Topics covered

• Introduction
• Magnetism as a quantum phenomenon
• Spin and orbital moments
• Paramagnetism/Diamagnetism
• Spin-orbit coupling
• Hundt’s rules and magnetic ions
• Magnetic interactions, dipolar, exchange
• Direct, indirect, super, and double exchange
• The Heisenberg Hamiltonian and ferro/antiferro magnetism
• Weiss model of ferromagnet
• Exchange coupling in metallic superlattices
• Domain walls
• Micromagnetics
• Kerr effect
• Magneto-crystalline anisotropy
Introduction

• Magnetic Moment
  – Interactions, ordering, temperature dependence

\[ \delta V \quad G \quad \parallel \quad oU \]
\[ \nabla \quad V \quad G \quad \parallel \quad oU \]

• Sources – intrinsic (spin), orbital
  Orbital moment \( m = \gamma L \)
  Einstein-de Haas experiment
The Bohr Magneton ($\mu_B$)

- Consider electron charge $e$, mass $m$ moving in a circular orbit radius $r$

- Angular momentum is quantized

\[ \mu = \pi r^2 l = -\frac{e u}{2m} = -\mu_B \approx 9.274 \times 10^{-24} \text{Am}^2 \]

- Leading to $\gamma = -\frac{e}{2m}$
Magnetism is a Quantum Phenomenon

- Magnetism is inherently a quantum phenomenon
- Von Leeuwen theorem

"At any finite temperature, and in all finite applied electrical or thermal fields, the net magnetization of a collection of electrons in thermal equilibrium vanishes identically."

- From classical mechanics

\[
\mathcal{Z} = \frac{1}{\mathcal{N}!} \int \exp\left(-\beta \mathcal{H}\right) d\mathcal{N} \prod_{i=1}^{\mathcal{N}} d\mathbf{r}_i d\mathbf{p}_i
\]

(Canonical momentum)

- \( \mathcal{Z} = \mathcal{N}! \exp\left(-\beta \mathcal{H}\right) \prod_{i=1}^{\mathcal{N}} d\mathbf{r}_i d\mathbf{p}_i \)
- Limits of integration are \(-\infty\) to \(\infty\)
- Simple change of variables shows partition function \( \mathcal{Z} \) is independent of \( A \)
Susceptibility/Magnetization and Field

• free space magnetic induction $B=\mu_0 H$, where $H$ is the magnetic field

• In a magnetic material $B=\mu_0 (H+M)$, $M$ is the magnetization, or magnetic dipole moment per unit volume

• In the special case of a linear material $M=\chi H$, $\chi$ is the susceptibility $B=\mu_0 (1+\chi)H$

• Consider a region of space with fields $B_0$ and $H_0$, $B_0 = \mu_0 H_0$.

• Now add in magnetic material. Fields inside the material $B_i$ and $H_i$ differ markedly from $B_0$ and $H_0$, and can be complicated to calculate except in simple cases e.g. slab, sphere… in which case $H_i=H_0-NM$, $N$ is the demagnetization factor =1/3 for a sphere.

• More complex shape need to satisfy Maxwell’s equations with $M=0$ outside the sample
Quantum Mechanics of Spin

- Orbital angular momentum
  - State defined by $l$ and $m_l$

- Spin angular momentum
  - State defined by $s$ and $m_s$

- Energy of a spin in a magnetic field $E = g\mu_B m_s B$

- $g \sim 2$, leads to Zeeman splitting
Electrons in a Magnetic Field

\[ H = Q S \left( \frac{p S + e A S}{2m} + V S + \mu B (\cdot + gS) \right) \cdot \mu + e^2 \]

- Now since \( G \ll + t \), we can choose gauge condition \( t \ G \ > \ + \frac{1}{4} \)
- Leads to

\[ Q \ \frac{\gg_0}{U} \ j \ \frac{1_U j}{Oc} \ >_R \ j \ MUblj^0 \ \frac{j^O}{kC} \]

- paramagnetism
- diamagnetism
Paramagnetism $J = 1/2$

- **Partition function**

  $$L \ G \ {^1K} \ _R \ i \ _R \ ^3b \ j \ {^1K} \ _R \ ^2/M \ _R \ i \ _R \ ^3b$$

  $$G \ \Omega \ \mu \ _R \ ^3O \ L$$

- **Free energy**

  $$^`G \ \mu \ _R \ ^3O \ L$$

- **Magnetization**

  $$^K \ G \ / \ F^F \ _R \ G \ :\ ^w \ _R \ ^3b$$

- **For high $T$, $M = g\mu_B B/k_B T$, $\chi = 1/T$ or Curie’s Law**

- **Can be generalized to other values of $J$ (Brillouin function)**
Diamagnetism

- Diamagnetic term in Hamiltonian

\[ g \circ G \frac{^0Q}{kC} \Rightarrow + \frac{1}{4}b^0 \]

- For \( B \) along the \( z \) axis

\[ S \sim G \frac{^0R^0Q}{kC} FM_U^0 j r_U^{OMF} G \frac{^0R^0Q}{\varepsilon_0C} FM_U^{OMF} \]

- For a solid with \( N \) ions in a volume \( V \), we get

\[ / G / \frac{\{ ^0>F_L^0 \}}{1} CC \]

- where \( Z_{\text{eff}} \) is the \# of outer shell electrons and \( r \) the ionic radius

- sign similar to Lenz’s law in induction
Spin Orbit Coupling

- Total angular momentum is the sum of both spin and orbital contributions

- The magnetic moment is given by

\[ \mu = gj(j + 1)\mu_B \]

\[ g_j = \frac{3}{2} + \frac{S(S+1)}{2J(J+1)} \]

- The spin and orbital moments are weakly coupled. This coupling falls out of the Dirac equation.

\[ > G > R \quad > _{R} \quad ^{2} l \quad j \quad M_{j} U b G \quad M_{m} > _{R} \quad d \]

- Lande g-factor

\[ M \cdot G \quad \langle j \quad \frac{a_{2} a_{j} \quad f b / \quad s_{2} s_{j} \quad f b \quad 0 m_{2} m_{j} \quad f b}{0 \cdot a \quad a \quad j \quad f b / \quad s_{2} s_{j} \quad f b \quad 0 m_{2} m_{j} \quad f b} \]
Classical View of Spin-Orbit

- Orbiting nucleus produces a magnetic field

\[ \mathbf{E} = -\frac{3}{2} \mathbf{v} \times \mathbf{r} \]

- where

\[ \mathbf{E} = \mathbf{v} \times \mathbf{r} \]

- \( \frac{1}{2} \) is the relativistic Thomas factor

\[ \mathbf{E} = c \frac{\alpha + \mathbf{C}}{\omega_0} \]

- where

\[ \mathbf{E} = \mathbf{v} \times \mathbf{r} \]

\[ \mathbf{E} = c \frac{\alpha + \mathbf{C}}{\omega_0} \]

- \( \frac{1}{2} \) is the relativistic Thomas factor
Magnetism of ions/Hundt’s rules

- Hundt’s rules used to determine total angular momentum. Minimize Coulomb energy taking into account the Pauli principle

  1. Maximise S (Pauli principle, minimizes U)
  2. Maximise L (keeps electrons I same orbit apart)
  3. Attempts to minimize spin-orbit interaction.
     - Shell less than half full $J=|L-S|$
     - Shell greater than half full $J=|L+S|$

- 3rd rule not always applicable in a solid since surrounding ions in the crystal provide an electrostatic field
Table 2.2 Magnetic ground states for 4f ions using Hund’s rules. For each ion, the shell configuration and the predicted values of $S$, $L^*$, and $J$ for the ground state are listed. Also shown is the calculated value of $p = \mu_{\text{eff}}/\mu_B = g_J |J(J+1)|^{1/2}$ using these Hund’s rules predictions. The next column lists the experimental value $p_{\text{exp}}$ and shows very good agreement, except for Sm and Eu. The experimental values are obtained from measurements of the susceptibility of paramagnetic salts at temperatures $k_B T \gg E_{\text{CEF}}$ where $E_{\text{CEF}}$ is a crystal field energy.

<table>
<thead>
<tr>
<th>ion</th>
<th>shell</th>
<th>S</th>
<th>L</th>
<th>J</th>
<th>term</th>
<th>$p$</th>
<th>$p_{\text{exp}}$</th>
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<tbody>
<tr>
<td>Ce$^{3+}$</td>
<td>4f$^1$</td>
<td>1/2</td>
<td>3</td>
<td>5/2</td>
<td>$^2F_{5/2}$</td>
<td>2.54</td>
<td>2.51</td>
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<td>4f$^2$</td>
<td>1</td>
<td>5</td>
<td>4</td>
<td>$^3H_4$</td>
<td>3.58</td>
<td>3.56</td>
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<tr>
<td>Nd$^{3+}$</td>
<td>4f$^3$</td>
<td>3/2</td>
<td>6</td>
<td>9/2</td>
<td>$^4I_{9/2}$</td>
<td>3.62</td>
<td>3.3–3.7</td>
</tr>
<tr>
<td>Pm$^{3+}$</td>
<td>4f$^4$</td>
<td>2</td>
<td>6</td>
<td>4</td>
<td>$^5I_4$</td>
<td>2.68</td>
<td>–</td>
</tr>
<tr>
<td>Sm$^{3+}$</td>
<td>4f$^5$</td>
<td>5/2</td>
<td>5</td>
<td>5/2</td>
<td>$^6I_{5/2}$</td>
<td>0.85</td>
<td>1.74</td>
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<tr>
<td>Eu$^{3+}$</td>
<td>4f$^6$</td>
<td>3</td>
<td>3</td>
<td>0</td>
<td>$^7F_0$</td>
<td>0.0</td>
<td>3.4</td>
</tr>
<tr>
<td>Gd$^{3+}$</td>
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<td>0</td>
<td>7/2</td>
<td>$^8S_{7/2}$</td>
<td>7.94</td>
<td>7.98</td>
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<td>4f$^8$</td>
<td>3</td>
<td>3</td>
<td>6</td>
<td>$^7F_6$</td>
<td>9.72</td>
<td>9.77</td>
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<td>4f$^9$</td>
<td>5/2</td>
<td>5</td>
<td>15/2</td>
<td>$^6H_{15/2}$</td>
<td>10.63</td>
<td>10.63</td>
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<tr>
<td>Ho$^{3+}$</td>
<td>4f$^{10}$</td>
<td>2</td>
<td>6</td>
<td>8</td>
<td>$^5I_8$</td>
<td>10.60</td>
<td>10.4</td>
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<td>Er$^{3+}$</td>
<td>4f$^{11}$</td>
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<td>6</td>
<td>15/2</td>
<td>$^4I_{15/2}$</td>
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<tr>
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<tr>
<td>Yb$^{3+}$</td>
<td>4f$^{13}$</td>
<td>1/2</td>
<td>3</td>
<td>7/2</td>
<td>$^2F_{7/2}$</td>
<td>4.53</td>
<td>4.5</td>
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<tr>
<td>Lu$^{3+}$</td>
<td>4f$^{14}$</td>
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<td>0</td>
<td>0</td>
<td>$^1S_0$</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Magnetic Ions in a solid

- Relative importance of crystal field terms and spin-orbit coupling determines the moment.

- Rare earth f-shell electrons
  - Angular momentum barrier confines electrons close to nucleus, moments localized & atomic
  - Spin-orbit important

- Transition metal d-shell electrons
  - Crystal field larger than spin orbit
  - Orbital moments quenched
Table 3.1 Magnetic ground states for 3d ions using Hund’s rules. For each ion, the shell configuration and the predicted values of $S$, $L$ and $J$ for the ground state are listed. Also shown is the calculated value of $p = \mu_{\text{eff}}/\mu_B$ for each ion using Hund’s rules predictions. This is given the symbol $p_1 = g_J[J(J+1)]^{1/2}$ and the next column lists the experimental values $p_{\text{exp}}$ which are derived from measurements on paramagnetic salts containing the relevant ions. This agrees much better with $p_2 = 2[S(S + 1)]^{1/2}$, which assumes orbital quenching, so that $L = 0$, $J = S$ and $g_J = 2$.

<table>
<thead>
<tr>
<th>ion</th>
<th>shell</th>
<th>$S$</th>
<th>$L$</th>
<th>$J$</th>
<th>term</th>
<th>$p_1$</th>
<th>$p_{\text{exp}}$</th>
<th>$p_2$</th>
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<tbody>
<tr>
<td>Ti$^{3+}$, V$^{4+}$</td>
<td>3d$^1$</td>
<td>$\frac{1}{2}$</td>
<td>2</td>
<td>$\frac{3}{2}$</td>
<td>$^2 D_{3/2}$</td>
<td>1.55</td>
<td>1.70</td>
<td>1.73</td>
</tr>
<tr>
<td>V$^{3+}$</td>
<td>3d$^2$</td>
<td>1</td>
<td>3</td>
<td>2</td>
<td>$^3 F_2$</td>
<td>1.63</td>
<td>2.61</td>
<td>2.83</td>
</tr>
<tr>
<td>Cr$^{3+}$, V$^{2+}$</td>
<td>3d$^3$</td>
<td>$\frac{3}{2}$</td>
<td>3</td>
<td>$\frac{3}{2}$</td>
<td>$^4 F_{3/2}$</td>
<td>0.77</td>
<td>3.85</td>
<td>3.87</td>
</tr>
<tr>
<td>Mn$^{3+}$, Cr$^{2+}$</td>
<td>3d$^4$</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>$^5 D_0$</td>
<td>0</td>
<td>4.82</td>
<td>4.90</td>
</tr>
<tr>
<td>Fe$^{3+}$, Mn$^{2+}$</td>
<td>3d$^5$</td>
<td>$\frac{5}{2}$</td>
<td>0</td>
<td>$\frac{5}{2}$</td>
<td>$^6 S_{5/2}$</td>
<td>5.92</td>
<td>5.82</td>
<td>5.92</td>
</tr>
<tr>
<td>Fe$^{2+}$</td>
<td>3d$^6$</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>$^5 D_4$</td>
<td>6.70</td>
<td>5.36</td>
<td>4.90</td>
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<tr>
<td>Co$^{2+}$</td>
<td>3d$^7$</td>
<td>$\frac{3}{2}$</td>
<td>3</td>
<td>$\frac{9}{2}$</td>
<td>$^4 F_{9/2}$</td>
<td>6.63</td>
<td>4.90</td>
<td>3.87</td>
</tr>
<tr>
<td>Ni$^{2+}$</td>
<td>3d$^8$</td>
<td>1</td>
<td>3</td>
<td>4</td>
<td>$^3 F_4$</td>
<td>5.59</td>
<td>3.12</td>
<td>2.83</td>
</tr>
<tr>
<td>Cu$^{2+}$</td>
<td>3d$^9$</td>
<td>$\frac{1}{2}$</td>
<td>2</td>
<td>$\frac{5}{2}$</td>
<td>$^2 D_{5/2}$</td>
<td>3.55</td>
<td>1.83</td>
<td>1.73</td>
</tr>
<tr>
<td>Zn$^{2+}$</td>
<td>3d$^{10}$</td>
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<td>0</td>
<td>0</td>
<td>$^1 S_0$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
Magnetic Interactions

• Dipole-Dipole forces (classical)

\[- G \frac{>_{F}}{YB^{\frac{1}{4}}} >_{\xi} o / \frac{<<}{1^{\frac{1}{4}}} ^{2} >_{\xi} 1^{\frac{1}{4}} 6^{2} o 1^{\frac{1}{4}} \]

• Size estimate for two atomic moments separated by 1 Angstrom E \sim 1K
Exchange

• The exchange interaction is a result of the Pauli principle and the Coulomb Interaction.
• Form antisymmetric wavefunctions as product of spatial and spin functions.
  – Singlet state has S=0

\[
\psi_s = \frac{1}{\sqrt{2}} \left[ \psi_a(r_1) \psi_b(r_2) + \psi_a(r_2) \psi_b(r_2) \right]
\]

\[
= \left( \begin{array}{c} \psi_a \psi_b \end{array} \right) \left( \begin{array}{c} 1 \ 1 \end{array} \right) = \frac{1}{\sqrt{2}} \left[ \psi_a(r_2) \psi_b(r_2) \right]
\]

– Triplet state has S=1

\[
\psi_t = \frac{1}{\sqrt{2}} \left[ \psi_a(r_1) \psi_b(r_2) - \psi_a(r_2) \psi_b(r_2) \right]
\]

\[
= \left( \begin{array}{c} \psi_a \psi_b \end{array} \right) \left( \begin{array}{c} 1 \ -1 \end{array} \right) = \frac{1}{\sqrt{2}} \left[ \psi_a(r_2) \psi_b(r_2) \right]
\]
Heisenberg Hamiltonian

- Energy of singlet & triplet states

\[ \begin{align*}
\mathcal{G}_v &= \mathcal{g}_v \\
\mathcal{G}_N &= \mathcal{g}_N
\end{align*} \]

- After some algebra we can show

\[ g \mathcal{G} \frac{f}{Y} 2\mathcal{g} j \ll \mathcal{G}_b \mathcal{U}_O \mathcal{U}_\epsilon \]

- Where we have used

  - For a singlet \( U_\epsilon \mathcal{U}_O \mathcal{G} / \ll \frac{f}{Y} \)

  - For a triplet \( U_\epsilon \mathcal{U}_O \mathcal{G} \frac{f}{Y} \)
Heisenberg Hamiltonian

\[ H = -Q \sum m_{ij} \cdot \hat{U}_i \hat{U}_j \]

- Two electrons on same atom, \( J \) usually positive. Spatial part of wavefunction antisymmetric lowers Coulomb Energy. (Hundt’s 1\textsuperscript{st} rule)

- Two electrons on different atoms is more complex. Some saving in kinetic energy to have a symmetric spatial wavefunction thus \( J \) can be negative
Direct Exchange

- Exchange interactions between electrons on neighboring sites
- In rare earths f-orbitals interact with each other weakly due to localization
- In transition metals d-d overlap is larger
- In these metals s-d and s-f interactions important for bonding and communicating exchange (indirect between d or f orbitals) important for RKKY like interactions in multilayers
Superexchange

- Found in magnetic ionic materials, eg. MnF$_2$ and usually antiferromagnetic
- Cannot be a direct exchange as the magnetic ions are too far apart
- Exchange is mediated through the non-magnetic ions orbitals
- Electron from non-metal hops onto metal ion and is coupled strongly, resulting single p-electron has direct exchange with the adjacent metal ion
- Coupling may be determined via Hundt’s rules parallel for ions with less than half filled d-shell antiparallel for ions with more than half filled d shell.
- Chromium telluride ferromagnetic, manganese telluride antiferromagnetic

<table>
<thead>
<tr>
<th>internal coupling</th>
<th>and exchange coupling of p-electron with other atom</th>
<th>coupling is</th>
</tr>
</thead>
<tbody>
<tr>
<td>parallel</td>
<td>ferromagnetic</td>
<td>antiferromagnet</td>
</tr>
<tr>
<td>parallel</td>
<td>anti-ferromagnet</td>
<td>ferromagnetic</td>
</tr>
<tr>
<td>antiparallel</td>
<td>ferromagnetic</td>
<td>ferromagnetic</td>
</tr>
<tr>
<td>antiparallel</td>
<td>anti-ferromagnet</td>
<td>antiferromagnet</td>
</tr>
</tbody>
</table>

H.A. Kramers, Physica 1, 182 (1934)
Double Exchange

- Occurs in some oxides where the magnetic ion can have mixed valence
- Leads to ferromagnetic coupling
- Examples include Fe$_2$O$_3$

![Electron hopping diagram]

Fe$^{2+}$ (3d$^6$)  Fe$^{3+}$ (3d$^5$)
Ferromagnetism

\[ g \ G / \ m_{U \cdot U_{B \cdot L_{U \cdot j \cdot M_{R}}}^{Q}} \ U_{U \cdot l} \]

- Mean field solution

\[ >_{c \ U \ G} / \ O \ Q \]
\[ m_{U \cdot c \ U \cdot c} \]

- Assuming \( S = 1/2 \)

\[ g \ G \ M_{R}^{Q} \ U_{U \cdot l^{2}}^{j} >_{v \ U} \]
\[ >_{v \ U} \ G \ '5 \]

\[ \frac{K}{K_{v \ W}} G :_{w}^{M_{R} a^{2} R j 'K b} \]
\[ \ \_{R^{3}} \]
Curie temperature

- Solve the two equations for appearance of non zero $M$

$$\frac{K}{K_v} G \otimes W^b$$
$$\frac{K}{K_v} G \frac{O_R^3}{M_R^* K_v}$$

- Leads to

$$3_s G \frac{M_i^*}{O_R^i} K_v G \frac{\mu_{iD}^0}{\ll R} G \frac{d m}{O_R^i}$$
- $z$ is # of nearest neighbors

- Susceptibility

$$/ - \frac{\xi}{3} / 3$$
Properties of some common ferromagnets

<table>
<thead>
<tr>
<th>Material</th>
<th>$T_c$ ($\text{p}$)</th>
<th>Moment in Bohr magnetons</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Q}^1$</td>
<td>$\text{FFY}$</td>
<td>$\text{O}&lt;0$</td>
</tr>
<tr>
<td>$\text{~}$</td>
<td>$\text{FF$$4Y}$</td>
<td>$\text{F}$</td>
</tr>
<tr>
<td>uB</td>
<td>$\text{c$&lt;$f}$</td>
<td>$\text{F}&lt;c$</td>
</tr>
<tr>
<td>$-g$</td>
<td>$\text{0k4}$</td>
<td>$\text{O}&lt;3$</td>
</tr>
<tr>
<td>5 $\text{U}_-$</td>
<td>$\text{3k}$ &amp; $\text{O}&lt;3$</td>
<td></td>
</tr>
<tr>
<td>$\times?$</td>
<td>$\text{O}$</td>
<td>$\text{F}$</td>
</tr>
<tr>
<td>$\times\text{U}$</td>
<td>$\text{F}$</td>
<td>$\text{c&lt;4}$</td>
</tr>
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</table>

Moment in Bohr magnetons
Stoner Criterion & Band magnetism

- Consider a density of electron states $g(E)$
- Move spin down electrons from $\uparrow \downarrow$ / $D\downarrow$ to spin up band at $\uparrow \uparrow \downarrow \downarrow$
- Change in KE
  $$D\downarrow \rightarrow G M^2 \downarrow \cdot \hbar D\downarrow \uparrow O + D\downarrow G \frac{f}{O} M^2 \downarrow \cdot \hbar D\downarrow O$$
- Change in PE
  $$D\downarrow \rightarrow G / \frac{B}{F} > F ^2 K \hbar o K G / \frac{f}{O} > F ^0 K \hbar o K G / \frac{f}{O} > F ^0 R \hbar o \uparrow \mu / \mu : b^0$$
- Where we used the molecular field = $'K$ and $\mu_7 / \mu$ : $G M^2 \downarrow \cdot \hbar D\downarrow$
- Change in total energy is
  $$\$ \rightarrow G \$ \rightarrow j \$ \rightarrow G \frac{f}{O} M^2 \downarrow \cdot \hbar^2 D\downarrow b^0 ^2 \uparrow \downarrow / \hbar M^2 \downarrow \cdot \hbar o$$
- Spontaneous ferromagnetism (Stoner criterion) is possible if
- $h M^2 \downarrow \cdot \hbar ; f$
Antiferromagnetism

- If the exchange interaction $J<0$ then nearest neighbor moments will align antiparallel.
- Often occurs for crystals with interpenetrating lattices.
- Can be treated via a Weiss mean field theory using the two sublattices.
- Leads to a susceptibility

\[
\chi = - \frac{\mathcal{E}}{3} \left( \frac{1}{j} \right)
\]

- $T_N$ is known as the Neel temperature shows this form but the extrapolated Weiss temperature differs from simple mean field Neel temperature. Need to include 2nd neighbor interactions (both sublattices).
Other magnetic ordering

- Ferrimagnetism – two sublattice moments with different values are coupled antiferromagnetically e.g. Fe₃O₄
- Helical ordering seen in some rare earth magnets e.g. Dy

\[
E = -2u S^2 (J_1 \Theta + J_2 \Theta^2)
\]

- Minimizing wrt \( \Theta \)

\[
\Theta = \frac{-J_1}{4J_2}
\]

- Leads to \( \Theta = 0 \) or \( \Theta = \frac{m_F}{Ym_0} \)

- Frustrated systems such as antiferromagnetism on a triangular lattice, spin glasses
Exchange coupling in Magnetic Superlattices

- Model proposed by Stiles (PRB 48, 7238, 1993)
- Based upon a quantum well model and the reflection coefficient for waves incident upon the well (see below) with $R<<1$
- Change in energy

$$
\Delta E(N) = \frac{\mu}{m_0} \left[ E - \epsilon_{F} \right] f(N) 
$$

- In 1-d for free electrons leads to

$$
\Delta E(N) = \frac{\mu}{m_0} \left[ E - \epsilon_{F} \right] f(N) 
$$

- Reason for the oscillations is the step function in occupation numbers at $k_F$
Exchange coupling

- Ferromagnetic state

\[ M \uparrow \quad M \uparrow \quad + \quad M \downarrow \quad M \downarrow \]

- Antiferromagnetic state

\[ M \uparrow \quad M \downarrow \quad + \quad M \downarrow \quad M \uparrow \]

- Exchange coupling

\[ m^2 \text{NbG} \left( \frac{uV}{B} \right. \left. + \right. \frac{h}{D} \right. \left. M \uparrow M \uparrow j M \uparrow M \downarrow / \right. \left. \text{OM} \uparrow M \uparrow M \downarrow \right. \left. - \right. \left. \text{OM} \uparrow M \downarrow M \downarrow \right. \left. + \right. \left. \frac{\xi}{N} dB \right. \left. \text{Nj} H_{\text{Fb}} \right. \]
3-d and realistic Fermi surfaces

- Moving from 1-d to 3-d for free electrons
  - Fermi surface spherical
  - Contributions from all $k_\parallel$
  - Contributions to integrand oscillate except when parts of Fermi surface are parallel (approximate with stationary phase integration)
  - Spanning vector of $2k_F$ determines oscillations just like 1-d model

- Realistic Fermi surface oscillations determined by spanning vectors in the growth direction that link parallel sheets of the Fermi surface

Stiles, PRB 48, 7238 (1993)
Fe/Au/Fe wedges

Data from Unguris et al. PRL 79, 2734 (1997)

SEMPA

MOKE

Theory: M.D. Stiles, J. Appl. Phys. 79(8), 5805 (1996)

Period and coupling strength in good agreement with measurement

Domain Walls

- Wall is region between two magnetic domains
  - Bloch wall (a) - spins rotate in plane parallel to the wall
  - Neel wall (b) - spins rotate in plane perpendicular to the wall

- Competition between exchange and anisotropy.

  Exchange wants a slowly varying wall since the energy rises as $\text{Si} \cdot \text{Sj}$

  Anisotropy wants to lock spins to a particular crystal direction
Wall size (Bloch)

- Suppose wall extends over N layers
- Anisotropy contributions – assuming uniaxial anisotropy

\[
Q' \quad / \quad pB^0 \quad 0_u \quad 5 \quad \left\{ \begin{array}{c}
V_B \\
B_F
\end{array} \right\} / \quad pB^0 \quad 0_00 \quad G \quad \left\{ \begin{array}{c}
/ \\
O
\end{array} \right\}
\]

- Exchange

\[
5 \quad ma^0 \quad 0^0 \quad \text{for small angles}
\]

\[
G \quad ma^0B^0 \quad \{ \quad \text{adding contribution from the N layers}
\]

- Total energy is sum of exchange and anisotropy

\[
\left\{ \begin{array}{c}
G \quad ma^0B^0 \\
\{ \quad \left\{ \quad / \\
O
\end{array} \right\}
\]
Wall size (cont.)

- Minimizing wrt N leads to

\[ N \frac{G \text{ Ba} \ Om_i}{\sigma_b} \]

- And

\[ N \frac{G \text{ Ba} \ Om_i}{3_{Rn} \ G \text{ Ba} \ Om_i} \]

- Where \( z_{i+1} \) is known as the exchange stiffness.
Domain Formation

- Creation of domain walls costs energy
- Dipolar energy reduced
- Domains are formed to balance these two effects
Micromagnetics

- Micromagnetics minimizes the energy of the system that includes exchange, anisotropy, external fields, and demagnetization (dipolar)
- Typically solved by breaking the sample into small elements and calculating the torque on the moment from an effective field determined from the energy function

\[
\mathcal{V} = \mathcal{G} \sum_{i=1}^{N} \mathbf{J} \mathbf{O} \mathbf{B} \mathbf{O} \mathbf{J} \mathbf{O} \mathbf{g} \mathbf{V} \mathbf{b} \mathbf{O} \mathbf{V}
\]

\[
\mathcal{V} = \sum_{i=1}^{N} \mathbf{J} \mathbf{b} \mathbf{j} \mathbf{b} \mathbf{j}
\]

- Damping is included to drive the solution to equilibrium
- In principle exchange, anisotropy can be found from electronic structure theory
- Several public domain codes oommf (NIST), magpar (Vienna)
  - http://magnet.atp.tuwien.ac.at/scholz/magpar/
  - http://math.nist.gov/oommf/
Calculation of hysteresis from 1st principles

Idealized model of the interface

HRTEM image of grain boundary in Co1Pd5

Calculated boundary exchange

Calculated hysteresis loop

- Anisotropy only perturbed right at boundary plane
- Exchange coupling falls off quickly
- Modeled distribution of grains and used calculated anisotropies and exchanges
Secondary Magnetic Properties

• magneto optics
  – Rotation of the plane of polarized light on either reflection/transmission
• magneto crystalline anisotropy
  – Energy cost as magnetization rotated wrt crystal axes
• magnetostriction
  – Change in shape of a sample as it is magnetized
• magnetoelastic effect
  – Influence of stress on magnetization

• all dependent on spin-orbit coupling
Kerr & Faraday effects

- Kerr effect – rotation of the plane of polarization of reflected light
- Faraday effect – rotation of the plane of polarization of transmitted light
- Key is the symmetry of the dielectric tensor
- Same as symmetry in Lorentz force
Example of Polar Kerr Effect

- M perpendicular to film, dielectric tensor

\[
\begin{bmatrix}
\alpha & \beta \\
\gamma & \delta
\end{bmatrix}
\]

- Maxwell’s equations

\[\begin{aligned}
\mathbf{D} &= \varepsilon_0 \mathbf{E} + \mathbf{J} \\
\mathbf{B} &= \mu_0 \mu_0 \mathbf{H} + \mathbf{M}
\end{aligned}\]

- Linear media

\[\begin{aligned}
\mathbf{H} &= \mu_0 \varepsilon_0 \mathbf{J} \\
\mathbf{D} &= \varepsilon_0 \mathbf{E} + \mathbf{J}
\end{aligned}\]
Polar Kerr Effect (cont)

- Consider incident plane waves
  \[ x \left( \frac{1}{2} \right) N b \ G \ x \sigma_{F}^{+} K \ \sigma_{J}^{+} \ 1^{1/4} / \ ; N b \]
  \[ Z \left( \frac{1}{2} \right) N b \ G \ \sigma_{F}^{+} K \ \sigma_{J}^{+} \ 1^{1/4} / \ ; N b \]

- Leads to modified Maxwell equation
  \[ \left\{ + \right. \ G \ \frac{F}{\alpha} \ \frac{T^{2}}{J} \ ; bG \ \frac{T}{j} \ \frac{UW^{3}}{2} ; b \]

- and
  \[ \left. \frac{F}{\alpha} \ \frac{H}{G} \ ; J \ \frac{L}{b} \right] \]

- At normal incidence for transverse waves
  \[ 2T / \ \mu_{0} b H \ G \ H \]

- Eigenvalue problem (circularly polarized light)
  \[ \mu_{0} G \ <_{\left( \right)} \ \right. \ \left. \ \left( \left( \right) \right) \ ; H \ G \ \right] \ & \ \right. \ \left( \left( \right) \right) \]
Polar Kerr effect (cont)

- Incident plane wave equals sum of left and right circularly polarized beams
- Each reflected from the surface (see Jackson) for reflection coefficients

\[ \alpha \frac{n}{\mu} \left( \frac{E}{j \mu} \right) L \left( \frac{E}{j \mu} \right) \left( \frac{1}{\mu} \right) \]

- After some simplifications we arrive at the standard formula

\[ \alpha \frac{n}{\mu} \left( \frac{E}{j \mu} \right) L \left( \frac{E}{j \mu} \right) \left( \frac{1}{\mu} \right) \]

- Formulae for different geometries more complicated (see chapter by J.M MacLaren in Magnetic Interactions and Spin Transport, eds Chtchelkanova, Wolf, Idzerda, pub. Kluwer, 2003.)
Density Functional Theory

- Based on two theorems by Hohenberg & Kohn
  - Ground state energy is a functional of the electron density
  - Energy minimized for the true density

- Made practical by Kohn-Sham
  - Find density from an effective single particle Schrödinger equation
  - Potential depends on electron density
  - Density determined from solutions (wavefunctions)
  - Potential includes electron-ion, electron-electron, and exchange-correlation potential.
  - Many accurate approximations to exchange & correlation
  - Solve self-consistently

- Extended to magnetic systems as spin-density functional theory
- Despite being a ground state theory, wavefunctions and eigenvalues of excited single particle states can explain properties like the Kerr effect
Kubo formula

- Linear response leads to the Kubo formula for the optical conductivity

\[ \sigma \times \beta = S_n e^2 m; f f \times \beta + 1 \Omega m \mu_0 dN e S; N \neq \sigma \times \beta = S_n e^2 / \tau \]

- This can be evaluated using single particle wavefunctions and operators using the momentum rather than current operators
Kubo formula (cont)

- Matrix elements include spin-orbit coupling
Example of Fe
Anisotropy

- Magnetization prefers to align with certain crystallographic directions – easy and hard axes
- Origin is spin orbit coupling
- Can be calculated using modern electronic structure methods
- Larger in technologically interesting superlattices where the symmetry is lower
- Often seen in superlattices is a sum of interface/surface and bulk contributions

\[ E = E_0 + L(r) I_0 q^2 + H(r) I_0 q^4 \]

- Neel model is a useful framework for understanding anisotropy – symmetry based expansion

\[ G \sim F \propto 2 \pi \rho^0 0 j Z 2 \pi \rho^y 0 j 0 0 0 \]
## Anisotropy for magnetic transition metals

<table>
<thead>
<tr>
<th>( \vec{p} \cdot \vec{V} )</th>
<th>( \omega^{1/4} )</th>
<th>( 2 &gt; 1 \mu )</th>
<th>( \vec{V} )</th>
<th>( \vec{t}_K )</th>
<th>( \vec{K}_F )</th>
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<tbody>
<tr>
<td>( \uparrow \downarrow Q^1 )</td>
<td>( \text{rF}^3 )</td>
<td>( \text{rF} )</td>
<td>( \text{rF} )</td>
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<tr>
<td>( \omega ), { \text{c} } , { \text{c} }</td>
<td>( \text{cF} )</td>
<td>( \text{r04} )</td>
<td>( \text{r04} )</td>
<td>( \text{rF} )</td>
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<td>( \omega ), { \text{c} } , { \text{c} }</td>
<td>( \text{F}^3 )</td>
<td>( \text{O}^0 )</td>
<td>( \text{F}^3 )</td>
<td>( \text{F} )</td>
<td>( \text{F} )</td>
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</tbody>
</table>

Column 1: Daalderop et al., PRB 41, 11919, 1990 (LMTO s,p,d partial waves)

Column 2: Daalderop et al., PRB 41, 11919, 1990 (LMTO s,p,d,f partial waves)


Column 4: Trygg et al., PRL 75, 2871 (1995)

Column 5: Trygg et al., PRL 75, 2871 (1995) (adding in orbital polarization)

Agreement ok, Ni LSD gives poor Fermi surface
Anisotropies for Superlattices

<table>
<thead>
<tr>
<th>${`z}g$</th>
<th>$0/_{\nu}2^{11/\Theta}zTV^0b$</th>
<th>$/_{\nu}2^{11/\Theta}zTV&lt;b$</th>
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<td>$w^{1/4}$</td>
<td>$1K,^{11/\Theta}V^1-$</td>
<td>$w^{1/4}$</td>
</tr>
<tr>
<td>$^{2}e^{2}f^{2}f^{2}b$</td>
<td>$f&lt;&lt;0$</td>
<td>$f&lt;&lt;$</td>
</tr>
<tr>
<td>$^{2}e^{2}f^{2}b$</td>
<td>$f&lt;&lt;Y$</td>
<td>$f&lt;&lt;$</td>
</tr>
<tr>
<td>$^{2}f^{2}f^{2}b$</td>
<td>$f&lt;&lt;$</td>
<td>$f&lt;&lt;$</td>
</tr>
</tbody>
</table>

- Theory Victora and MacLaren, PRB, 47 11919 (1993)
- Experiment Engel et al. PRL, 67, 1910 (1991)
- Interface term well described (larger)
- Volume term less accurate (smaller)
Other results - Co/Pd

(†) Draaisma et al., JMMM 66, 351 (1987)
Theory Daalderop et al. in “Ultrathin magnetic films”, Springer Verlag, 1994
Neel Model & Disorder

• Disorder at the interface is seen to reduce the anisotropy
• Disorder – $P_j = \text{probability of a magnetic atom on a particular site.}$

$$2K_i = \sum_{j=1}^{n} P_j^2 W_{0}^f + 2(1 - P_j)P_j W_{0}^m + P_j P_{j+1} W_{1}^f +$$

$$P_{j} (1 - P_{j+1}) W_{1}^m + (1 - P_{j}) P_{j+1} W_{1}^m$$

• For pure materials $K=0$, so

$$W_{0}^f = -W_{1}^f; W_{0}^m = -W_{1}^m$$

hence

$$2K_i = K_p \sum_{j=1}^{n} (P_j - P_{j+1})^2$$
Application to FePd

- Hirotsu’s data for L10 FePd (private communication)
  - $K_p = 2.6 \times 10^7$ ergs/cc
  - $K_i = 1.0 \times 10^7$ ergs/cc
  - LRO = 0.65

- Neel theory for $K_i \approx 0.65^2 \times 2.6 \times 10^7$ ergs/cc $\approx 1.1 \times 10^7$ ergs/cc

- $K_i/K_p$ can also be derived from XRD diffraction intensities (MacLaren, Victora, Sellmyer, unpublished)

- Calculated $K_p$ for $a = 0.386$ nm, $c/a = 0.968$ $1.2 \times 10^7$ ergs/cc