form gases, liquids or solids, and how they aggregate themselves in living organisms.

The Pauli Exclusion Principle explains the degenerate white dwarf (a type of star) as if two identical particles are forced to have the same quantum numbers, they respond with a repelling outward force, known as "degeneracy pressure" or "Pauli repulsion".

The Pauli exclusion principle is one of the most important principles because the three types of particles (electrons, protons and neutrons) from which ordinary matter is made up concludes that all material particles exhibit space-occupying behavior.