

MAGNETISM OF ATOMS – QUANTUM-MECHANICAL BASICS

Janusz Adamowski

AGH University of Science and Technology, Kraków, Poland

- The magnetism of materials can be derived from the magnetic properties of atoms.
- The atoms as the quantum objects subject to **the laws of quantum mechanics**.
- $\Rightarrow$ The magnetism of materials possesses **the quantum nature**.
- In my lecture, I will give a brief introduction to the **basic quantum mechanics** and its application to a description of the magnetism of atoms.

The observable part of the Universe (light matter) consists of massive particles and mass-less radiation.

Both particles and radiation possess the quantum nature.

Experimental background of quantum physics

- distribution of black-body radiation (Planck's law, 1900)
- photoelectric effect
- discrete emission and absorption spectra of atoms
- existence of spin (Stern- Gerlach experiment and spin Zeeman effect)
- ...
- nanoelectronic/spintronic devices
- quantum computer

Outline of lecture

- 1** Quantum states, wave functions, eigenvalue equations
 - 1.1** Orbital momentum
 - 1.2** Spin
 - 1.3** Magnetic moments
 - 1.4** Spin-orbit coupling
- 2** Atoms
 - 2.1** Hydrogen atom
 - 2.2** Many-electron atoms
 - 2.3** Pauli exclusion principle, Hund's rules, periodic table of elements
- 3** Exchange interaction
- 4** Summary
 - 4.1** Spintronics
 - 4.2** Negative absolute temperature

1 Quantum states, wave functions, eigenvalue equations

Quantum states of quantum objects (electrons, protons, atoms, molecules) are described by **the state vectors** being the elements of the abstract Hilbert space $\mathcal{H}$.

State vectors in **Dirac (bracket) notation**:
ket vectors

$$|\varphi\rangle, |\psi\rangle, |\chi\rangle, \dots$$

bra vectors

$$\langle\varphi|, \langle\psi|, \langle\chi|, \dots$$

Scalar product

$$\langle\varphi|\psi\rangle = c$$

c = complex number

How can we connect the abstract state vectors with the quantum phenomena that take place in the real/laboratory space?

In order to answer this question we introduce the state vector $|\mathbf{r}\rangle$ that describes the state of the single particle in the well-defined position $\mathbf{r} = (x, y, z)$ and calculate the scalar product

$$\langle\mathbf{r}|\psi\rangle \stackrel{def}{=} \psi(\mathbf{r}) . \quad (1)$$

$\Rightarrow$ Eq. (1) defines the **wave function** of the particle.

Physical interpretation of wave function

The wave function determines the probability density of finding the particle in quantum state $|\psi\rangle$ in position $\mathbf{r}$

$$\varrho(\mathbf{r}) = |\psi(\mathbf{r})|^2 . \quad (2)$$

Probability of finding a particle in space region $\Delta\tau$ in state $|\psi\rangle$

$$P_{\Delta\tau} = \int_{\Delta\tau} d^3r |\psi(\mathbf{r})|^2 \quad (3)$$

Normalization of wave function

$$\int_{\infty} d^3r |\psi(\mathbf{r})|^2 = 1 . \quad (4)$$

In Eq. (4), the integration runs over the entire space.

In quantum theory, we associate the **operators** $\hat{\Omega}$ to classical dynamic quantities Ω by the **quantization procedure**.

For example,

linear momentum $\mathbf{p} \longrightarrow \hat{\mathbf{p}} = -i\hbar\nabla$

angular momentum $\mathbf{l} \longrightarrow \hat{\mathbf{l}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$

energy (Hamilton function) $H(\mathbf{r}, \mathbf{p}) \longrightarrow \hat{H}(\hat{\mathbf{r}}, \hat{\mathbf{p}})$

$\hat{H}$ = operator of energy = Hamiltonian

$\hbar = h/(2\pi)$

h = Planck constant = 6.626×10^{-34} Js

Eigenvalue equation

The eigenvalue equation

$$\hat{\Omega}|\nu\rangle = \omega_\nu|\nu\rangle \quad (5)$$

is satisfied for operator $\hat{\Omega}$ of measurable quantity Ω if the quantum system is in state $|\nu\rangle$.

In Eq. (5), ω_ν is the **eigenvalue** (real number) that is the exact result of the measurement of quantity Ω for the quantum system in its **eigenstate** $|\nu\rangle$.

The quantum states are specified by the **quantum numbers** ν .

E.g., for the electron in atom

$$\nu = (n, l, m, s) ,$$

(n, l, m) = orbital quantum numbers

s = spin quantum number

for the electron in a crystalline solid

$$\nu = (k_x, k_y, k_z, s) ,$$

$(k_x, k_y, k_z) = \mathbf{k}$ = wave vector.

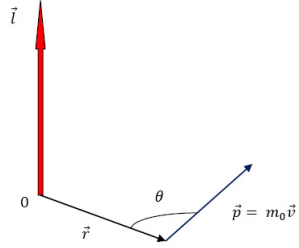


Figure 1: Classical orbital (angular) momentum $\mathbf{l} = \mathbf{r} \times \mathbf{p}$.

1.1 Orbital momentum

Quantum operator of angular momentum has the vector form

$$\hat{\mathbf{l}} = (\hat{l}_x, \hat{l}_y, \hat{l}_z) \quad (6)$$

Eigenvalue equation for the z component of the angular momentum

Operator of the z component of the angular momentum in spherical coordinates

$$\hat{l}_z = -i\hbar \frac{\partial}{\partial \varphi}$$

Eigenequation for $\hat{l}_z$

$$-i\hbar \frac{d\Phi(\varphi)}{d\varphi} = \lambda \Phi(\varphi) \quad (7)$$

Solutions of Eq. (7)

$$\Phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

Eigenvalues of the z component of the angular momentum

$$\lambda = m\hbar$$

$$m = 0, \pm 1, \pm 2, \dots \pm l \equiv -l, \dots, -1, 0, +1, \dots, +l$$

$m =$ **magnetic quantum number**

For given l the magnetic quantum number m takes on $2l + 1$ values.

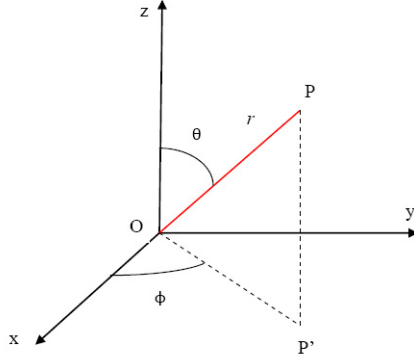


Figure 2: Spherical coordinates.

Eigenvalues of the square of orbital momentum

$$I^2 = l(l+1)\hbar^2$$

l = **azimuthal (orbital) quantum number**

For the electron in atom, $l = 0, 1, \dots, n-1$,
where n is the **principal quantum number**
that determines the **electronic shell** in atom.

$$n = 1, 2, 3, \dots \equiv K, L, M, \dots$$

Spatial quantization of angular momentum

For the electron in atom we can simultaneously measure the eigenvalues of square of orbital momentum $\hat{I}^2$ and one of its components, e.g., $\hat{l}_z$.

As results of these measurements we obtain

$$I^2 = l(l+1)\hbar^2$$

and

$$l_z = m\hbar$$

These results can be illustrated by the **vector model**.

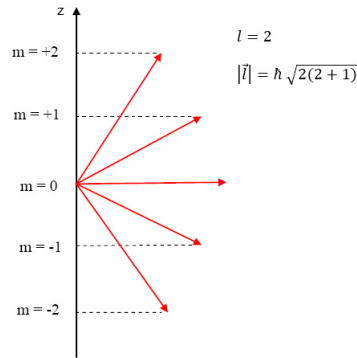


Figure 3: Vector model for $l = 2$.

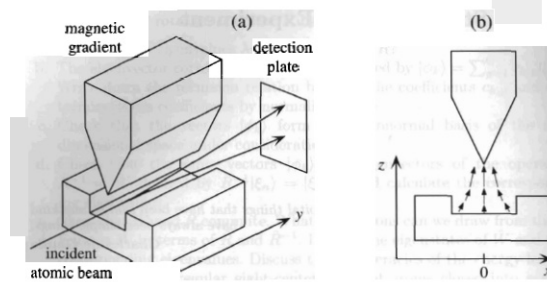


Figure 4: The first experimental observation of spin: Stern-Gerlach experiment.

1.2 Spin

Spin is a purely quantum variable that describes the inner properties of the electron (proton, neutron) (not connected with any rotation).

There is no classical quantity that corresponds to spin, although spin shows some formal similarity to the orbital momentum.

For electron, proton, neutron, the z component of the electron spin takes **only two values**

$$s_z = s\hbar = \pm\hbar/2.$$

$$s = \pm 1/2 = \text{spin quantum number}$$

The square of spin

$$\mathbf{s}^2 = s(s+1)\hbar^2 \quad (8)$$

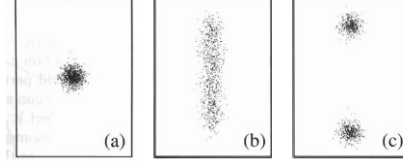


Figure 5: Results of the Stern-Gerlach experiment observed for: (a) atomic beam without the magnetic field, (b) classical magnetic moment, (c) atomic beam in nonhomogeneous magnetic field.

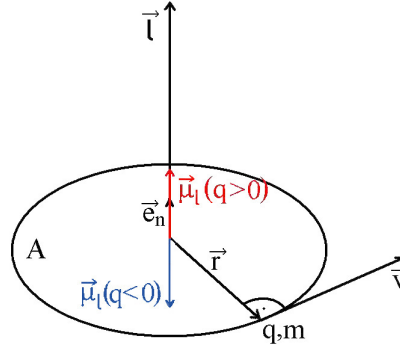


Figure 6: Magnetic orbital moment μ_l of particle with electric charge q and mass m rotating on the orbit with radius r .

1.3 Magnetic moments

Orbital magnetic moment of the electron

$$\mu_l = \gamma_l \mathbf{l}, \quad (9)$$

γ_l = orbital giromagnetic factor

For electron in atom

$$\gamma_l = \frac{q_e}{2m_e} = -\frac{e}{2m_e} \quad (10)$$

charge of electron $= q_e = -e < 0$, e = elementary charge

Spin magnetic moment of the electron

$$\mu_s = -g\mu_B \mathbf{s}. \quad (11)$$

$\mu_B = e\hbar/(2m_e) =$ Bohr magneton $g =$ Lande factor

In vacuum, $g = 2 + \mathcal{O}(10^{-3})$,

in semiconductors, g can be negative ($g = -0.44$ in GaAs) and can be very large ($g \sim 500$ in GaMnAs). In a general case, the electron possesses the total angular momentum

$$\mathbf{J} = \mathbf{l} + \mathbf{s} .$$

Then, the total magnetic moment $\boldsymbol{\mu}_J$ of the electron with $\mathbf{J}$ is given by

$$\boldsymbol{\mu}_J = \boldsymbol{\mu}_l + \boldsymbol{\mu}_s \tag{12}$$

Interaction energy of the magnetic moment $\boldsymbol{\mu}_J$ with the external magnetic field

$$\Delta U_J = -\boldsymbol{\mu}_J \cdot \mathbf{B} . \tag{13}$$

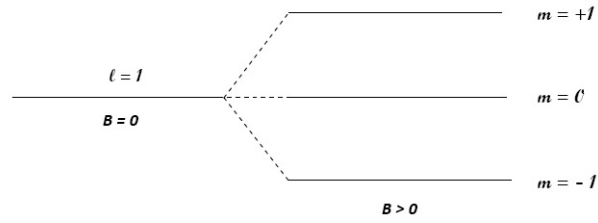


Figure 7: Splitting of energy level with $l = 1$ in external magnetic field B .

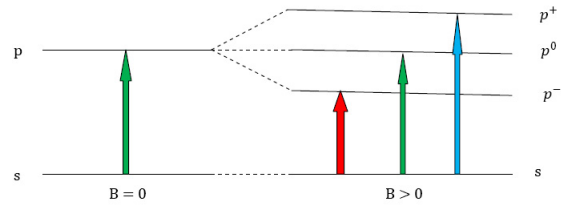


Figure 8: Normal Zeeman effect: transitions $s \rightarrow p$.

Normal Zeeman effect

For $\mathbf{J} = \mathbf{l}$: interaction energy of orbital magnetic moment $\boldsymbol{\mu}_l$ with magnetic field $\mathbf{B} = (0, 0, B)$

$$\Delta U_l = -\mu_{l,z} B$$

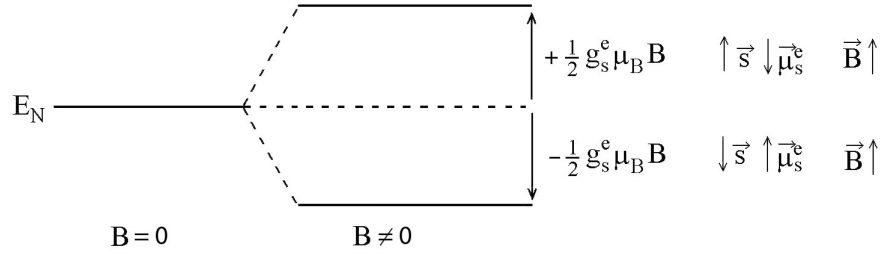


Figure 9: Spin Zeeman effect: spin splitting of energy level E_N in external magnetic field B .

Spin Zeeman effect

For $\mathbf{J} = \mathbf{s}$: interaction energy of the electron with spin $\mathbf{s}$ with the magnetic field $\mathbf{B} = (0, 0, B)$

$$\Delta U_s = \pm |\mu_{s,z}| B$$

1.4 Spin-orbit coupling

Classical electrodynamics[†]

If the electron with charge $q_e = -e$, spin $\mathbf{s}$ and rest mass m_{e0} moves with linear momentum $\mathbf{p}$ in external magnetic ($\mathbf{B}$) and electric ($\mathbf{F}$) fields (measured in the laboratory frame), then – in the electron frame – the following additional magnetic field acts on the electron:

$$\mathbf{B}_{SO} = -\frac{1}{2m_{e0}c^2}\mathbf{p} \times \mathbf{F} . \quad (14)$$

Eq. (14) results from the Lorentz transformation of the electric and magnetic fields.

Magnetic field $\mathbf{B}_{SO}$ describes the **spin-orbit (SO) interaction**.

[†]The same result can be obtained in the framework of quantum electrodynamics.

$$\mathbf{B}_{total} = \mathbf{B} + \mathbf{B}_{SO} \quad (15)$$

Interaction energy of the electron spin with the total magnetic field

$$E_{spin} = -\boldsymbol{\mu}_s \cdot \mathbf{B}_{total} = E_Z + E_{SO} , \quad (16)$$

$E_Z =$ **energy of spin Zeeman interaction**,

$$E_Z = -\boldsymbol{\mu}_s \cdot \mathbf{B} , \quad (17)$$

$E_{SO} =$ **energy of spin-orbit interaction**

$$E_{SO} = \frac{1}{2m_{e0}c^2}\boldsymbol{\mu}_s \cdot (\mathbf{F} \times \mathbf{p}) . \quad (18)$$

If the electric field is **central**, i.e., $\mathbf{F}(\mathbf{r}) = F_r(r)(\mathbf{r}/r)$, then Eq. (18) transforms into

$$E_{SO} = -\frac{e\hbar F_r}{2m_{e0}^2c^2r}\mathbf{s} \cdot \mathbf{l} , \quad (19)$$

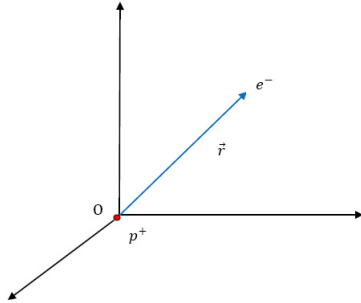
$\mathbf{s}$ = electron spin $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ = orbital angular momentum

$\Rightarrow E_{SO}$ in form (19) explains the name: **spin-orbit interaction**.

Energy of spin-orbit interaction in atoms

$$E_{SO} = \alpha \mathbf{s} \cdot \mathbf{l}$$

α = spin-orbit coupling constant



Hydrogen atom consists of positively charged proton p^+ and negatively charged electron e^- .

2 Atoms

2.1 Hydrogen atom

Potential energy of proton-electron Coulomb attraction

$$U_C(\mathbf{r}) = -\frac{\varkappa e^2}{r} \quad (20)$$

e = elementary charge
The coupling constant

$$\varkappa = \frac{1}{4\pi\varepsilon_0} = 8.988 \times 10^9 \frac{\text{Jm}}{\text{C}^2}. \quad (21)$$

The Schrödinger equation for hydrogen atom

$$\left(-\frac{\hbar^2}{2m_0} \nabla^2 - \frac{\varkappa e^2}{r} \right) \psi_\nu(\mathbf{r}) = E_\nu \psi_\nu(\mathbf{r}), \quad (22)$$

m_0 = rest mass of the electron

Solutions of the Schrödinger equation for the hydrogen atom

Wave function of the ground state

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_B^3}} e^{-r/a_B} \quad (23)$$

$\nu = (n, l, m) = (1, 0, 0) \equiv 1s$

Bohr radius $= a_B = \frac{\hbar^2}{\varkappa m_0 e^2}$

$a_B = 0.529 \text{ \AA} = \text{atomic unit of length}$

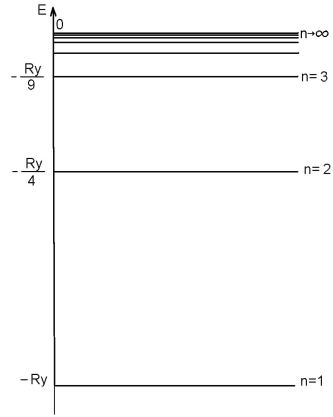


Figure 10: Energy levels of the bound states of the hydrogen atom.

Energy eigenvalues (for bound states)

$$E_n = -\frac{Ry}{n^2} . \quad (24)$$

$$Ry = \frac{\varkappa^2 m_0 e^4}{2\hbar^2} = 13.6058 \text{ eV}$$

Ry = **Rydberg constant**

The energy of electron quantum states in hydrogen atom is independent of the (l, m, s) quantum numbers, which means that these states are **degenerate**.

2.2 Many-electron atoms

Spectroscopic notation

l	0	1	2	3	4	5	6	...
<i>symbol</i>	<i>s</i>	<i>p</i>	<i>d</i>	<i>f</i>	<i>g</i>	<i>h</i>	<i>i</i>	...

Arbitrary atom consists of the nucleus with Z protons (the nuclear charge $Q_j = +Ze$) and Z electrons with charge $Q_{el} = -Ze$.

In one-electron approximation, we treat each electron as a particle being independent of other electrons that moves in an effective central field generated by the nucleus and other electrons.

Potential energy of the electron

$$U_{eff}(r) \neq U_C(r) . \quad (25)$$

The one-electron states in the many-electron atom are determined by quantum numbers (n, l, m, s) .

Quantum numbers (n, l, m) define the **(space) orbital**.

The state with given (n, l, m, s) is called the **spinorbital**.

The energy levels of electrons in many-electron atoms

$$E = E_{nlm}$$

in general depend on the quantum numbers (n, l, m) , which means that the degeneracy typical to hydrogen atom is lifted.

2.3 Pauli exclusion principle, Hund's rules, periodic table

The electrons possess the fundamental quantum property:

Pauli exclusion principle.

For electrons in many-electron atoms this principle is formulated as follows:

The quantum state $|n, l, m, s\rangle$ can be occupied by at most one electron.

The Pauli principle for the orbitals:

the given space orbital $|n, l, m\rangle$ can be occupied by at most two electrons with different spins $s_z = \pm\hbar/2$.

The construction of the **periodic table of elements** is based on the Pauli exclusion principle.

The maximal numbers N_l of electrons that can occupy the one-electron states for the successive values of angular quantum number l

$\Rightarrow$ **occupation numbers of atomic subshells**

l	$N_l = 2(2l + 1)$
0	2
1	6
2	10
3	14
4	18
...	...

The maximal numbers N_n of electrons that can occupy the one-electron shells for the successive values of principal quantum number n

$\Rightarrow$ **occupation numbers of atomic shells**

n	$N_n = 2n^2$
1	2
2	8
3	18
4	32
...	...

According to the spectroscopic notation we denote the states with different values of the total orbital momentum L as follows:

$$\begin{array}{cccccccc} L = & 0 & 1 & 2 & 3 & 4 & 5 & \dots \\ \text{symbol} & S & P & D & F & G & H & \dots \end{array}$$

For a description of electron states in many-electron atoms we introduce:

Multiplicity $= 2S + 1$

S = total spin quantum number ($S = 0, 1/2, 1, 3/2, \dots$)

Total angular momentum of N electrons in the atom

$$J = L + S \tag{26}$$

$$J = 0, 1/2, 1, 3/2, \dots$$

Atomic terms

Atomic term is defined by the quantum numbers (L, S, J) that determine the ground-state energy of atom.

Notation for atomic terms:

$$(\text{electron configuration})^{(2S+1)}L_J$$

where for L we use the letters $S, P, D, \dots$

Hund's rules

The Hund's rules determine the ground state of the atom, i.e., the state with the lowest energy.

Hund's rules: general formulation

If the one-electron orbital is degenerate (or is almost degenerate), the ground state corresponds to the **orbitals** with the **same orientation of spins**.

In other words, for the given electron configuration the ground state possesses the **maximal multiplicity** ($2S + 1$).

Hund's rules: detailed formulation

For a given electronic configuration determined by quantum numbers (L, S) :

- (1) the ground state possesses the maximal possible multiplicity ($2S + 1$),
- (2) if there exist several states with the same maximal multiplicity, the ground state possesses the maximal value of total orbital quantum number L ,
- (3) if the open subshell is filled by the number of electrons less than $(1/2)$ of the maximal subshell occupation number, the ground state possesses the total momentum quantum number $J = |L - S|$.

Electronic structure of atoms of elements for the two first periods in the periodic table

Z	symbol	electron configuration	atomic term	ionization energy [eV]
1	H	$1s$	$^2S_{1/2}$	13.6
2	He	$(1s)^2$	1S_0	24.6
3	Li	$(1s)^2 2s^1$	$^2S_{1/2}$	5.4
4	Be	$(1s)^2 2s^2$	1S_0	9.3
5	B	$(1s)^2 2s^2 2p^1$	$^2P_{1/2}$	8.3
6	C	$(1s)^2 2s^2 2p^2$	3P_0	11.3
7	N	$(1s)^2 2s^2 2p^3$	$^4S_{3/2}$	14.5
8	O	$(1s)^2 2s^2 2p^4$	3P_2	13.6
9	F	$(1s)^2 2s^2 2p^5$	$^2P_{3/2}$	17.4
10	Ne	$(1s)^2 (2s^2 2p^6)$	1S_0	21.6

Configurations of outer electron subshells for iron subgroup

^{21}Sc	^{22}Ti	^{23}V	^{24}Cr	^{25}Mn	^{26}Fe	^{27}Co	^{28}Ni
$3d4s^2$	$3d^2 4s^2$	$3d^3 4s^2$	$3d^5 4s$	$3d^5 4s^2$	$3d^6 4s^2$	$3d^7 4s^2$	$3d^8 4s^2$
$^2D_{3/2}$	3F_2	$^4F_{3/2}$	7S_3	$^6S_{5/2}$	5D_4	$^4F_{9/2}$	3F_4

Inner shell electron configuration = electron shell of ^{18}Ar .

3 Exchange interaction

Exchange interaction for two electrons localized on two different atoms

We consider two electrons localized on two identical atoms in positions $\mathbf{R}_a$ and $\mathbf{R}_b$. We assume that the electrons occupy the same one-electron orbital (n, l, m) localized on each atom a and b .

The electrons can possess either parallel or antiparallel spins.

For parallel spins the two-spin state is **the triplet state**

$$|\uparrow\uparrow\rangle \equiv \chi_T$$

for antiparallel spins the two-spin state is **the singlet state**

$$|\uparrow\downarrow\rangle \equiv \chi_S$$

The total two-electron wave function has to be **antisymmetric** with respect to the interchange of electron coordinates (we interchange both the spatial and spin variables).

$$\Psi(\zeta_1, \zeta_2) = -\Psi(\zeta_2, \zeta_1), \quad (27)$$

where $\zeta = (x, y, z, \sigma) = (\mathbf{r}, \sigma)$, σ = spin coordinate

For $\Psi_{total} = \psi_{space}\chi_{spin}$ the antisymmetry (68) leads to one of the properties: either

$$\Psi_{total} = \psi_{space, antisym}\chi_T \quad (28)$$

or

$$\Psi_{total} = \psi_{space, sym}\chi_S \quad (29)$$

$\Rightarrow$ the symmetry of the spatial two-electron wave function depends on the symmetry of the associated two-spin state.

The two-electron spatial states can be written down in either of two forms

$$\Psi_S(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}(\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)) \quad (30)$$

if the electrons are in the spin singlet state S ,

$$\Psi_T(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}(\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) - \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)) \quad (31)$$

if the electrons are in the spin triplet state T .

The energies of electron-electron interaction calculated for singlet (30) and triplet (31) states differ by the quantity

$$J_{ab} = \int d^3r_1 d^3r_2 \psi_a^*(\mathbf{r}_1)\psi_b^*(\mathbf{r}_2) \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) \quad (32)$$

Quantity (32) is called **exchange integral**.

It describes the purely quantum-mechanical **exchange interaction**.

Ferromagnetism

The ferromagnetic properties of materials can be described by the **Heisenberg model**.

Heisenberg Hamiltonian

$$H = - \sum_{\langle a,b \rangle} J_{ab} \mathbf{S}_a \cdot \mathbf{S}_b . \quad (33)$$

In Eq. (33), the sum runs over all different pairs of atoms $\langle a, b \rangle$.

J_{ab} = **exchange integral**

$\mathbf{S}_a, \mathbf{S}_b$ = effective spins of atoms localized in positions $\mathbf{R}_a$ and $\mathbf{R}_b$.

Assume that $J_{ab} > 0$.

If the spins are parallel, i.e., $\uparrow\uparrow$, $\mathbf{S}_a \cdot \mathbf{S}_b > 0$, therefore, according to (33), the energy contribution is negative, i.e., we are dealing with the effective attraction.

$\Rightarrow$ ferromagnetism

For $\uparrow\downarrow$ $\mathbf{S}_a \cdot \mathbf{S}_b < 0$, therefore, the energy contribution is positive (effective repulsion)

$\Rightarrow$ diamagnetism

Important remark:

The value of exchange integral J results from the **Coulomb electrostatic interactions** and one-electron atomic wave functions.

$\Rightarrow$ the electrostatic interactions between electrons and nuclei are responsible for the ferromagnetism.

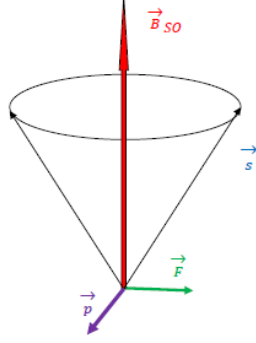


Figure 11: Precession of electron spin $\vec{s}$ in the spin-orbit magnetic field $\vec{B}_{SO}$. If the electron moves in x direction (i.e., along the nanowire axis) and electric field $\vec{F}$ generated by the gate is oriented in the y direction, i.e., $\vec{F} = (0, F_y, 0)$, then $\vec{B}_{SO} = (0, 0, B_{SO})$.

4 Summary

4.1 Application: Spintronics

Spin precession resulting from the spin-orbit coupling

The spin-orbit interaction leads to the precession of the electron spin around spin-orbit magnetic field $\vec{B}_{SO}$.

The precession around the $\vec{B}_{SO}$ can be controlled by the electric field $\vec{F}$ that is generated by the external gate voltage V_g .

$\Rightarrow$ all electric devices

Spintronic devices

- spin filter (analog of the light polarizator)
- spin splitter (analog of the birefractive crystal)
- spin transistor (analog of the electro-optical modulator)

Example: nanowire-based spin splitter

Spin splitting generated in a Y-shaped semiconductor nanostructure with a quantum point contact

P. Wójcik,^{a)} J. Adamowski,^{b)} M. Wołoszyn, and B. J. Spisak

AGH University of Science and Technology, Faculty of Physics and Applied Computer Science,
al. Mickiewicza 30, Kraków, Poland

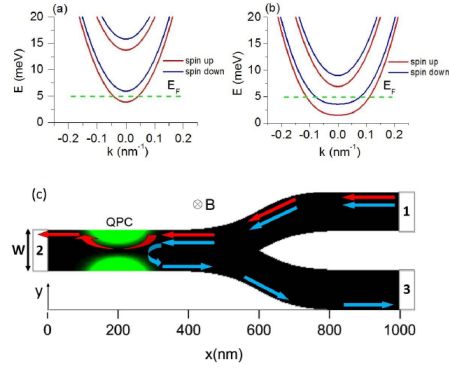


Figure 12: Dispersion relation $E(k)$ for spin-up and spin-down electrons calculated for (a) the center of the QPC and (b) the contacts (1, 2, 3). (c) Schematic of the Y-shaped nanowire structure with the QPC. Red (blue) arrows show the spin-up and spin-down currents, magnetic field $\mathbf{B} = (0, 0, B)$.

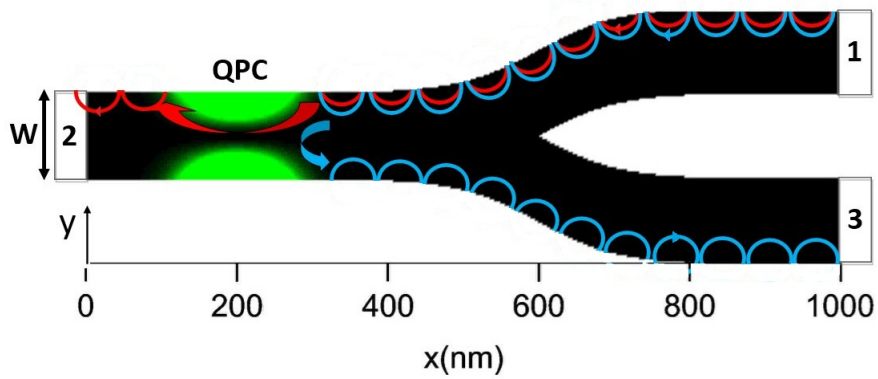


Figure 13: Spin transport via the edge states. Red (blue) arrows correspond to the spin-up (down) current.

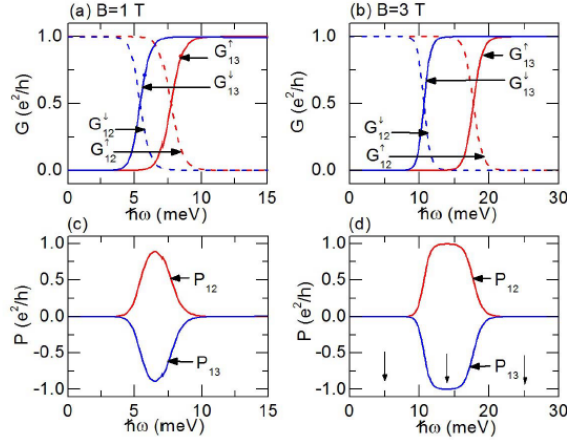


Figure 14: Spin conductance G and spin polarization $P = G_{\uparrow} - G_{\downarrow}$ for (a) $B = 1$ T and (b) $B = 3$ T as a function of the confinement energy $\hbar\omega$ of the electron in the QPC.

4.2 Basic research: Negative absolute temperature

(4.B) Basic research: Negative absolute temperature

Formal definition of temperature

$$T = (\partial S / \partial E)^{-1} \quad (34)$$

S = entropy, E = total energy

Usually,

$$\partial S / \partial E > 0 \implies T > 0.$$

However, in spin systems in the external magnetic field, we can obtain

$$\partial S / \partial E < 0 \implies T < 0.$$

Negative absolute temperature has been realized in the spin nuclear system in the external magnetic field (in NMR-type apparatus).

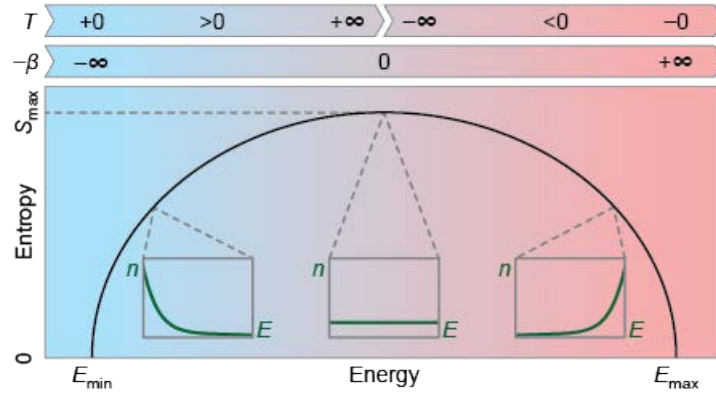


Figure 15: Entropy vs energy. S. Braun & U. Schneider, Ludwig-Maximilians University, Munich.

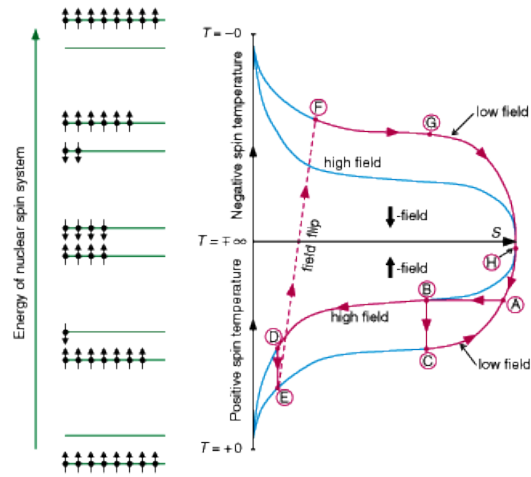


Figure 16: Experimental realization of nano- and picokelvin negative temperatures in silver and rhodium. O.V. Lounasmaa et al.

Hypothetical existence of the negative absolute temperature in the Universe

Observable/non-observable structure of the Universe:

light matter ($\sim 5\%$ of the total energy of the Universe) + **dark matter** (23%) + **dark energy** (72%)

The observed **expansion of the Universe** is in contradiction to the attractive character of the gravitational forces.

Hypothesis

The dark energy possesses the negative absolute temperature, which leads to the effective repulsion that causes the accelerated expansion of the Universe.