The Degenerate Fermi Gas, Pauli Blocking, and Compact Objects

Part I: The Degenerate Fermi Gas

by Dwight E. Neuenschwander, Professor Emeritus, Southern Nazarene University

Bosons and Fermions

Since the most stable equilibrium configuration of a system is the state of lowest energy, why don't all the electrons in an atom reside in the 1s orbital? Of course, if they did, there would be no chemistry, no biology, and no life. There would be no metals to conduct electricity. All white dwarf and neutron stars would collapse into black holes. The universe would be very different indeed, and we would not be here to appreciate it! The Pauli exclusion principle asserts that electrons do not all collapse into an atom's 1s orbital because only two electrons can live there, and then only when they have opposite spins, to not occupy the same space-spin state.

Elementary particles, and composites made of them, fall into two categories: bosons and fermions. Identical bosons (named after Satyendra Nath Bose, 1894–1974) readily share the same state. In contrast, identical fermions (named after Enrico Fermi, 1901–1954) occupy states in solitude. Here's an analogy: In the restaurants of some countries, the *maître d'* will seat your party at a table already occupied by strangers if the table has a sufficient number of empty chairs. But in other cultures, new diners expect to be seated at empty tables even when occupied tables contain surplus seats. Bosons are analogous to the first group of diners; fermions to the second group.

The exclusion principle that applies generally to identical fermions grew out of the realization that the discrete quantum states for electrons in atoms could not, by themselves, explain the periodic table of the elements. The crucial clue toward a resolution came in 1924 when Edmund Stoner (1899–1968) published a paper giving the first correct extension to multielectron atoms of Niels Bohr's model of the hydrogen atom.[1] From Stoner's paper, Wolfgang Pauli (1900–1958) realized that the sequence of closed-shell electron numbers 2, 8, 18,... is equivalent to a rule asserting that no quantum state can hold more than one electron.[2] But to implement this rule he had to postulate the existence of an extra quantum number to account for a pair of electrons in the same *spatial* state, so each electron in that spatial state could have a unique set of quantum numbers. The extra quantum number was forthcoming from Samuel Goudsmit (1902–1978) and George Uhlenbeck (1900–1988) in the autumn of 1925. Passing a beam of free electrons through a magnetic field, the beam split into two.[3] This splitting—two energy possibilities revealed for electrons interacting with a magnetic field—is evidently a property of the electrons themselves. Therefore, for electrons bound in an atom—where an ambient magnetic field exists because of the relative motion between the nucleus and an electron—each spatial state should be split into a pair of states, one for each electron in the pair. Thanks to this response of the electron's magnetic dipole moment when placed in a magnetic field, this new quantum number was identified with the electron's intrinsic angular momentum, or spin, because the spin angular momentum is proportional to its magnetic dipole moment.

One may define an elementary particle as a state of definite mass and spin. The intrinsic angular momentum, the spin $\mathbf{S}$ carried by a particle, like any angular momentum, is quantized in units of Planck's quantum $\hbar$. This occurs because a generic angular momentum $\mathbf{L}$ is defined by $\mathbf{L} \equiv \mathbf{r} \times \mathbf{p}$, where $\mathbf{r}$ denotes the particle's position and $\mathbf{p}$ its linear momentum. But in quantum mechanics the position and momentum variables do not commute, as in $p_x x - x p_x = \hbar/i$, which shows up in angular momentum components as the cyclic commutation relation such as $L_x L_y - L_y L_x = i\hbar L_z$. From these relations it follows that a spin vector $\mathbf{S}$ is described by a quantum number s, where $|\mathbf{S}|^2 = \hbar^2 s(s+1)$, where the options for s are $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$.[4]

Thanks to the commutation relations, only $|\mathbf{S}|^2$ and just one component of $\mathbf{S}$ can be simultaneously measured (the component parallel to an ambient magnetic field is a typical choice). That distinguished component will have values $\hbar m_s$ where $m_s = s,\ s-1,\ s-2, \ldots, -(s-1),\ -s$, making $2s+1$ possible values of m_s, the multiplicity. The electron beams that were split into two by Goudsmit and Uhlenbeck tell us that $2 = 2s+1$, so that $s = \frac{1}{2}$ for the electron.

All particles that carry odd-half-integer spin, $1/2, 3/2, 5/2, \ldots$, are fermions, and particles that carry integer spin $0, 1, 2, 3, \ldots$ are bosons. Identical fermions will not be found in the same quantum space-spin state, whereas identical bosons "like" to be in the same quantum state. Illustrations of boson collective behavior are found in Bose-Einstein condensation, superfluidity, and superconductivity. A classic electromagnetic wave is, in a quantum mental picture, a swarm of spin-0 photons all in the same energy, momentum, and polarization state. Illustrations of the aloof behavior of fermions range from the

electronic configuration of atoms and conduction electrons in metals to white dwarf and neutron stars, where fermion aloofness exhibits a pressure that prevents these compact objects from undergoing gravitational collapse—provided the star's mass does not exceed certain limits.

The assertion that no two identical fermions will be in the same quantum state, and any number of identical bosons can be in the same quantum state, finds formal expression in Pauli's spin-statistics theorem of 1940.[5] The *theorem* shows that this *postulate* about how the spin of identical particles determines how they populate quantum states is *consistent* with relativistic quantum field theory.[6, 7]

Because electrons have spin-1/2, they are fermions, and therefore only two electrons can be in the same spatial state if their spin orientations are opposite relative to, say, an ambient magnetic field. If a system consists of N electrons, at absolute zero the N-electron system's ground state will be the configuration of Fig. 1(a). The electrons "stack up," and the electrons at the top of the "stack" have the *Fermi energy* E_F. The fact that electrons cannot coalesce into the same state suggests that some kind of pressure keeps them apart.

When the system is excited by thermal or other energy input, some electrons are kicked above the Fermi energy, leaving electron vacancies, or "holes," beneath it.

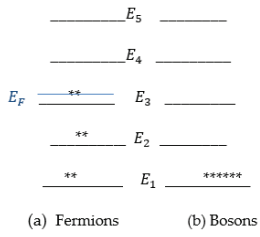


Figure 1: The zero-temperature ground states for a system of six identical particles: fermions [(a), left] and bosons [(b), right]. The energy labels in the center are eigenvalues of the single-particle spatial states, with E_1 the single-particle ground state. The fermions must have opposite spin to not be in the same space-spin state. Each E_i can therefore accept two fermions (although there is a slight energy difference—an energy level splitting—for the oppositely oriented spins, e.g., the spin-orbit interaction). The energy of the most energetic electrons in the multifermion system's ground state defines the Fermi energy E_F.

The Fermi Surface

Consider a system of N freely mobile spin-½ fermions, such as the loosely bound valence electrons in a good conductor that collectively form an electron gas. Examples are found in the conduction electrons in a metal and the gas of electrons permeating completely ionized carbon atoms in a white dwarf star. These electrons, each of mass m, are enclosed within a finite volume and may therefore be modeled as otherwise free particles in a three-dimensional box having rigid walls enclosing the volume $V = L^3$. The time-independent Schrödinger equation yields, for one electron, the standing-wave "eigenstates," the normalized quantum spatial states:[8]

$$\psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{8}{V}} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right), \qquad (1)$$

where $n_i = 1,2,3,\ldots$ (a general electron state is a superposition of eigenstates, just as the music emitted by a violin is a superposition of a harmonic series of standing waves). This state, when squared, gives its contribution to the probability density for locating the electron within the box. The energy eigenvalues corresponding to the spatial-only states of Eq. (1) are

$$E_{n_x n_y n_z} = \frac{\pi^2 \hbar^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right), \qquad (2)$$

where $k_i = n_i \pi / L$ denotes the wave number of a de Broglie wave, and $k_i = 2\pi/\lambda_i$, where λ_i denotes the de Broglie wavelength of one of the standing waves.

Including the electron's spin state $\chi_\pm$ (plus for spin-up, minus for spin-down) creates the space-spin eigenstate $\psi_{n_x n_y n_z}(x,y,z)\chi_\pm$. The spin-orbit interaction, where the electron's magnetic dipole moment $\boldsymbol{\mu}$ contributes the potential energy $-\boldsymbol{\mu} \cdot \mathbf{B}$ because of its interaction with magnetic field $\mathbf{B}$ produced by the relative motion between the electron and the nucleus, gives a slight energy splitting for electrons having opposite spins but residing in the same spatial state $\psi_{n_x n_y n_z}(x,y,z)$.

Note that the energy eigenvalues of Eq. (2) are highly degenerate, e.g., $E_{112} = E_{121} = E_{211}$, even though the corresponding eigenstates are different. The state (111) is the ground state of a single particle, but the question that needs answering for the multiparticle system is this: What is the ground state for the entire system of N identical electrons? The ground state, of course, would occur at absolute zero, $T = 0$. If the free particles were distinguishable particles or identical bosons, then, at absolute zero when they have negligible thermal energy $k_B T$ to bounce them along (where k_B denotes Boltzmann's constant), they would all coalesce into their (111) states and the state of the system would be as in Fig. 1(b).

But with a system of identical fermions, we need to find the number of single-particle states from E_{111} to E_F. Since the states are identified by sets of integers, this means counting the number of possibilities for (n_x, n_y, n_z) that can fit within the energy range $0 < E \leq E_F$. To proceed, since $E = \mathbf{p}^2/2m$ for a single free particle, make an orthogonal coordinate system (p_x, p_y, p_z) in momentum space, or, equivalently, since $p_i = \hbar k_i$, make an orthogonal coordinate system in k-space, where $(k_x, k_y, k_z) = (\pi/L)(n_x, n_y, n_z)$. Thus, any ordered triplet (n_x, n_y, n_z) designates a lattice point in k-space (Fig. 2) that corresponds to one of the single-particle spatial states of Eqs. (1) and (2). The volume of one lattice cell in k-space (also called reciprocal space) is π^3/V because adjacent n_i differ by π/L.

Suppose L is sufficiently large that the k-space lattice spacing becomes infinitesimal. Since each n_i in Eq. (2) is positive, the N free-electron states occupy the (+++) octant of a sphere of radius k_F, where $E_F = \hbar^2 k_F^2/2m$. Invoking the fact that electrons carry spin-½, two opposite-spin electrons may live at each lattice site. Therefore, within the octant bounded by the Fermi surface, the number of lattice sites is

$$(2)\left(\frac{1}{8}\right)\left(\frac{4\pi}{3}k_F^3\right) = N\left(\frac{\pi^3}{V}\right), \tag{3}$$

where the term on the right arises because the volume within the octant equals the number N of fermions times the reciprocal volume π^3/V of one lattice cell. Therefore, for the wave number of the Fermi momentum we find

$$k_F = \left(3\pi^2\,\frac{N}{V}\right)^{1/3}. \tag{4}$$

The quantity $\hbar k_F = p_F$ is called the Fermi momentum and the surface $k = k_F$ in k-space is called the Fermi surface. It forms the boundary between occupied and unoccupied states when the system of N identical fermions is in its lowest energy state, the ground state at $T = 0$. The energy of an electron at the Fermi surface, the Fermi energy E_F, is

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(3\pi^2\frac{N}{V}\right)^{2/3}. \tag{5}$$

The total energy of all the electrons within the Fermi surface—energy here called E_{Pauli} because it's due to the Pauli exclusion principle—is given by

$$E_{Pauli} = \int_0^{k_F} E(k)d\kappa = \int_0^{k_F}\left(\frac{\hbar^2 k^2}{2m}\right)d\kappa, \tag{6}$$

where $d\kappa$ denotes the number of states from k to $k + dk$.

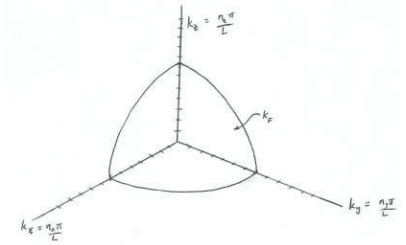


Figure 2: The k-space, showing the Fermi surface $k = \sqrt{k_x^2 + k_y^2 + k_z^2} = k_F$ for free, nonrelativistic identical fermions. The lattice sites are labeled with integers (n_x, n_y, n_z). Author image.

To evaluate $d\kappa$ is to count the number of lattice points in a shell of thickness dk in k-space. As noted above, since L is large compared to an atom's size, $k_i = n_i\pi/L$ approaches a continuum as the difference between two adjacent lattice points becomes very small. Then, the number of states between k and $k + dk$ equals the volume of the spherical shell of radius k and thickness dk. The number of lattice points with their corresponding states equals this volume divided by the volume of a unit cell, π^3/V. In addition, since each lattice point corresponds to a state $\psi_{n_x n_y n_z}(x, y, z)$ of Eq. (1) and an electron has spin-½, each lattice site can accommodate two electrons. Thus, we can say

$$d\kappa = (2)\,\frac{\frac{1}{8}(4\pi k^2\,dk)}{\pi^3/V} = \frac{Vk^2dk}{\pi^2}. \tag{7}$$

Insert Eq. (7) into Eq. (6) to complete the integration,

$$E_{Pauli} = \int_0^{k_F}\left(\frac{\hbar^2 k^2}{2m}\right)\frac{Vk^2dk}{\pi^2} = \frac{\hbar^2 V}{10m\pi^2}\,k_F^5. \tag{8}$$

Using Eq. (4), Eq. (8) may also be written

$$E_{Pauli} = \frac{\hbar^2(3\pi^2 N)^{5/3}}{10\pi^2 m\,V^{2/3}}. \tag{9}$$

We must keep in mind that as the *ground-state* energy of the N-identical spin-½ particle system, Eq. (9) describes its energy at absolute zero. However, it will turn out that Eq. (9) approximately holds even in the thermodynamic environments of white dwarf stars! While their temperatures are many orders of magnitude above absolute zero (e.g., white dwarf stars are typically built of carbon, and to fuse helium to carbon in a star before it becomes a white dwarf requires a temperature of about 100 MK), we shall see how a comparison of the Pauli energy of Eq. (9) to core thermal energy $\frac{3}{2}k_BT$ allows Eq. (9) to be a useful approximation even in those extreme environments.

In Part 2 we will examine how the degeneracy in a gas of fermions leads to a pressure that keeps the fermions from collapsing into a common ground state and see the role of this pressure in compact objects—white dwarfs and neutron stars.

Acknowledgment

With great appreciation I thank Curtis McCully for reading a preliminary draft of this manuscript and making useful suggestions.

References

1. Edmund C. Stoner, "The Distribution of Electrons Among Atomic Levels," *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 48 (1924): 719–736.
2. Wolfgang Pauli, "Über den Zusammenhang des Abschlusses der Elektronengruppen im Atom mit der Komplexstruktur der Spektren," *Zeitschrift für Physik*, 31 (1925): 765–783.
3. G. Uhlenbeck and S. Goudsmit, "Replacement of the Hypothesis of a Non-Mechanical Constraint by the Requirement of an Internal Property of Each Individual Electron," *Die Naturwisenchaften* (1925): 953; "Spinning Electrons and the Structure of Spectra," *Nature* 117 (1926): 264.
4. D. Neuenschwander, "Elegant Connections in Physics: Angular Momentum and 'Spin,'" *The SPS Observer*, Fall 2000, 10-14.
5. Wolfgang Pauli, "The Connection Between Spin and Statistics," *Phys Rev.* 58 (1940): 716–722.
6. George Sudarshan and Ian Duck, *Pauli and the Spin-Statistics Theorem* (Singapore: World Scientific, 1998).
7. D. Neuenschwander, "Elegant Connections in Physics: The Spin-Statistics Theorem and Identical Particle Distribution Functions," *Radiations*, Fall 2003, 27-32.
8. David Saxon, *Elementary Quantum Mechanics* (San Francisco: Holden-Day, 1968), 265-267.