Electron Spin

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Outline

- The Quantum concept
- The Stern - Gerlach experiment
- Introducing the electron spin
  - superposition of states (quantum mechanics with spins)
  - entanglement
  - Fermions and bosons, Pauli Principle, exchange interaction
- Magnets

Color code: Single electron, two electrons, many electrons

The quantum concept

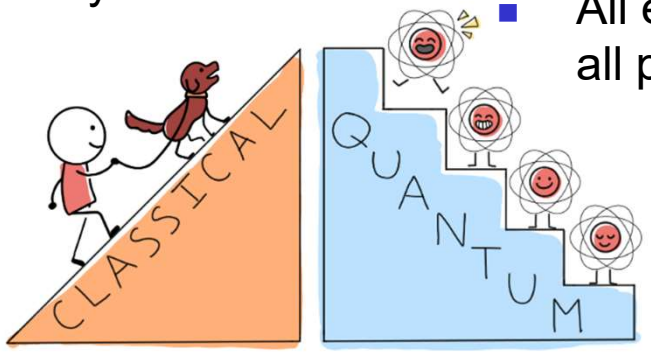
Classical

- A planet has a well-defined orbit, we can always tell where is it.
- Given accurate initial conditions, we can calculate the position of an object precisely.
- The position and velocity of a ball can be known with great accuracy.

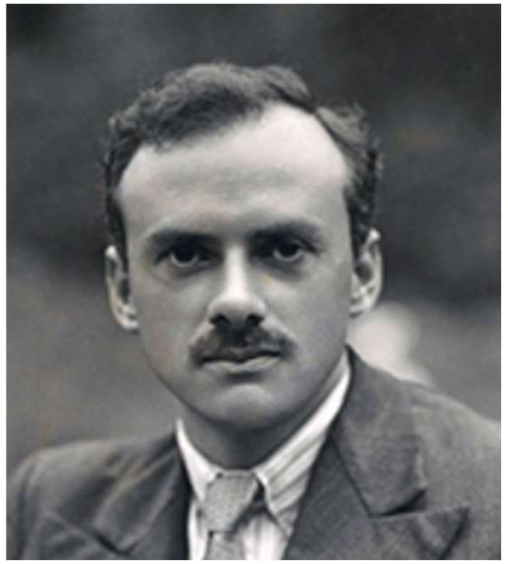
- The total energy of an orbiting planet may be set to a continuous range of energies
- No two balls are exactly the same

Quantum

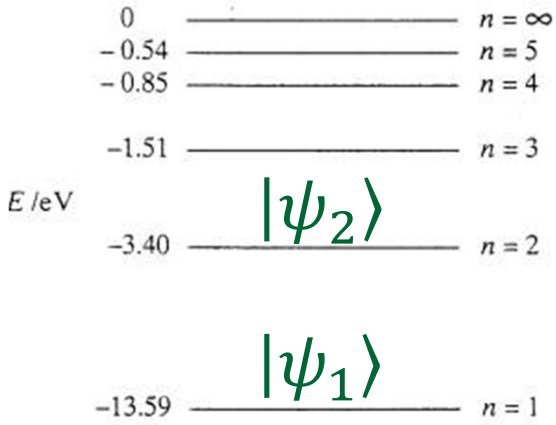
- When a particle propagates, we cannot tell where is it.
- We can only calculate the probability of finding the particle in a given position.
- The position and velocity of a particle cannot be known with great accuracy.
- The energy of the electron in an atom is precisely defined, and the energy levels are separated by large gaps
- All electrons are exactly identical in all properties.



Wavefunction



In quantum mechanics we need to introduce the concept of wavefunction, that is something we can never measure directly. It is a computational tool. Measurable quantities involve combination of two wavefunctions. Paul Dirac invented a simple way to capture the essence of the project without too much math; he introduced the bra ⟨| and ket |⟩ symbols. The wavefunction is denoted by $|\psi\rangle$ or $\langle\psi|$, and the measured quantity is a complete bracket: $\langle\psi|something|\psi\rangle$, where "something" can be position, energy, momentum, e.t.c.



There are some very simple rules for working with wavefunctions, illustrated by wavefunctions belonging to energy levels in hydrogen.

$\langle\psi_1|\psi_1\rangle = \langle\psi_2|\psi_2\rangle = 1$ and $\langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle = 0$

In practice this simple notation stands for complicated integrals, but we do not need to go there.

Key concept: A particle has a wave function that we cannot measure. Measurable quantities are obtained by calculating brackets.

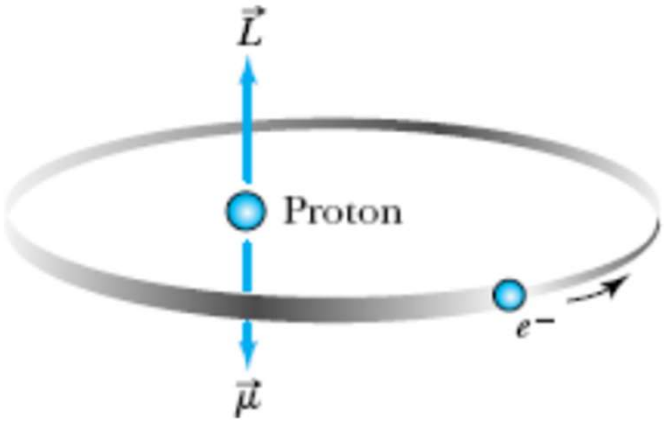
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Angular momentum, magnetic moment

Rotational motion. Pick the z axis perpendicular to the cirlce. The z component of the angular momentum is L_z

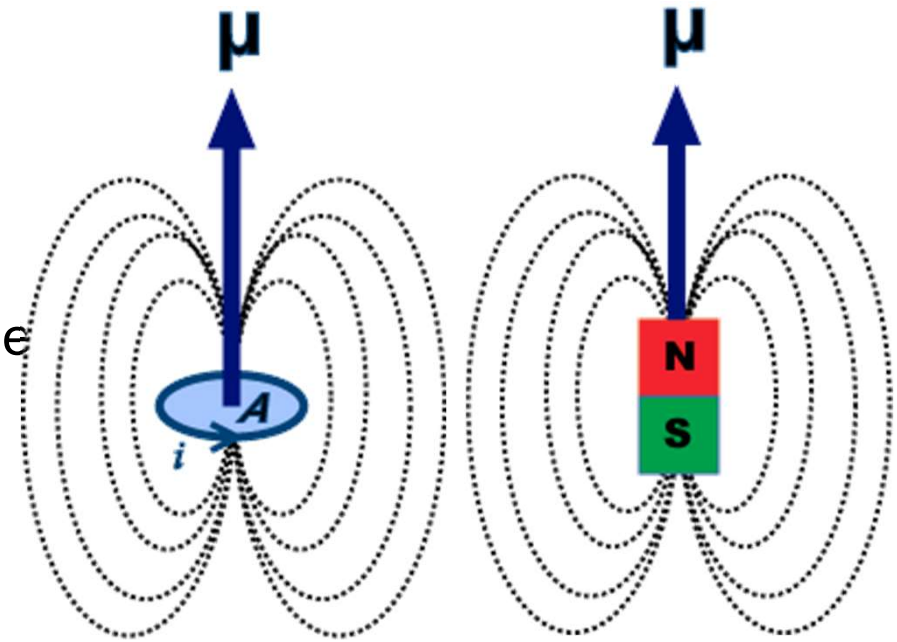


Current loop.

Acts like a small magnet.

The strength of the magnet is called magnetic moment, μ

For a current loop $\mu = IA$



For an electron on a circular orbit a simple calculation shows that the z component of the magnetic moment is

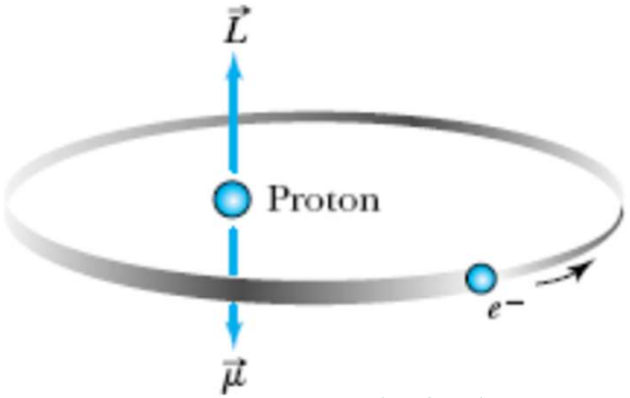
$$\mu_z = \frac{e}{2m} L_z$$

Birth of quantum mechanics

Quantum mechanics tells us the z component of the angular momentum is very precisely determined ("quantized"):

$$L_z = m_z h/2\pi,$$

where m_z is an integer, and $h = 6.626 \times 10^{-3}\ kg\ m^2/s$ is the Planck's constant. Therefore μ_z is also quantized, $\mu_z = m_z \frac{eh}{4\pi m}$. The spacing between the quantized value is called "Bohr magneton", $\mu_B = \frac{eh}{4\pi m}$. This idea was first introduced by Niels Bohr in the 1920's. In Bohr's model, in the lowest energy state of hydrogen $m_z = -1, 0, 1$ are possible.



$m_z = -1, 0, 1$



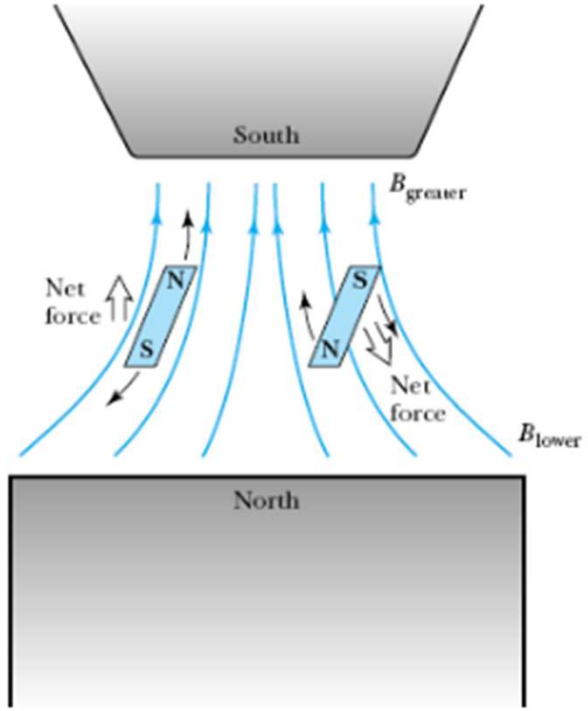
$m = 10^{30}$

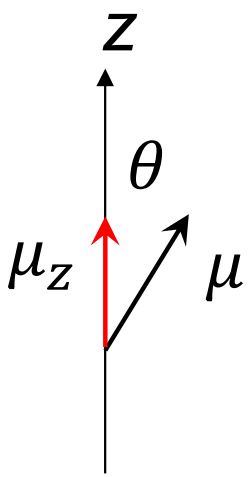
Large quantum number → classical physics

Magnetic moment in an inhomogeneous B field

Atom beam passes through inhomogeneous magnetic field. Each atom is a tiny magnet.

Top: stronger field





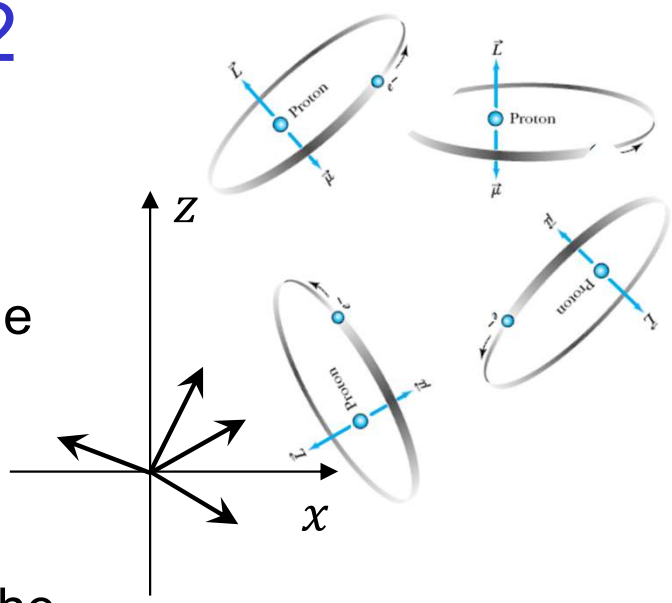
Bottom: weaker field

Left: N – South attraction is stronger than S – North attraction → net force up. In general, the net force is proportional to $\mu \cos\theta = \mu_z$

Stern Gerlach experiment, 1922

Imagine a beam of H atoms coming from a hot source. If there is no quantization, the magnetic moments point in random directions. We expect a continuous band of hits on the photo plate, with the upper and lower limits corresponding to

$\theta = 0^o$ and $\theta = 180^o$

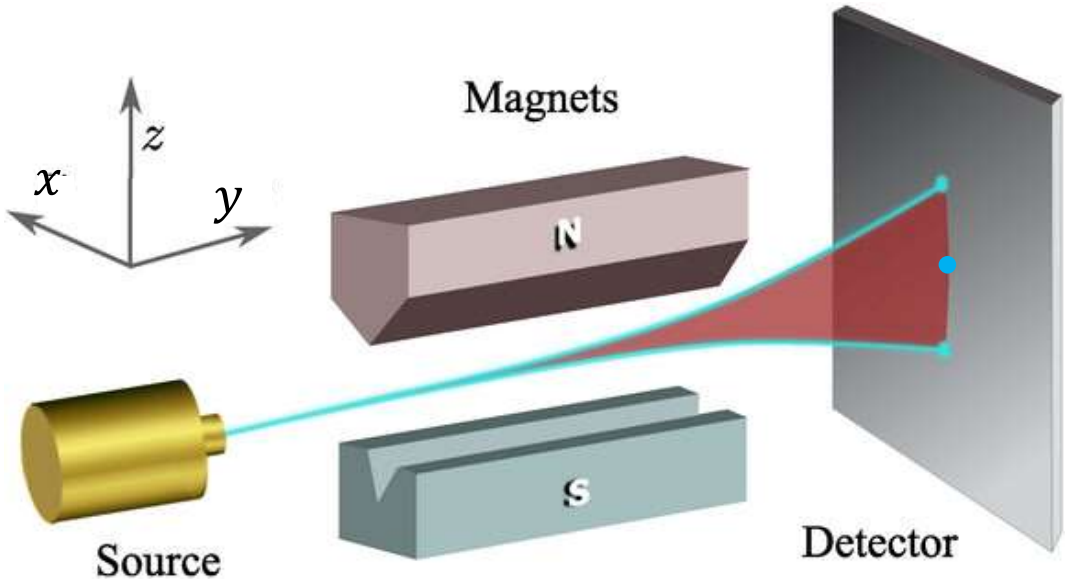


Alternative: Bohr is right and the *z* component of the angular momentum is quantized. μ_z is also quantized:

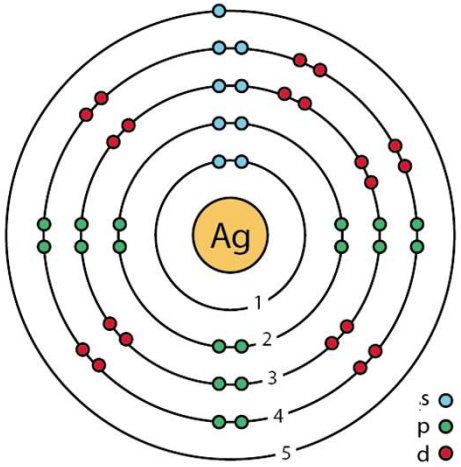
$\mu_z = -\mu_B$, $\mu_z = 0$, or $\mu_z = \mu_B$

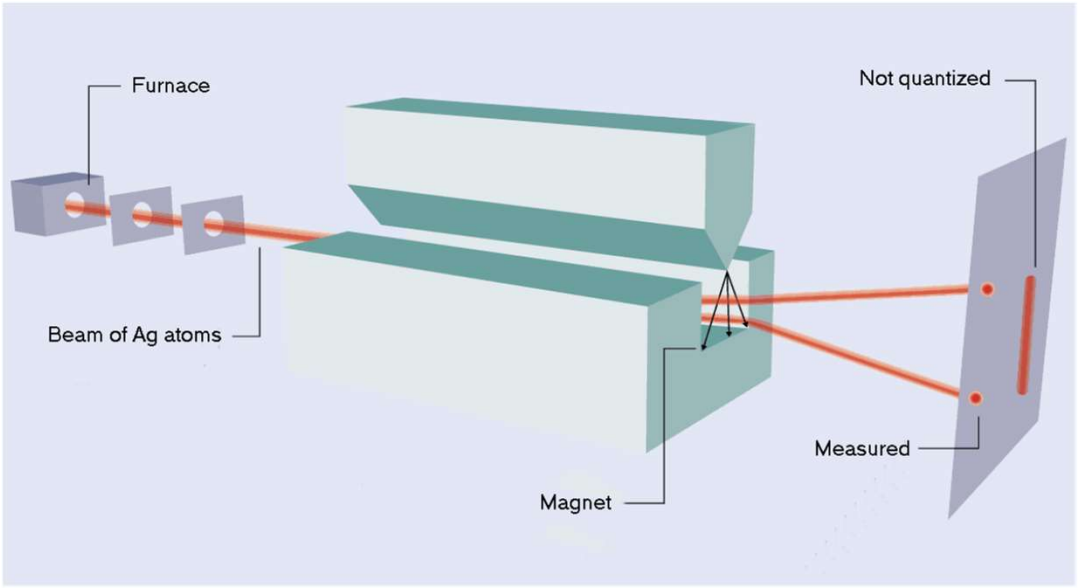
We have only 3 possible μ_z

We get 3 dots on the screen.



The right experiment, with wrong theory





The experiment was first done with silver beam. Result: Not a continuous line, proving that the z component of the angular momentum is indeed quantized. So far so good. But….

Instead of 3 dots they observed only 2. Big mystery.

Perhaps silver is more complicated than hydrogen? Experiment repeated with H, result is the same.

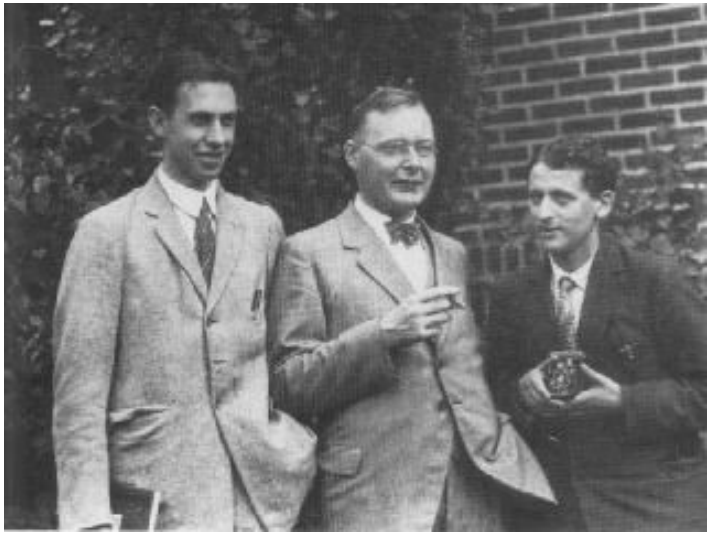
Electron Spin

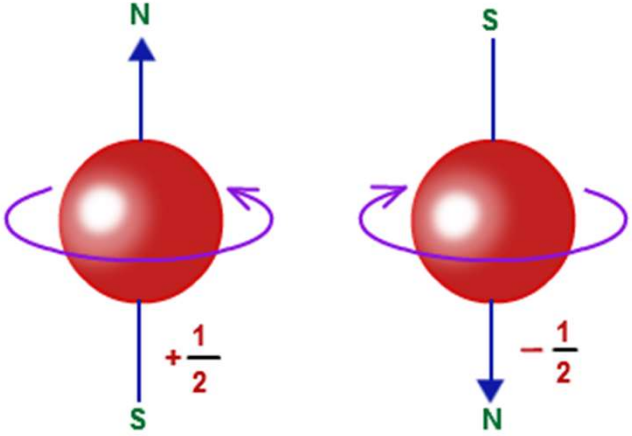
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Discovery of the electron spin

https://lorentz.leidenuniv.nl/history/spin/spin.html#:~:text=Discovery%20of%20electron%20spin&text=This%20photograph%20was%20taken%20around,moment%20of%20one%20Bohr%20magneton.





George Uhlenbeck (left) and Samuel Goudsmit (right) proposed the idea that each electron spins with an angular momentum of $L = \frac{1}{2}\left(\frac{h}{2\pi}\right)$ *and carries a magnetic moment of* $\mu_B = \frac{eh}{4\pi m}$. *At the time of their discovery, Uhlenbeck and Goudsmit were studying in Leiden with Paul Ehrenfest. At the center is Hendrik Kramers, another of Ehrenfest's students, who came to the same idea a few month before but never published it, because it seemed way too crazy.*

In the rest of the lecture we will use units of $\frac{h}{2\pi}$ for the angular momentum. In these units the z component of the electron spin is +1/2 or -1/2

Electron spin

Explains the S-G experiment, because the z component has only two values, $\mu_z = \frac{1}{2}\mu_B$ and $\mu_z = -\frac{1}{2}\mu_B$. We call this spin up and spin down.

Usual notation: ↑ and ↓

There is still something wrong here, we do not see any evidence for the orbital magnetic moment.

Resolution: The Bohr model is not the final story. Full blown quantum mechanics (the Schrödinger equation) tells us that in the ground state of hydrogen the electron has zero angular momentum. It does not circulate the nucleus, and therefore it does not create orbital magnetic moment.

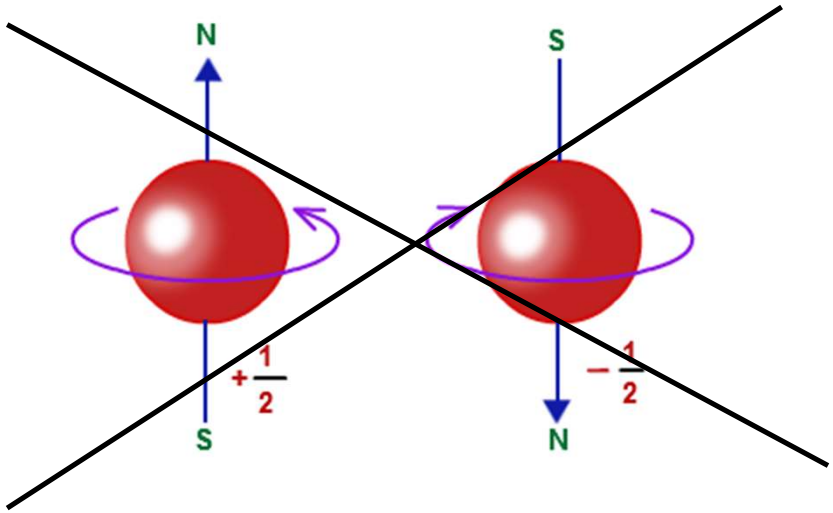
There is also another twist with the magnitude and direction of the angular momentum vector, but we do not need to get there – we will talk only about the *z* component.

-- Topics for another lecture series

Electron spin: charged rotating ball

Charged rotating ball explains the angular momentum and the magnetic moment as well. Minor problem: as far as we know the electron is a point. It does not have a radius.

This is why the idea was considered crazy. Even in the 1920's there was an upper limit to the electron size, and a quick calculation showed that to "explain" the magnetic moment, the electron's "surface" must move faster than the speed of light.



What explains the electron spin?

1905 Einstein's special relativity

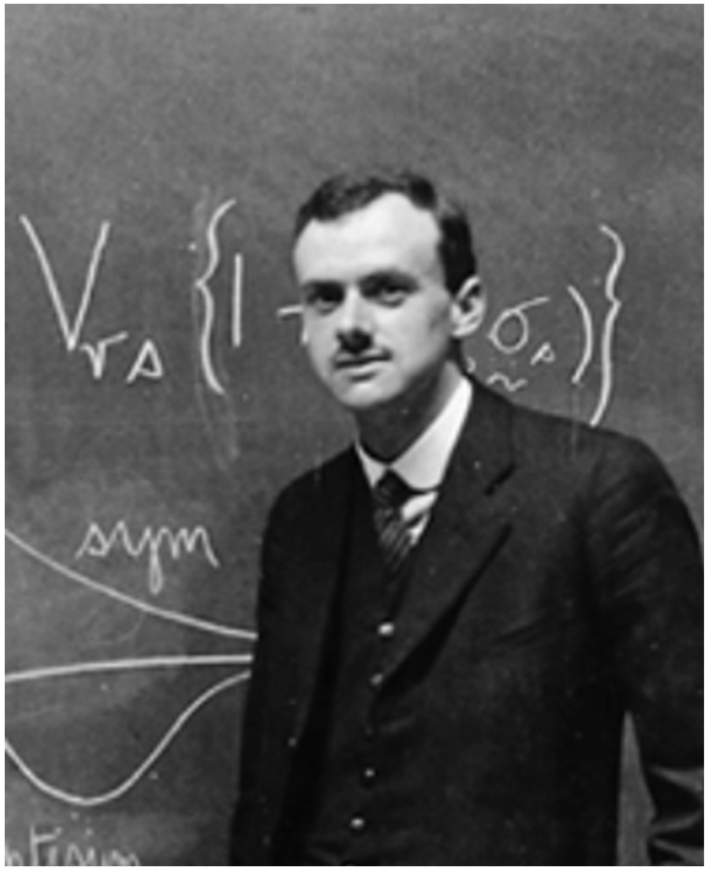
1926 Schrödinger's quantum mechanics

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\Psi(x,t)$$

The Schrödinger equation is not compatible with relativity

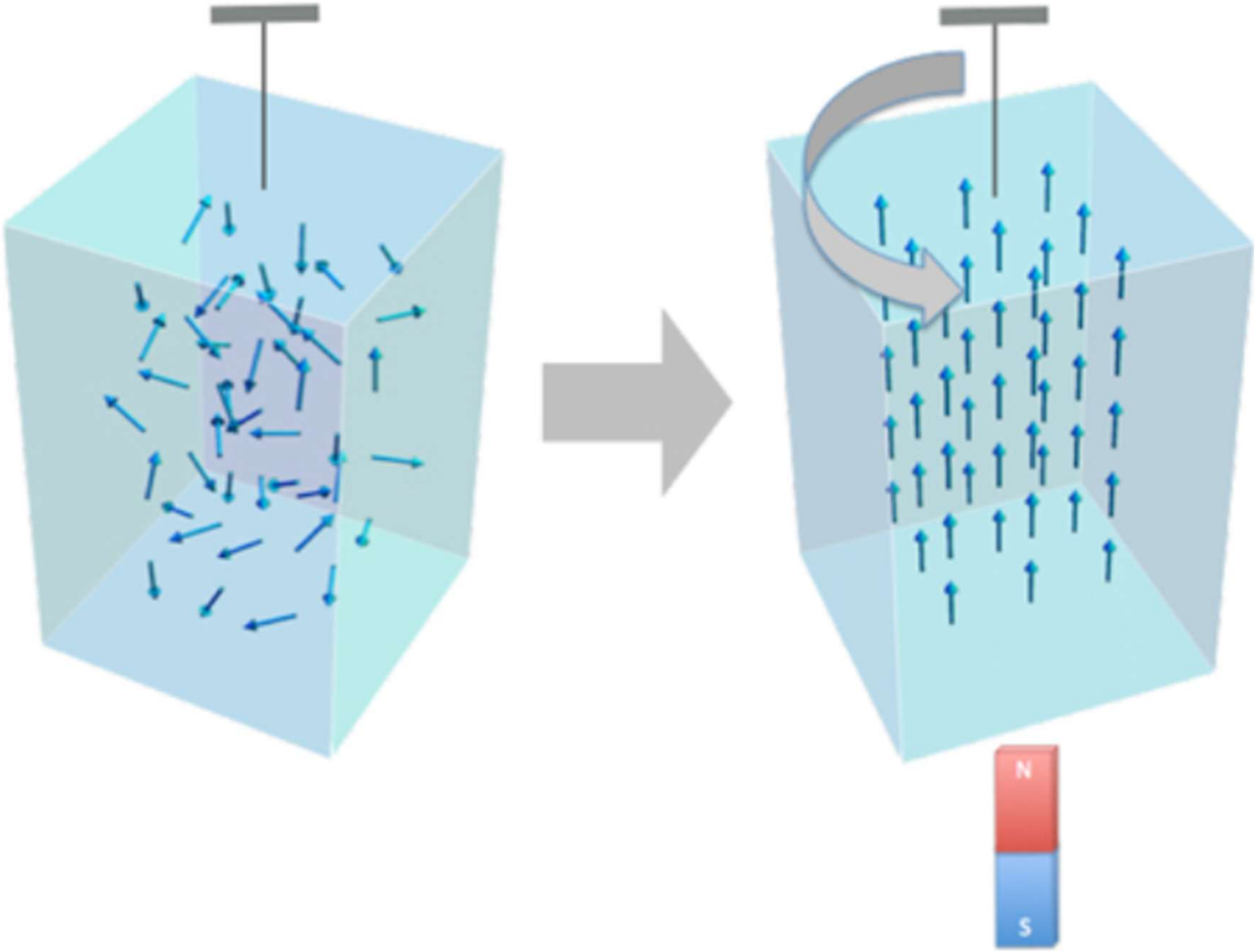
1928 Dirac solves the problem.

$$\left(\beta mc^2 + c\sum_{n=1}^{3}\alpha_n p_n\right)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$



In addition to being compatible with relativity, the Dirac equation also explained the electron spin, and predicted the existence of anti-particles. The positron, the anti-particle of the electron was discovered in 1932.

Einstein de Haas experiment



Electron Spin

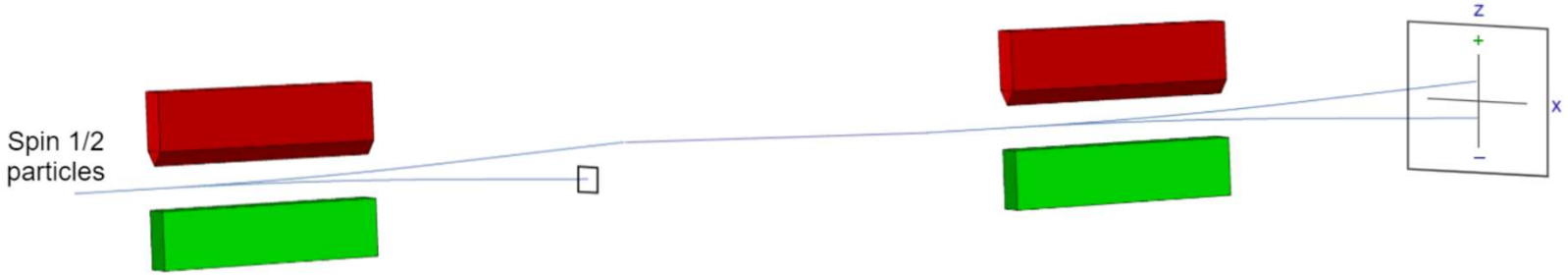
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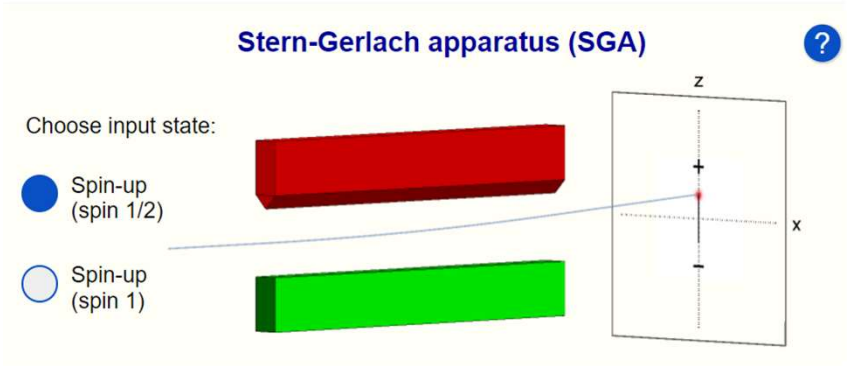
  superposition of states (quantum mechanics with spins)

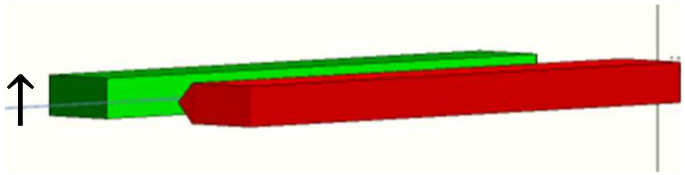
Experimenting with spins

Create a spin – polarized beam with a Stern Gerlach Apparatus (SGA), and send it to a second SGA

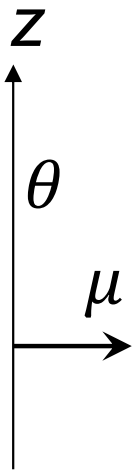


What happens if we rotate the second SGA? Start with 90^0 rotation.





$\frac{\hbar}{2}$ $means$ $\mu_z = -\frac{1}{2}\mu_B$



$\mu_z = 0$

All simulations in this section are from the St. Andrews University' QuVis WEB page: https://www.st-andrews.ac.uk/physics/quvis/

Conclusions of experiment 1

The measurement apparatus has its own up and down states, we will denote them “+” and “-” as seen on the screen.

An ↑ beam goes fully to the + state on the screen if $\theta = 0$, but it splits evenly between + and – if $\theta = 90°$.

Even with perfect instrumentation there are statistical fluctuations. They can be reduced by increasing the number of measurements.

We need quantum mechanics to describe and predict experimental results.

Quantum mechanics for spin



Let us invent a simple math for spin wavefunctions. For spins there are two principal wavefunctions, $|\uparrow\rangle$ and $|\downarrow\rangle$, representing the spin up and down states. All other wavefunctions are linear combinations of these two:

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$$

To calculate the probability of finding the spin in the "up" state we need to calculate the product

$$\langle\psi|\psi\rangle$$

and evaluate the result (see next page)

Rules of the game: $\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1$; $\langle\uparrow|\downarrow\rangle = \langle\downarrow|\uparrow\rangle = 0$

Spin wavefunction

Recall: $|\psi\rangle = a|\uparrow\rangle + b\,|\downarrow\rangle$

How about the probabilities?

$\langle\psi|\psi\rangle = a^2\langle\uparrow|\uparrow\rangle + b^2\,\langle\downarrow|\downarrow\rangle$, the other terms that contain $\langle\uparrow|\downarrow\rangle = \langle\downarrow|\uparrow\rangle = 0$

The probability of being in the up state is $P_\uparrow = a^2$

The probability of being in the down state is $P_\downarrow = b^2$

If we add up these probabilities we will get the probability of finding the spin in either the up or the down state. But the spin has only two choices, so this probability is 1.

The spin is either up or down, so $a^2 + b^2 = 1$.

We will only use the case of $a = b = 1/\sqrt{2}$.

Superposition of states

If we stay with a=b, there are two possible wavefunctions

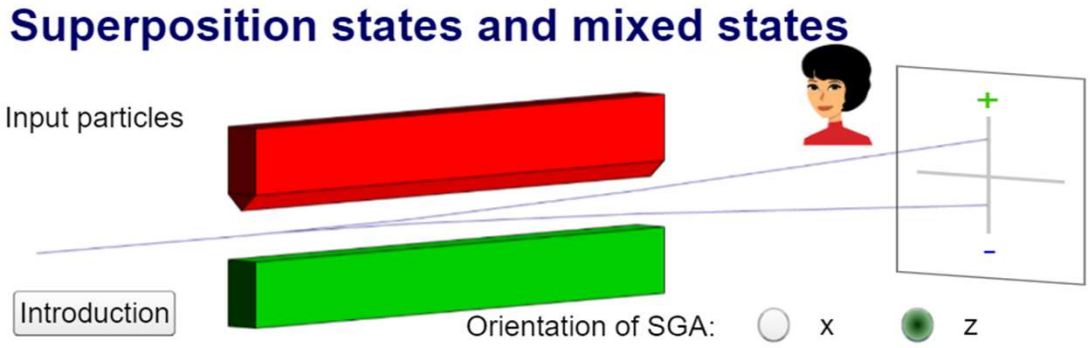
$|\psi_+\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, and $|\psi_-\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$

Note that we can place a "-" in front of the $\frac{1}{\sqrt{2}}$, but that will not influence the quantity we can measure, the probability, because when we do the brackets we get $(-1)^2=1$.

The $|\psi_+\rangle$ and the$|\psi_-\rangle$states are created by the "superposition" of the up and down states, with equal weight. This can be done for a single spin. Each electron in the beam is in this state.

If we have many electrons, we can create a beam, where half of the spins are up, and the other half is down. This is a 50% - 50% mixture. We can do this only if we have many spins.

Experiment with superposition of states



$P_\uparrow = a^2 = \frac{1}{2}, \quad P_\downarrow = b^2 = \frac{1}{2}$ agrees with experiment

Most importantly, when the SGA is in the x direction the superposition state $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ yielded only "+" results, as if the electron spin is in the x direction.

The superposition $\frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$ looks like spins in the –x direction.

By combining up and down state wavefunctions, we can recover a continuum of spin directions.

$$|\psi\rangle = a|\uparrow\rangle + b\,|\downarrow\rangle,\ a^2 + b^2 = 1,\ a = \cos\phi,\ b = \sin\phi\ ,\ \phi = \theta/2$$

Spinors

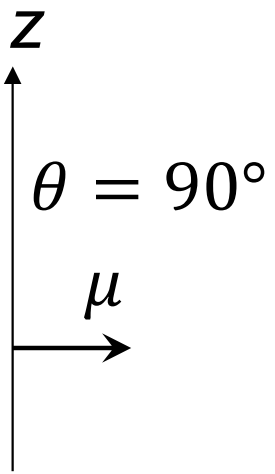
$|\psi\rangle = a|\uparrow\rangle + b\,|\downarrow\rangle$

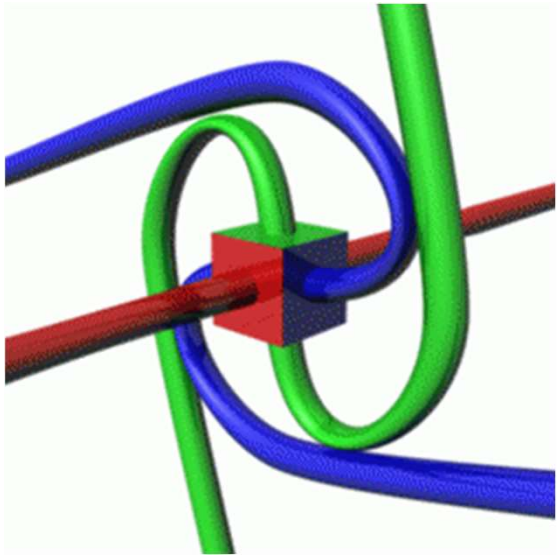
$a^2 + b^2 = 1,\ \ a = \cos\phi,\ b = \sin\phi$

Spin in +x direction :

$\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

$a = b = 1/\sqrt{2}$ → $\phi = 45°$





https://commons.wikimedia.org/wiki/User:JasonHise

In general, $\phi = \theta/2$

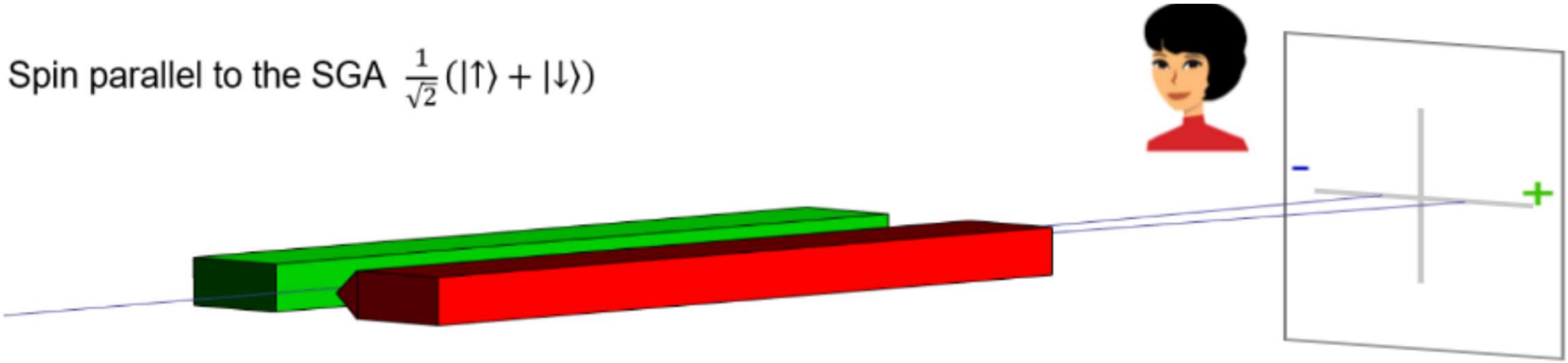
Let us start with $|\psi\rangle = |\uparrow\rangle,\ \ (\theta = 0°)$ and rotate the spin by 360°.

$\phi = \frac{\theta}{2} = 180°.$ → $|\psi'\rangle = -|\uparrow\rangle$. The wavefunction gets a "-" sign! Does not matter for measurable quantities, since $\langle\psi'|\psi'\rangle = (-1)^2\langle\uparrow|\uparrow\rangle$, but strange. We need a 720° rotation to get back the $|\uparrow\rangle$.

Mathematics: spinors.

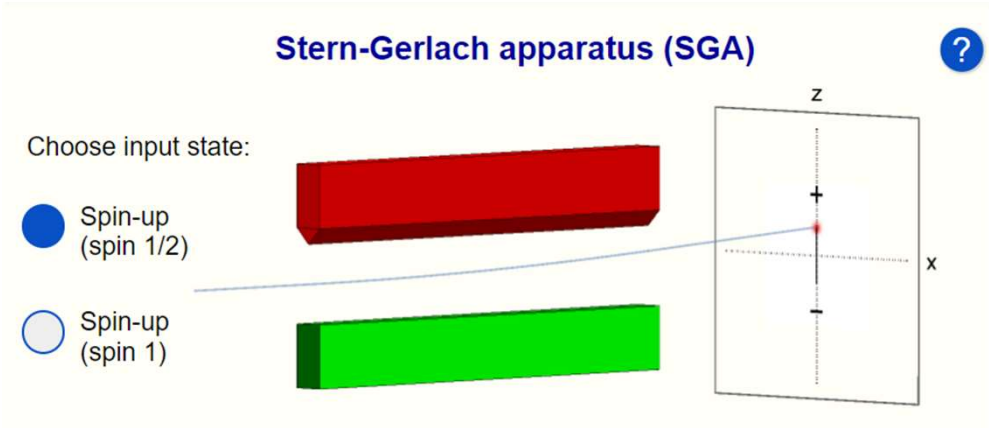
Explaining experiment 1

Spin parallel to the SGA $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$



Parallel → single dot on screen

Perpendicular → two dots



Electron Spin

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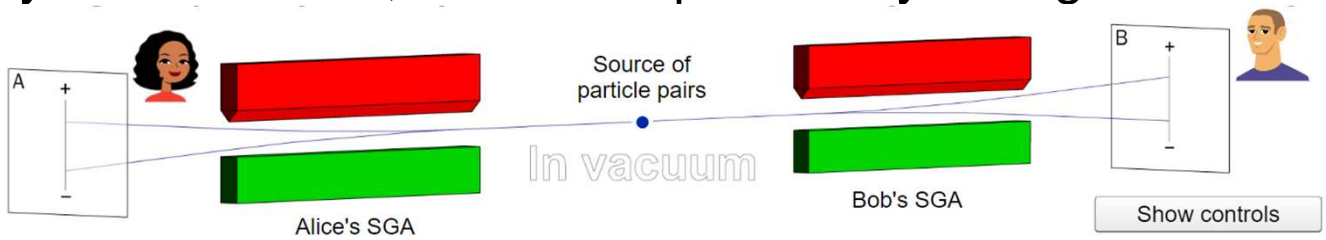
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    entanglement

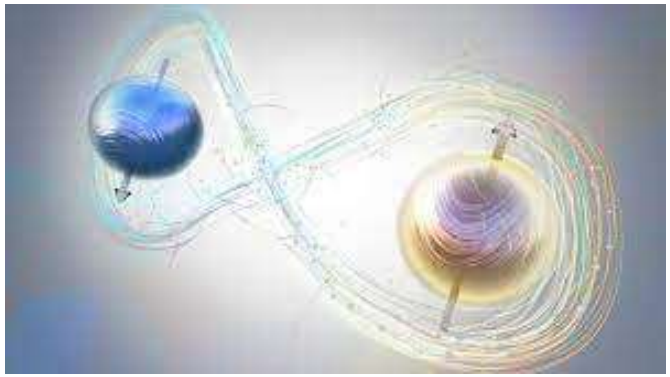
Entanglement

Create a source that emits two electrons in opposite directions. the process is such that the total angular momentum is zero, and therefore the two electrons must have opposite spins. The spin orientation is measured at the same time by Alice and Bob, who are separated by a large distance.



Naturally, if Bob measures a spin up, Alice has to get spin down.
There are two possible ways to achieve this.

1./ At the time the electrons are created the spin direction is firmly decided. If one of the electron comes with up spin, the other one will have down spin.



2./ The electrons are in a superposition of up and down spins, so that the sum is zero. The actual spin direction is decided only when the measurement happens.

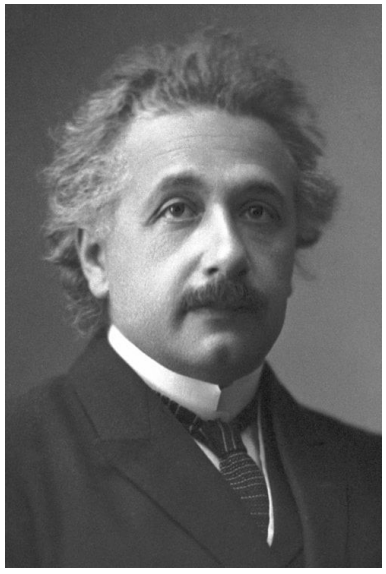
Einstein's protest



As quantum mechanics emerged, leading scientists tried to understand the nature of the wave function. The "Copenhagen interpretation" emerged. According to this, Option 2 is the reality, Option 1 is wrong.

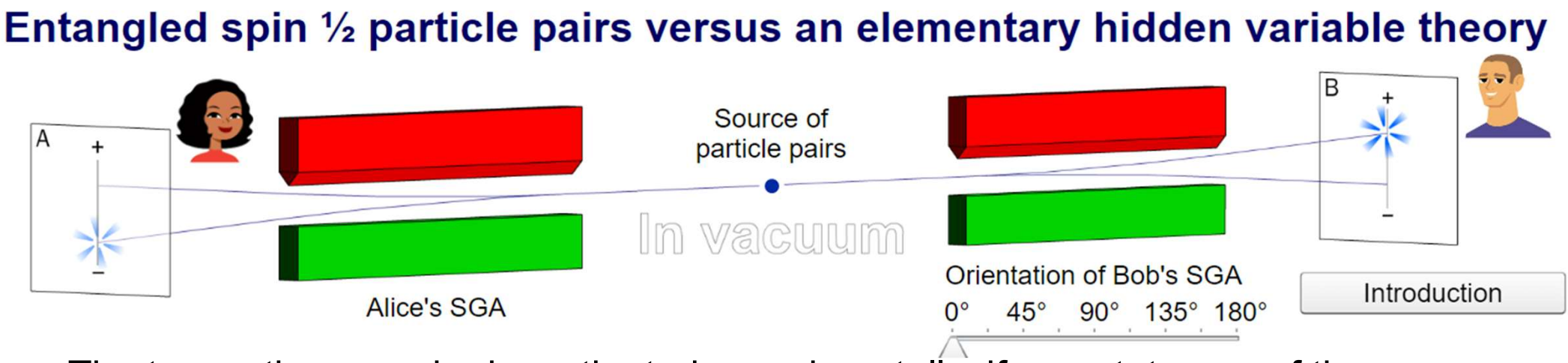
Einstein claimed that this is impossible because it will lead to a violation of his most fundamental discovery that no object or information can propagate faster than the speed of light. He called it a "spooky action at a distance". (He also disliked the idea that the wavefunction determines probabilities only. He said: "God does not play dice".)





Einstein was wrong

Today, entangled electrons and, more conveniently, entangled photon pairs are regularly produced. The key to accepting this is in the recognition that the measurement of the spins of electrons does not involve transmission of information.



The two options can be investigated experimentally, if we rotate one of the SGAs. For parallel and perpendicular SGAs the result does not distinguish between 1. and 2. For 45^0 angle we get a pronounced difference.

Entanglement is the key to quantum computing and quantum information processing

Electron Spin

Laszlo Mihaly,

Department of Physics and Astronomy, Stony Brook University

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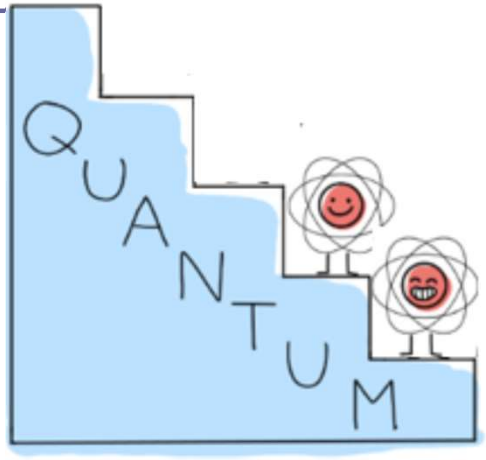
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  Fermions and bosons, Pauli Principle, exchange interaction

Fermions and bosons (no spin!)

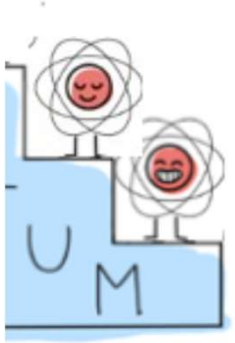


Imagine a system where the electron can occupy different energy levels and we have two electrons, electron A and electron B. We place electron A on the level 1 and electron B on level 2. The corresponding wavefunction is $|\psi_{12}\rangle$. (The first index tells you where is electron A, and the second one tells you where is electron B.) If we interchange the two electrons, we get another wavefunction, $|\psi_{21}\rangle$. To calculate brackets, the old rules apply:

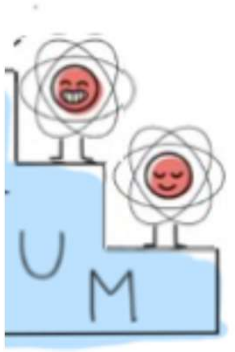
$\langle\psi_{21}|\psi_{21}\rangle = \langle\psi_{21}|\psi_{21}\rangle = 1, \quad \langle\psi_{12}|\psi_{21}\rangle = \langle\psi_{21}|\psi_{12}\rangle = 0$

If we look at the probabilities, we find that for a given wavefunction we know for sure where is electron A and where is electron B

$P_{12} = \langle\psi_{12}|\psi_{12}\rangle = 1$ and $P_{21} = \langle\psi_{21}|\psi_{21}\rangle = 1$



$|\psi_{12}\rangle$



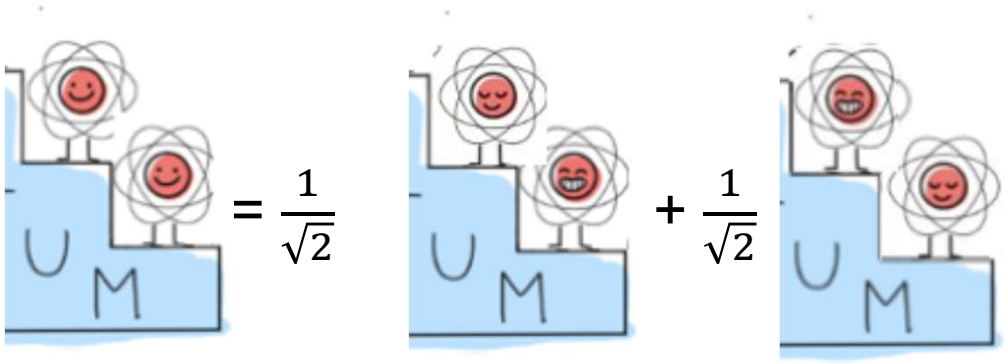
$|\psi_{21}\rangle$

But wait!! The two electrons look and behave exactly the same! We should not be able to know. Electrons A and B should have 50%-50% chance of being on levels 1 and 2.

Bosons

There is an easy fix for this:

$$|\psi_+\rangle = \frac{1}{\sqrt{2}}(|\psi_{12}\rangle + |\psi_{21}\rangle)$$



The probabilities are

$$\langle\psi_+|\psi_+\rangle = \frac{1}{2}\langle\psi_{21}|\psi_{21}\rangle + \frac{1}{2}\langle\psi_{12}|\psi_{12}\rangle$$

We have the 50% - 50% split. And we cannot tell which electron is where.

Fermions

Same combination, but with a – sign.

$$|\psi_-\rangle = \frac{1}{\sqrt{2}}(|\psi_{12}\rangle - |\psi_{21}\rangle)$$

If you do the calculation, you get the same result as before

$$\langle\psi_-|\psi_-\rangle = \frac{1}{2}\langle\psi_{21}|\psi_{21}\rangle + \frac{1}{2}\langle\psi_{12}|\psi_{12}\rangle$$

Because the terms that carry the "–" sign are 0. $\langle\psi_{12}|\psi_{21}\rangle = \langle\psi_{21}|\psi_{12}\rangle = 0$

This is what electrons do.

In general, there is a class of particles that carry a + sign when we interchange them. The are called Bosons. Examples are the particle of light (photon) or a hydrogen atom. Bosons carry an angular momentum that is integer (in units of $\frac{h}{2\pi}$)

Electrons bring a – sign to the wavefunction upon interchange. These kind of particles are called Fermions. They all have a spin that is 1/2, 3/2, … generally integer+1/2.

Pauli exclusion principle (with spin)

What happens if try to put two electrons on the same energy level?

$|\psi_-\rangle = \frac{1}{\sqrt{2}}(|\psi_{12}\rangle - |\psi_{21}\rangle)$ → $|\psi_-\rangle = \frac{1}{\sqrt{2}}(|\psi_{11}\rangle - |\psi_{11}\rangle) == 0$

Impossible, there is no wavefunction. This is the Pauli exclusion principle.

For a moment we forgot that the electron has spin. Let' add it back. $|\psi_{12}\uparrow\downarrow\rangle$ means this: electron A is in state 1 with spin up; electron B is in state 2 with spin down.

Parallel spins: $|\psi_-\rangle = \frac{1}{\sqrt{2}}(|\psi_{11}\uparrow\uparrow\rangle - |\psi_{11}\uparrow\uparrow\rangle) == 0$

Opposite spins: $|\psi_-\rangle = \frac{1}{\sqrt{2}}(|\psi_{11}\uparrow\downarrow\rangle - |\psi_{11}\downarrow\uparrow\rangle) \neq 0$

Two electrons can be in the same state as long as the spins are opposite.

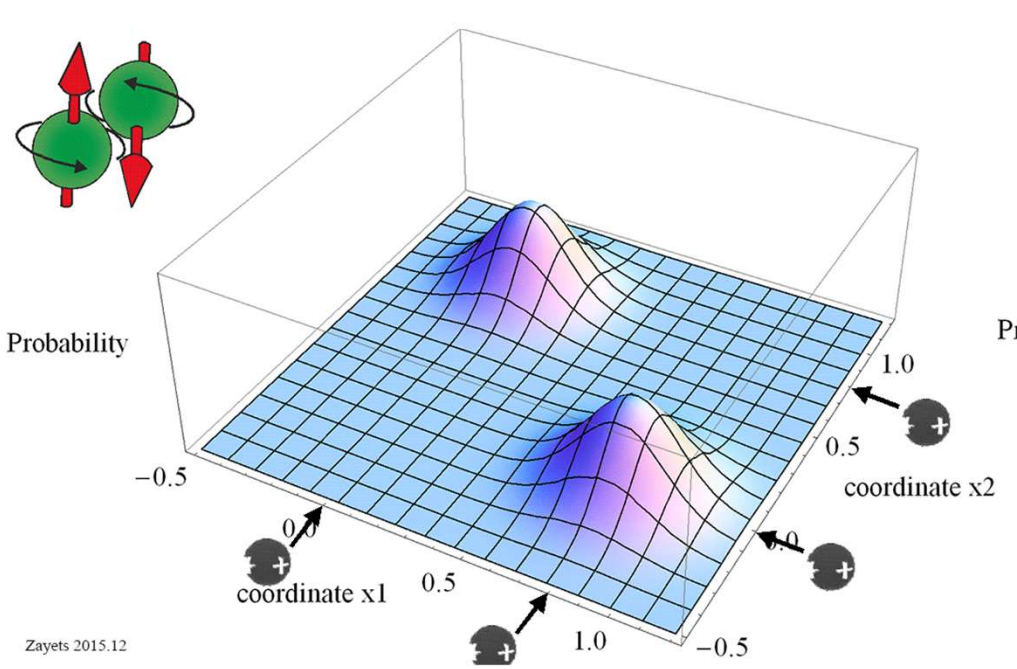
Exchange interaction

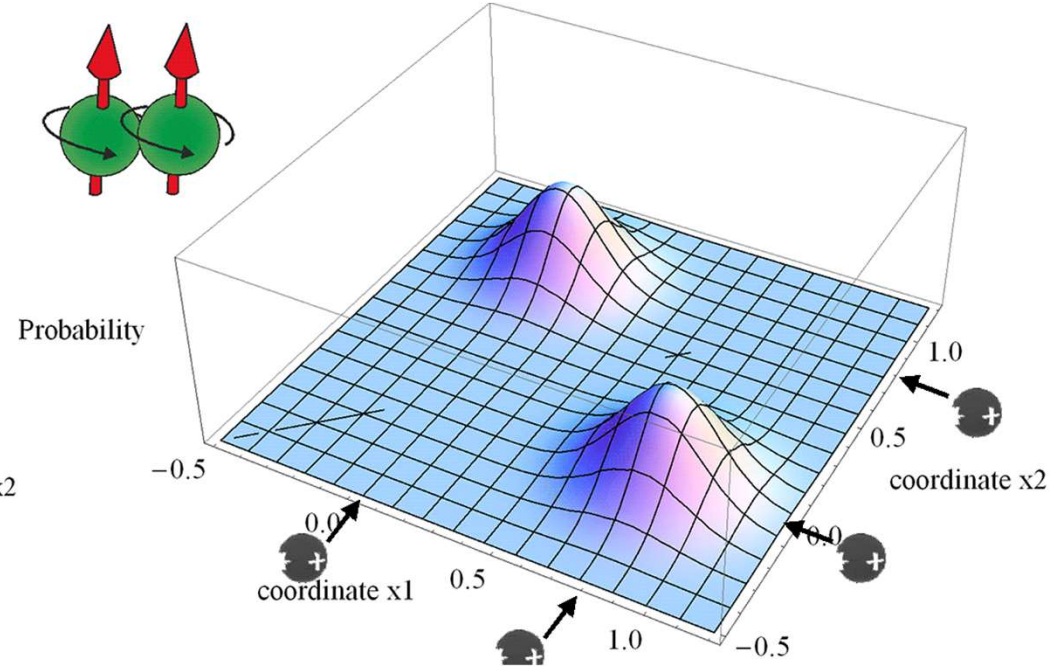
Electrons with parallel spins do not want to be at the same place.

It looks like they repel each other.

This has nothing to do with the Coulomb interaction between the electrons; it is a new, quantum mechanical effect.

Also: https://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/FermionsBosons/FermionsBosons.html





Electron Spin

Outline

- The Quantum concept
- The Stern - Gerlach experiment
- Introducing the electron spin
  - superposition of states (quantum mechanics with spins)
  - entanglement
  - Fermions and bosons, Pauli Principle, exchange interaction
- Magnets

Magnets

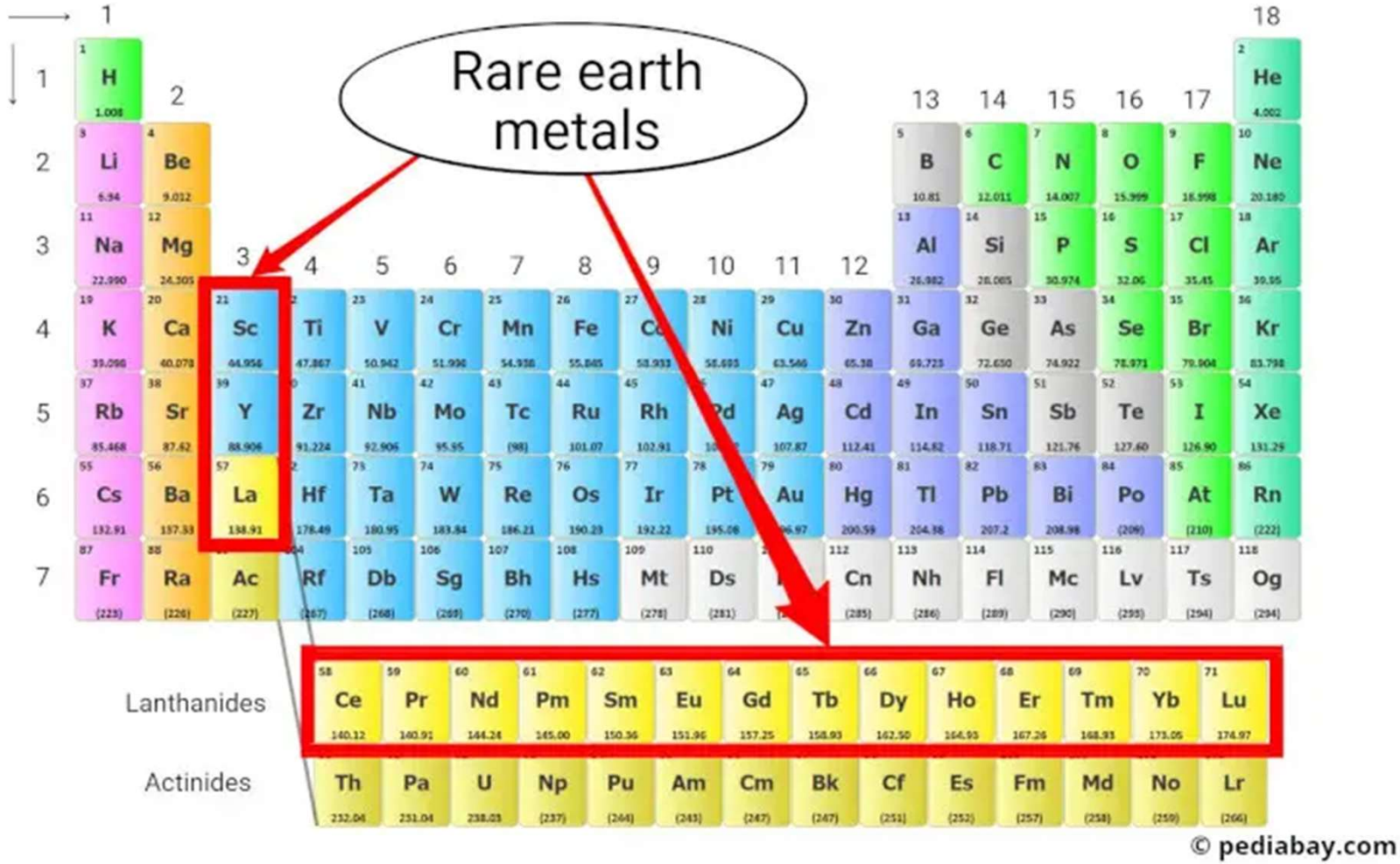
Rare-earth magnet revolution



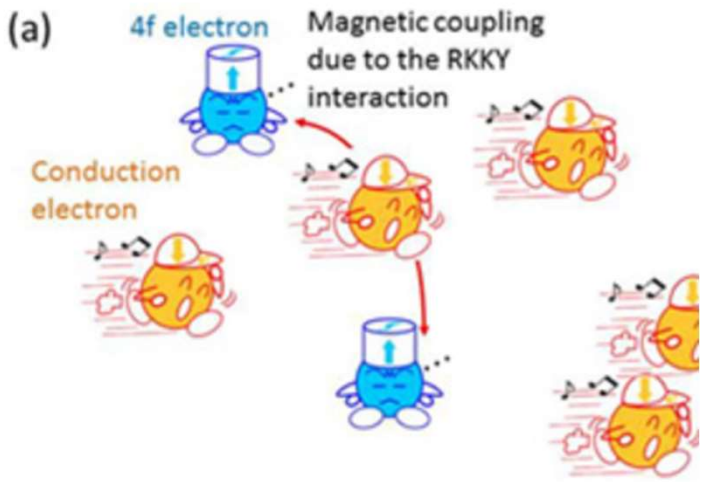







Rare earth metals
Lanthanides
Actinides
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Rare earth magnets: exchange interaction



Rare earth atoms have so called *f* electrons that are tightly bound to the atom, with spins lining up parallel, generating a large localized magnetic moment. They also have loosely bound *s* (conduction) electrons that move around the metal from one atom to the next.

If the spin on one of the *f* electron points up, the exchange interaction will polarize the s elctron spins downwards. As these electrons visit the next atoms's *f* electrons the exchange interaction will turn the spin upwards. As a result the *f* electron spins all line up in the same direction → magnetic moments add up.

