Pauli exclusion principle

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The Pauli exclusion principle is a quantum mechanical principle formulated by the Austrian physicist Wolfgang Pauli in 1925. In its simplest form for electrons in a single atom, it states that no two electrons can have the same four quantum numbers; that is, if \( n, l, \) and \( m_l \) are the same, \( m_s \) must be different such that the electrons have opposite spins. More generally, no two identical fermions (particles with half-integer spin) may occupy the same quantum state simultaneously. A more rigorous statement of this principle is that for two identical fermions, the total wave function is anti-symmetric.

In contrast, integer spin particles, bosons, are not subject to the Pauli exclusion principle. For bosons, any number of identical particles can occupy the same quantum state, as with, for instance, lasers and Bose-Einstein condensation.

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Overview

The Pauli exclusion principle is one of the most important principles in physics, mainly because the three types of particles from which the ordinary atom is made—electrons, protons, and neutrons—are all subject to it; consequently, all material particles exhibit space-occupying behavior. The Pauli exclusion principle underpins many of the characteristic properties of matter, from the large-scale stability of matter to the existence of the periodic table of the elements.

Fermions, particles with antisymmetric wave functions, obey the Pauli exclusion principle. Apart from the familiar electron, proton and neutron, these include neutrinos and quarks (from which protons and neutrons are made), as well as some atoms like helium-3. All fermions possess "half-integer spin",
meaning that they possess an intrinsic angular momentum whose value is $\hbar = \hbar/2\pi$ (reduced Planck's constant) times a half-integer (1/2, 3/2, 5/2, etc.). In the theory of quantum mechanics, fermions are described by antisymmetric states. Particles with integer spin have a symmetric wave function and are called bosons; in contrast to fermions, they may share the same quantum states. Examples of bosons include the photon, the Cooper pairs (which are responsible for superconductivity), and the W and Z bosons.

**History**

In the early 20th century, it became evident that atoms and molecules with even numbers of electrons are more stable than those with odd numbers of electrons. In the famous 1916 article *The Atom and the Molecule* (http://dbhs.wvusd.k12.ca.us/webdocs/Chem-History/Lewis-1916/Lewis-1916.html) by Gilbert N. Lewis, for example, the third of his six postulates of chemical behavior states that the atom tends to hold an even number of electrons in the shell and especially to hold eight electrons which are normally arranged symmetrically at the eight corners of a cube (see: cubical atom). In 1919, the American chemist Irving Langmuir suggested that the periodic table could be explained if the electrons in an atom were connected or clustered in some manner. Groups of electrons were thought to occupy a set of electron shells about the nucleus.[1] In 1922, Niels Bohr updated his model of the atom by assuming that certain numbers of electrons (for example 2, 8 and 18) corresponded to stable "closed shells".

Pauli looked for an explanation for these numbers, which were at first only empirical. At the same time he was trying to explain experimental results in the Zeeman effect in atomic spectroscopy and in ferromagnetism. He found an essential clue in a 1924 paper by E.C.Stoner which pointed out that for a given value of the principal quantum number (n), the number of energy levels of a single electron in the alkali metal spectra in an external magnetic field, where all degenerate energy levels are separated, is equal to the number of electrons in the closed shell of the rare gases for the same value of n. This led Pauli to realize that the complicated numbers of electrons in closed shells can be reduced to the simple rule of one per state, if the electron states are defined using four quantum numbers. For this purpose he introduced a new two-valued quantum number, identified by Samuel Goudsmit and George Uhlenbeck as electron spin.

**Connection to quantum state symmetry**

The Pauli exclusion principle with a single-valued many-particle wavefunction is equivalent to the assumption that the wavefunction is antisymmetric. An antisymmetric two-particle state is represented as a sum of states in which one particle is in state $|x\rangle$ and the other in state $|y\rangle$:

$$|\psi\rangle = \sum_{x,y} A(x,y) |x,y\rangle$$

and antisymmetry under exchange means that $A(x,y) = -A(y,x)$. This implies that $A(x,x)=0$, which is Pauli exclusion. It is true in any basis, since unitary changes of basis keep antisymmetric matrices antisymmetric.
although strictly speaking, the quantity $A(x,y)$ is not a matrix but an antisymmetric rank two tensor.

Conversely, if the diagonal quantities $A(x,x)$ are zero in every basis, then the wavefunction component:

$$A(x, y) = \langle \psi | x, y \rangle = \langle \psi | (|x\rangle \otimes |y\rangle)$$

is necessarily antisymmetric. To prove it, consider the matrix element:

$$\langle \psi | (|x\rangle + |y\rangle) \otimes (|x\rangle + |y\rangle) \rangle$$

This is zero, because the two particles have zero probability to both be in the superposition state $|x\rangle + |y\rangle$. But this is equal to

$$\langle \psi | x, x \rangle + \langle \psi | x, y \rangle + \langle \psi | y, x \rangle + \langle \psi | y, y \rangle$$

The first and last terms on the right hand side are diagonal elements and are zero, and the whole sum is equal to zero. So the wavefunction matrix elements obey:

$$\langle \psi | x, y \rangle + \langle \psi | y, x \rangle = 0.$$

or

$$A(x, y) = -A(y, x)$$

The Pauli principle in advanced quantum theory

According to the spin-statistics theorem, particles with integer spin occupy symmetric quantum states, and particles with half-integer spin occupy antisymmetric states; furthermore, only integer or half-integer values of spin are allowed by the principles of quantum mechanics. In relativistic quantum field theory, the Pauli principle follows from applying a rotation operator in imaginary time to particles of half-integer spin. Since, nonrelativistically, particles can have any statistics and any spin, there is no way to prove a spin-statistics theorem in nonrelativistic quantum mechanics.

In one dimension, not only fermions, but also bosons can obey the exclusion principle. A one dimensional Bose gas with delta function repulsive interactions of infinite strength is equivalent to a gas of free fermions. The reason for this is that in one dimension, exchange of particles requires that they pass through each other, and for infinitely strong repulsion, this cannot happen. This model is described by a quantum nonlinear Schroedinger equation. In momentum space the exclusion principle is valid also for finite repulsion in Bose gas with delta function interactions,[2], as well as for interacting spins and Hubbard model in one dimension, as well as for other models solvable by Bethe ansatz. The ground state in models solvable by Bethe ansatz is a Fermi sphere.

Consequences

Atoms and the Pauli principle

The Pauli exclusion principle helps explain a wide variety of physical phenomena. One particularly important consequence of the principle is the elaborate electron shell structure of atoms and the way atoms share electrons, explaining the variety of chemical elements and their chemical combinations. An electrically neutral atom contains bound electrons equal in number to the protons in the nucleus. Since electrons are fermions, the Pauli exclusion principle forbids them from occupying the same quantum state, so electrons have to "stack"
within an atom, i.e. have different momenta while at the same place.

For example, consider a neutral helium atom, which has two bound electrons. Both of these electrons can occupy the lowest-energy (1s) states by acquiring opposite spin. This does not violate the Pauli principle because spin is part of the quantum state of the electron, so the two electrons are occupying different quantum states. However, the spin can take only two different values (or eigenvalues). In a lithium atom, which contains three bound electrons, the third electron cannot reside in a 1s state, and must occupy one of the higher-energy 2s states instead. Similarly, successively larger elements produce successively higher-energy shells. The chemical properties of an element largely depend on the number of electrons in the outermost shell, which gives rise to the periodic table of the elements.

**Solid state properties and the Pauli principle**

In conductors and semi-conductors, free electrons have to share entire bulk space. Thus, their energy levels stack up, creating band structure out of each atomic energy level. In strong conductors (metals) electrons are so degenerate that they can not even contribute much to the thermal capacity of a metal. Many mechanical, electrical, magnetic, optical and chemical properties of solids are the direct consequence of Pauli exclusion.

**Stability of matter**

The stability of the electrons in an atom itself is not related to the exclusion principle, but is described by the quantum theory of the atom. The underlying idea is that close approach of an electron to the nucleus of the atom necessarily increases its kinetic energy, an application of the uncertainty principle of Heisenberg. However, stability of large systems with many electrons and many nuclei is a different matter, and requires the Pauli exclusion principle.

It has been shown that the Pauli exclusion principle is responsible for the fact that ordinary bulk matter is stable and occupies volume. This suggestion was first made in 1931 by Paul Ehrenfest, who pointed out that the electrons of each atom cannot all fall into the lowest-energy orbital and must occupy successively larger shells. Atoms therefore occupy a volume and cannot be squeezed too closely together.

A more rigorous proof was provided in 1967 by Freeman Dyson and Andrew Lenard, who considered the balance of attractive (electron-nuclear) and repulsive (electron-electron and nuclear-nuclear) forces and showed that ordinary matter would collapse and occupy a much smaller volume without the Pauli principle. The consequence of the Pauli principle here is that electrons of the same spin are kept apart by a repulsive exchange interaction, which is a short-range effect complemented by the long-range electrostatic or coulombic force. This effect is therefore partly responsible for the everyday observation in the macroscopic world that two solid objects cannot be in the same place in the same time.

However, Dyson and Lenard did not consider the extreme magnetic or gravitational forces which occur in some astronomical objects. In 1995, Elliott Lieb and coworkers showed that the Pauli principle still leads to stability in intense magnetic fields such as in neutron stars, although at a much higher density than in ordinary matter. It is a consequence of General Relativity that in sufficiently intense gravitational fields, matter collapses to form a black hole.

**Astrophysics and the Pauli principle**

Astronomy provides another spectacular demonstration of this effect, in the form of white dwarf stars and neutron stars. For both bodies, the usual atomic structure is disrupted by large gravitational forces, leaving the
constituents supported by "degeneracy pressure" alone. This exotic form of matter is known as degenerate matter. In white dwarfs, atoms are held apart by electron degeneracy pressure. In neutron stars, which exhibit even more intense gravitational forces, electrons have merged with protons to form neutrons. Neutrons are capable of producing an even higher degeneracy pressure, albeit over a shorter range. This can stabilize neutron stars from further collapse, but at a smaller size and higher density than with a white dwarf. Neutrons are the most "rigid" objects known; their Young modulus (or more accurately, bulk modulus) is 20 orders of magnitude larger than that of diamond. However, even this enormous rigidity can be overcome by the gravitational field of a massive star or by the pressure of a supernova, leading to the formation of a black hole.

See also

- Exchange force
- Exchange interaction
- Exchange symmetry
- Hund's rule
- Fermi hole

References

5. ^ As described by FJ Dyson (J.Math.Phys. 8, 1538-1545 (1967) ), Ehrenfest made this suggestion in his address on the occasion of the award of the Lorentz Medal to Pauli.

External links

The Exclusion Principle (http://www.energyscience.org.uk/essays/ese06.htm) (1997), Pauli's exclusion rules vs. the Aspden exclusion rules (plus the radiation factor, Larmor radiation formula, elliptical motion, the quantum states, occupancy of electron shells, nature of ferromagnetism, ...).

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