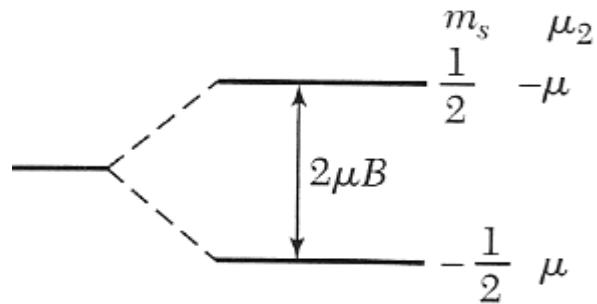


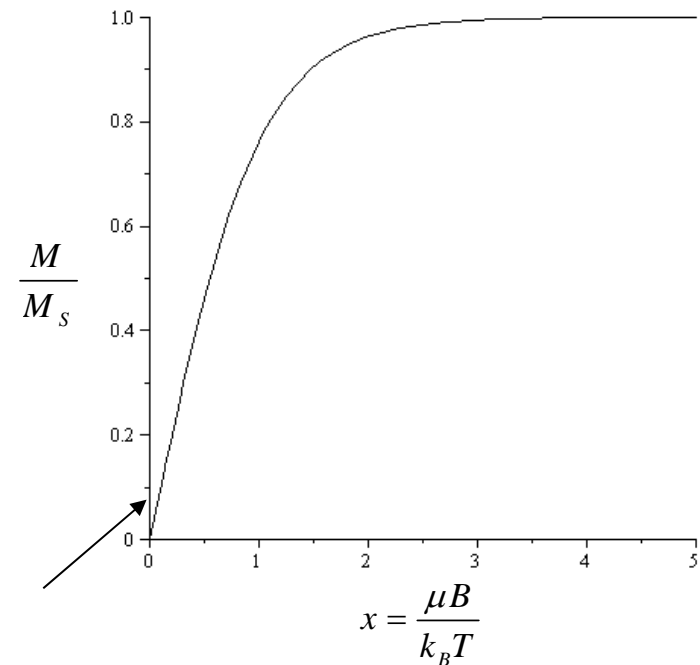
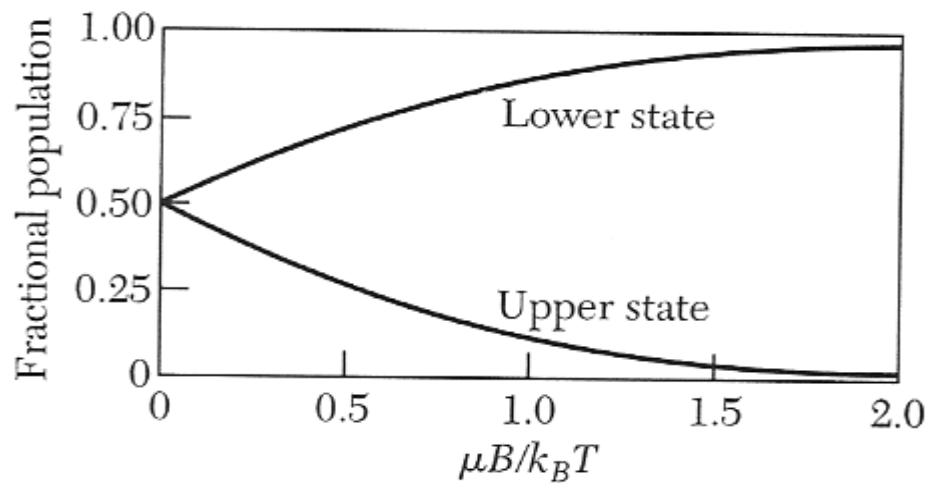
Magnetism

Paramagnetism, spin 1/2



$$M = N\mu \tanh\left(\frac{\mu B}{k_B T}\right) \approx \frac{N\mu^2 B}{k_B T} = \frac{CB}{T}$$

for $\mu B \ll k_B T$ Curie law

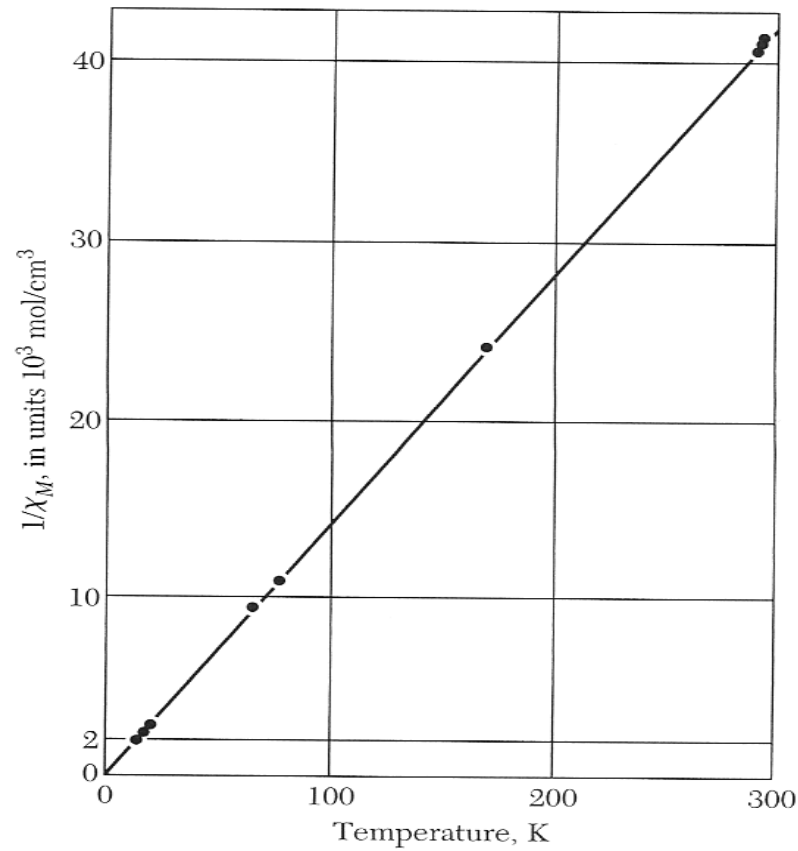


Curie law

for $\mu B \ll k_B T$ $M = CB / T$

$$\chi \propto \left. \frac{dM}{dB} \right|_{B=0} = \frac{C}{T}$$

C is the Curie constant



Atomic physics

In atomic physics, the possible values of the magnetic moment of an atom in the direction of the applied field can only take on certain values.

Total angular momentum

$$J = L + S \quad \text{Orbital } L + \text{ spin } S \text{ angular momentum}$$

Magnetic quantum number

$$m_J = -J, -J + 1, \dots, J - 1, J$$

Allowed values of the magnetic moment in the z direction

$$\mu_z = m_j g_J \mu_B$$

Lande g factor \swarrow \nwarrow Bohr magneton

$$g_J \approx \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

Brillouin functions

Average value of the magnetic quantum number

$$\langle m_J \rangle = \frac{\sum_{-J}^J m_J e^{-E(m_J)/k_B T}}{\sum_{-J}^J e^{-E(m_J)/k_B T}} = \frac{\sum_{-J}^J m_J e^{-m_J g_J \mu_B B / k_B T}}{\sum_{-J}^J e^{-m_J g_J \mu_B B / k_B T}} = -\frac{1}{Z} \frac{dZ}{dx}$$

Lande g factor

$$x = g_J \mu_B B / k_B T$$

Bohr magneton

$$Z = \sum_{-J}^J e^{-m_J x} = \frac{\sinh\left(\left(2J+1\right)\frac{x}{2}\right)}{\sinh\left(\frac{x}{2}\right)}$$

check by synthetic
division

Brillouin functions

$$Z = \sum_{-J}^J e^{-m_J x} = \frac{\sinh\left(\left(2J+1\right)\frac{x}{2}\right)}{\sinh\left(\frac{x}{2}\right)}$$

$$J = 1/2$$

$$e^{\frac{x}{2}} - e^{-\frac{x}{2}} \left(\frac{e^{\frac{x}{2}} + e^{-\frac{x}{2}}}{e^x - e^{-x}} \right) \frac{e^x - 1}{e^x - 1}$$

$$\frac{1 - e^{-x}}{1 - e^{-x}}$$

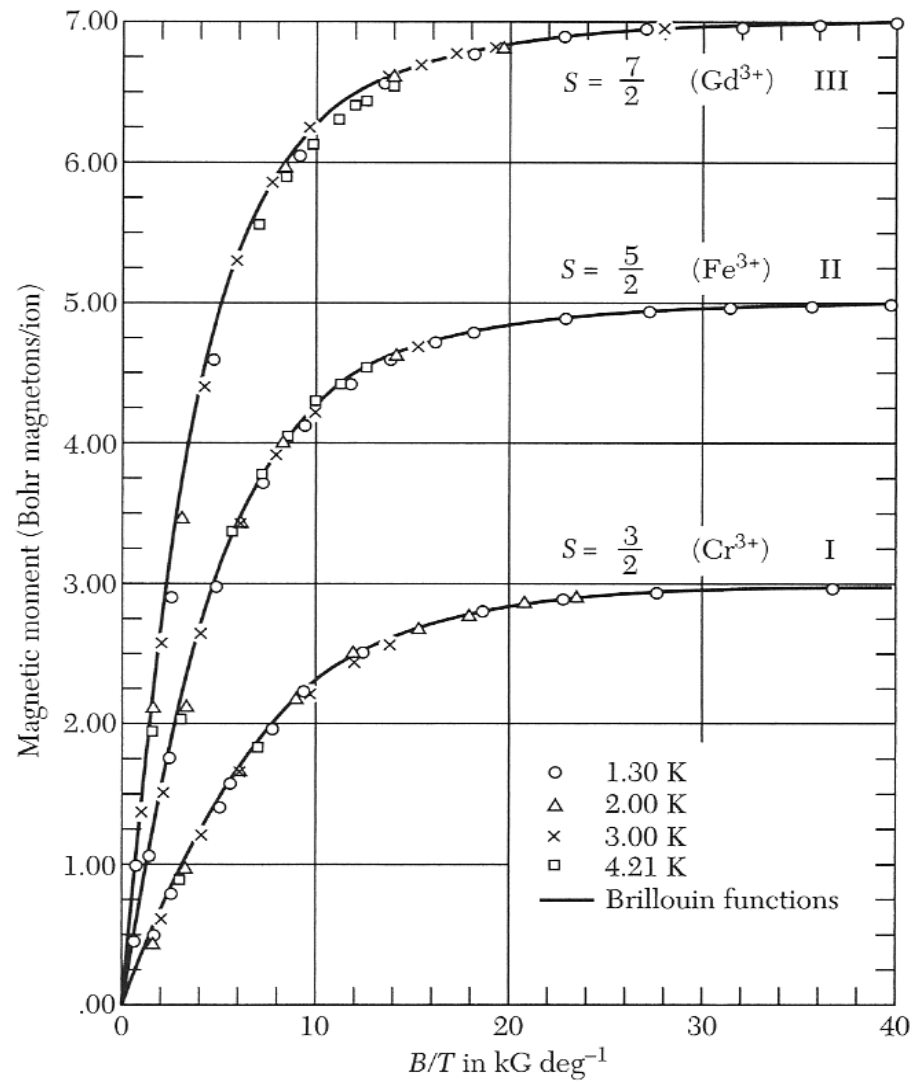
$$0$$

$$M = Ng_J \mu_B \langle m_J \rangle = -Ng_J \mu_B \frac{1}{Z} \frac{dZ}{dx}$$

Brillouin function

$$M = Ng \mu_B J \left(\frac{2J+1}{2J} \coth\left(\frac{2J+1}{2J} \frac{g \mu_B JB}{k_B T}\right) - \frac{1}{2J} \coth\left(\frac{1}{2J} \frac{g \mu_B JB}{k_B T}\right) \right)$$

Paramagnetism



Hund's rules from atomic physics

Hund calculated the energies of atomic states:

$$\frac{\langle \psi_{Ne3s} | H | \psi_{Ne3s} \rangle}{\langle \psi_{Ne3s} | \psi_{Ne3s} \rangle} < \frac{\langle \psi_{Ne3p} | H | \psi_{Ne3p} \rangle}{\langle \psi_{Ne3p} | \psi_{Ne3p} \rangle} < \frac{\langle \psi_{Ar4s} | H | \psi_{Ar4s} \rangle}{\langle \psi_{Ar4s} | \psi_{Ar4s} \rangle} < \frac{\langle \psi_{Ne3d} | H | \psi_{Ne3d} \rangle}{\langle \psi_{Ne3d} | \psi_{Ne3d} \rangle}$$

H includes $e-e$ interactions

He formulated the following rules:

Electrons fill atomic orbitals following these rules:

1. Maximize the total spin S allowed by the exclusion principle
2. Maximize the orbital angular momentum L
3. $J=|L-S|$ when the shell is less than half full, $J=|L+S|$ when the shell is more than half full.

Hund's rules (f - shell)

n	$l_z = 3, 2, 1, 0, -1, -2, -3$	S	$L = \Sigma l_z $	J
1	↓	1/2	3	5/2
2	↓ ↓	1	5	4
3	↓ ↓ ↓	3/2	6	9/2
4	↓ ↓ ↓ ↓	2	6	4
5	↓ ↓ ↓ ↓ ↓	5/2	5	5/2
6	↓ ↓ ↓ ↓ ↓ ↓	3	3	0
7	↓ ↓ ↓ ↓ ↓ ↓ ↓	7/2	0	7/2
8	↑↑ ↑ ↑ ↑ ↑ ↑	3	3	6
9	↑↑ ↑↑ ↑ ↑ ↑ ↑ ↑	5/2	5	15/2
10	↑↑ ↑↑ ↑↑ ↑ ↑ ↑ ↑ ↑	2	6	8
11	↑↑ ↑↑ ↑↑ ↓↓ ↑ ↑ ↑	3/2	6	15/2
12	↑↑ ↑↑ ↓↓ ↓↓ ↓↓ ↑ ↑	1	5	6
13	↑↑ ↓↓ ↓↓ ↓↓ ↓↓ ↓↓ ↑	1/2	3	7/2
14	↑↑ ↓↓ ↓↓ ↓↓ ↓↓ ↓↓ ↓↓ ↓	0	0	0

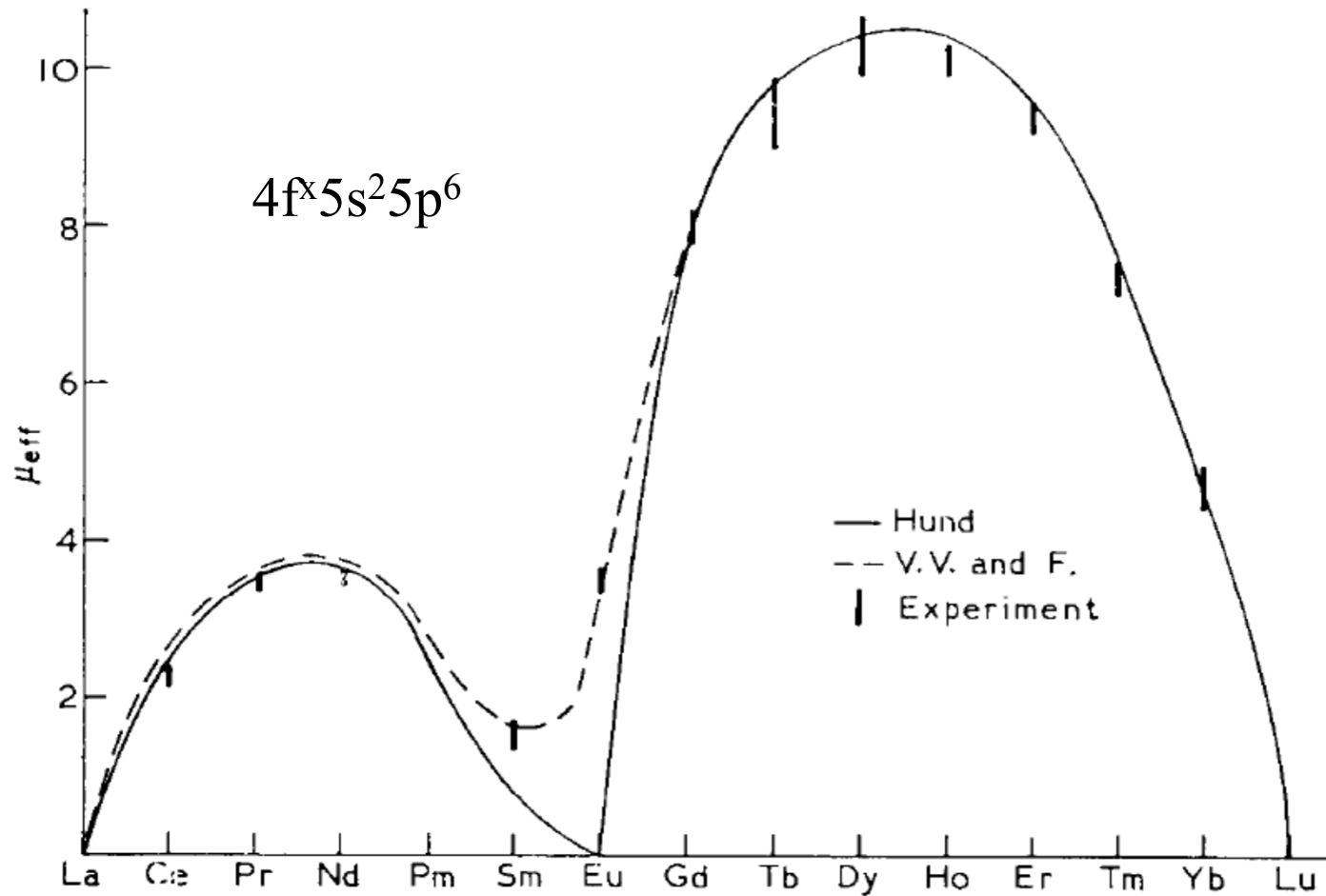
$J = |L - S|$

$J = L + S$

The half filled shell and completely filled shell have zero total angular mo.

Quantum Mechanics: The Key to Understanding Magnetism

John H. van Vleck



Pauli paramagnetism

Paramagnetic contribution due to free electrons.

Electrons have an intrinsic magnetic moment μ_B .

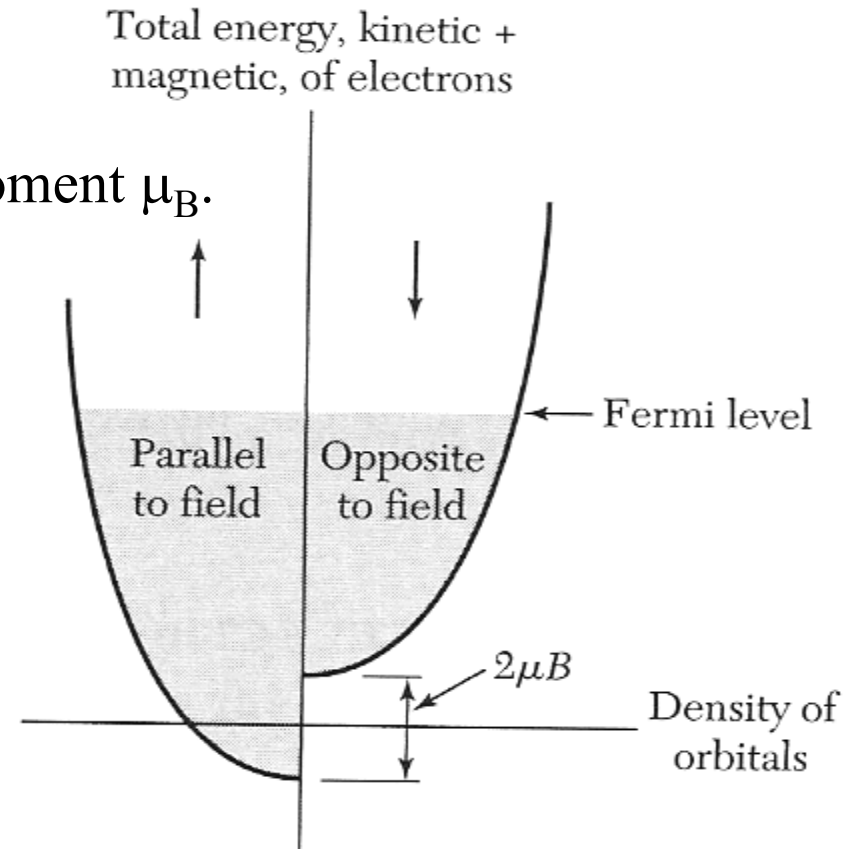
$$n_+ \approx \frac{1}{2}n + \frac{1}{2}\mu_B BD(E_F)$$

$$n_- \approx \frac{1}{2}n - \frac{1}{2}\mu_B BD(E_F)$$

$$M = \mu_B(n_+ - n_-)$$

$$M = \mu_B^2 D(E_F) B = \mu_0 \mu_B^2 D(E_F) H$$

$$\chi = \frac{dM}{dH} = \mu_0 \mu_B^2 D(E_F)$$



If E_F is 1 eV, a field of $B = 17000$ T is needed to align all of the spins.

Pauli paramagnetism is much smaller than the paramagnetism due to atomic moments and almost temperature independent because $D(E_F)$ doesn't change very much with temperature.

Paramagnetism

In paramagnetism the field aligns local magnetic moments

Paramagnetism due to atomic magnetic moments:

- Determine total angular momentum J

- Quantized values the magnetic moment in the direction of the field

- Use Brillouin functions to describe the field and temperature dependence of the magnetization

Pauli paramagnetism (another component to paramagnetism)

- Due to alignment of electron spins in a free electron gas

Ferromagnetism

Below a critical temperature (called the Curie temperature) a magnetization spontaneously appears in a ferromagnet even in the absence of a magnetic field.

Iron, nickel, and cobalt are ferromagnetic.

Ferromagnetism overcomes the magnetic dipole-dipole interactions. It arises from the Coulomb interactions of the electrons. The energy that is gained when the spins align is called the exchange energy.

Schrödinger equation for two particles

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2} \right) \psi + V_1(\vec{r}_1)\psi + V_2(\vec{r}_2)\psi + V_{1,2}(\vec{r}_1, \vec{r}_2)\psi = E\psi$$

$\psi(\vec{r}_1, \vec{r}_2) = \psi_1(\vec{r}_1)\psi_2(\vec{r}_2)$ is a solution to the noninteracting Hamiltonian, $V_{1,2} = 0$

$$\psi_A(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)) \begin{pmatrix} \uparrow\uparrow \\ \frac{1}{\sqrt{2}} (\uparrow\downarrow + \downarrow\uparrow) \\ \downarrow\downarrow \end{pmatrix}$$

$$\psi_S(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) + \psi_1(\vec{r}_2)\psi_2(\vec{r}_1)) \frac{1}{\sqrt{2}} (\uparrow\downarrow - \downarrow\uparrow)$$

Exchange (Austauschwechselwirkung)

$$\psi_A(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_1(\vec{r}_2)\psi_2(\vec{r}_1))$$

$$\begin{aligned} \langle \psi_A | H | \psi_A \rangle &= \frac{1}{2} [\langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) | H | \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \rangle - \langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) | H | \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \rangle \\ &\quad - \langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) | H | \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \rangle + \langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) | H | \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \rangle] \end{aligned}$$

$$\psi_S(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) + \psi_1(\vec{r}_2)\psi_2(\vec{r}_1))$$

$$\begin{aligned} \langle \psi_S | H | \psi_S \rangle &= \frac{1}{2} [\langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) | H | \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \rangle + \langle \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) | H | \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \rangle \\ &\quad + \langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) | H | \psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \rangle + \langle \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) | H | \psi_1(\vec{r}_2)\psi_2(\vec{r}_1) \rangle] \end{aligned}$$

The difference in energy between the ψ_A and ψ_S is twice the **exchange energy**.

Exchange

The exchange energy can only be defined when you speak of multi-electron wavefunctions. It is the difference in energy between the symmetric solution and the antisymmetric solution. There is only a difference when the electron-electron term is included. Coulomb repulsion determines the exchange energy.

In ferromagnets, the antisymmetric state has a lower energy. Thus the state with parallel spins has lower energy.

In antiferromagnets, the symmetric state has a lower energy. Neighboring spins are antiparallel.

Mean field theory (Molekularfeldtheorie)

Heisenberg Hamiltonian $H = -\sum_{i,j} J_{i,j} \vec{S}_i \cdot \vec{S}_j - g \mu_B B \sum_i \vec{S}_i$

Exchange energy

Mean field approximation

$$H_{MF} = \sum_i \vec{S}_i \cdot \left(\sum_{\delta} J_{i,\delta} \langle \vec{S} \rangle + g \mu_B \vec{B} \right)$$

δ sums over the neighbors of spin i

Looks like a magnetic field B_{MF}

$$\vec{B}_{MF} = \frac{1}{g \mu_B} \sum_{\delta} J_{i,\delta} \langle \vec{S} \rangle$$

magnetization $\longrightarrow \vec{M} = g \mu_B \frac{N}{V} \langle \vec{S} \rangle$

eliminate $\langle S \rangle$