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Magnetism and Matter

MM-2: Electronic and magnetic properties

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1. Elliott-Yafet Parameter & spin-relaxation

Unquenching the orbital moment by spin-orbit interaction

The spin-orbit interaction is in the wave function!

1st order perturbation theory: $|o\rangle^{(1)} = |o\rangle + \sum_u \frac{\langle u|\xi \vec{L}\cdot\vec{S}|o\rangle}{(\epsilon_u - \epsilon_o)}|o\rangle$

Orbital moment: $^{(1)}\langle o|\vec{L}|o\rangle^{(1)} \propto -\sum_{u(u\neq o)} \frac{\langle o|\vec{L}|u\rangle\langle u|\xi \vec{L}\cdot\vec{S}|o\rangle}{(\epsilon_u - \epsilon_o)}|o\rangle$

MAE due to MCA: $E_{\mathrm{MCA}} \propto \langle H_{\mathrm{SO}}\rangle \quad \propto \quad \xi\,\langle o|\vec{L}|o\rangle^{(1)}\langle\vec{S}\rangle$

(2nd order perturbation)

$$\propto \quad -\sum_{u(u\neq o)} \frac{|\langle u|\xi \vec{L}\cdot\vec{S}|o\rangle|^2}{(\epsilon_u - \epsilon_o)}$$

$|o\rangle :=$ occupied, ground states

$|u\rangle :=$ unoccupied, excited states

For d-states $|o\rangle, |u\rangle \in (|xy;\uparrow\rangle, |xz;\uparrow\rangle, |yz;\uparrow\rangle, |x^2-y^2;\uparrow\rangle, |3z^2-r^2;\uparrow\rangle$
$|xy;\downarrow\rangle, |xz;\downarrow\rangle, |yz;\downarrow\rangle, |x^2-y^2;\downarrow\rangle, |3z^2-r^2;\downarrow\rangle)$

Concept of spin relaxation

Injection of spin population

Equilibration of spin population

Bloch equation:

$$\frac{d\langle \mathbf{s} \rangle}{dt} = -\gamma \, \mathbf{B} \times \langle \mathbf{s}(t) \rangle - \frac{1}{T_1} \langle \mathbf{s}(t) \rangle$$

For B=0:

$$\langle \mathbf{s}(t) \rangle = \langle \mathbf{s}(0) \rangle \exp(-t/T_1)$$

Spin degeneracy in nonmagnetic solid without spin orbit interaction

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degenerate states

$$\left\{ \begin{array}{l} \psi_{\mathbf{k}\uparrow}(\mathbf{r}) = a_{\mathbf{k}\nu}(\mathbf{r})|\uparrow\rangle\, e^{i\mathbf{k}\cdot\mathbf{r}} \\ \psi_{\mathbf{k}\downarrow}(\mathbf{r}) = a_{\mathbf{k}\nu}(\mathbf{r})|\downarrow\rangle\, e^{i\mathbf{k}\cdot\mathbf{r}} \end{array} \right.$$

Spin mixing by spin-orbit coupling (Elliott, 1954)

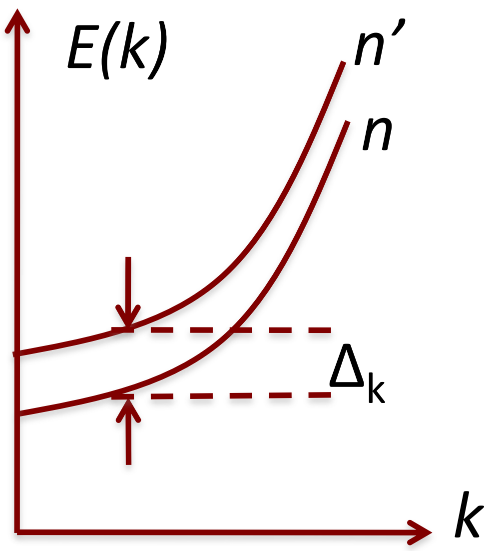
degenerate states

$$\begin{cases} \psi_{\mathbf{k}\uparrow}(\mathbf{r}) = \Big(a_{\mathbf{k}}(\mathbf{r})|\uparrow\rangle + b_{\mathbf{k}}(\mathbf{r})|\downarrow\rangle\Big)e^{i\mathbf{k}\cdot\mathbf{r}} \\ \psi_{\mathbf{k}\downarrow}(\mathbf{r}) = \Big(a^*_{-\mathbf{k}}(\mathbf{r})|\downarrow\rangle - b^*_{-\mathbf{k}}(\mathbf{r})|\uparrow\rangle\Big)e^{+i\mathbf{k}\cdot\mathbf{r}} \end{cases}$$

Usually:

$$|a|^2 \approx 1$$
$$|b|^2 \ll 1$$

$|b^2|$: Elliott-Yafet parameter



$$H_{\mathrm{SOC}} = \xi(r)\ \mathbf{L}\cdot\mathbf{S}$$

Perturbation theory:

$$b_{\mathbf{k}} = \frac{(\mathring{\Psi}^{\downarrow}_{n'\mathbf{k}}|H_{\mathrm{SOC}}|\mathring{\Psi}^{\uparrow}_{n\mathbf{k}})}{\Delta_{\mathbf{k}}}\ e^{-i\mathbf{kr}}\ \mathring{\Psi}^{\downarrow}_{n'\mathbf{k}}$$

Rule of thumb:

Δ small → $|b^2|$ large

Importance for spin relaxation (Elliott 1954; Yafet 1963)

degenerate states

$$\begin{cases} \psi_{\mathbf{k}\uparrow}(\mathbf{r}) = \Big(a_{\mathbf{k}}(\mathbf{r})|\uparrow\rangle + b_{\mathbf{k}}(\mathbf{r})|\downarrow\rangle\Big)e^{i\mathbf{k}\cdot\mathbf{r}} \\ \psi_{\mathbf{k}\downarrow}(\mathbf{r}) = \Big(a^*_{-\mathbf{k}}(\mathbf{r})|\downarrow\rangle - b^*_{-\mathbf{k}}(\mathbf{r})|\uparrow\rangle\Big)e^{+i\mathbf{k}\cdot\mathbf{r}} \end{cases}$$

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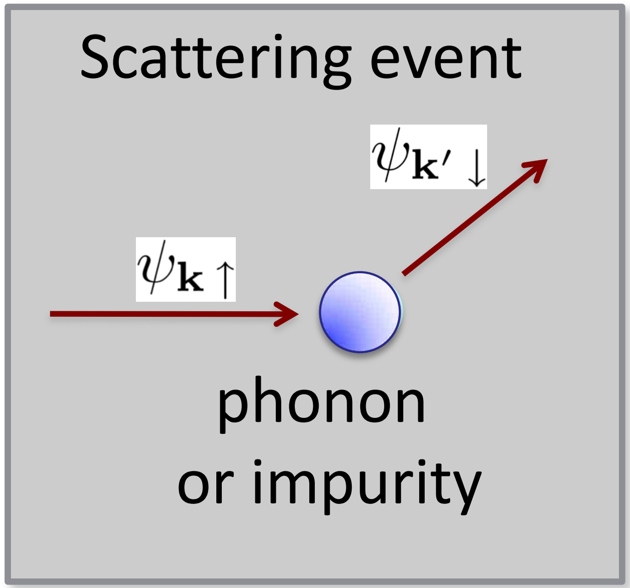


Spin-flip probability: momentum scattering × spin overlap

$$P^{\uparrow\downarrow}_{\mathbf{k}\mathbf{k}'} \sim |T_{\mathbf{k}\mathbf{k}'}|^2 \times |\langle a_{\mathbf{k}}|b_{\mathbf{k}'}\rangle|^2 \propto |b_{\mathbf{k}'}|^2$$

+ (impurity spin-orbit effects)

Spin-relaxation rate:

$$T_1^{-1} = \sum_{\mathbf{k}\mathbf{k}'}(P^{\uparrow\downarrow}_{\mathbf{k}\mathbf{k}'} + P^{\downarrow\uparrow}_{\mathbf{k}\mathbf{k}'})$$

Example:
Elliott-Yafet parameter in Cu, Au

degenerate states

$$\begin{cases} \psi_{\mathbf{k}\uparrow}(\mathbf{r}) = \Big(a_{\mathbf{k}}(\mathbf{r})|\uparrow\rangle + b_{\mathbf{k}}(\mathbf{r})|\downarrow\rangle\Big)e^{i\mathbf{k}\cdot\mathbf{r}} \\ \psi_{\mathbf{k}\downarrow}(\mathbf{r}) = \Big(a^*_{-\mathbf{k}}(\mathbf{r})|\downarrow\rangle - b^*_{-\mathbf{k}}(\mathbf{r})|\uparrow\rangle\Big)e^{+i\mathbf{k}\cdot\mathbf{r}} \end{cases}$$

Usually:

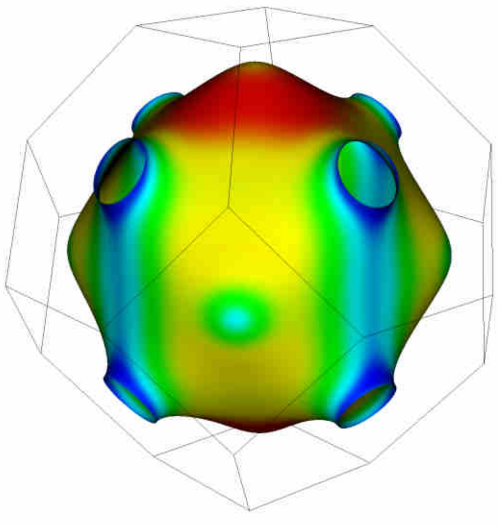
$|a|^2 \approx 1$

$|b|^2 \ll 1$

$|b^2|$: Elliott-Yafet parameter

fcc Cu

Fermi surface



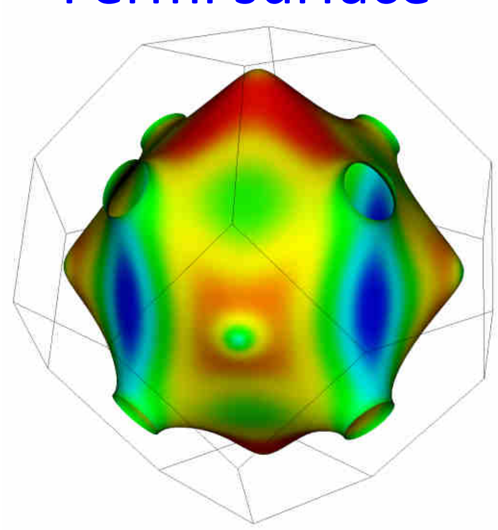
$\langle|b^2_{\mathbf{k}}(\langle s\rangle||[001])|\rangle_{\mathrm{FS}}$

fcc Cu	fcc Au
0.004	0.094
Average: 0.002	Average: 0.022
0.001	0.021

different scale

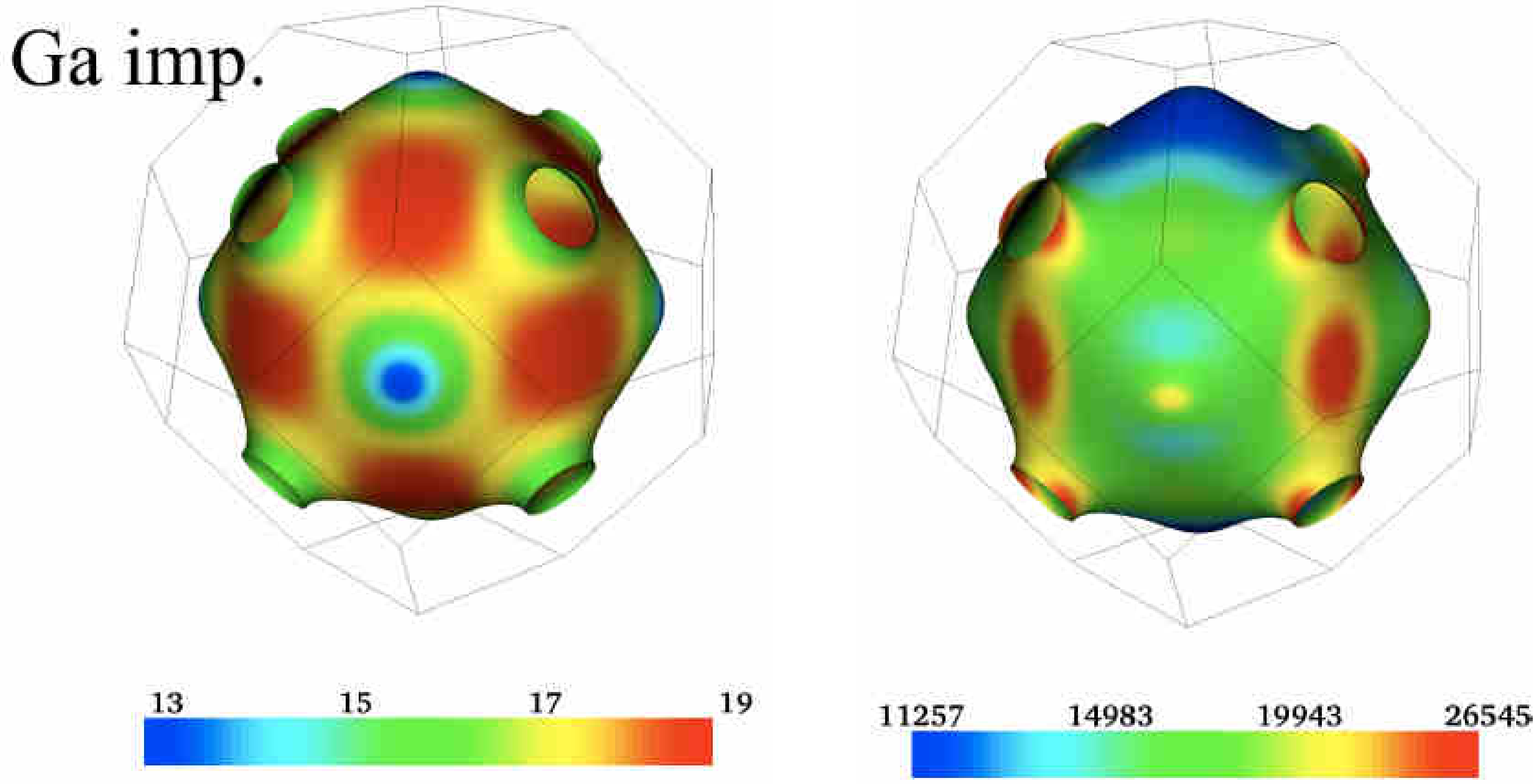
fcc Au

Fermi surface



Momentum and spin relaxation time

1% Ga impurities in Cu

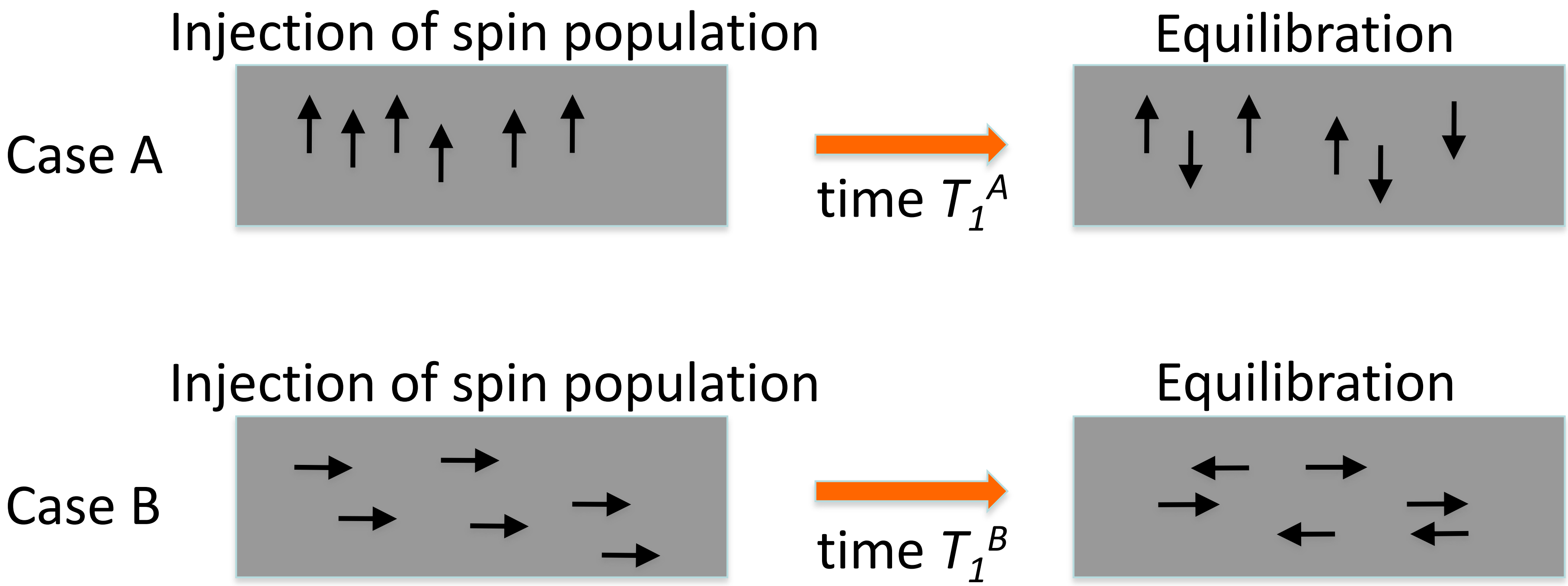


Momentum relaxation time (fs) Spin relaxation time (fs)

Relative difference: Factor 1000

Swantje Heers, PhD Thesis, FZJ 2011 (see also D. Fedorov et al, PRB 2008)

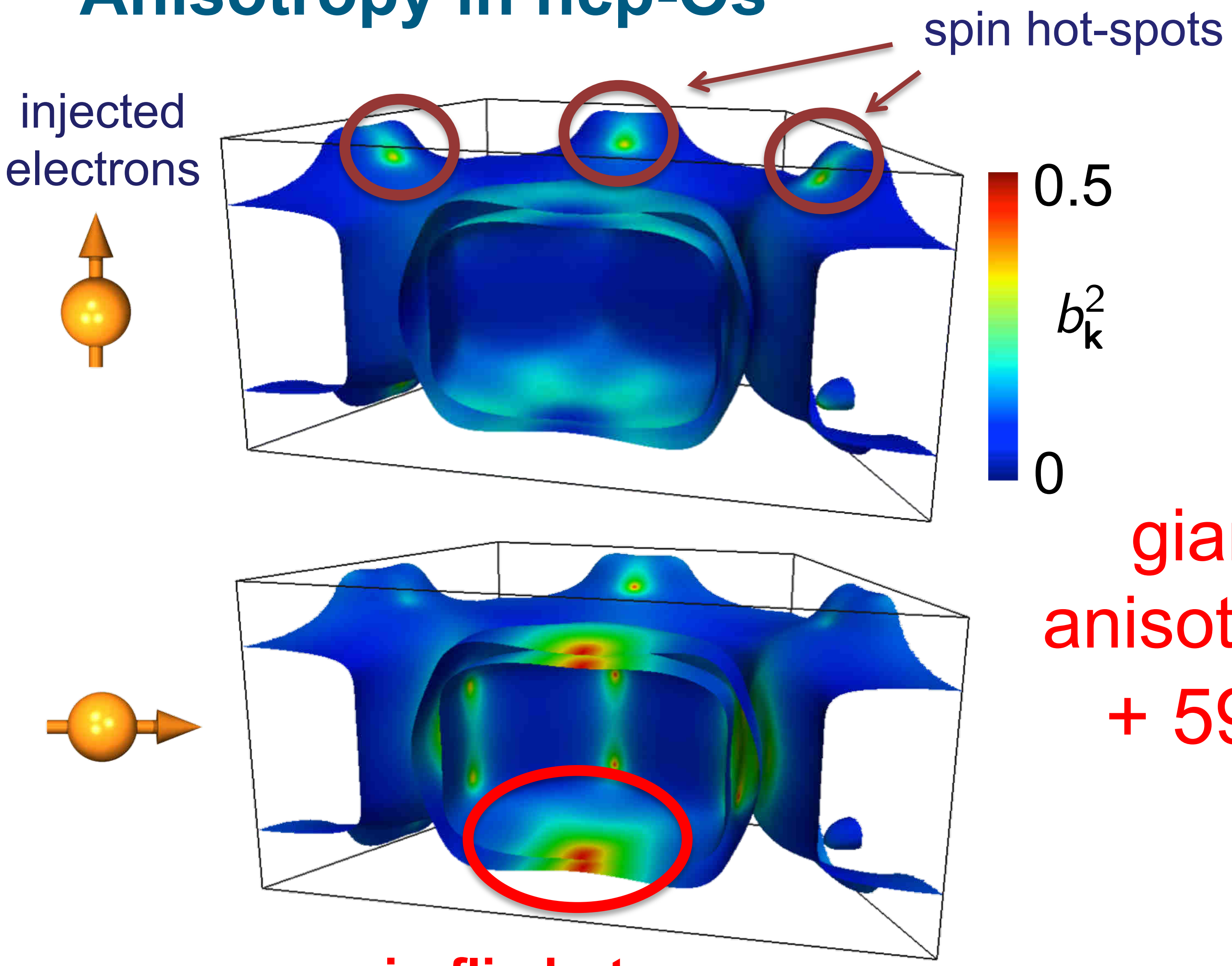
Gedanken-experiment



Should we expect that $T_1^A \neq T_1^B$?

Yes, if the material structure is anisotropic:
Anisotropy of Elliott-Yafet parameter b^2 !

Anisotropy in hcp-Os



$$\frac{1}{T_1} \sim \langle b_{\mathbf{k}}^2 \rangle_{\mathrm{FS}}$$

$$= 0.048 \approx \frac{1}{20}$$

giant anisotropy + 59%

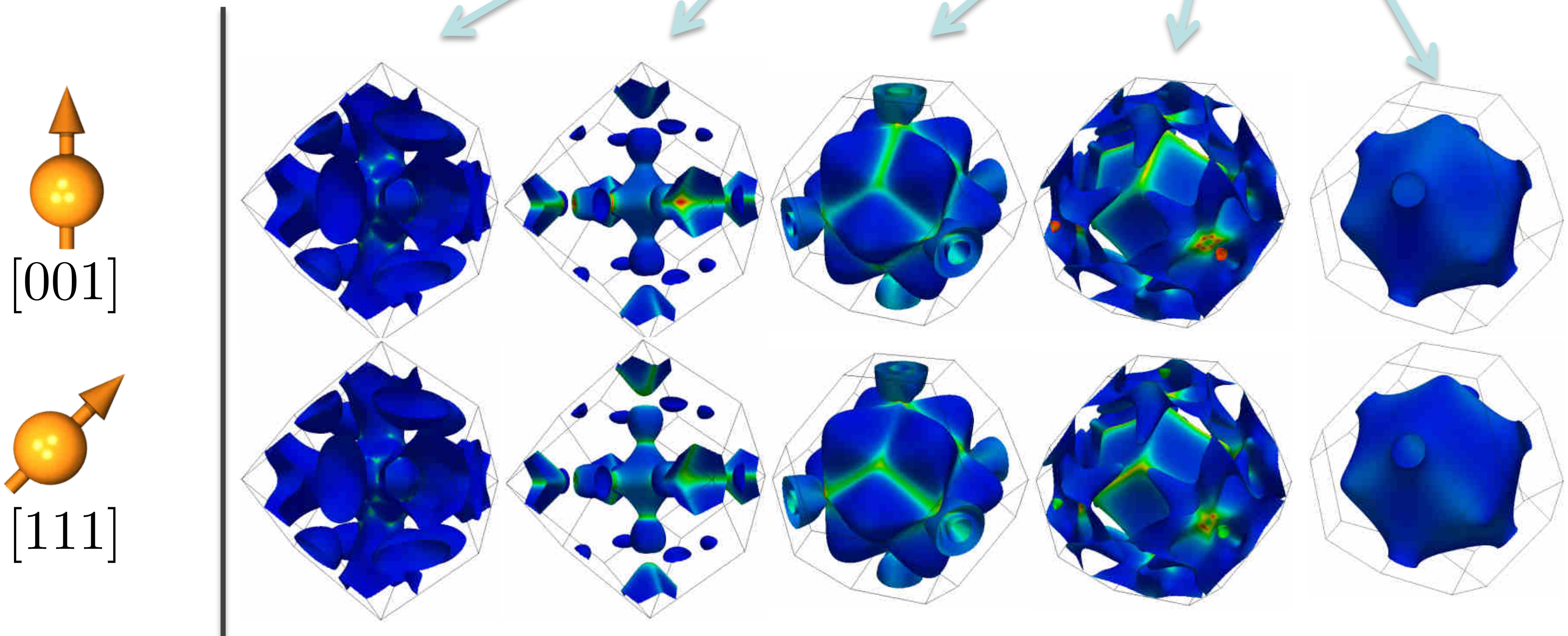
$$0.077 \approx \frac{1}{13}$$

Zimmermann *et al.*, **PRL** (2012)

Trends across the periodic table

cubic

57	…	71	72	73	74	75	76	77	78	79
La		Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au



Anisotropy	0.2%	**5.7%**	0.9%	0.4%	0.1%

Zimmermann *et al.*, **PRL** (2012)

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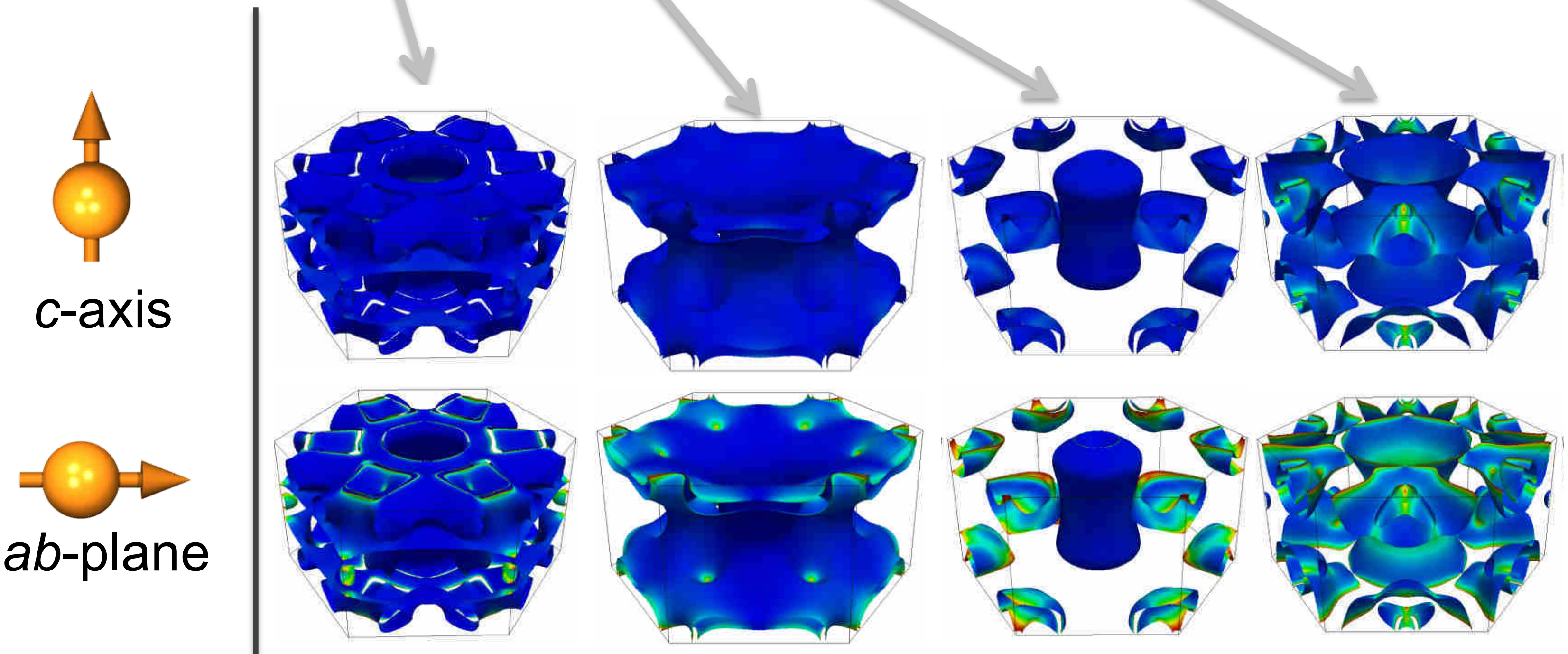
Trends across the periodic table

hexagonal

57	…	71	72	73	74	75	76	77	78	79
La		Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au



Anisotropy	150%	200%	**830%**	88%

Zimmermann *et al.*, **PRL** (2012)

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Spin-Orbit Coupling: Space Inversion Symmetry

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Elemental solids (Cu, Si, Al….)

For a given band ν the following two states have the same energy $\epsilon_{\mathbf{k}\nu}$

$$\Psi_{\mathbf{k}\nu\uparrow}(\mathbf{r}) = [a_{\mathbf{k}\nu}(\mathbf{r})|\uparrow\rangle + b_{\mathbf{k}\nu}(\mathbf{r})|\downarrow\rangle]e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\Psi_{\mathbf{k}\nu\downarrow}(\mathbf{r}) = [a^*_{-\mathbf{k}\nu}(\mathbf{r})|\downarrow\rangle - b^*_{-\mathbf{k}\nu}(\mathbf{r})|\uparrow\rangle]e^{i\mathbf{k}\cdot\mathbf{r}}$$

Proof:

$$\Psi_{\mathbf{k}\nu\uparrow}(\mathbf{r}) = [a_{\mathbf{k}\nu}(\mathbf{r})|\uparrow\rangle + b_{\mathbf{k}\nu}(\mathbf{r})|\downarrow\rangle]e^{i\mathbf{k}\cdot\mathbf{r}}$$

time reversal ↓ $-i\sigma_y\hat{C}$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$[a^*_{\mathbf{k}\nu}(\mathbf{r})|\downarrow\rangle - b^*_{\mathbf{k}\nu}(\mathbf{r})|\uparrow\rangle]e^{-i\mathbf{k}\cdot\mathbf{r}}$$

space inversion ↓ $\mathbf{k} \rightarrow -\mathbf{k}$

$$[a^*_{-\mathbf{k}\nu}(\mathbf{r})|\downarrow\rangle - b^*_{-\mathbf{k}\nu}(\mathbf{r})|\uparrow\rangle]e^{i\mathbf{k}\cdot\mathbf{r}}$$

q.e.d.

What happens when space inversion symmetry broken

(GaAs, InSb, interfaces, surfaces, ...)

Time reversal + space inversion symmetry

$$\epsilon_{\mathbf{k}\uparrow} = \epsilon_{\mathbf{k}\downarrow}$$

Time reversal only !

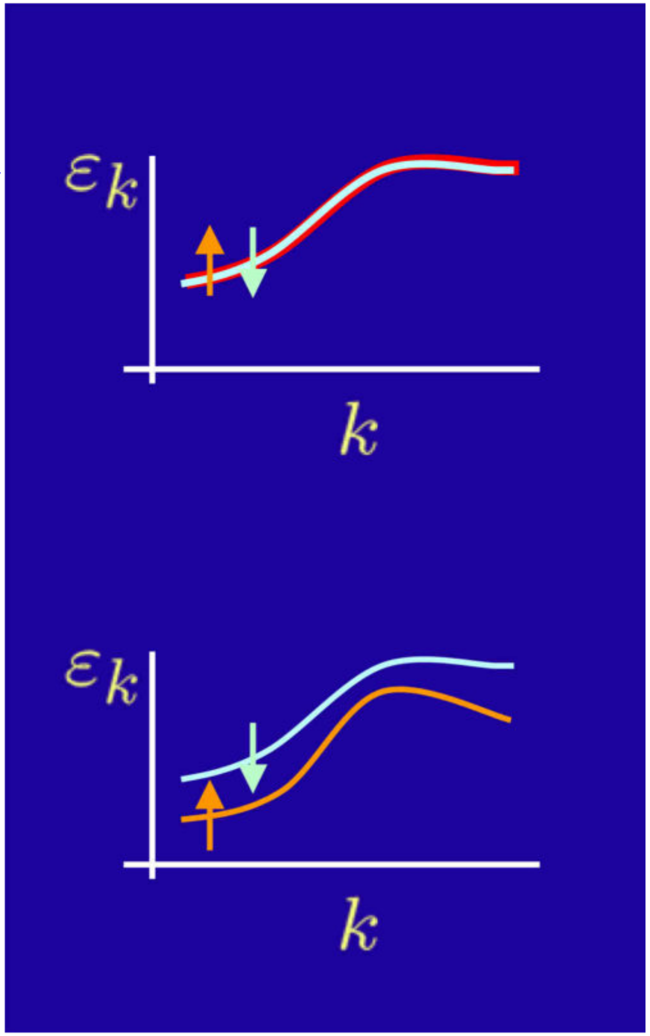
$$\epsilon_{\mathbf{k}\uparrow} = \epsilon_{-\mathbf{k}\downarrow} \quad , \quad \epsilon_{\mathbf{k}\uparrow} \neq \epsilon_{\mathbf{k}\downarrow}$$

Effective spin-orbit ("magnetic") field Ω:

$$H_1(\mathbf{k}) = \frac{\hbar}{2}\Omega(\mathbf{k}) \cdot \sigma$$

Time reversal symmetry:

$$\Omega(-\mathbf{k}) = -\Omega(\mathbf{k})$$



I. Z˘uti´c, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004).