

HOB-02: Energetics of spin-flop and spin-flip transitions in homogeneous antiferromagnets

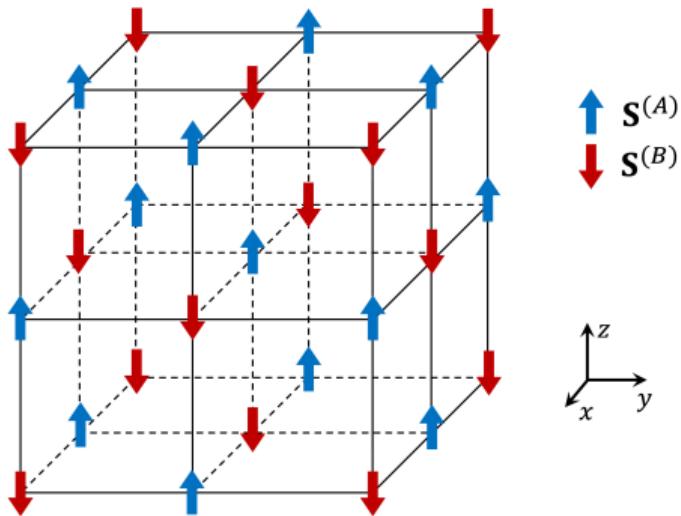
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7-Oct-2022

Two-lattice AFM



In macrospin model $S^{(A)}$ and $S^{(B)}$ are each homogeneous, and represented by micromagnetic variables

$$\mathbf{M}_A = \langle S^{(A)} \rangle, \quad \mathbf{m}_A = \mathbf{M}_A / |\mathbf{M}_A|$$

$$\mathbf{M}_B = \langle S^{(B)} \rangle, \quad \mathbf{m}_B = \mathbf{M}_B / |\mathbf{M}_B|$$

For AFMs, $|\mathbf{M}_A| = |\mathbf{M}_B|$.

Macrospin model

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$$E = -h_0(\mathbf{m}_A \cdot \hat{\mathbf{z}} + \mathbf{m}_B \cdot \hat{\mathbf{z}}) - \frac{1}{2}h_k \left[(\mathbf{m}_A \cdot \hat{\mathbf{z}})^2 + (\mathbf{m}_B \cdot \hat{\mathbf{z}})^2 \right] + h_e(\mathbf{m}_A \cdot \mathbf{m}_B)$$

where

$$m_i = \mathbf{M}_i/M_s$$

h_0 = applied field $h_0\hat{\mathbf{z}}$ (WLOG $h_0 \geq 0$)

h_k = anisotropy coefficient,

$h_k > 0 \implies$ easy z -axis,

$h_k < 0 \implies$ easy xy -plane

h_e = AFM exchange coefficient, > 0 .

Reduced form (divide by h_e):

$$\bar{E} = -\bar{h}_0(\mathbf{m}_A \cdot \hat{\mathbf{z}} + \mathbf{m}_B \cdot \hat{\mathbf{z}}) - \frac{1}{2}\bar{h}_k \left[(\mathbf{m}_A \cdot \hat{\mathbf{z}})^2 + (\mathbf{m}_B \cdot \hat{\mathbf{z}})^2 \right] + (\mathbf{m}_A \cdot \mathbf{m}_B)$$

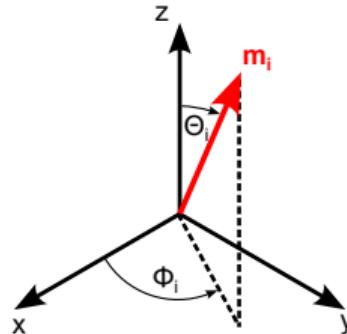
Macrospin model
Critical points
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Critical energy configurations

Introduce spherical coordinates

$$m_i = (\sin \Theta_i \cos \Phi_i, \sin \Theta_i \sin \Phi_i, \cos \Theta_i),$$

$i = A$ or B , and find critical points by setting



$$\frac{\partial E}{\partial \Theta_A} = 0, \quad \frac{\partial E}{\partial \Phi_A} = 0, \quad \frac{\partial E}{\partial \Theta_B} = 0, \quad \frac{\partial E}{\partial \Phi_B} = 0.$$

Note: Φ_i appears only in the exchange term, and

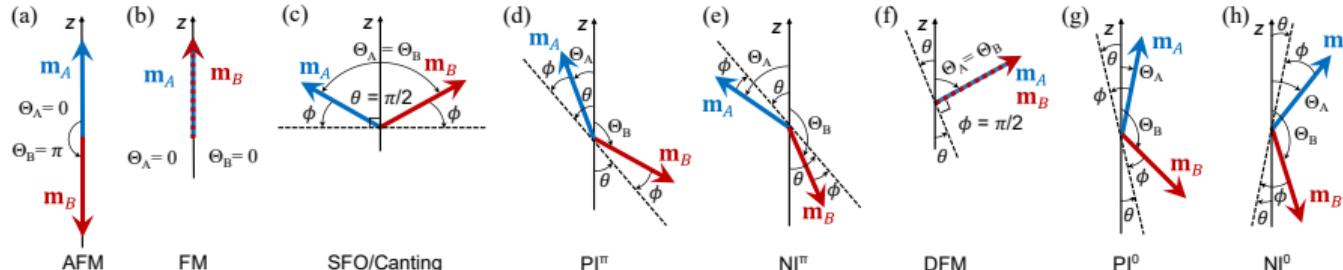
$$\frac{\partial E}{\partial \Phi_i} = 0 \implies |\Phi_A - \Phi_B| = 0 \text{ or } \pi$$

$\implies m_A$ and m_B lie in some plane \perp to xy -plane
(WLOG say xz -plane)

Critical energy catalog

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Spin-Flop/Spin-Flip

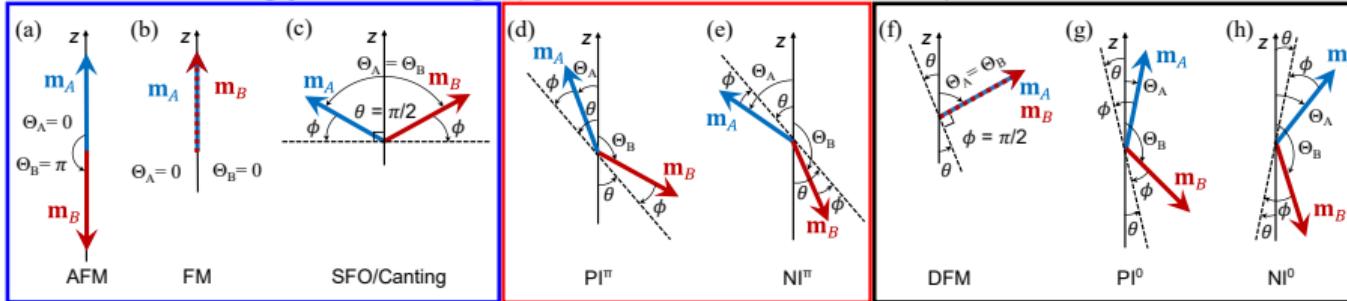
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- (a) AFM: $\Theta_A = 0, \Theta_B = \pi$
- (b) spin-up FM: $\Theta_A = \Theta_B = 0$
- (c) SFO ($h_k > 0$) or canting ($h_k < 0$): $|\Phi_B - \Phi_A| = \pi, \Theta_A = \Theta_B$
- (d) PI $^\pi$: $|\Phi_B - \Phi_A| = \pi, \Theta_A + \Theta_B \leq \pi$
- (e) NI $^\pi$: $|\Phi_B - \Phi_A| = \pi, \Theta_A + \Theta_B > \pi$
- (f) DFM: $\Phi_B - \Phi_A = 0, \Theta_A = \Theta_B$
- (g) PI 0 : $\Phi_B - \Phi_A = 0, \Theta_A + \Theta_B \leq \pi$
- (h) NI 0 : $\Phi_B - \Phi_A = 0, \Theta_A + \Theta_B > \pi$.

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Critical energy catalog (2nd derivative test)



Local Minima

Transition Saddles

Local Maxima and
Non-Transition Saddles

- (a) AFM: $\Theta_A = 0, \Theta_B = \pi$
- (b) spin-up FM: $\Theta_A = \Theta_B = 0$
- (c) SFO ($h_k > 0$) or canting ($h_k < 0$): $|\Phi_B - \Phi_A| = \pi, \Theta_A = \Theta_B$
- (d) PI $^\pi$: $|\Phi_B - \Phi_A| = \pi, \Theta_A + \Theta_B \leq \pi$
- (e) NI $^\pi$: $|\Phi_B - \Phi_A| = \pi, \Theta_A + \Theta_B > \pi$
- (f) DFM: $\Phi_B - \Phi_A = 0, \Theta_A = \Theta_B$
- (g) PI 0 : $\Phi_B - \Phi_A = 0, \Theta_A + \Theta_B \leq \pi$
- (h) NI 0 : $\Phi_B - \Phi_A = 0, \Theta_A + \Theta_B > \pi$.

Stability regime for energy critical points

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Parameter regime		Phase name	Stable field interval
$h_k > 0$	$h_k < 2h_e$	AFM	$0 \leq h_0 \leq h_{cr3}$
		SFO	$h_{cr2} \leq h_0 \leq h_{cr1}$
		FM, spin-up	$h_0 \geq h_{cr1}$
	$h_k \geq 2h_e$	AFM	$0 \leq h_0 \leq h_{cr3}$
		FM, spin-up	$h_0 \geq h_{cr1}$
		FM, spin-down	$h_0 \leq -h_{cr1}$
$h_k < 0$		IPAFM	$h_0 = 0$
		Canting	$0 < h_0 \leq h_{cr1}$
		FM, spin-up	$h_0 \geq h_{cr1}$

Where

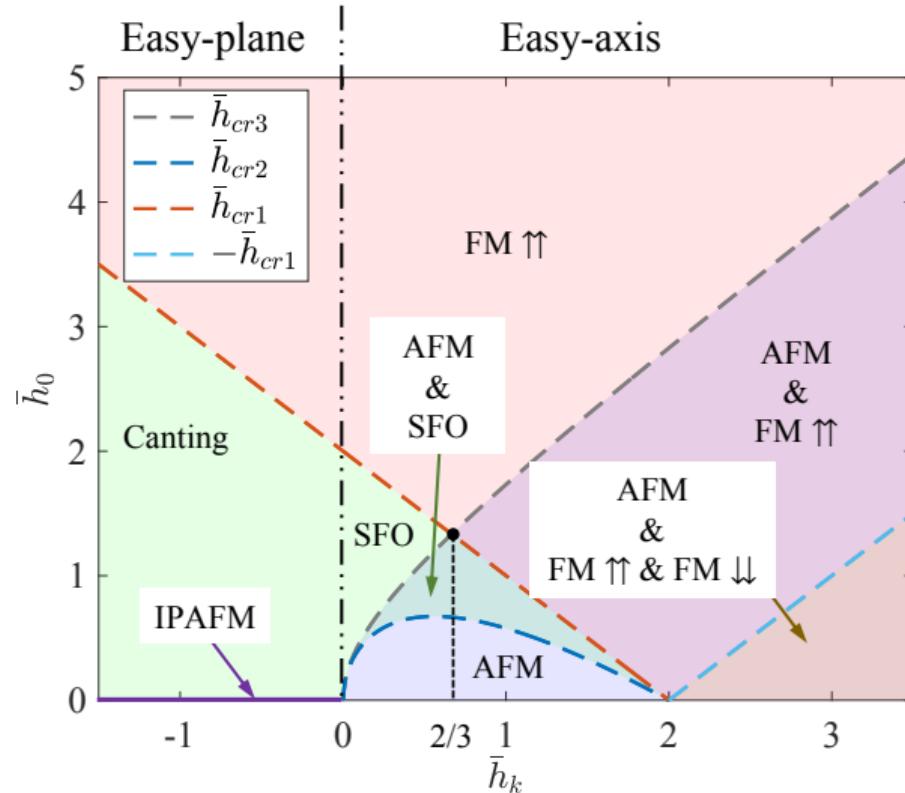
$$h_{cr1} \equiv 2h_e - h_k, \quad h_{cr2} \equiv (2h_e - h_k) \sqrt{\frac{h_k}{2h_e + h_k}}$$

$$h_{cr3} \equiv \sqrt{h_k(2h_e + h_k)}$$

Phase diagram: Local minima

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Mapping model parameters to critical states

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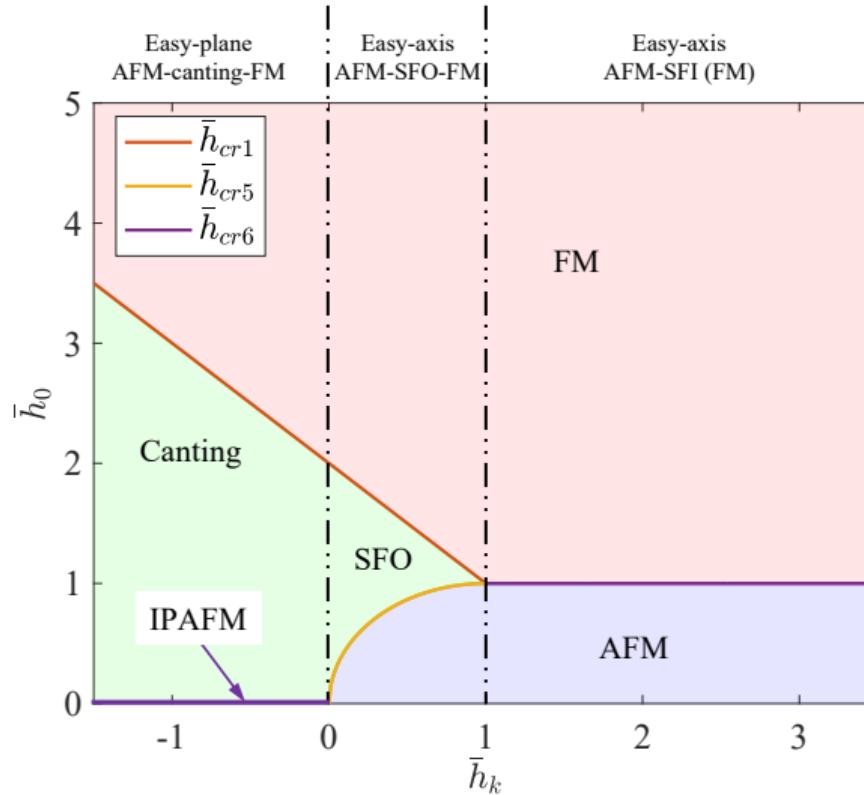
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Phase name	Phase configuration
SFO ($h_k > 0$) or canting ($h_k < 0$)	$\theta = \pi/2, \phi = \arcsin\left(\frac{h_0}{2h_e - h_k}\right)$
PI $^\pi$, $\phi \geq 0$	$\theta = \arctan\left(\sqrt{\left[2h_e h_k + h_k^2 \mp h_0 \sqrt{h_k(2h_e + h_k)}\right] / \left[-2h_e h_k + h_k^2 \pm h_0 \sqrt{h_k(2h_e + h_k)}\right]}\right),$ $\phi = \arctan\left(\sqrt{\left[2h_e h_k + h_k^2 \mp h_0 \sqrt{h_k(2h_e + h_k)}\right] / \left[2h_e h_k + h_k^2 \pm h_0 \sqrt{h_k(2h_e + h_k)}\right]}\right),$ <p style="text-align: center;">upper (lower) sign for $h_k > 0$ ($h_k < 0$)</p>
NI $^\pi$, $\phi < 0$	$\theta = \arctan\left(\sqrt{\left[2h_e h_k + h_k^2 \pm h_0 \sqrt{h_k(2h_e + h_k)}\right] / \left[-2h_e h_k + h_k^2 \mp h_0 \sqrt{h_k(2h_e + h_k)}\right]}\right),$ $\phi = \arctan\left(-\sqrt{\left[2h_e h_k + h_k^2 \pm h_0 \sqrt{h_k(2h_e + h_k)}\right] / \left[2h_e h_k + h_k^2 \mp h_0 \sqrt{h_k(2h_e + h_k)}\right]}\right),$ <p style="text-align: center;">upper (lower) sign for $h_k > 0$ ($h_k < 0$)</p>

Phase diagram: Global minima

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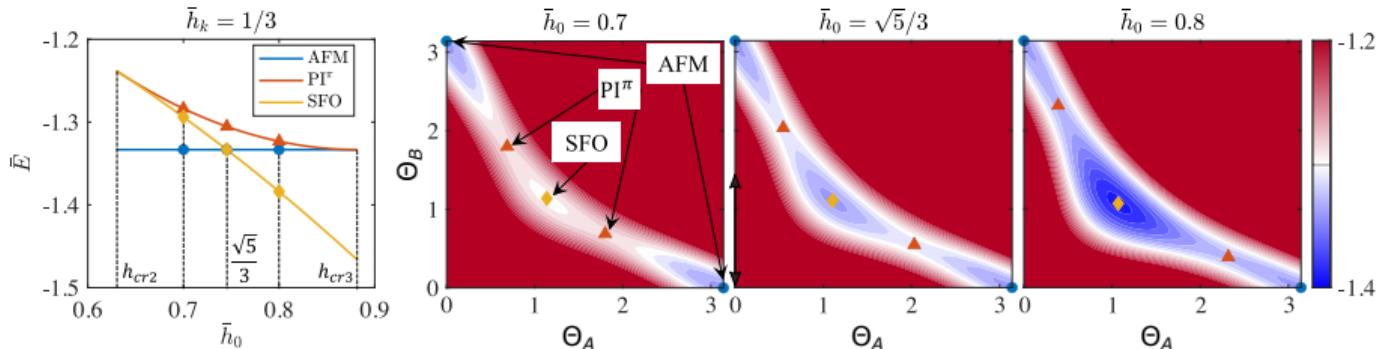


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Phase transitions, $\bar{h}_k = 1/3$

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- Critical energy configurations for two-lattice macrospin AFM system fully cataloged.
- Critical points identified as local or global minima, maxima, or saddle points including pertinent parameter ranges.
- Formulae for mapping material parameters and applied field to m_A and m_B are obtained.
- Phase diagrams showing local minimum and global minima have been created.
- Contour plots illustrating phase transitions as a function of applied field provided for several \bar{h}_k values.

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