Exchange, antisymmetry and Pauli repulsion

Can we 'understand' or provide a physical basis for the Pauli exclusion principle?

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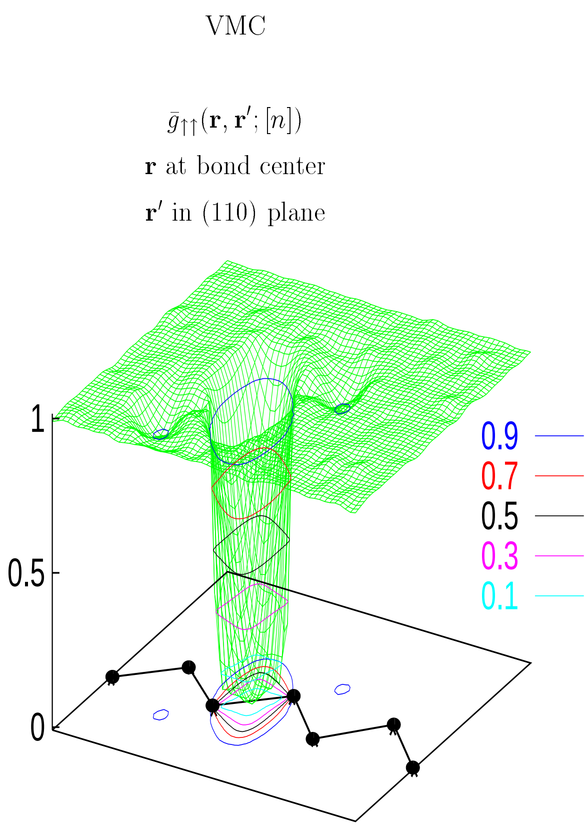
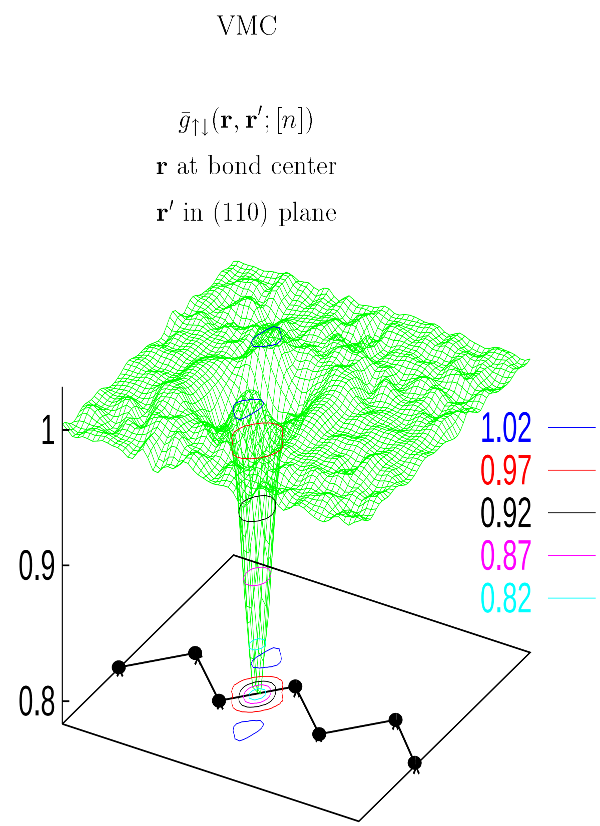
Pair correlation functions in silicon





Why is the parallel spin hole wider and deeper than the antiparallel one? Nobody knows, other than to say ‘because of the Pauli exclusion principle’, or ‘due to statistical repulsion’, or ‘because fermions cannot be in the same state’, or whatever.

The Exclusion Principle

Long standing, unsolved theoretical problem of atomic physics: *why is that electrons within an atom do not all collect in the lowest energy orbital?* In 1925 Pauli published a limited version of the Exclusion Principle from studies of fine structure of atomic energy levels and earlier suggestions of E.C. Stoner:

Pauli's Principle: *In an atom there cannot be two or more electrons with the same quantum numbers*.

Then realised that the Principle applies not just to electrons but to all *fermions* of same type. If we say quantum particles are **identical** when they have same mass, charge, spin, etc., then fermions are sometimes defined to be those identical quantum particles that, when part of a quantum system consisting of two or more of the same particles, the system has a wavefunction that is antisymmetrical in its form. Consequent generalization of Pauli's Principle:

Exclusion Principle: *In a quantum system, two or more fermions of the same kind cannot be in the same (pure) state.*

The antisymmetrical form of the wavefunction is generally taken as a 'brute fact', i.e. as a defining characteristic of fermions or as a feature of nature that cannot be otherwise explained. The exclusion principle acts primarily as a selection rule for non-allowed quantum states and cannot be deduced as a theorem from the axioms of Orthodox Quantum Theory.

References:

Quantum Causality by P. Riggs (2009)
Pauli's Exclusion Principle - the origin and validation of a scientific principle, by M. Massimi (2005)

"*The reason why the Pauli Exclusion Principle is true and the physical limits of the principle are still unknown.*" (NASA website)

Indistinguishability

Standard approach: justify Exclusion Principle by appealing to assumed 'indistinguishability' of identical particles. Consider two spinless non-interacting identical particles at $\mathbf{x}_1$ and $\mathbf{x}_2$ with wave functions $\psi_A(\mathbf{x}_1)$ and $\psi_B(\mathbf{x}_2)$. Assume composite system wave function $\psi(\mathbf{x}_1, \mathbf{x}_2) = \psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2)$.

Claim since particles indistinguishable, coords are just labels whose exchange is not meaningful. Thus require the 2-particle wave function to give same probability density after such exchange, i.e.

$$|\psi(\mathbf{x}_1, \mathbf{x}_2)|^2 = |\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2)|^2 = |\psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)|^2 = |\psi(\mathbf{x}_2, \mathbf{x}_1)|^2$$

Not true in general! So use technique of *linearly combining* wave functions. Since $\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2)$ and $\psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)$ are both solutions of Schrödinger equation, so is any linear combination. Two possibilities for composite system wave function:

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}}[\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) \pm \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)]$$

If $\pm$ is positive, Ψ said to be symmetric with respect to coord exchange since $\Psi(\mathbf{x}_1, \mathbf{x}_2) = \Psi(\mathbf{x}_2, \mathbf{x}_1)$. If $\pm$ is negative, Ψ said to be antisymmetric since $\Psi(\mathbf{x}_1, \mathbf{x}_2) = -\Psi(\mathbf{x}_2, \mathbf{x}_1)$.

Observed fact: only symmetrical and antisymmetrical wave functions are 'found' in nature. Both types satisfy required probability density equality, but only antisymmetrical ones entail the Exclusion principle (if $\mathbf{x}_1 = \mathbf{x}_2$ then $\Psi = 0$, i.e. there is no corresponding quantum state.)

Conclusion: Exclusion Principle arises from the wave function of system of fermions being antisymmetric (Dirac 1926, Heisenberg 1926). However, note the Exclusion Principle is not *equivalent* to the condition that fermionic systems have antisymmetrical wave functions (as commonly asserted) but *follows* from this condition. Thus, indistinguishability is not enough.

The spin-statistics theorem and relativistic invariance

Often claimed antisymmetric form of fermionic Ψ arises from *relativistic invariance* requirement, i.e. it is conclusively established by the spin-statistics theorem of quantum field theory (Fierz 1939, Pauli 1940). Not so - relativistic invariance merely *consistent* with antisymmetric wave functions. Consider:

Postulate 1: *Every type of particle is such that its aggregates can take only symmetric states (boson) or antisymmetric states (fermion).*

All known particles are bosons or fermions. All known bosons have integer spin and all known fermions have half-integer spin. So there must be - and there is - a connection between statistics (i.e. symmetry of states) and spin. But what does Pauli's proof actually establish?

- Non-integer-spin particles (fermions) cannot consistently be quantized with symmetrical states (i.e. field operators cannot obey boson commutation relationship)
- Integer-spin particles (bosons) cannot be quantized with antisymmetrical states (i.e. field operators cannot obey fermion commutation relationship).

Logically, this does not lead to Postulate 1 (even in relativistic QM). If particles with integer spin cannot be fermions, it does not follow that they are bosons, i.e. it does not follow that symmetrical/antisymmetrical states are the only possible ones (see e.g. 'parastatistics'). Pauli's result shows that if only symmetrical and antisymmetrical states possible, then non-integer-spin particles should be fermions and integer-spin particles bosons. But point at issue is whether the existence of only symmetrical and antisymmetrical states can be derived from some deeper principle.

Actually, fact that fermionic wave function is antisymmetric - rather than symmetric or some other symmetry or no symmetry at all - has not been satisfactorily explained. *Additional postulate of orthodox QM*. Furthermore, antisymmetry cannot be given physical explanation as wave function only considered to be an abstract entity that does not represent anything physically real.

Does Pauli exclusion principle *need* a physical explanation?

"..[the Exclusion Principle] remains an independent principle which excludes a class of mathematically possible solutions of the wave equation. .. the history of the Exclusion Principle is thus already an old one, but its conclusion has not yet been written. .. it is not possible to say beforehand where and when one can expect the further development.." [Pauli, 1946]

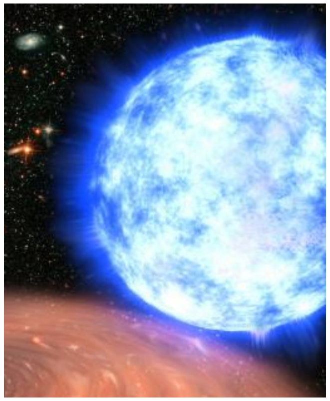
" I was unable to give a logical reason for the Exclusion Principle or to deduce it from more general assumptions. .. in the beginning I hoped that the new quantum mechanics [would] also rigorously deduce the Exclusion Principle." [Pauli, 1947]

"It is still quite mysterious why or how fermions with common values in their internal degrees of freedom [i.e spin] will resist being brought close together, as in the dramatic example of the formation of neutron stars, this resistance resulting in an effective force, completely different from the other interactions we know.." [Omar, 2005]

"..The Pauli Exclusion Principle is one of the basic principles of modern physics and, even if there are no compelling reasons to doubt its validity, it is still debated today because an intuitive, elementary explanation is still missing.." [Bartalucci *et al.*, 2006]

"The Exclusion Principle plays an important role in quantum physics and has effects that are almost as profound and as far-reaching as those of the principle of relativity... [the Exclusion Principle] enacts vetoes on a very basic level of physical description." [Henry Margenau]

An example: electron degeneracy pressure



When a typical star runs out of fuel it collapses in on itself and eventually becomes a *white dwarf*. The material no longer undergoes fusion reactions, so the star has no source of energy, nor is it supported against gravitational collapse by the heat generated by fusion. It is supported only by *electron degeneracy pressure*. This is a force so large that it can stop a star from collapsing into a black hole, yet no-one seems to know what it is.. Which of the four fundamental forces is responsible for it? None of them seems to have the right characteristics..

Degenerate matter: At very high densities *all* electrons become free as opposed to just conduction electrons like in a metal. When this happens, degeneracy pressure (which is essentially independent of temperature) becomes bigger than the usual thermal pressure.

Usual explanation: *Electron degeneracy pressure is a quantum-mechanical effect arising from the Pauli exclusion principle. Since electrons are fermions, no two electrons can be in the same state, so not all electrons can be in the minimum-energy level. Rather, electrons must occupy a band of energy levels. Compression of the electron gas increases the number of electrons in a given volume and raises the maximum energy level in the occupied band. Therefore, the energy of the electrons will increase upon compression, so pressure must be exerted on the electron gas to compress it. This is the origin of electron degeneracy pressure.* [Wikipedia]

All explanations apparently boil down to "because of the Pauli Exclusion Principle", or "because fermions can't be in the same state". The origin of the Pauli repulsion which prevents particles being in the same state (that is, having identical probability distributions) is thus *not understood*.

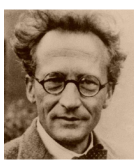
Required characteristics of 'Pauli repulsion' force supporting a white dwarf?

All discussions of degeneracy pressure talk about electrons as objectively-existing point particles, so we shall also make this assumption (it then follows that the electrons must have *trajectories*).

Strategy: Work with statistical distribution ρ since particle positions unknown. Assuming *classical* Newtonian trajectories, derive differential equation giving time evolution of ρ. Can we deduce from this anything about form of force in *quantum* case?

- Probability distribution ρ must obey usual continuity equation $\partial\rho/\partial t = -\nabla\cdot(\rho\mathbf{v})$ so that it remains normalized as it changes shape over time (here $\mathbf{v}$ is velocity vector).
- Assume particles obey classical dynamics. To calculate trajectories, don't use Newtonian $\mathbf{F} = m\mathbf{a}$ formulation; instead use the *entirely equivalent* Hamilton-Jacobi equation $-\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V$- where S is related to the 'action'.

For convenience, combine continuity and classical Hamilton-Jacobi equations (two *real* equations, note) into a single *complex* equation. To do this, introduce general complex function $\Psi = re^{i\theta} = \sqrt{\rho}e^{\frac{iS}{\hbar}}$ with $\hbar$ an arbitrary constant giving a dimensionless exponent. Complex equation that results is:



$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V - Q\right)\Psi \qquad \text{with} \qquad Q = -\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}.$$

This is the *time-dependent Schrödinger equation* - straight out of QM - with one difference: something like a potential ('Q') is subtracted off the Hamiltonian. Note Ψ has same interpretation as in QM: a particle probability density. Tells us that if particles are to follow Newtonian trajectories, must subtract off an extra 'quantum force' $-\nabla Q$ (apparently due to a 'wave field' pushing the particles) from the usual classical force. Could this 'fifth force' be responsible for Pauli repulsion?

Electron trajectories? What do we think about this in TCM?

But do electrons really have trajectories? This is really a question of the *interpretation* of QM, but since essentially no-one thinks about that here, let's see what we *actually do in practice* in TCM.

Density functional theory people:

- Create movies using *ab initio* molecular dynamics, where the nuclear positions are evolved using Newton's equations. We therefore believe that nuclei are point particles with classical trajectories.
- The electrons have a sort of fuzzy charge density which is a 'solution to the Schrödinger equation' (in the Kohn-Sham sense) for a sequence of nuclear positions. So - because electrons are very light - either we don't believe they have trajectories at all, or we believe they move much faster than the nuclei and their (presumably non-classical) trajectories are 'smeared out'.
- Sometimes, for very light atoms such as H, we think that *quantum effects* such as zero-point motion or tunnelling are important. We then might do e.g. *ab initio* path integral molecular dynamics (e.g. Matt Probert's implementation in CASTEP).[1]
- The 'exchange potential' - which gives rise to so-called 'quantum effects that cannot be described classically' - is presumably some kind of approximation to Q?

"*If we were to name the most powerful assumption of all, which leads one on and on in an attempt to understand life, it is that all things are made of atoms, and that everything that living things do can be understood in terms of the jigglings and wigglings of atoms.*" [Feynman]

[1] It can be shown that Feynman path-integral QM - where you sum over the infinite number of possible trajectories each weighted by an expression involving the classical Lagrangian $T - V$ - is equivalent to just using a single term involving the trajectory that the electron actually follows along with the new 'quantum Lagrangian' $T - V - Q$. In principle one could just calculate $-\nabla Q$ to correct the quantum H atom trajectories.

Electron trajectories? What do we think about this in TCM?

Quantum Monte Carlo people:

- Both nuclei and electrons are treated as point particles (though the nuclei are usually clamped).
- We can compute forces (albeit with some difficulty) and if we bothered to implement coupled DMC-MD in CASINO [as Wagner and Mitas did with their code] then we would move the nuclei along classical trajectories just as with DFT. Widely differing timescales make it difficult to treat nuclei and electrons on the same quantum footing.
- In QMC the point electrons do not move along trajectories (we instead move them along a stochastic random walk to sample the distribution). However it can be shown that diffusion Monte Carlo is in principle a stochastic quantum trajectory method in imaginary time (this would be more apparent if we ever used time-dependent probability distributions).

Conclusions:

- Neither DFT people or QMC people are Copenhagenists, since such people explicitly state - as part of the ontology - that quantum particles *do not have positions* unless they are measured. It is explicitly understood that hidden variables descriptions (and particle positions and their consequent trajectories are hidden variables) are impossible.
- The 'quantum force' depends inversely on the mass. So when we decide whether particles follow classical trajectories, we appear to have developed a mental facility for estimating the size of Q. Clearly for heavier particles, Q will be small and the trajectories approximately classical. For lighter particles, this is not so and we must use quantum methods to calculate their dynamics.
- There is no justification for saying that in TCM we do not believe in the reality of particle trajectories (either for electrons or nuclei). We may therefore proceed with a clear conscience to understand the Exclusion Principle using an argument based on particle trajectories.

Indistinguishability and wave field overlap

Unfortunately, if particles have a continuous existence, then the usual way of arguing in terms of permutation invariance and so on becomes invalid. We can no longer assume identical particles are *always* indistinguishable, since they may be distinguished by their spatial relations (trajectories).

Permutation invariance postulate: *If Ψ is the state of a composite system whose components are identical particles, then expectation value of any obervable A is the same for all permutations of Ψ.*

This allows for quantum states that are symmetric, antisymmetric, and of higher symmetry, and so we must supplement this with the following (experimentally-derived) postulate:

Symmetrization postulate: *The only possible states of a system of identical particles are described by state vectors (wave functions) that are either completely symmetrical or completely antisymmetrical.*

In a realist approach the wave function antisymmetry is a conceptual problem since, if the wave field is a physical field that propagates through space, it should be representable by functions without any particular symmetry. In our arguments we instead use the criterion that *particles are indistinguishable if their individual wave fields spatially overlap (either now or at some particular time in the past)*.

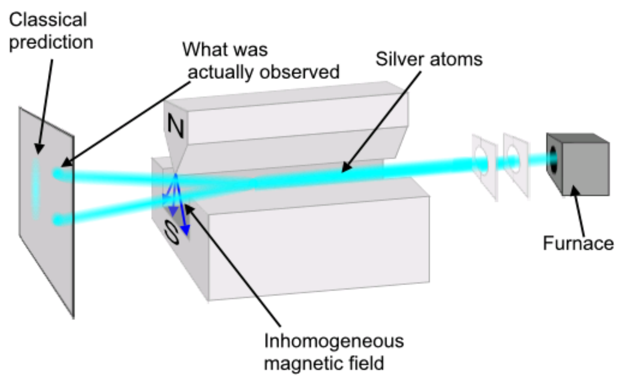
Justification: work out expectation value of square of distance between two particles for product wave function $\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2)$ and for an antisymmetrized one $\frac{1}{\sqrt{2}}[\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)]$:

$$\langle(\mathbf{x}_1 - \mathbf{x}_2)^2\rangle = \langle\mathbf{x}^2\rangle_A + \langle\mathbf{x}^2\rangle_B - 2\langle\mathbf{x}\rangle_A\langle\mathbf{x}\rangle_B + 2|\langle\mathbf{x}\rangle_{AB}|^2$$

where $\langle\mathbf{x}\rangle_{AB} = \int \mathbf{x}\Psi_A^*(\mathbf{x})\Psi_B(\mathbf{x})\,\mathrm{d}\mathbf{x}$ is measure of overlap between wave fields Ψ_A and Ψ_B, and e.g. $\langle\mathbf{x}\rangle$ is the expectation value of $\mathbf{x}$ in the (single particle) state denoted A. If no overlap, then the antisymmetrized result (blue + green) reduces to the product one (blue only). The fermions are then distinguishable, in which case particles must be widely separated and have remained so.

Spin

To do this properly we need a realistic explanation of *spin*, since the Exclusion Principle prescribes that if the fermions of a particular physical system share the same set of quantum numbers (and this includes the spin quantum number) then they cannot be at the same location.



Initial concept of spin had its origin in the experiments of Stern and Gerlach in which a beam of silver atoms was split in two by passage through a non-uniform magnetic field. In 1925 Uhlenbeck and Goudsmit proposed that an electron had a magnetic dipole moment which they explained using the classical idea of an extended particle (in this case, an electron) spinning about an axis through its centre. They used this idea to explain the results of the Stern-Gerlach experiments.

It has become clear that what is called the 'spin of a quantum particle' cannot be the rotational angular momentum of a spinning particle. In other words, spin cannot be due to an extended body rotating about an axis through its centre of mass. The reasons against the axial rotation explanation are readily provided:

- the rotation of an extended particle would not require an additional variable for its specification;
- the spin's vector does not depend on the particle's position and momentum;
- angular momentum due to rotation about the centre of mass cannot take half-odd-integer values;
- the rate of rotation required to give results in agreement with experiment would need tangential velocities exceeding the speed of light in vacuum.

Pauli theory of spin

In order to meet the need for incorporating spin into Orthodox QM, much attention was given to developing spinor representations and spin algebra as a way of dealing with an aspect of quantum systems (i.e. spin) that was not properly understood. E.g., the Pauli equation $i\hbar(\partial\Psi/\partial t) = \mathbf{H}\Psi)$ for a single spin-$\frac{1}{2}$ particle has a *two-component* spinor wavefunction Ψ and the following Hamiltonian:

$$\mathbf{H} = \frac{-\hbar^2}{2m}\left[\nabla - \frac{ie}{\hbar c}\mathbf{A}\right]^2 + \mu\mathbf{B}\cdot\sigma + eA_0 + V$$

with $\mathbf{A}$ and A_0 being the electromagnetic potentials, $\mathbf{B} = \nabla \times \mathbf{A}$ an external magnetic field and V a (classical) scalar potential. The vector quantity σ has Pauli's 'spin matrices' as its components:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

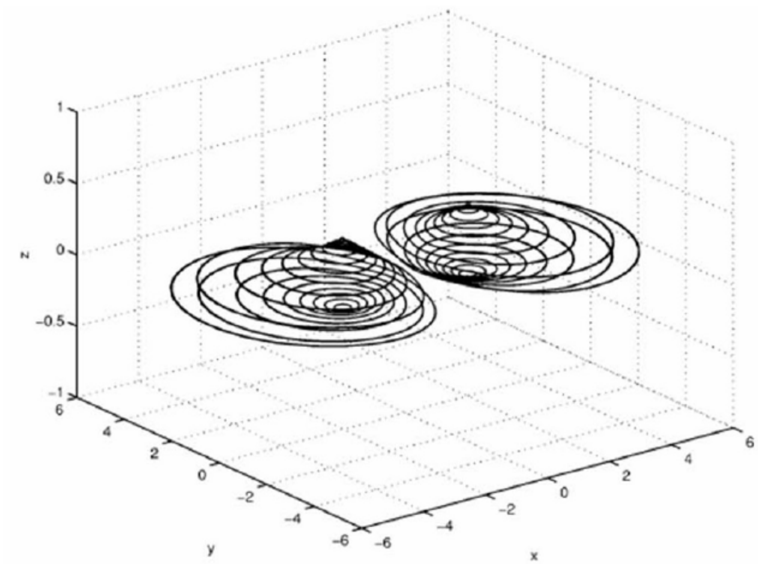
where $\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2$. These matrices are operators that represent the spin observables, e.g. z-component of spin given by $s_z = \frac{1}{2}\hbar\sigma_z$. Eigenfunctions of spin representing 'up' and 'down' spin given by following two-component spinor wave functions: $\chi_1 = \begin{pmatrix} 1 & 0 \end{pmatrix}$ and $\chi_2 = \begin{pmatrix} 0 & 1 \end{pmatrix}$. General expression for system not in eigenstate is the superposition $\chi = a\chi_1 + b\chi_2$ where a, with complex b. These functions give required measured values of spin, i.e. $\pm(\hbar/2)$ with certainty when system is in an eigenstate, or with probability $|a|^2$ for up and $|b|^2$ for down when in a superposition.

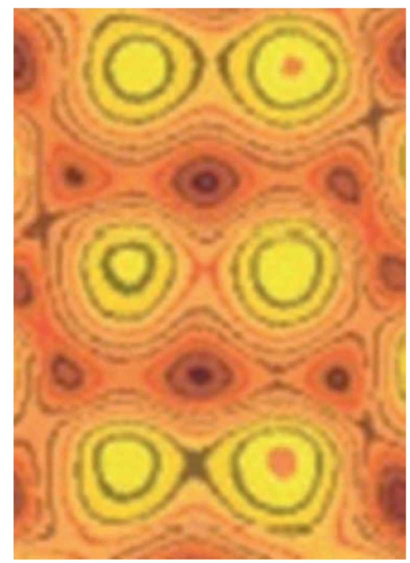
Although it is the case that spinor methods have been formally successful, they are really a technical means of not addressing the underlying nature of the spin phenomenon. Indeed, the Pauli equation does not provide any insight into the origin or characteristics of spin:

Pauli's theory does not explain the origin of the spin, nor does it give any reason for its magnitude. It merely provides a method for incorporating it into quantum mechanics. [Lindsay and Margenau, 1957]

Spin with trajectories

- We have seen that if we accept particles have a continuous objective existence, then in QM it appears as if they are acted on by a force $-\nabla V - \nabla Q$, with the Q bit having its origin in an accompanying wave field mathematically represented by Ψ. The wave field ought therefore to be a reservoir of potential energy, and can receive or impart energy and momentum to the particles.
- Q is the potential energy of the wave field and represents the amount of energy available to the particle/configuration at its specific position in the field.
- There is no spin in the non-relativistic Schrödinger theory. However, if we take the non-relativistic limit of the relativistic trajectory equations, we find that Q develops a spin dependence.





"*In classical physics the aim of research was to investigate objective processes occurring in space and time. In the quantum theory, however, the situation is completely different. The very fact that the formalism of quantum mechanics cannot be interpreted as visual description of a phenomenon occurring in space and time shows that quantum mechanics is in no way concerned with the objective determination of space-time phenomena*" [Heisenberg, 1965]. Hmmm..

An important inference about the nature of spin

- We have seen that spin cannot arise from electron rotation, nor do electrons appear to have internal structure. Moreover, the fact that the quantum potential Q (which represents a portion of the wave field's energy) has a *spin dependence* implies that spin must be a *property of the wave field*.
- Is there a precendent for this? Yes! In electromagnetic theory - spin is part of an electromagnetic wave's angular momentum, the part which is dependent on the wave's polarization (see e.g. Jackson electromagnetism textbook 1975, p. 333, Ohanian 1986 - see next page).

Consider, for example, a circularly-polarized plane electromagnetic wave with a vector potential $\mathbf{A}$ given by:

$$\mathbf{A} = (\hat{\mathbf{x}} \pm i\hat{\mathbf{y}}) \left(i\frac{E_0}{\omega} \right) \exp \left[i\omega \left(t - \frac{x}{c} \right) \right]$$

where E_0 is the electric field strength, ω is the angular frequency, and $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are Cartesian unit vectors. The polarization-dependent part of the wave's angular momentum (i.e. its spin s) is:

$$s = \pm \frac{1}{\mu_0 c^2} \int \frac{E_0^2}{\omega} \hat{\mathbf{z}} \, \mathrm{d}^3\mathbf{x}$$

Nice paper

What is spin?

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According to the prevailing belief, the spin of the electron or of some other particle is a mysterious internal angular momentum for which no concrete physical picture is available, and for which there is no classical analog. However, on the basis of an old calculation by Belinfante [Physica **6**, 887 (1939)], it can be shown that the spin may be regarded as an angular momentum generated by a circulating flow of energy in the wave field of the electron. Likewise, the magnetic moment may be regarded as generated by a circulating flow of charge in the wave field. This provides an intuitively appealing picture and establishes that neither the spin nor the magnetic moment are "internal"—they are not associated with the internal structure of the electron, but rather with the structure of its wave field. Furthermore, a comparison between calculations of angular momentum in the Dirac and electromagnetic fields shows that the spin of the electron is entirely analogous to the angular momentum carried by a classical circularly polarized wave.

I. INTRODUCTION

When Goudsmit and Uhlenbeck proposed the hypothesis of the spin of the electron, they had in mind a mechanical picture of the electron as a small rigid body rotating about its axis. Such a picture had earlier been considered by Kronig and discarded on the advice of Pauli, Kramers, and Heisenberg, who deemed it a fatal flaw of this picture that

See also "What is spin?", A. Gsponer, arXiv:physics/0308027v3 (2003).

Spin and polarization

"The lack of a concrete picture of the spin leaves a grievous gap in our understanding of quantum mechanics ... spin could be regarded as due to a circulating flow of energy, or a momentum density in the electron wave field ... this picture of the spin is valid not only for electrons ..." [Ohanian, 1986]

- In this picture wave fields must have states of polarization, similarly to the case of an electromagnetic wave. However, it is obvious that in non-relativistic QM wavefunctions are *scalar* waves describing spinless quantum states. It might thus be objected that if wave fields have states of polarization, then QM wave functions would have to represent *vector* waves, and this might conflict with the representation of quantum systems with spin by spinors.
- However, there is more than one formal way to achieve this representation. In particular, *either vector waves or scalar waves plus spinors can be used*. Indeed, spinors are used this way in classical wave theory [see e.g. Rogalski/Palmer *Advanced University Physics* p.401-403 (2006)]. As previously noted, the representation of spin by spinors is only a method of dealing with the spin phenomenon without needing an understanding of its fundamental nature.
- The explanation of spin as the polarization-dependent part of the wave field's angular momentum has not only *not been accepted* by most physicists who are aware of this explanation, it is almost universally ignored. The principal reason for this is probably that, in orthodox QM, the wave field is generally not considered to be a real field, but to be a representation of our *knowledge* (or something similar).

The exclusion principle in a trajectory theory

- Let's delay discussion of why fermionic wave functions are antisymmetric, and for the moment just accept that they are. What then is the causal mechanism which explains the Exclusion Principle?
- Normally ones says things like "*A system in an antisymmetric state exhibits what is called statistical repulsion*" [Park, 1974]. Strange notions such as 'statistical repulsion' come from dismissing any possibility of a realistic, causal description of quantum phenomena and leaves this kind of correlated particle motion completely unexplained. However, if we accept that electrons have trajectories..

  "*The symmetrization or antisymmetrization of the wavefunction has nothing to do with the 'indistinguishability', but in fact, implies the introduction of forces between the particles making up the system, which bring about correlations in their motion.*" [Holland, 1993]
- When we analyze possible trajectories, we find they cannot pass through the nodal surface of the wave field (where the wave amplitude is zero) because the quantum force is always directed away from these nodes. Antisymmetrical wave fields have nodal surfaces, symmetrical ones do not. This is the basis of the exclusion principle for fermions.

Let's try to show this mathematically!

Fermionic repulsion in a trajectory theory

A total antisymmetrical wave function for a many-electron system can occur in a number of ways. For 2 electrons there are 3 states of interest where the electrons 'avoid each other'. Collectively called the 'triplet state' with total z-components of spin $\hbar$, $-\hbar$, 0. Their wave functions (which are products of space and spin) all have antisymmetrical spatial components so $\Psi = 0$ if $\mathbf{x}_1 = \mathbf{x}_2$ and are given by:

$$\begin{aligned}
\Psi &= \{\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)\}\,\alpha(1)\alpha(2) \\
\Psi &= \{\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)\}\,\beta(1)\beta(2) \\
\Psi &= \{\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)\}\,\{\alpha(1)\beta(2) + \alpha(2)\beta(1)\}
\end{aligned}$$

Now let the spatial part be written in complex polar form: $\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1) = Re^{i\frac{S}{\hbar}}$. When this is zero the amplitude R must be zero (since $e^{i\frac{S}{\hbar}}$ cannot be zero by definition). Thus, as a nodal region of the wave field is approached, the value of R will tend to zero. The (repulsive) quantum force on each particle is $\mathbf{F}_i = (\mathrm{d}\mathbf{p}_i/\mathrm{d}t) = -\nabla_i Q$ where $Q = -\hbar^2/2mR(\nabla_1^2 R + \nabla_2^2 R)+$ spin-dependent terms. Finding the negative gradient of Q (ignoring the spin-dependent terms since the spatial terms will dominate as R tends to zero) gives:

$$\mathbf{F}_i = \frac{\hbar^2}{2mR^2}\sum_{j=1}^{2}\left[R\nabla_i(\nabla_j^2 R) - (\nabla_i^2 R)(\nabla_j R)\right]$$

It can be seen that as $R \longrightarrow 0$ then $\mathbf{F}_i \longrightarrow \infty$. The 'Pauli repulsion' force $\mathbf{F_i}$ exerted by the wave field on the two fermions prevents them coming into close proximity of each other when their 'spins are the same' (i.e. in cases where the spatial part of Ψ is antisymmetric). More generally, the dynamics as shown by this trajectory theory prevent fermions occupying the same quantum state.

Towards a fundamental basis for the exclusion principle

Must now explain why Ψ in a fermionic system takes an antisymmetric form. Some considerations:

- In a realist theory where the wave field objectively exists, the antisymmetrical form should be explicable in terms of the well-established behaviour of physical waves. If fermions are localized particles as we postulate, then the Exclusion Principle must also be a *non-local* effect.
- The Exclusion Principle is normally assumed to apply to all physical situations involving fermions of the same kind, but it has been argued that its applicability should be restricted; there are certain kinds of *non-stationary* state for which it produces paradoxical results. Reasonable statement: Exclusion Principle applies to *a system of identical fermions that has constraints imposed upon it which are necessary but not always sufficient for the establishment of a stationary state*.

Physically, a stationary state results when two travelling waves that are propagating in opposite directions superpose (due to restriction in a finite spatial region such as a box or an atom). Clearly the Exclusion Principle does not apply to widely-separated fermions of the same kind; need wave-field overlap.

But if only one of these waves was π out of phase with the other then wouldn't their sum be an antisymmetric function?

Modelling of fermionic wave fields

Consider system of two neutrons (to avoid electrical interaction) in a large box. Particles initially moving and well-separated with non-overlapping travelling wave fields. Initial wave function of product form. Let us make the radical assumption that the antisymmetrical form of the wave function develops over the course of time, rather than being fundamental.

So what happens when the neutrons come close enough together for wave field overlap? Without invoking the antisymmetry assumption, there is *no obvious expression* for the form of the two-neutron wave function when the individual wave fields first overlap.

Speculation: After some time, the initial wave field Ψ_I of the two neutron system will be successively reflected from the ends of the box. In the case of a fermionic wave field, reflection at a rigid wall causes a change of the wave field's phase of π radians. This is a well-known effect when a physical wave is reflected from a fixed boundary. However, it is the *polarization* of the incident wave field (and not the total spin) that determines whether there is a change of phase on reflection. (Spin part of wave field doesn't change on reflection). Interference between incident and reflected wave fields produces stationary state within the box, and the total wave function will have an antisymmetric form due to the negative sign in the reflected wave. (A similar argument can be made for atoms).

Difficult to analytically model this behaviour, since do not yet know valid mathematical description of the *initial overlap* of individual non-stationary wave fields. In the literature, it is simply *assumed* that the overall Ψ for a combined system is antisymmetric without showing how this is achieved.

Ultimately made difficult by the non-local nature of the interactions between entangled particles, which is what happens when your wave function is a function of the positions of all the particles. We do not currently know the 'means' by which the non-local connections are actualized. It would help if we did.

Experimental tests

An explanation of the Exclusion Principle does not seem to be possible within Orthodox Quantum Theory. In the absence of any theoretical basis for the Exclusion Principle, a series of further experiments are being planned and conducted by the Violation of the Pauli Exclusion Principle (VIP) Experimental Group:

"*The Pauli Exclusion Principle is one of the basic principles of modern physics and is at the very basis of our understanding of matter: thus it is fundamental importance to test the limits of its validity .. the VIP (Violation of the Pauli Exclusion Principle) experiment, where we search for anomalous X-rays emitted by copper atoms in a conductor: any detection of these anomalous X-rays would mark a Pauli-forbidden transition. .. VIP is currently taking data at the Gran Sasso underground laboratories, and its scientific goal is to improve by at least four orders of magnitude the previous limit on the probability of Pauli violating transitions..*" [Curceanu *et al.*, 2008].

In this talk a basis for the Exclusion Principle has been set out which provides the intuitive and relatively simple explanation that has been missing since Pauli first postulated the Principle. Further, this basis clearly allows the possibility that the Exclusion Principle might be violated in some extreme circumstances.

Conclusions

All QM textbooks describe the effects of the Exclusion Principle but its explanation is either avoided or put down to symmetry considerations. The importance of the Exclusion Principle as a foundational pillar of modern physics cannot be overstated since, for example, atomic structure, the rigidity of matter, stellar evolution and the whole of chemistry depend on its operation.

In this talk, I have shown that (1) the simple assumption that fermions are point particles with a continuous objective existence, and (2) the equations of non-relativistic QM, allow us to deduce:

- *..that a mathematically well-defined 'fifth force', non-local in character, appears to act on the particles and causes their trajectories to differ from the classical ones.*
- *..that this force appears to have its origin in an objectively-existing 'wave field' mathematically represented by the usual QM wave function.*
- *..that indistinguishability arguments are invalid under these assumptions; rather antisymmetrization implies the introduction of forces between particles.*
- *..the nature of spin.*
- *..that the action of the force prevents two fermions from coming into close proximity when 'their spins are the same', and that in general, this mechanism prevents fermions from occupying the same quantum state. This is a readily understandable causal explanation for the Exclusion principle.*

If we allow ourselves to assume that antisymmetry of the wave field is not fundamental, but develops naturally over the course of time, then we can see the character of the reason for fermionic wave functions having the symmetry behaviour they do. Mathematical details tricky.

Note we get a lot of stuff for a little assumption. Maybe this is rubbish but it's still very interesting!

Acknowledgement

The slides for this talk are largely based on the discussion in Chapter 6 of P. Riggs's book 'Quantum Causality' (2009).

The reader may also be interested in the slides available on the web site of my graduate lecture course, where there is also an extensive bibliography (click 'Further Reading').

www.tcm.phy.cam.ac.uk/~mdt26/pilot_waves.html

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