# PHY331
Magnetism

Lecture 8

Last week….

- We discussed domain theory of Ferromagnetism.
- We saw there is a motion of domain walls with applied magnetic field.
- Stabilization of domain walls due to competition between magnetostatic energy, anisotropy energy and exchange energy.
- This results in the formation of domains having finite wall thickness.

This week…

- We will discuss the mechanisms at the atomic length-scale that cause spontaneous magnetization.

- Will show that the magnetic field from a single dipole is not sufficient to align its neighbours.

- Rather it is the energy of exchanging electrons that 'forces' dipoles to align.

- Find lowest ground state is always spin-parallel.

What *mechanisms* (on an atomic scale) can *cause* the *spontaneous magnetisation*?

We need an *alignment* of *neighbouring magnetic dipoles*

1) The magnetic dipole field
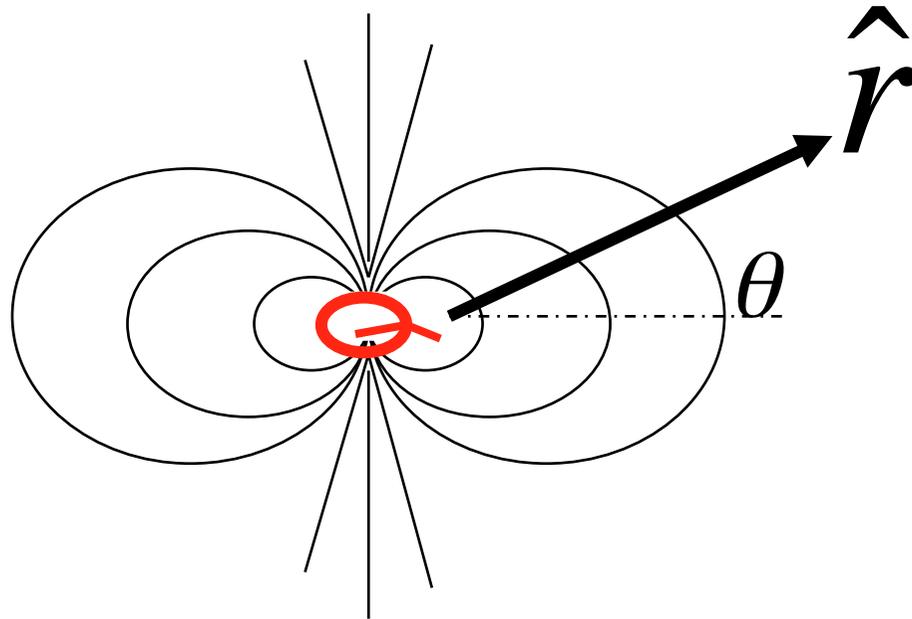
We know the equation for spatial variation the magnetic $V_M(r,\theta)$ potential in the magnetic dipole field

$$V_M(r,\theta) = \frac{\underline{\mu}\cdot\hat{r}}{4\pi r^2}$$

from which we can obtain the B field,

$$\underline{B}(r,\theta) = \frac{\mu_0\mu}{4\pi r^3}\left(2\cos\theta\,\hat{r} + \sin\theta\,\hat{\theta}\right)$$

Is this field strong enough to align a *neighbouring dipole*?

we can calculate its value, or *alternatively* use the result that the *magnetic energy* must equal the *thermal energy* when we reach the **Curie temperature** T_C

$$\left| -\underline{\mu}\cdot\underline{B} \right| \approx k_B T_C$$

we know $\mu_J = J g \mu_B$ and k_B is a constant, so we can calculate B at the first (atomic) neighbour distance, either,

$B(r_0, 0)$ on axis   or $B(r_0, 90^\circ)$ alongside

For α–Fe $\qquad \mu_{Fe} = 2.2\mu_B$

$\mu_B = 9.27 \times 10^{-24}$ J T^{-1}

$\mu_0 = 4\pi \times 10^{-7}$ h m^{-1} (N A^{-2})

$k = 1.38 \times 10^{-23}$ J K^{-1}

$r_0 = 2.5 \times 10^{-10}$ m

so that, $\qquad \mu_{Fe} \dfrac{\mu_0 \mu_{Fe}}{4\pi r_0^3} \approx k T_C$

gives, $\qquad T_C^{Fe} \approx 0.2\,\text{K}$ (Thermal effects should destroy alignment at 0.2K)

But we know that $\quad T_C^{Fe} = 1043K$

so we can work the equation backwards to get the actual magnitude of the aligning field B

$$\left| \underline{\mu} \, \underline{B} \right| = kT$$

$$(2.2 \times 9.27 \times 10^{-24}) \times B \ = \ 1.38 \times 10^{-23} \times 1043$$

or $$B_{\text{int}}^{Fe} \approx 705 \text{ T}$$

This is often referred to as the **"Internal Field"**.

Clearly, it is ***significantly larger*** than the magnetic fields that are created in most laboratories.

We can conclude that if magnetic dipole interactions were responsible for ferromagnetism, then the ferromagnetic state would not exist above a few Kelvin

Where next?

- So what does cause spontaneous alignment of magnetic dipoles in a ferromagnet?

- Need to look for an explanation involving quantum mechanics.

Pauli Exclusion Principle

For two identical fermions, total wavefunction is antisymmetric under exchange of particles

Two states, ψ_1 and ψ_2
Two particles, a and b

$$\Psi = \psi_1(a)\psi_2(b) - \psi_1(b)\psi_2(a)$$

If $\psi_1 = \psi_2$ (same quantum state), and
$a = b$ (identical particles)

Then $\Psi = 0$ (the state does not exist)

"−" sign tells us that the state is antisymmetric

2) The (quantum mechanical) exchange interaction

This is an extension of the discussions about the **orbital wave functions in an H_2^+ molecule**, concerning the **alignment of neighbouring electron spins.**

We have two hydrogen atoms labelled A and B, so their **orbital wavefunctions** can be written ϕ_A and ϕ_B
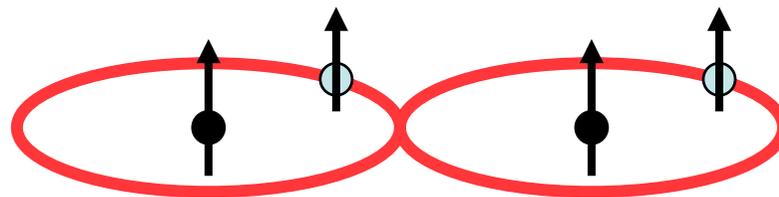
The **total wave function*** must include, **both** the **orbital motion** and the **spin motion**

$$\Phi_{total} = \varphi_{symm}^{orbit} \times \chi_{antisymm}^{spin}$$

$$\Phi_{total} = \varphi_{antisymm}^{orbit} \times \chi_{symm}^{spin}$$

But what does this mean in practice? There are **four ways** of writing the **total wave function**

$$\Phi_{total} = \left[\phi_A(1)\phi_B(2)+\phi_A(2)\phi_B(1)\right]_{symm} \times \left[\alpha(1)\beta(2)-\alpha(2)\beta(1)\right]_{anti}$$

$$\uparrow_1\downarrow_2 - \uparrow_2\downarrow_1$$

This is a **singlet state** with the **electron spins antiparallel,**

$$\Phi_{total} = \left[\phi_A(1)\phi_B(2) - \phi_A(2)\phi_B(1)\right]_{anti} \times \left[\alpha(1)\alpha(2)\right]_{symm}$$

$$\uparrow_1 \uparrow_2$$

$$\Phi_{total} = \left[\phi_A(1)\phi_B(2) - \phi_A(2)\phi_B(1)\right]_{anti} \times \left[\beta(1)\beta(2)\right]_{symm}$$

$$\downarrow_2 \downarrow_1$$

$$\Phi_{total} = \left[\phi_A(1)\phi_B(2) - \phi_A(2)\phi_B(1)\right]_{anti} \times \left[\alpha(1)\beta(2) + \alpha(2)\beta(1)\right]_{symm}$$

$$\uparrow_1 \downarrow_2 + \uparrow_2 \downarrow_1$$

This are a ***triplet states*** with the ***electron spins parallel***

- As electrons are Fermions, the Pauli Exclusion Principle dictates that the overall wavefunction of a multi-electron state must be anti-symmetric with respect to particle exchange.
- The overall quantum state is defined by spatial coordinates and spin-coordinates of electron and hole.
- Thus the spatial wavefunction must have opposite symmetry to spin-wavefunction to ensure overall state is antisymmetric:

$$\Psi = \psi_{spatial}(r_1, r_2)\psi_{spin}$$

S	M_S	ψ_{spin}	ψ_{spatial}
0	0	$\frac{1}{\sqrt{2}}(\uparrow_1 \downarrow_2 - \downarrow_1 \uparrow_2)$ **—**	$\frac{1}{\sqrt{2}}\left(u_A(r_1)u_B(r_2) + u_B(r_1)u_A(r_2)\right)$ **+**
1	+1	$\uparrow_1 \uparrow_2$ **+**	**—**
	0	$\frac{1}{\sqrt{2}}(\uparrow_1 \downarrow_2 + \downarrow_1 \uparrow_2)$	$\frac{1}{\sqrt{2}}\left(u_A(r_1)u_B(r_2) - u_B(r_1)u_A(r_2)\right)$
	−1	$\downarrow_1 \downarrow_2$	

Key points:

- Singlets and triplets have different spatial wavefunctions.
- Singlet spatial wavefunctions are symmetric.
- Triplet spatial wavefunctions are anti-symmetric.
- So what…! Has important consequences for the energy of singlet and triplet states.

- Sketch the spatial distribution for an electron in a symmetric and anti-symmetric wave-function in the confining potential of 2 atoms.
- Probability distribution given by $\left|\psi_{spatial}\right|^2$

Spatial
Symmetric
Spin antisymmetric
(SINGLET)
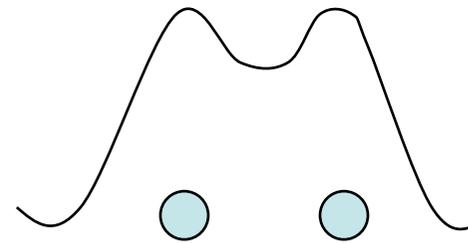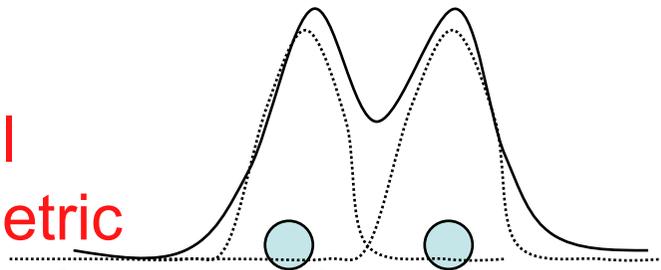
Spatial
Anti-symmetric
Spin symmetric
(TRIPLET)
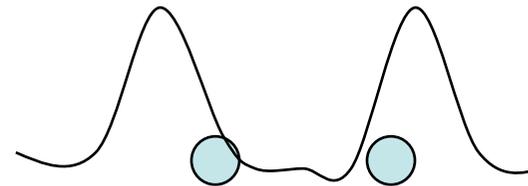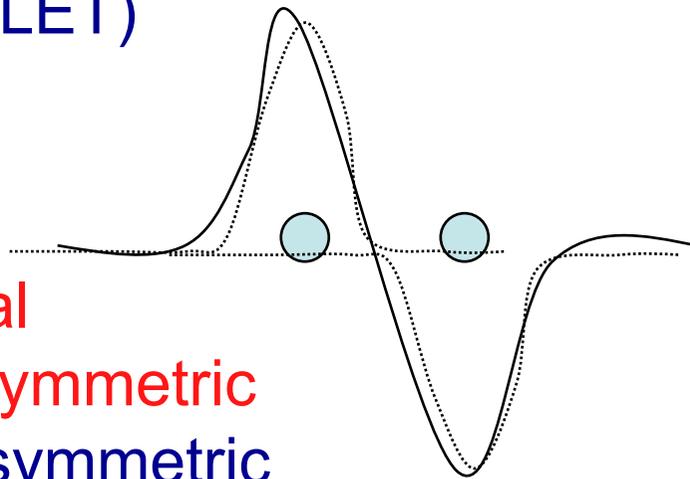
$\left|\psi_{spatial}\right|^2$

$\left|\psi_{spatial}\right|^2$

The exchange energy

Much smaller overlap in distribution for two electrons in an anti-symmetric spatial wavefunction.

Therefore much smaller Coulomb repulsion between 2 electrons in a triplet wavefunction.

Energy of triplet state is significantly lower than that of the singlet state. This energy difference is termed the exchange energy J.

Thus lowest ground state energy associated with a spin-parallel triplet state - feromagnetic alignment between neighbouring atoms.

Best condition for a feromagnetic state is when J is positive.

Of course, some this disagreement can be expected, since in metals like *iron* and *nickel*, the ferromagnetism is likely to be due to the *conduction electrons (i.e. not localised states).*

However, *direct exchange* is an important mechanism in *insulator (ferro) magnetic materials*, where the electrons are *localised* on each atom

MnO
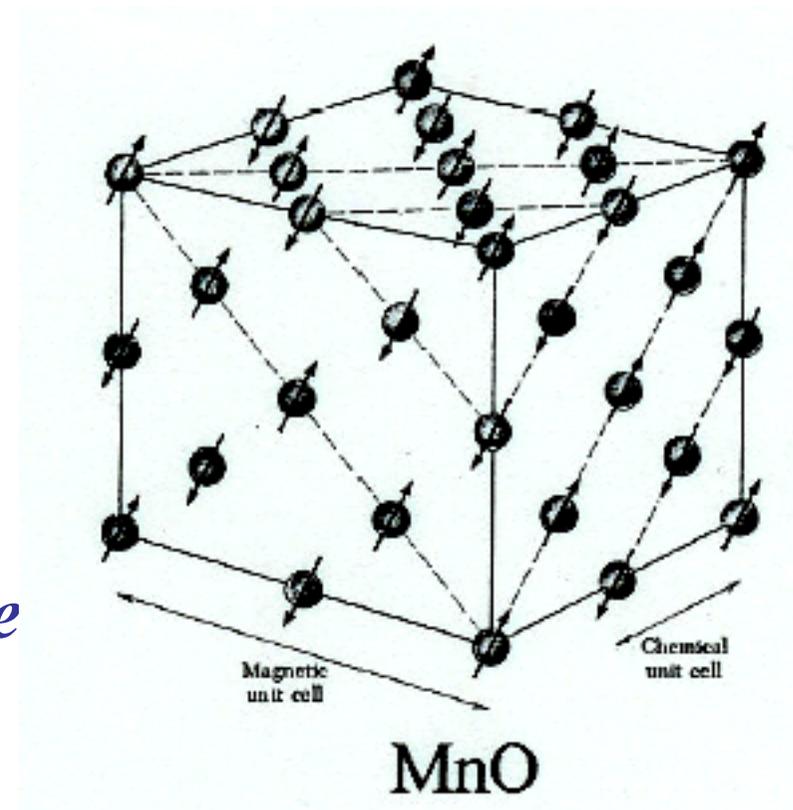
Summary…

- We showed that the magnetic field from a single dipole is not sufficient to align its neighbours. E.g. would require very large fields (100's of T) to align electron spins. If such effect were the correct explanation, ferromagnetism would not exist above a few kelvin.

- Rather it is the energy of exchanging electrons that 'forces' dipoles to align. Find lowest ground state is always spin-parallel.