## Magnetism and the lattice

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The crystal field is a real poteshal due to electrostatic freids from neighbouring ions. The eigenfunction cannot be $e^{i m \phi}$
because require real solutions.
) Recall: particle in a box
Solutions are real: $\cos k x$ and $\sin k x$
$\ldots$ but not $e^{i k x}$.
$\therefore$ make linear combinations: $e^{i k x_{ \pm}} e^{-i k k_{x}}$
Similary, crystal field states can be $e^{i m \phi} \neq e^{-i m \phi}$

|  | A parable: p -orbitals |  |
| :---: | :---: | :---: |
| $\cos \theta$ | $\sin \theta \cos \phi$ | $\sin \theta \sin \phi$ |
| real eigenfunction, for $V(r)$ which is real |  |  |

$\frac{\text { Spin-orbit interaction }}{\lambda \vec{S} \cdot \vec{L}_{r}}$
acts on spin on $\psi(\vec{r})$
If states are $\approx$ atomic states, and s.0.
acts as a perturbation, can focus on
$\lambda S^{z} L^{z}$
note $L_{z}=-i \hbar \frac{\partial}{\partial \phi}$ which has eigenfunction
$\hat{L_{z}} e^{i m \phi}=m \hbar e^{i m \phi} \quad e^{i m \phi}$

This is the origin of ORBITAL QUENCHING
$\because$ relevant states are of the form
$|m\rangle \pm|-m\rangle$, and hence $\langle\psi| \vec{h}|\psi\rangle=0$.
Notice this in Sd transition metal ions
(where $L=0, J=S$ and $g=2$ ), but
NOT in $4 f$ lanthanide ions. Why?

| ion | shell | S | L | J | term | $p_{1}$ | $p_{\exp }$ | $p_{2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{Ti}^{3+}, \mathrm{V}^{4+}$ | $3 \mathrm{~d}^{1}$ | $\frac{1}{2}$ | 2 | $\frac{3}{3}$ | ${ }^{2} D_{2 / 2}$ | 1.55 | 1.70 | 1.73 |


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| $\mathrm{~V}^{3+}$ | $3 \mathrm{~d}^{2}$ | 1 | 3 | 2 | ${ }^{3} F_{2}$ | 1.63 | 2.61 | 2.83 |
| $\mathrm{C}^{3+}$, | $\mathrm{V}^{2+}$ | $31^{3}$ | 3 | 3 |  | ${ }^{4} 5$ | 0.75 |  |

$\begin{array}{ccccccccc}\mathrm{Cr}^{\mathrm{s}+}, \mathrm{V}^{2+} & 3 \mathrm{~d}^{3} & \frac{3}{2} & 3 & \frac{3}{2} & { }^{4} F_{3 / 2} & 0.77 & 3.85 & 3.87 \\ \mathrm{Mn}^{3+}, \mathrm{Cr}^{2+} & 3 \mathrm{~d}^{4} & 2 & 2 & 0 & { }^{5} D_{0} & 0 & 4.82 & 4.90\end{array}$
$\begin{array}{ccccccccc}\mathrm{Fe}^{3+}, \mathrm{Mn}^{2+} & 3 \mathrm{~d}^{5} & \frac{5}{2} & 0 & \frac{5}{2} & { }^{6} 5_{5 / 2} & 5.92 & 5.82 & 5.92 \\ \mathrm{Fe}^{2+} & 3 \mathrm{~d}^{6} & 2 & 2 & 4 & { }^{5} D_{4} & 6.70 & 5.36 & 4.90\end{array}$
$\begin{array}{lllllllll}\mathrm{Ni}^{2+} & 3 \mathrm{~d}^{8} & \frac{5}{2} & 3 & \frac{9}{2} & { }^{4} F_{9 / 2} & 6.63 & 4.90 & 3.87 \\ & 1 & 3 & 4 & { }^{3} F_{4} & 5.59 & 3.12 & 2.83\end{array}$

## A parable: p-orbitals

$$
\left.\begin{array}{cl}
Y_{l m}(\theta, \phi) \quad l=1 & m=0 \\
& \cos \theta \\
m=1 & \sin \theta \mathrm{e}^{i \phi} \\
m=-1 & \sin \theta \mathrm{e}^{-i \phi} \\
\hat{L}_{z}=-i \hbar \frac{\partial}{\partial \phi} \text { imaginary, } & |m\rangle \text { eigenfunctions }
\end{array}\right] \begin{array}{ll}
\left|p_{z}\right\rangle=|0\rangle & \begin{array}{l}
\text { note that these contain } \\
\text { the eigenfunction }|m\rangle \text { and }
\end{array} \\
\left|p_{x}\right\rangle=\frac{|1\rangle+|-1\rangle}{\sqrt{2}} \quad|-m\rangle \text { in equal mixtures }
\end{array}
$$



Jahn-Teller distortion in a $3 \mathrm{~d}^{4}$ ion

distortion parameter $=q$
energy $=a q^{2}-b q$
(elastic) (elechonic)


$$
\begin{array}{cc}
\mathrm{LaMnO}_{3} & \mathrm{Mn}^{3+} 3 d^{4} \\
3 d \Rightarrow & \\
\text { note } \mathrm{Mn}^{4+}\left(3 d^{3}\right) \text { has No Jaha-Teller } \\
\text { distortion } \Rightarrow \text { CMR }
\end{array}
$$

Goodenough-Kanamori-Anderson (GKA) rules

1. Exchange interaction of two half-filled orbitals is strong and antiferromagnetic
2. If this overlap is at $90^{\circ}$, exchange interaction is weak and ferromagnetic
3. Exchange interaction of half-filled with empty (or doubly-occupied) orbital is weak and ferromagnetic





Hamiltonian is

$$
H=-D S_{z}^{2}+\text { other terms }
$$

so for $D>0$, ground state is $S_{z}= \pm 10$



## Outline

1. Orbitals and the crystal field
2. Magnetocrystalline anisotropy and domains
3. Magnetostriction and magnetoelasticity


$$
\left.\begin{array}{l}
\text { Magnetocrystalline anisotropy } \quad \vec{M}=\left(M_{1}, M_{2}, M_{3}\right) \\
\text { Anisotropy energy } E_{a} \quad \alpha_{1}=\cos \theta_{1}=\frac{M_{1}}{\sqrt{M_{1}^{2}+M_{2}^{2}+M_{3}^{2}}} \\
\text { Cubic crystal: } E_{a} \text { only depends on even power of of } \alpha_{i} \\
\text { direction of } \vec{M}
\end{array}\right\} \begin{aligned}
& \text { and must be invariant to cosines interhaige of } \alpha_{i} \\
& \Rightarrow \text { can't have } E_{a}=K \alpha_{1}^{2} \text {, must be } K\left(\alpha_{1}^{2}+\alpha_{2}^{2}+\alpha_{3}^{2}\right) \\
& \text { BUT } \alpha_{1}^{2}+\alpha_{2}^{2}+\alpha_{3}^{2}=1 .
\end{aligned}
$$



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