Entropic effects and solitons in thermally activated magnetic transitions

Louise Desplat

Photo credit: https://h2obyjoanna.wordpress.com/

Ackowledments

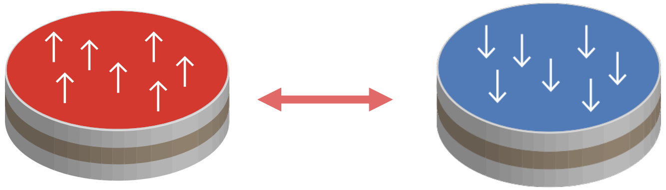
Prof. Robert L. Stamps

Dr. Joo-Von Kim

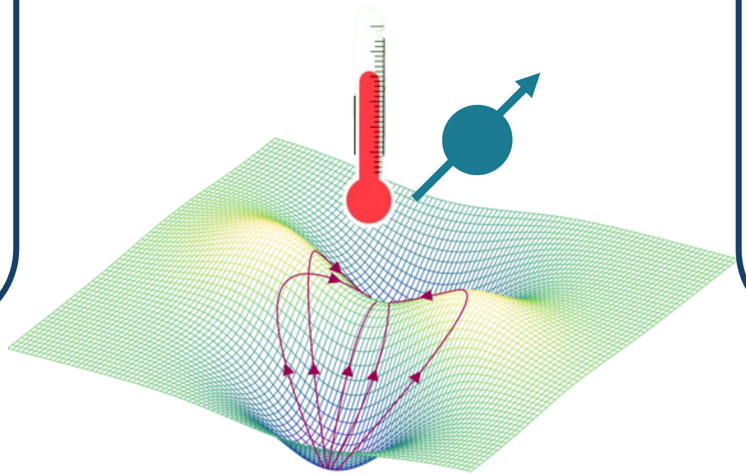
Prof. Dieter Suess
Dr. Christoph Vogler

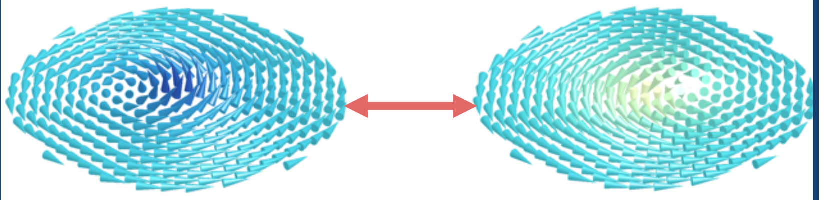
Computing thermal activation rates in magnetism

An overview

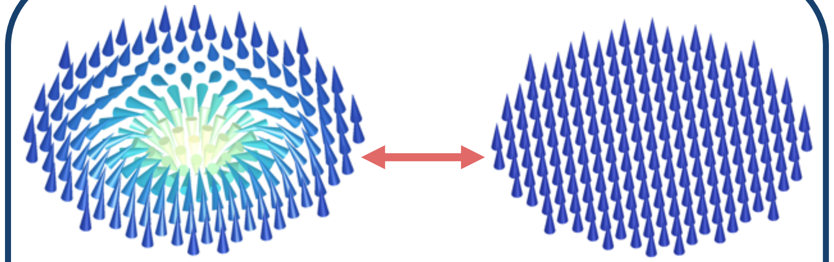


Magnetization reversal in a tunnel junction

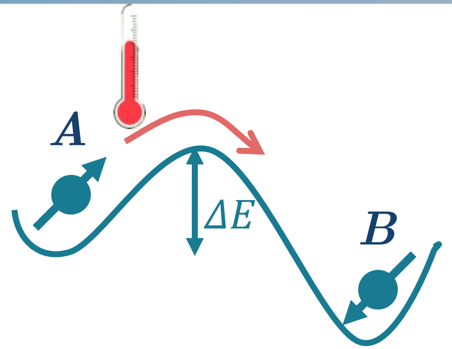




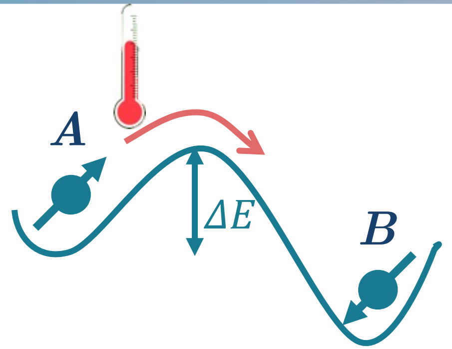
Vortex core reversal



Nucleation/annihilation of a skyrmion



Arrhenius law: $k_{AB} = f_0 \, e^{-\beta \Delta E}$



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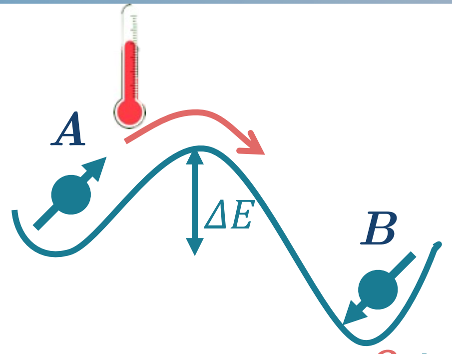
Usual practise in magnetism

$f_0 \sim$ GHz – THz, ΔE determines stability



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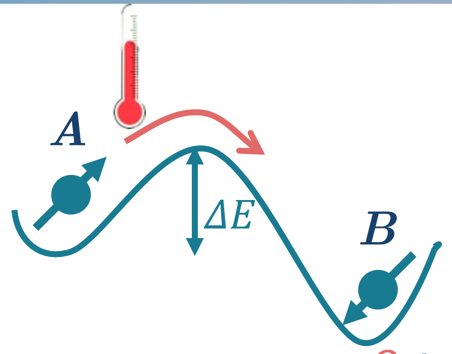
Usual practise in magnetism

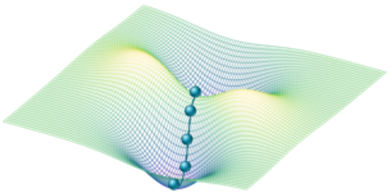
$f_0 \sim$ GHz – THz, ΔE determines stability

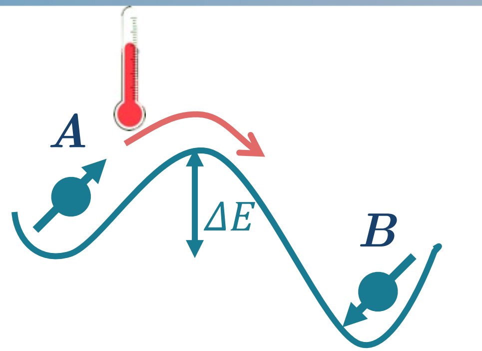
→ **Incomplete**



Arrhenius law: $k_{AB} = f_0 \, e^{-\beta \Delta E}$

① **Kramers method**





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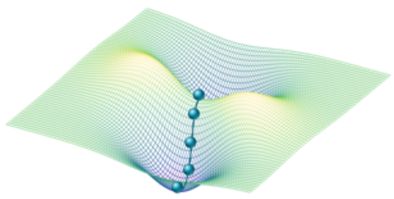
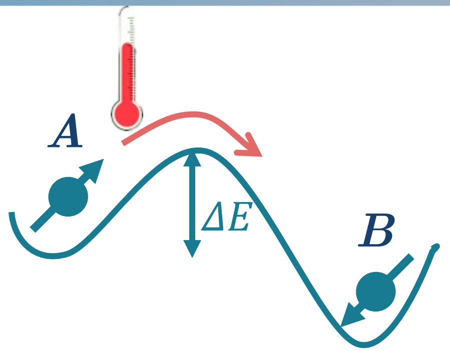


OR



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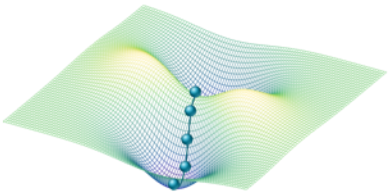
① **Kramers method**

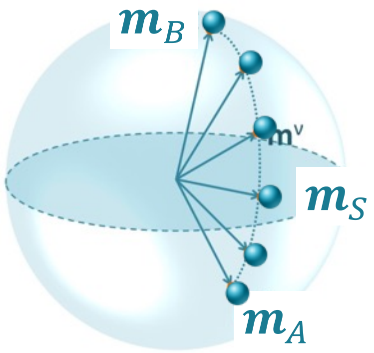


OR

② **Sampling the dynamics**

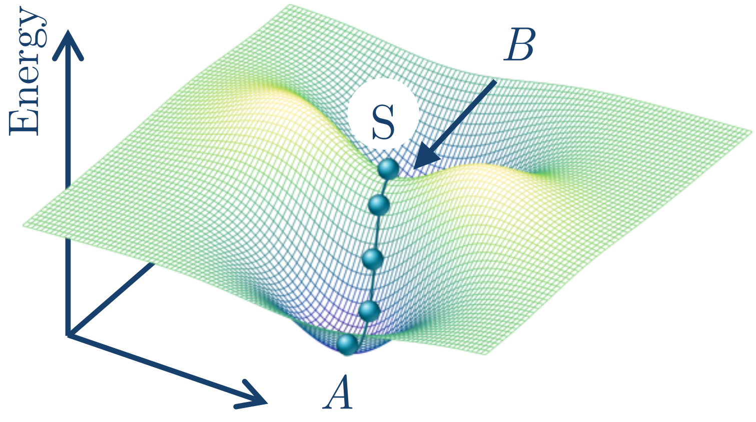
❖ Search for transition pathways: GNEB

Bessarab *et al.*, *Comp. Phys. Comm.* ***196*** (2015)

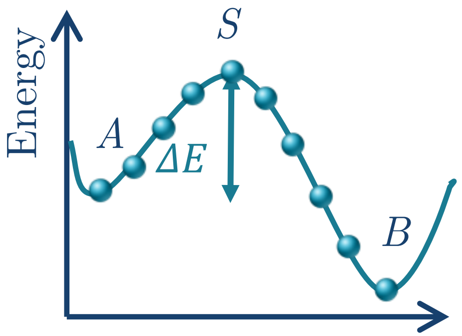


$\boldsymbol{m} \in S^2$

geodesic



nudged elastic band



Reaction coordinate

❖ Evalute the prefactor: Langer's theory

- ✓ No barrier recrossings
- ✓ Quasi equilibrium
- ✓ Intermediate to high damping

Dynamical contribution: rate of growth of unstable mode at S

$$k_{AB} = \frac{\lambda_+}{2\pi} \Omega_0 \, e^{-\beta \Delta E}$$

Entropic contribution $\Omega_0 = \sqrt{\frac{\det H^A}{\det' H^S}} \propto e^{\frac{\Delta S}{k_B}}$

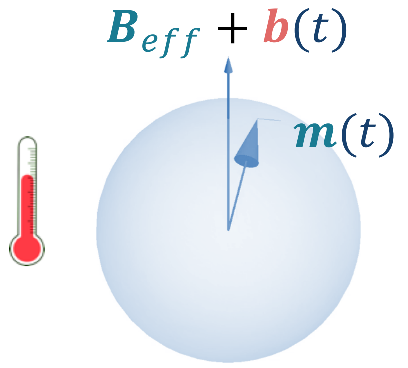
where $H_{ij} = \frac{\partial^2 E}{\partial \boldsymbol{m}_i \partial \boldsymbol{m}_j}$ is the Hessian matrix

$$H\chi = \lambda\chi$$

Langer, *Ann. of Phys.* **54** (1969)

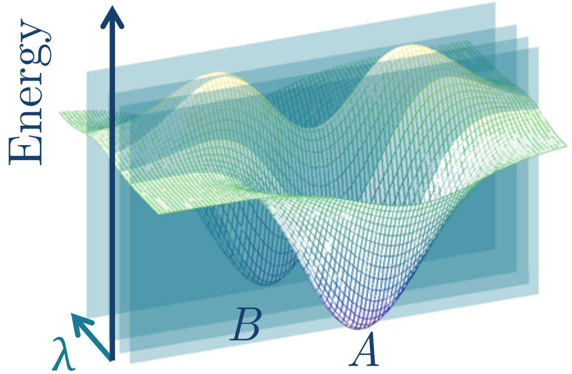
❖ **Langevin dynamics:** stochastic Laudau-Lifshitz-Gilbert equation

$$\frac{d\boldsymbol{m}}{dt} = \gamma \boldsymbol{m} \times (\boldsymbol{B}_{eff} + \boldsymbol{b}(t)) - \gamma \frac{\alpha}{\mu_S} \boldsymbol{m} \times (\boldsymbol{m} \times (\boldsymbol{B}_{eff} + \boldsymbol{b}(t)))$$

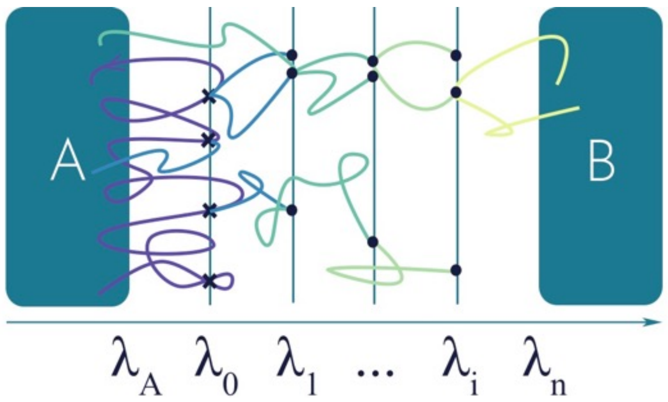


- **However: brute-force sampling: $k^{-1} \leq$ ns**

❖ **Sampling rare events: Forward flux sampling (FFS)**



- Transition path ensemble between stationary states A and B
- In or out of equilibrium
- Define interfaces between A and B
- Langevin trial runs → compute partial flux of trajectories p_i



$$k_{AB} = \Phi_{A0} \prod_{i=0}^{n-1} p_i$$

Rate of crossing of interface Λ_0 coming from region A

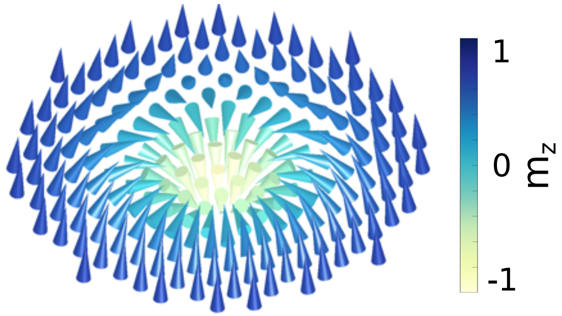
Probability that a trajectory that has crossed interface λ_i will cross λ_{i+1} before returning to A

Allen *et al. Phys. Rev. Lett.* *94* (2005)

Thermal stability of magnetic skyrmions

Entropic narrowing

- **Topologically nontrivial solitonic textures**

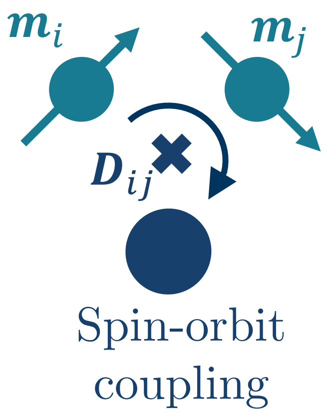


$$\pi_2(S^2) = \mathbb{Z}$$

Topological charge $N = \frac{1}{4\pi}\int d\boldsymbol{r}^2 \ \boldsymbol{m}\cdot(\partial_x \boldsymbol{m}\times\partial_y \boldsymbol{m})$

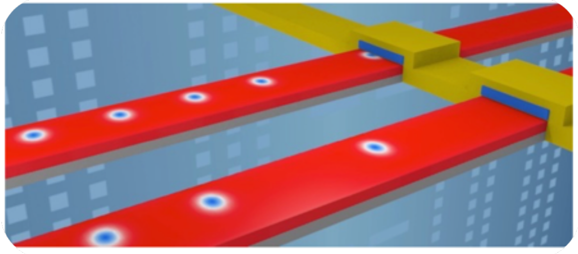
- Stabilized by the chiral **Dzyaloshinskii-Moriya interaction (DMI)**

$$\mathcal{H}_{DMI} = -\boldsymbol{D}_{ij}\cdot(\boldsymbol{m}_i\times\boldsymbol{m}_j)$$



Levy & Fert, *Phys. Rev. Lett.* **44** (1980)
Bogdanov & Yablonskii, *Zh. Eksp. Teor. Fiz* **95** (1989)

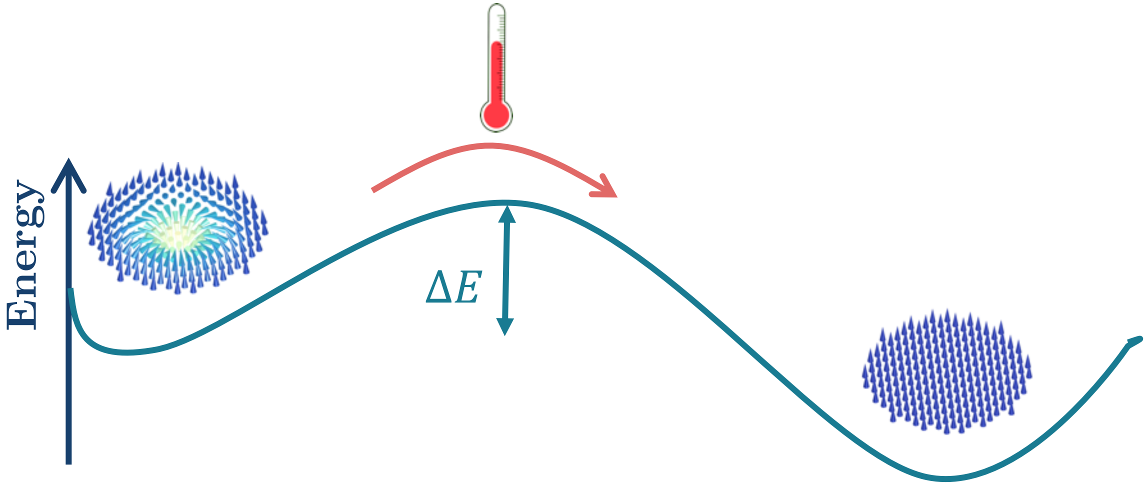
- Envisioned as information carriers in future spintronics devices



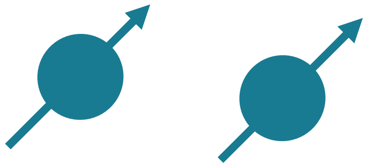
Skyrmion racetrack

Sampaio *et al. Nat. Nanotechnol.* **8** (2013)
Prychynenko *et al. Phys. Rev. Appl.* **9** (2018)
Pinna *et al. Phys. Rev. Appl.* **9** (2018)

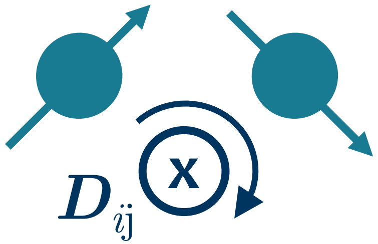
- **Continuum limit**: topological protection
- **Discrete lattice:** *skyrmions are metastable*



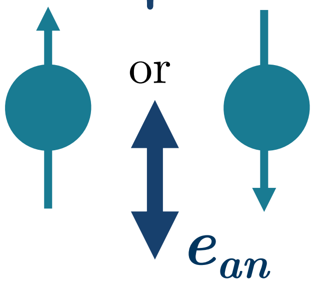
$$\mathcal{H} = -\sum_{ij} J_{ij}(\boldsymbol{m}_i \cdot \boldsymbol{m}_j) - \sum_{ij} \boldsymbol{D}_{ij} \cdot (\boldsymbol{m}_i \times \boldsymbol{m}_j) - K \sum_i m_{zi}^2 - \mu_s B_z \sum_i m_{zi}$$



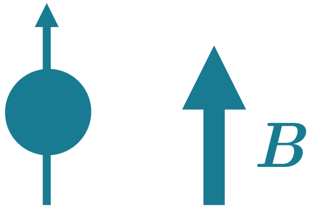
Heisenberg exchange



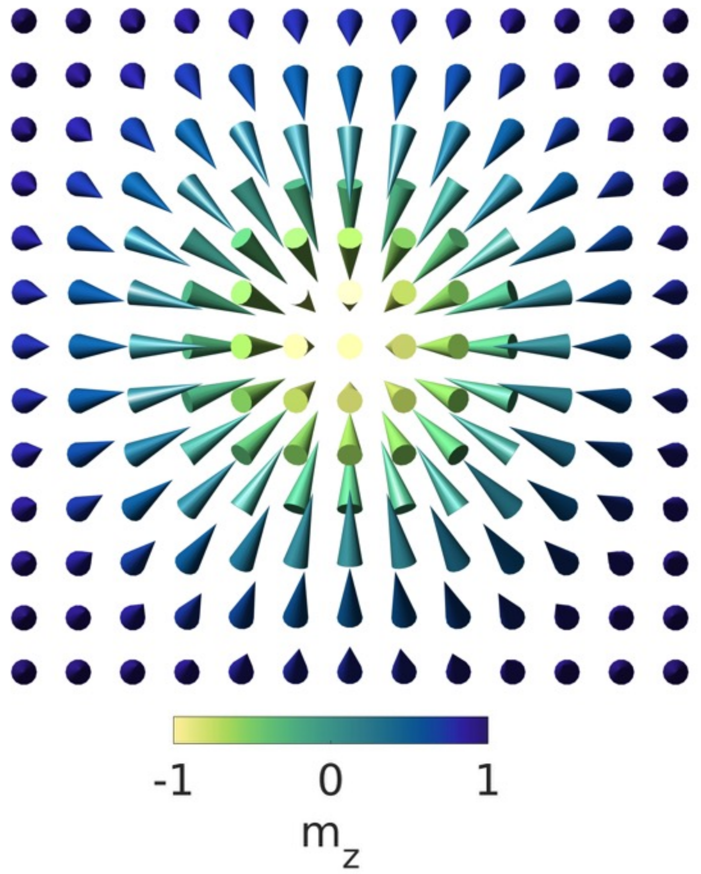
Dzyaloshinskii-Moryia Interaction (DMI)



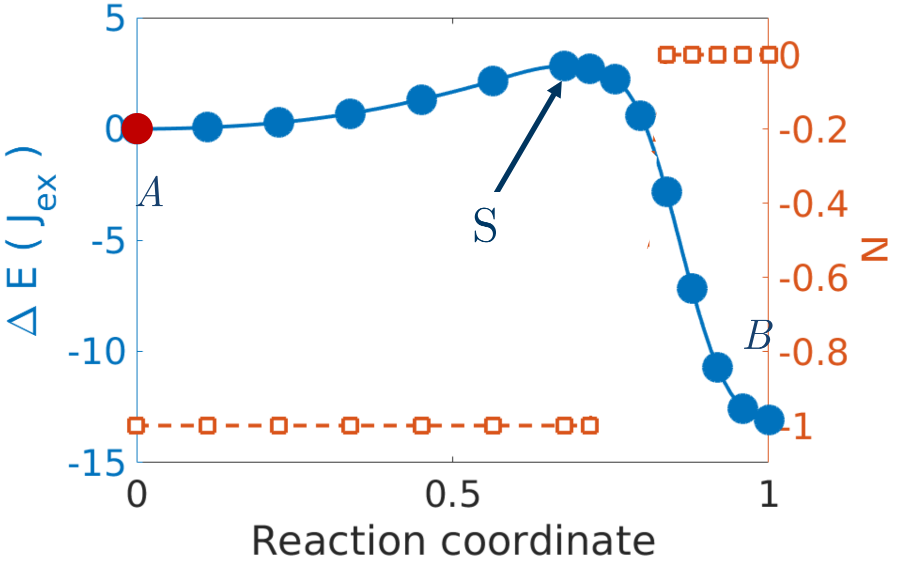
Magnetic anisotropy



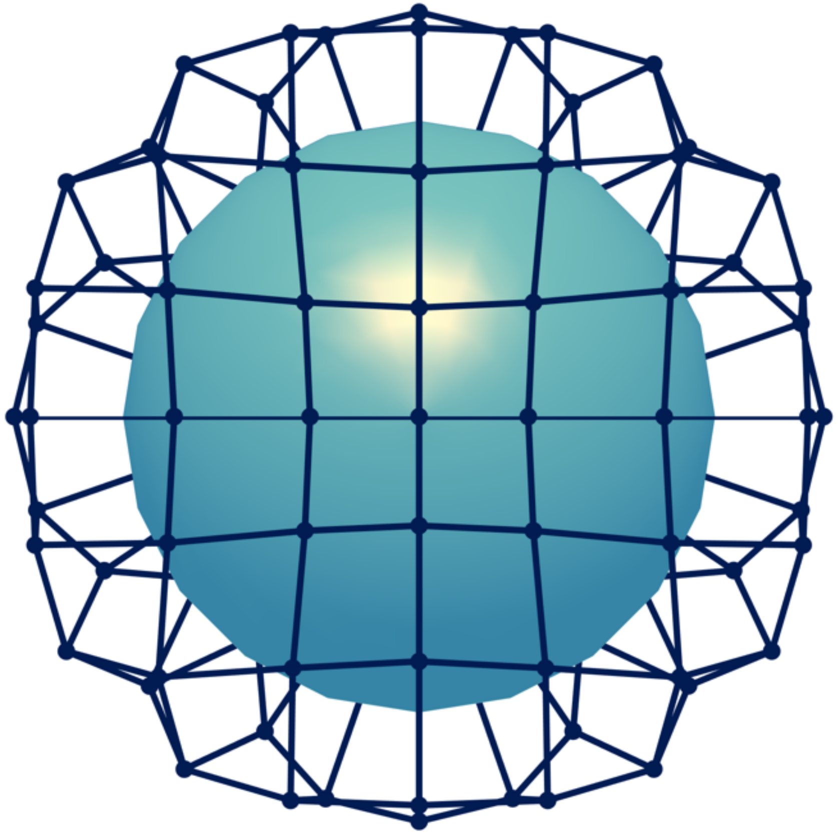
Zeeman



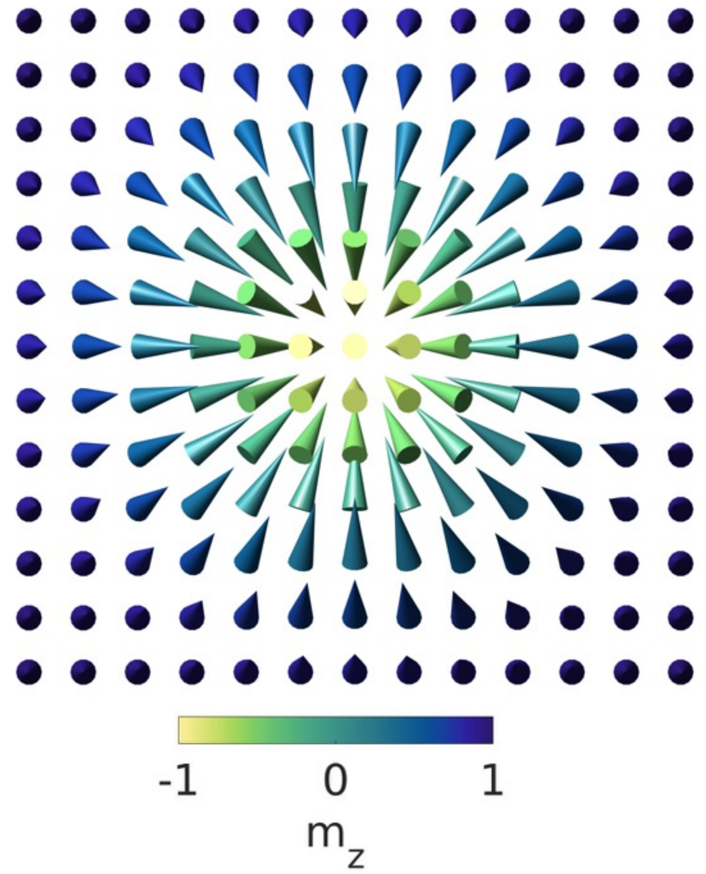
Energy profile



Projection on the unit sphere



Desplat *et al.* *PRB* **98**, 134407 (2018)



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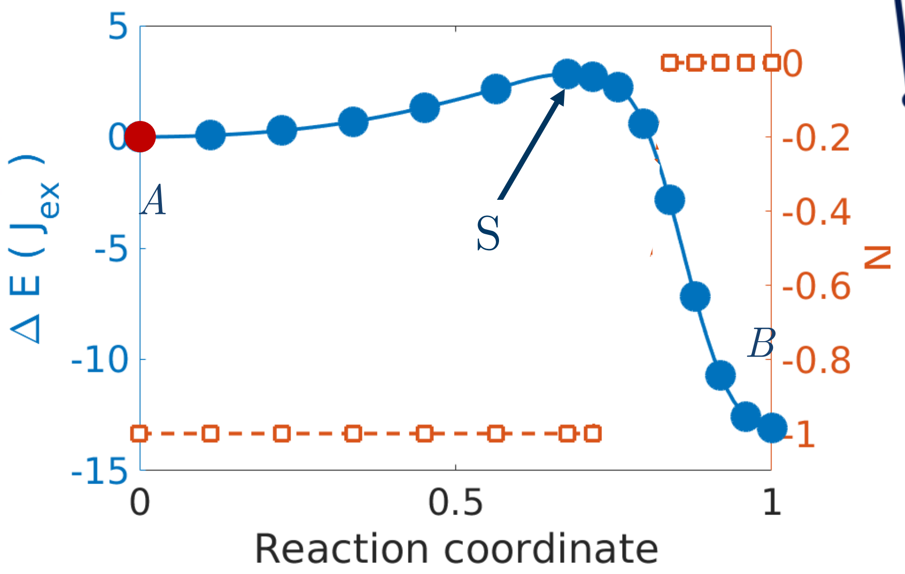

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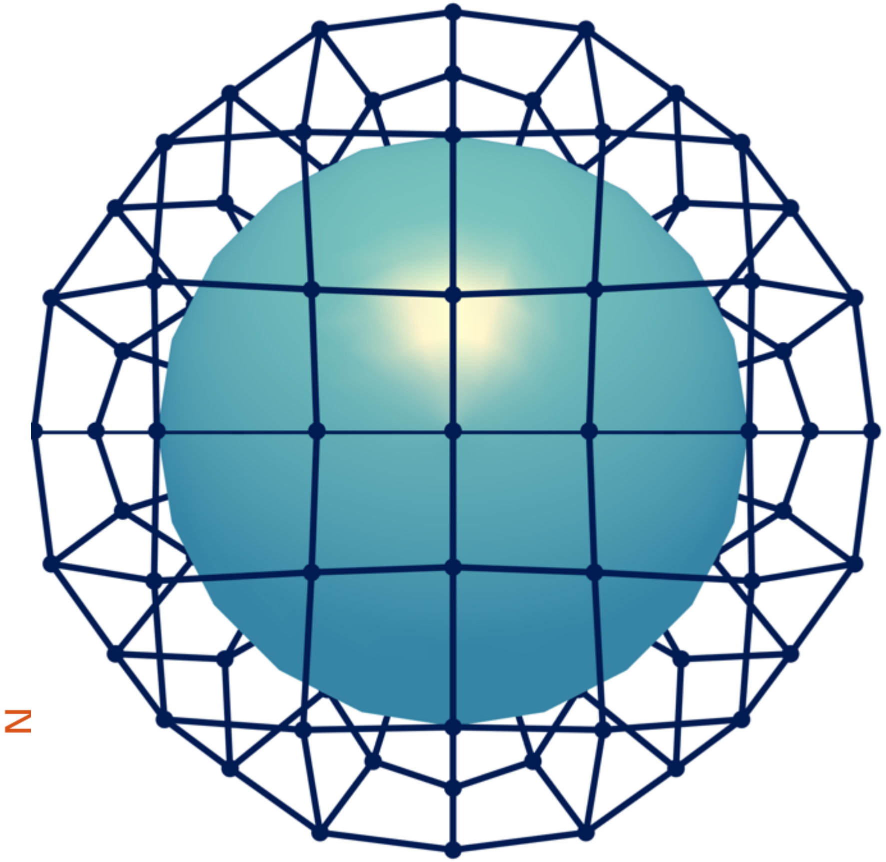

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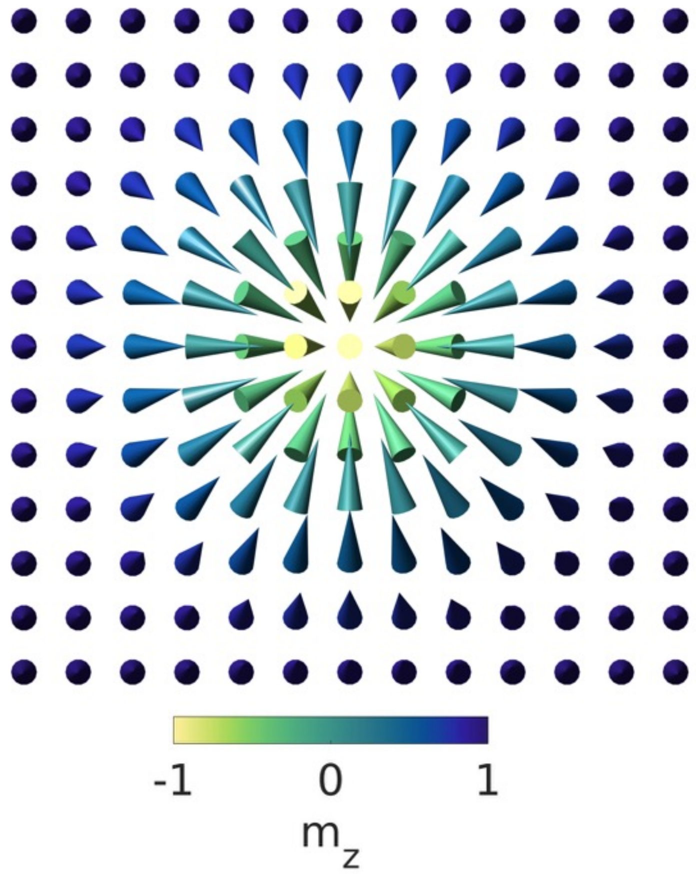

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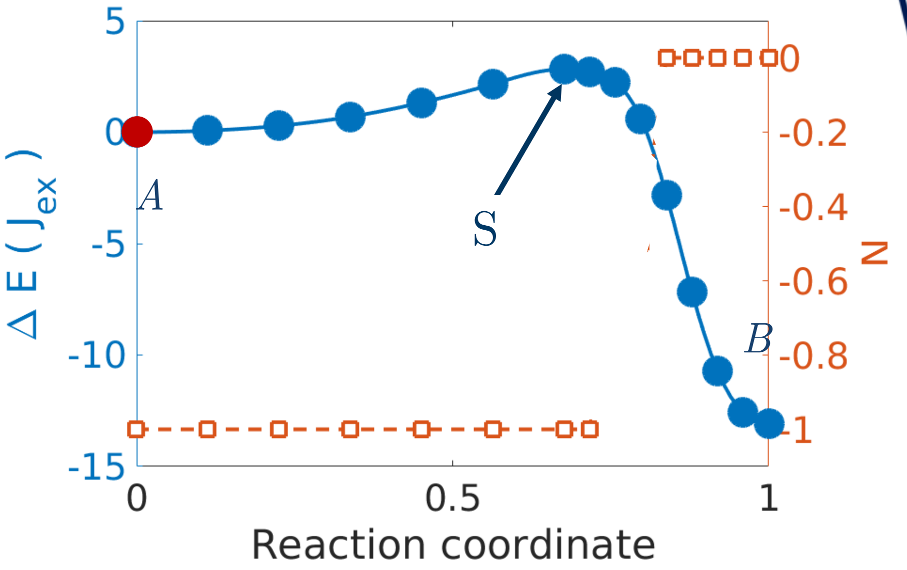

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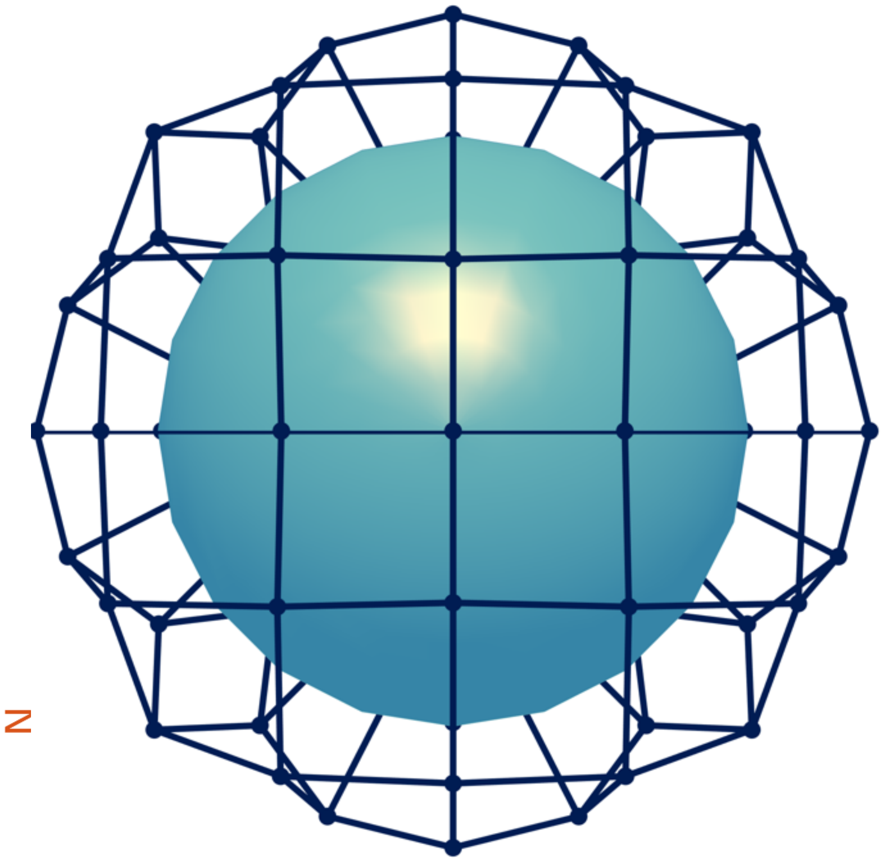

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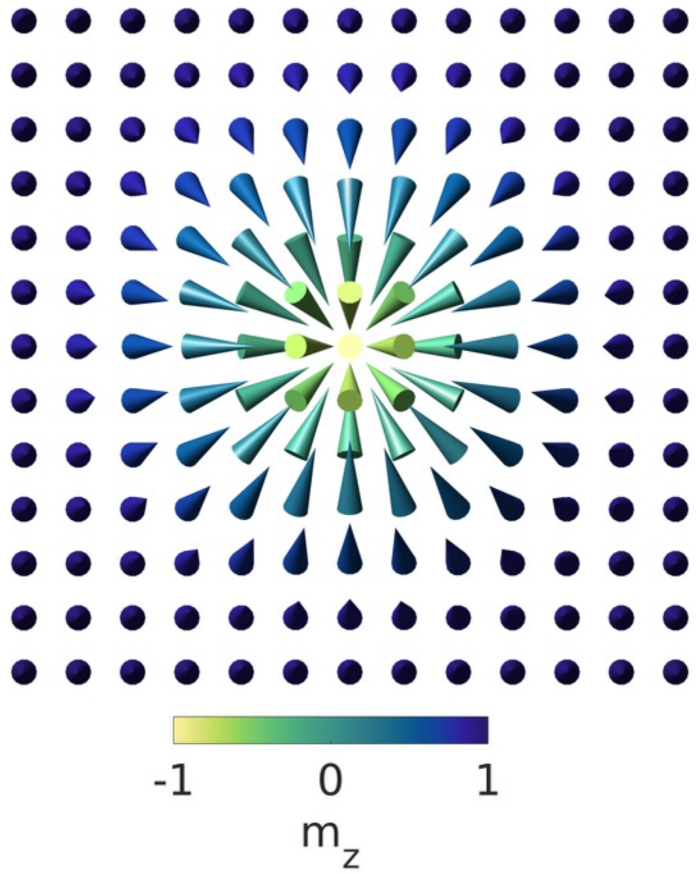

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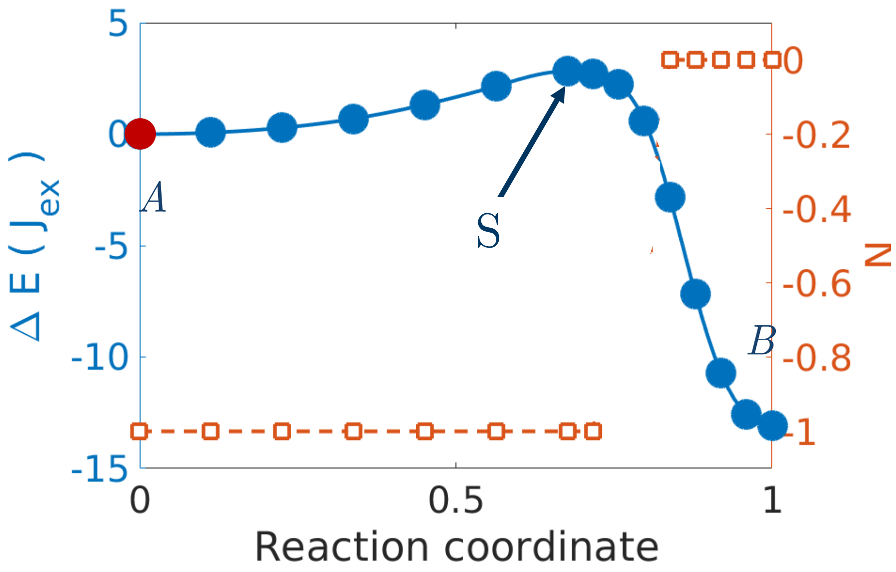

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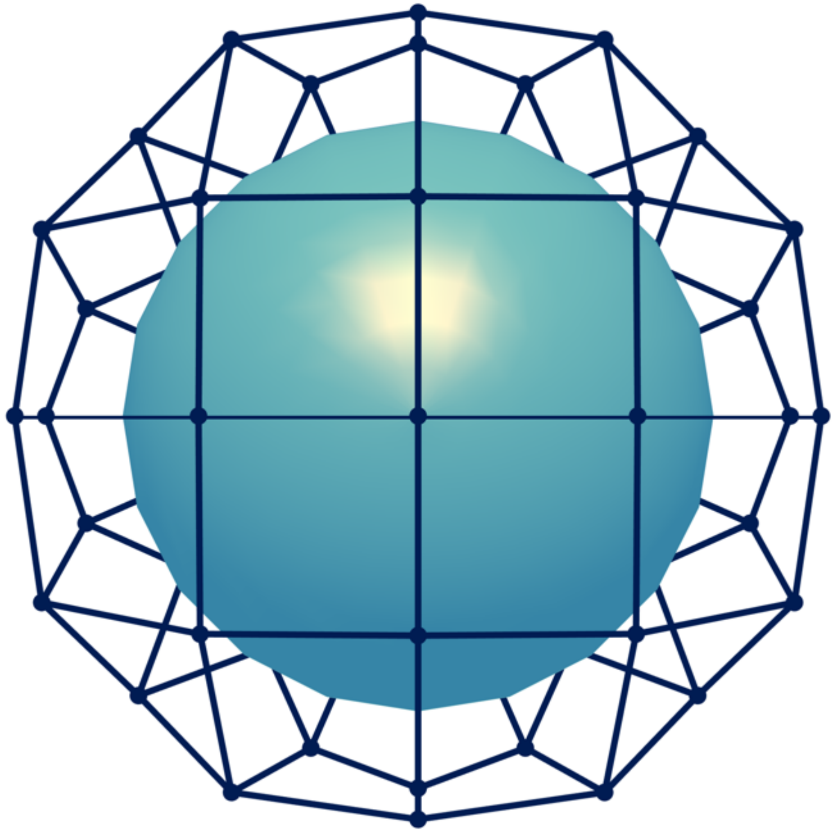

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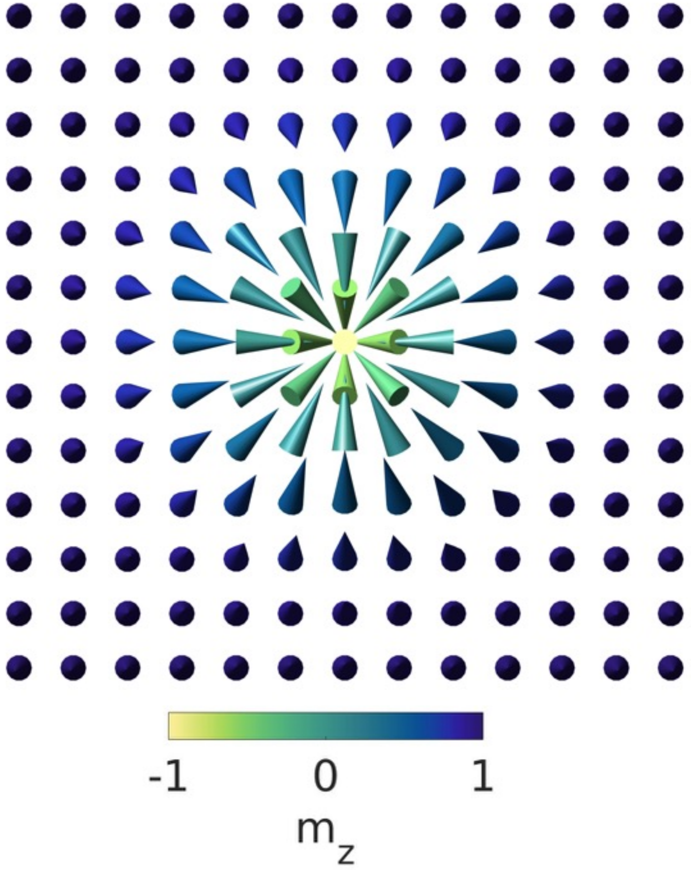

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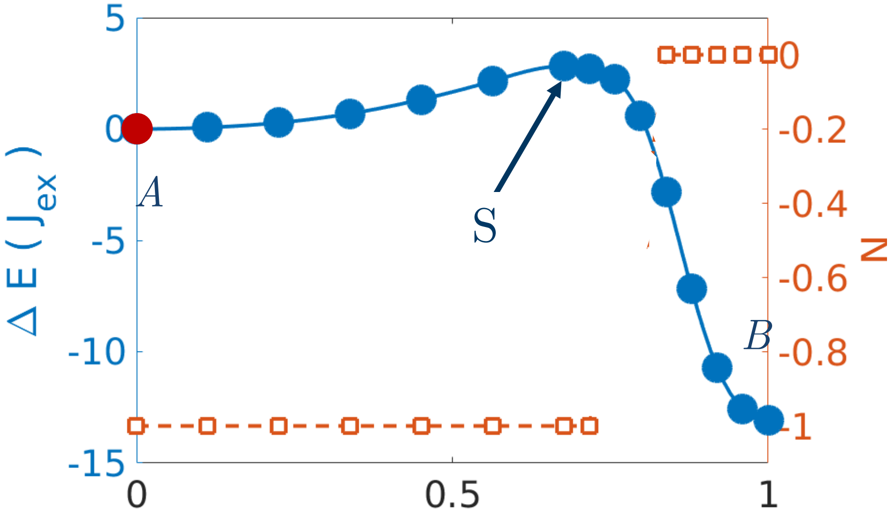

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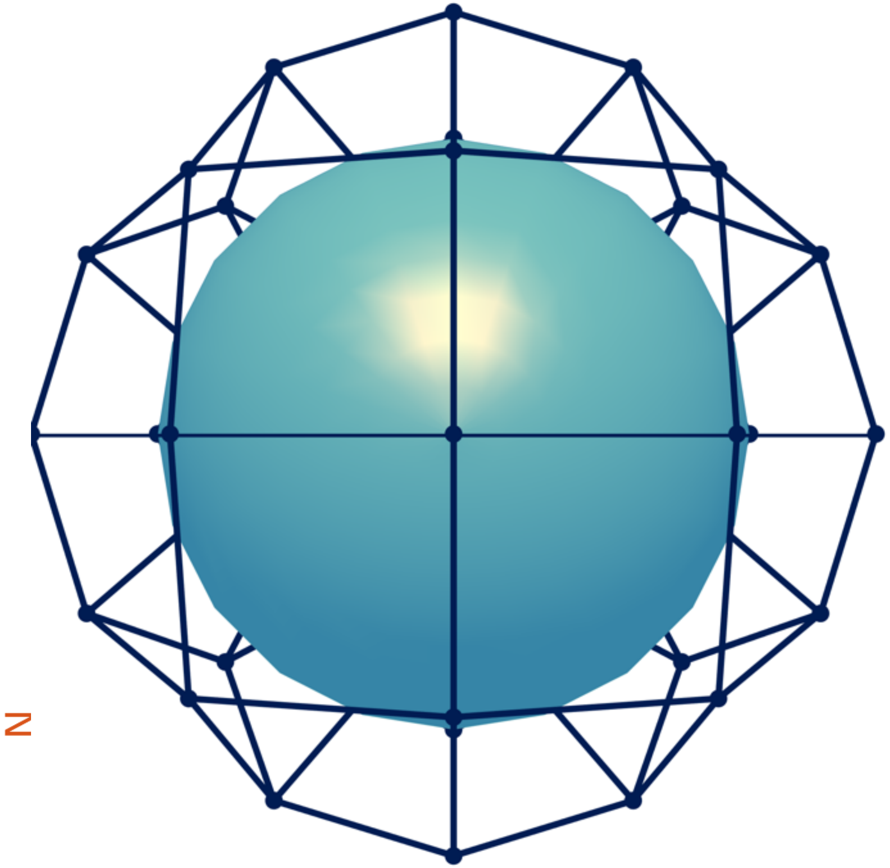

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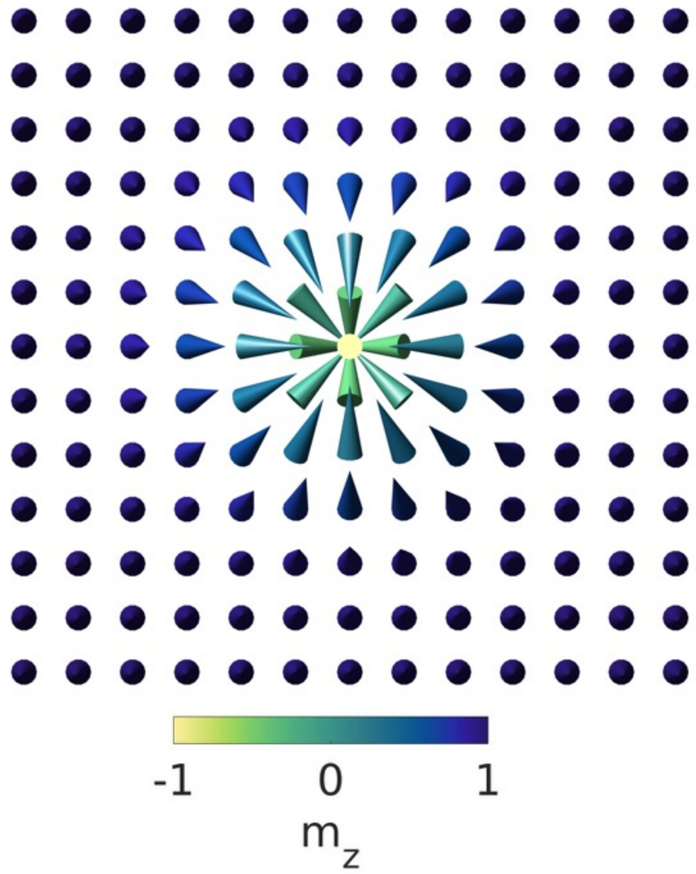

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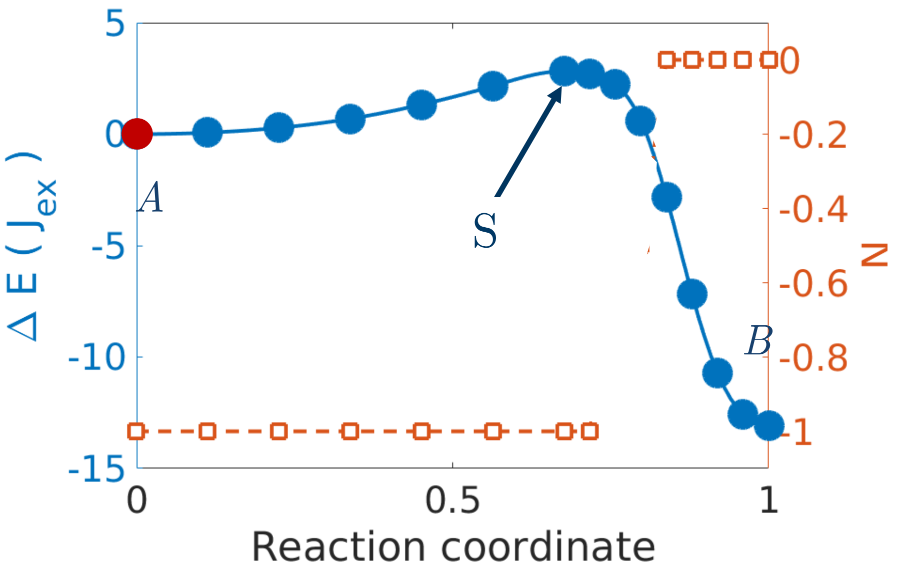

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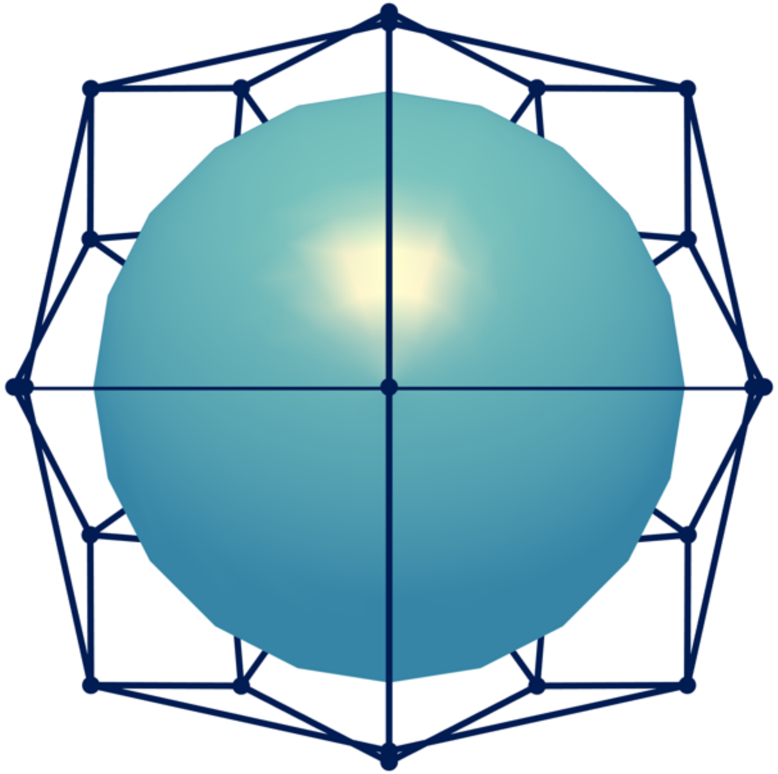

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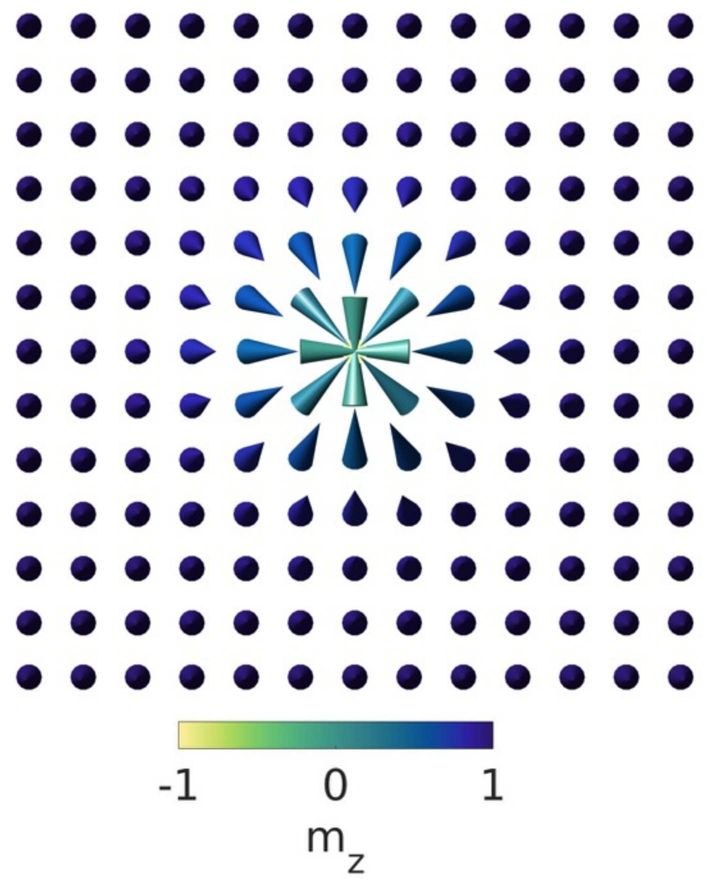

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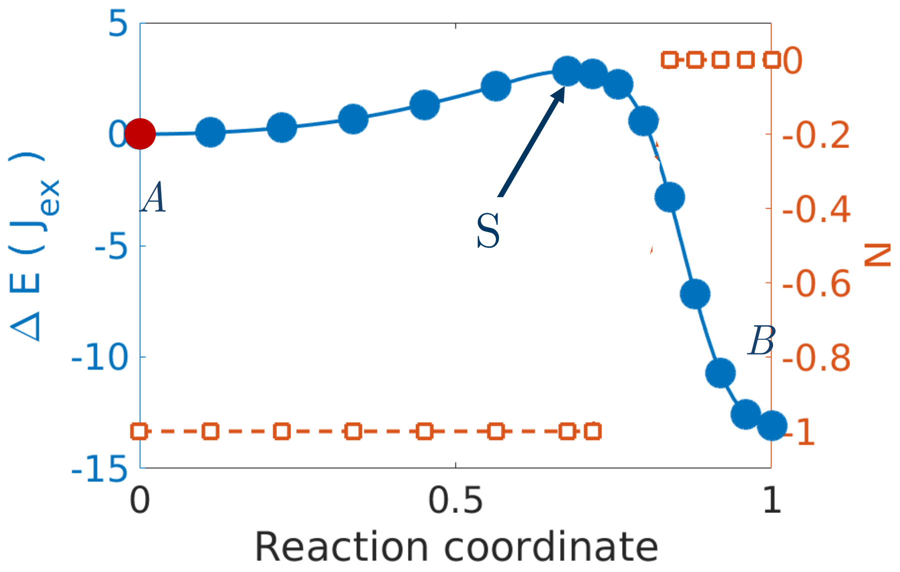

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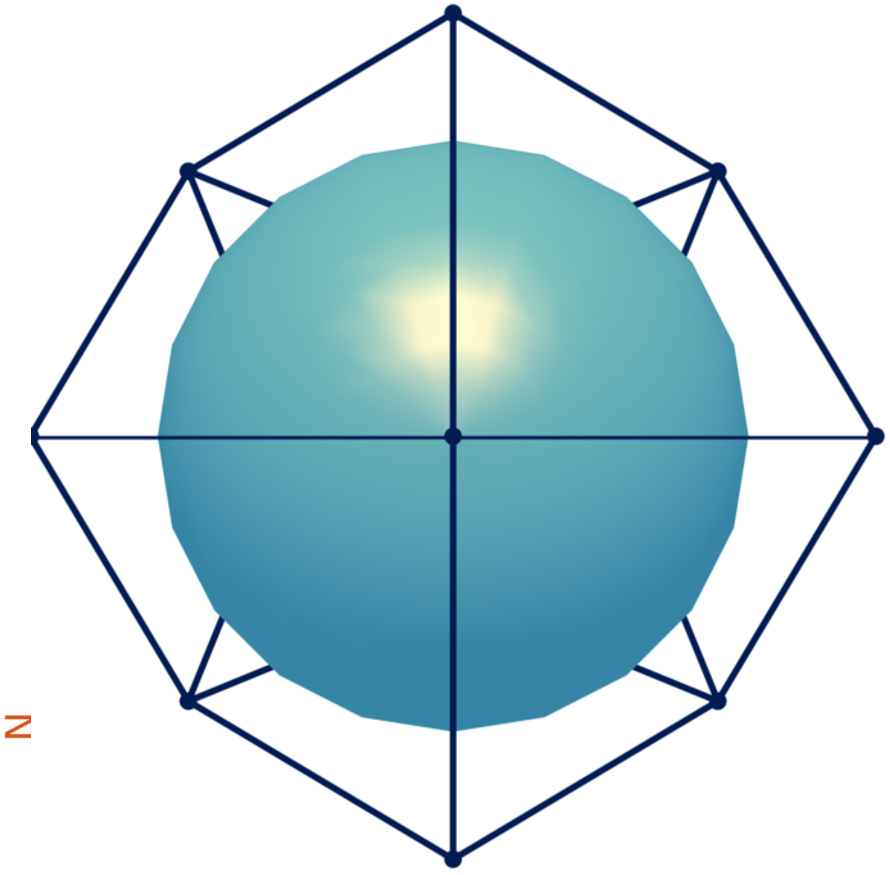

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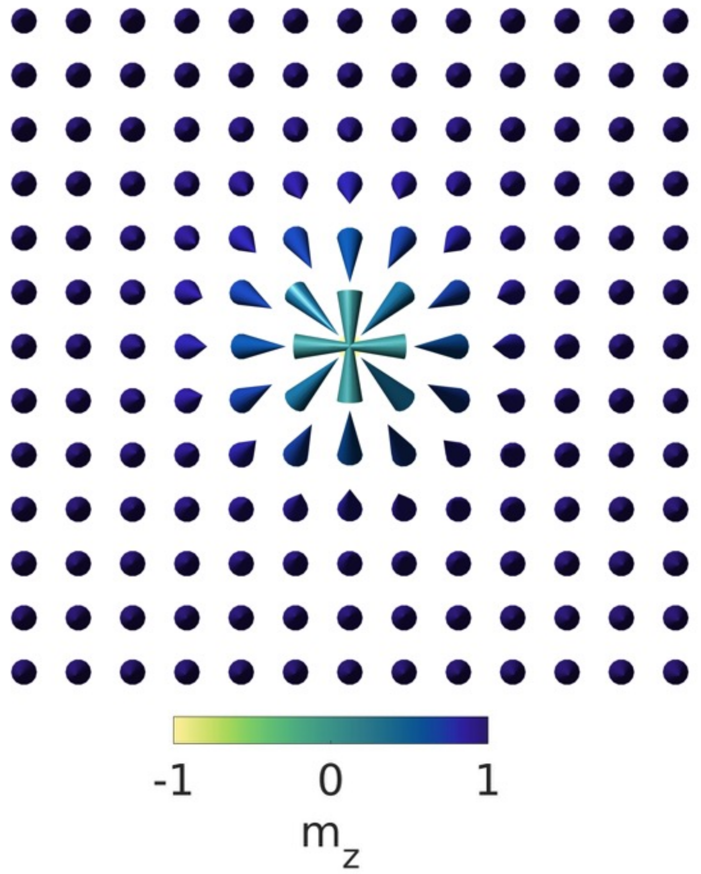

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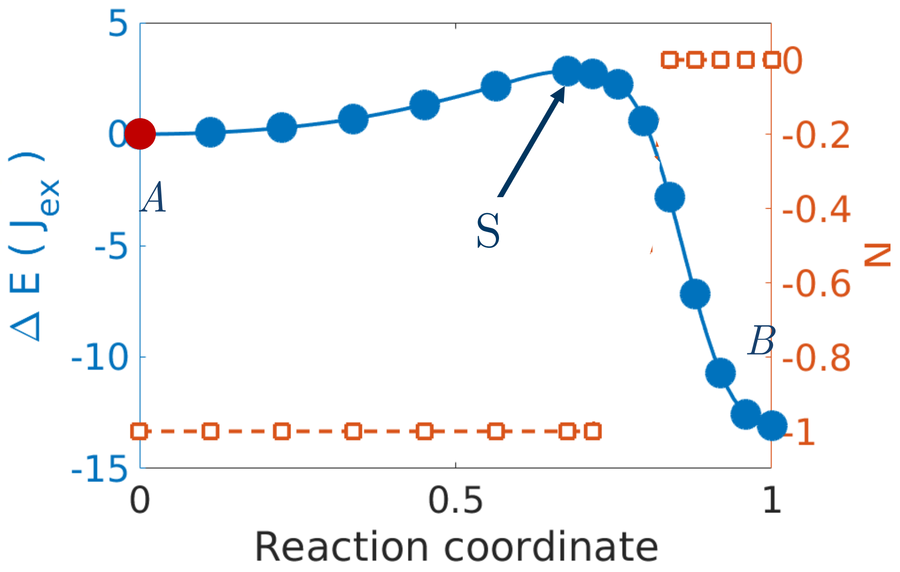

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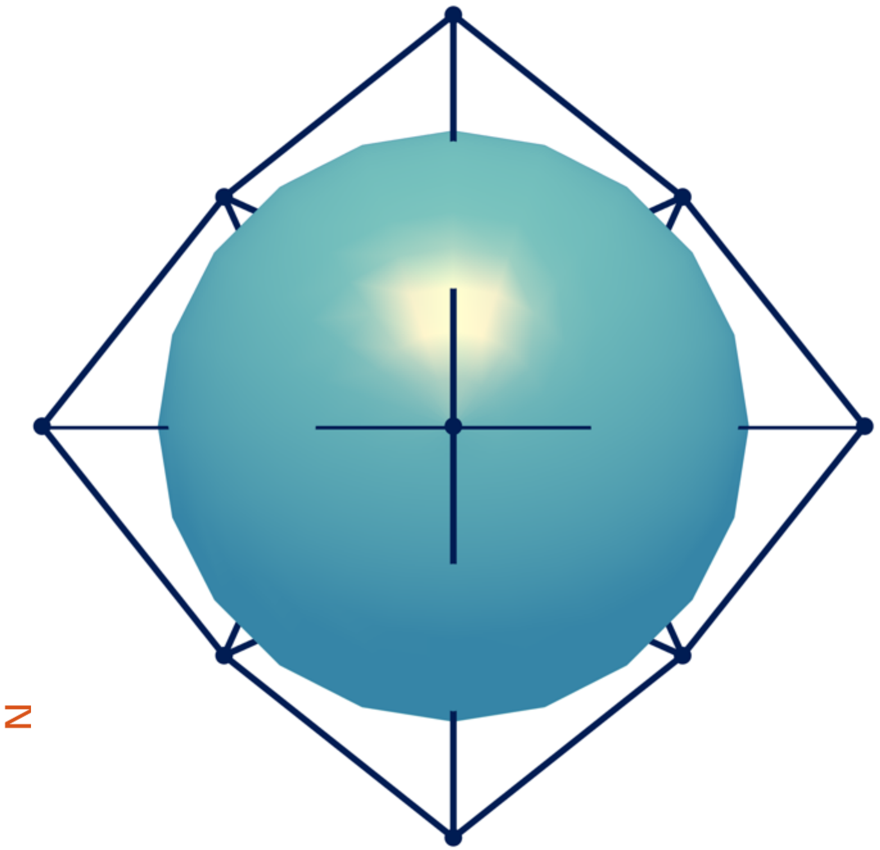

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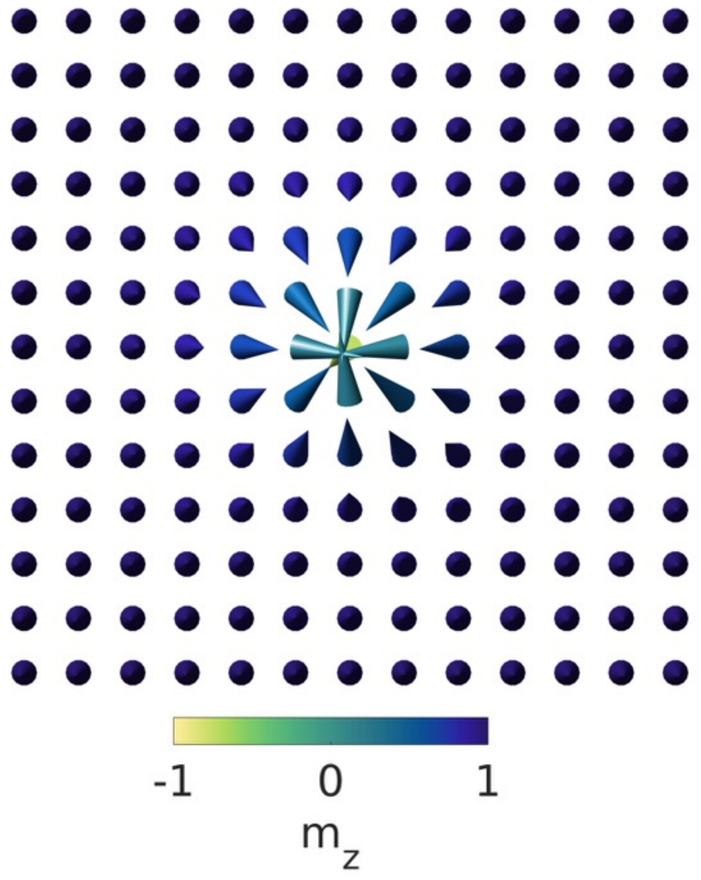

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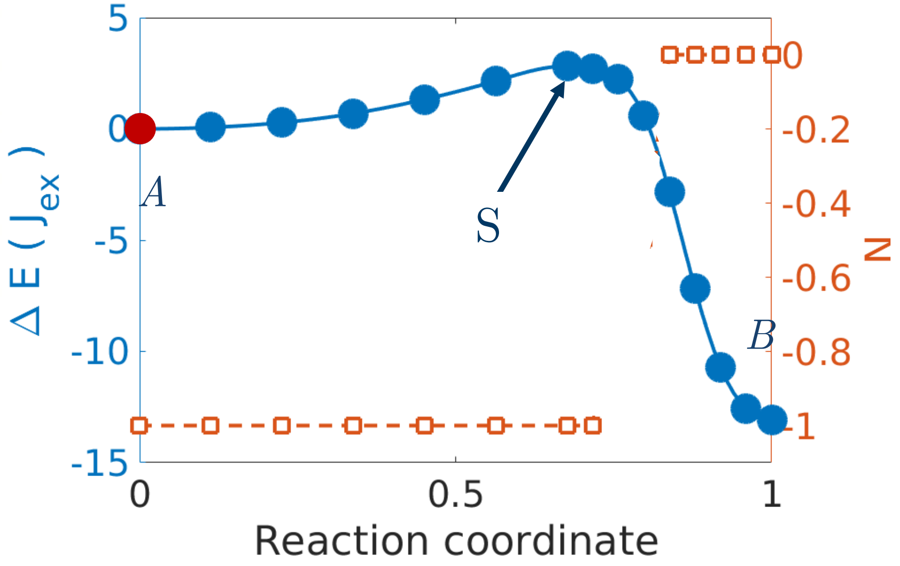

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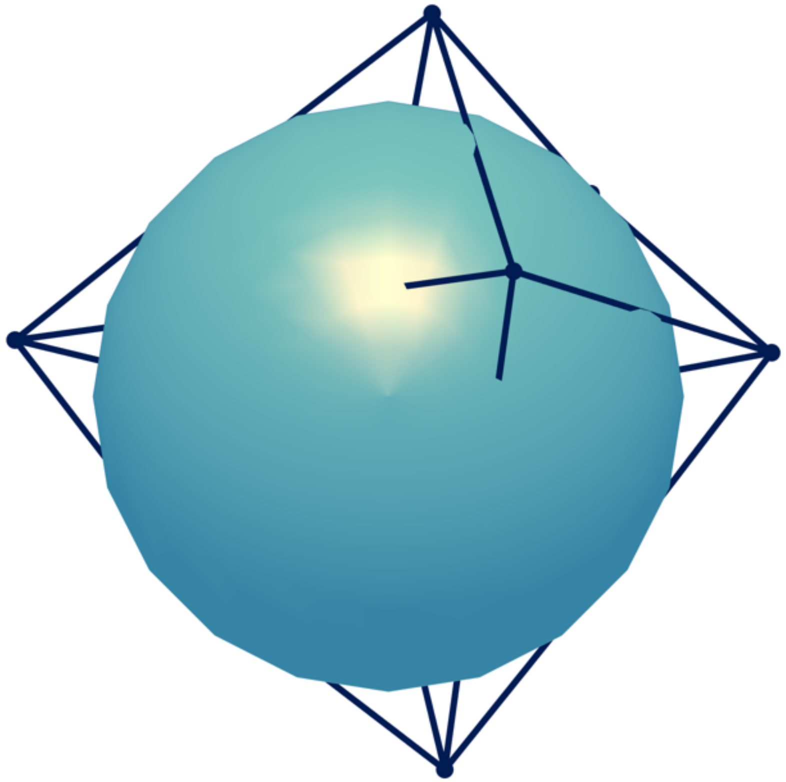

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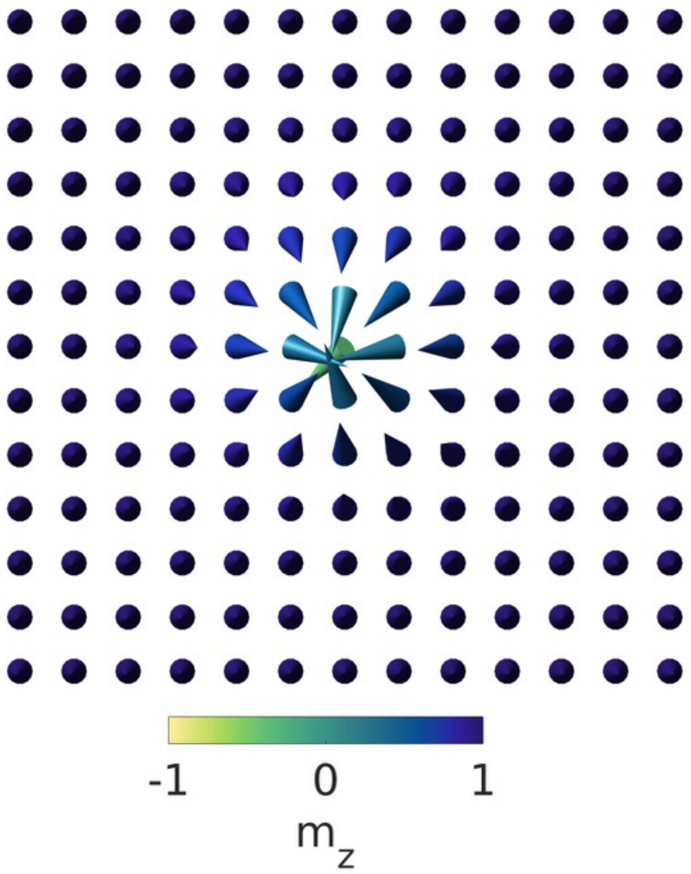

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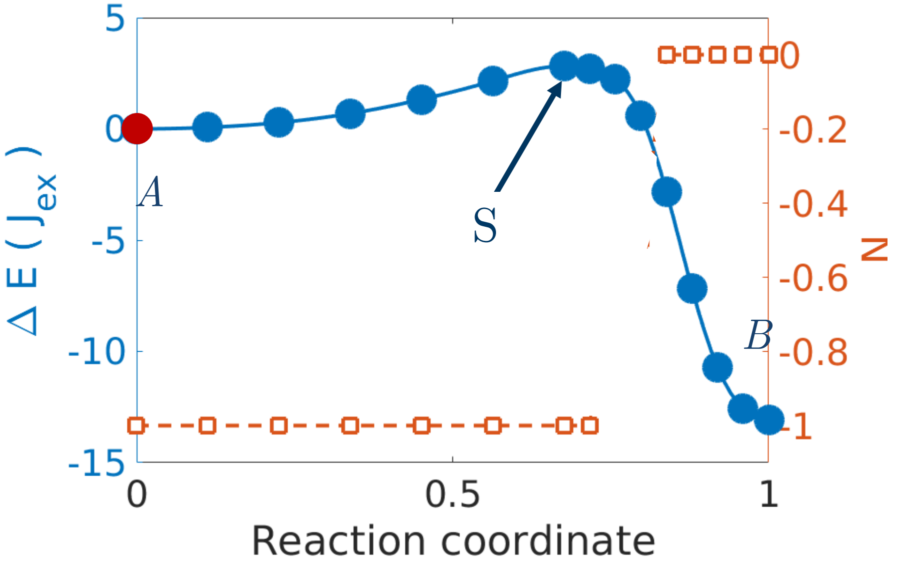

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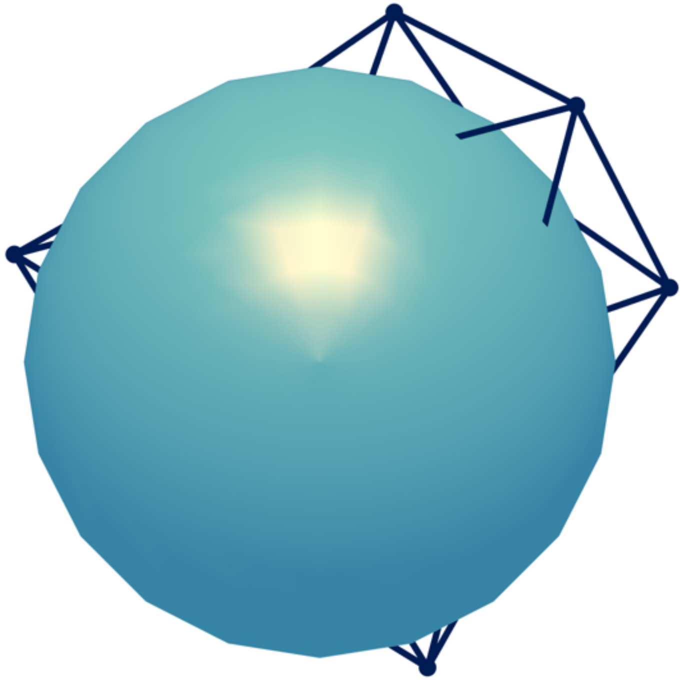

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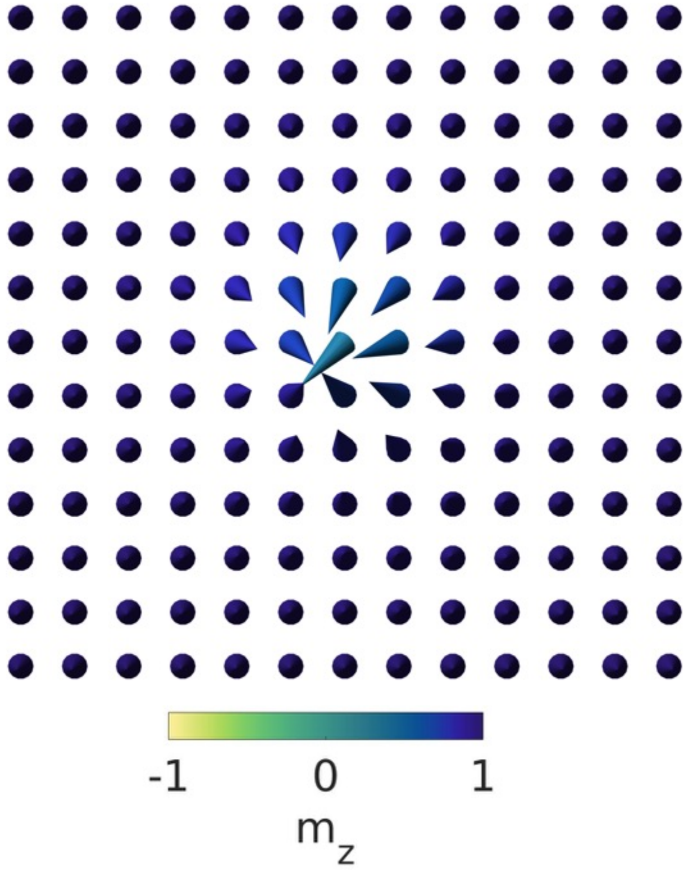

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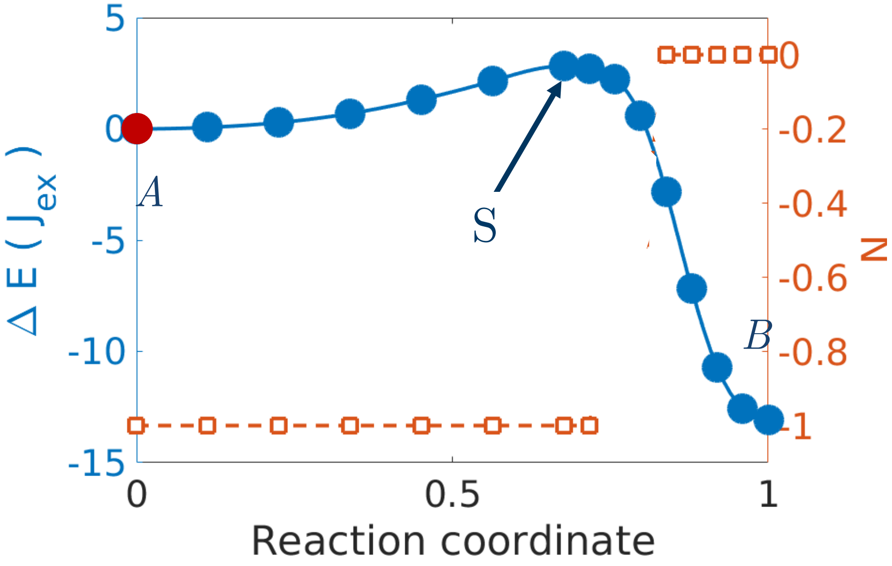

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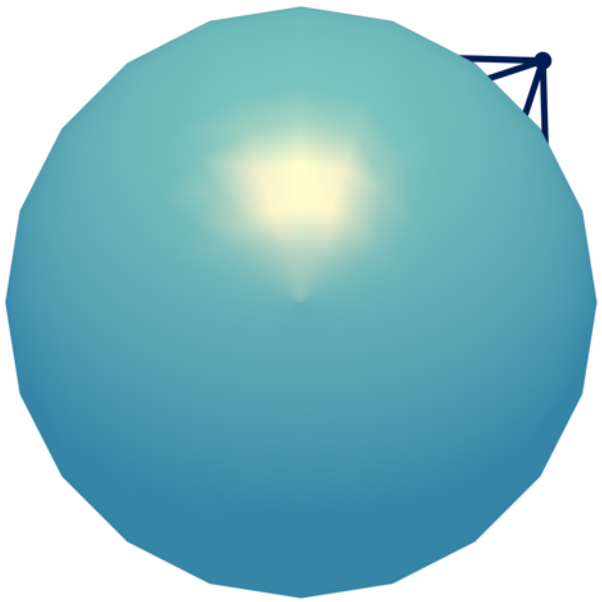

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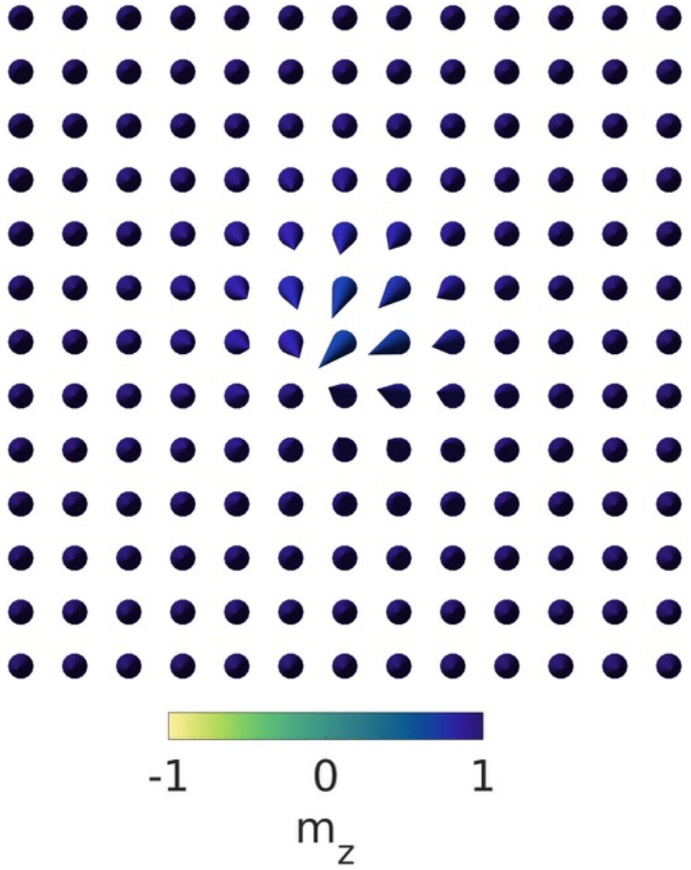

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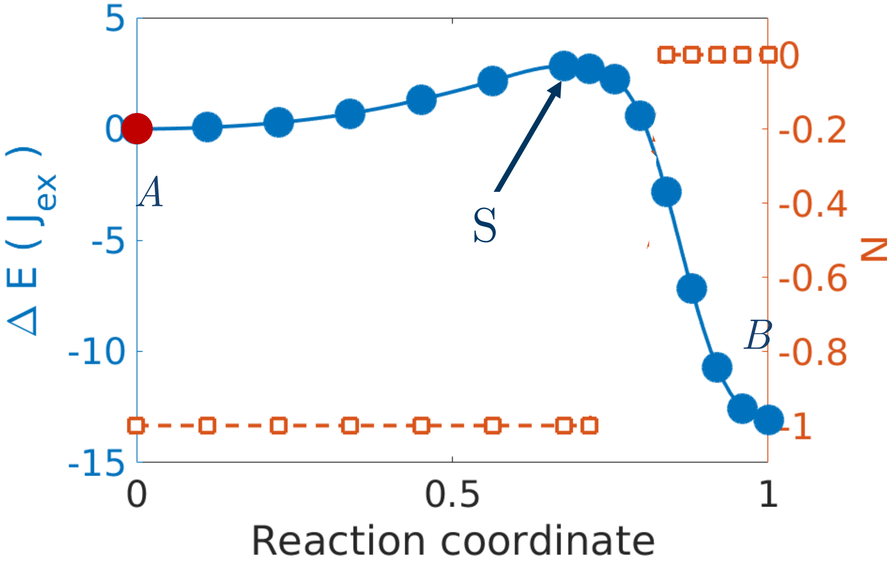
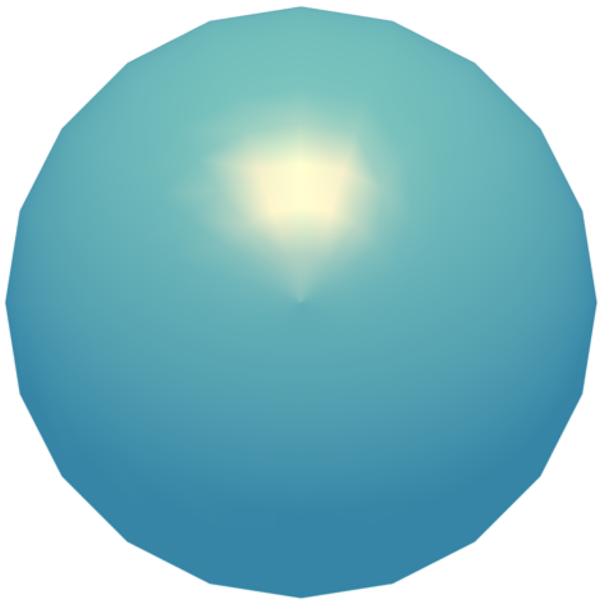
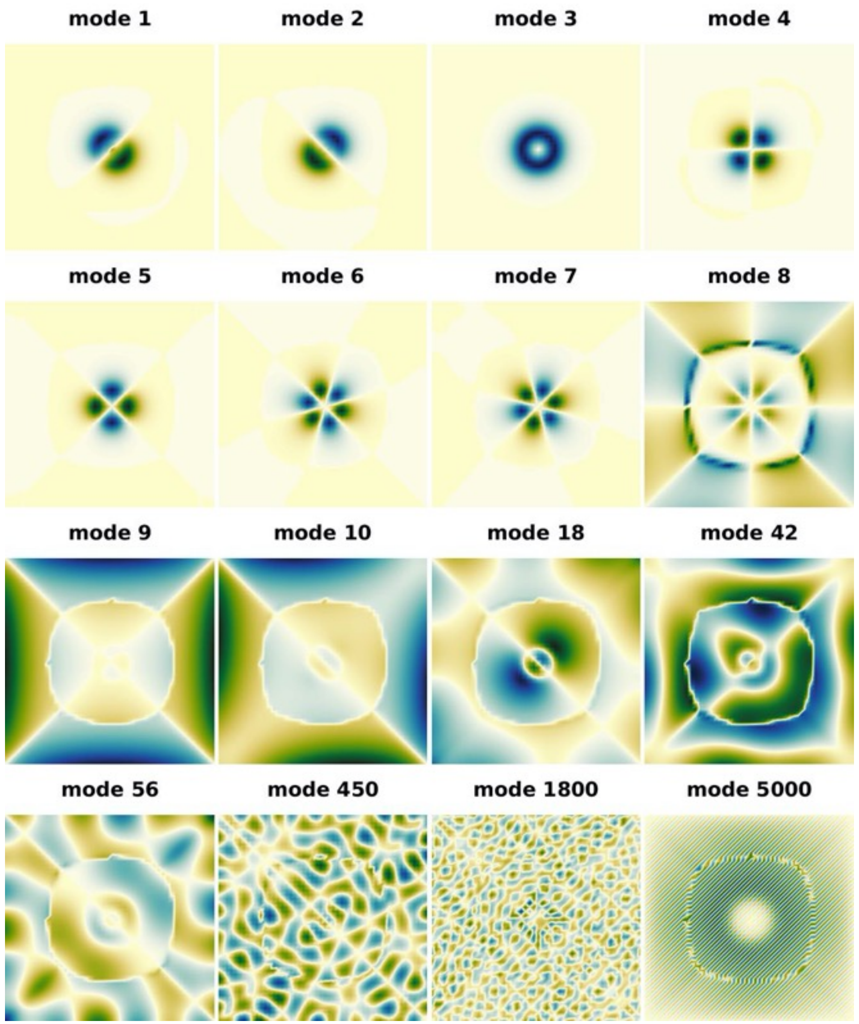


Projection on the unit sphere

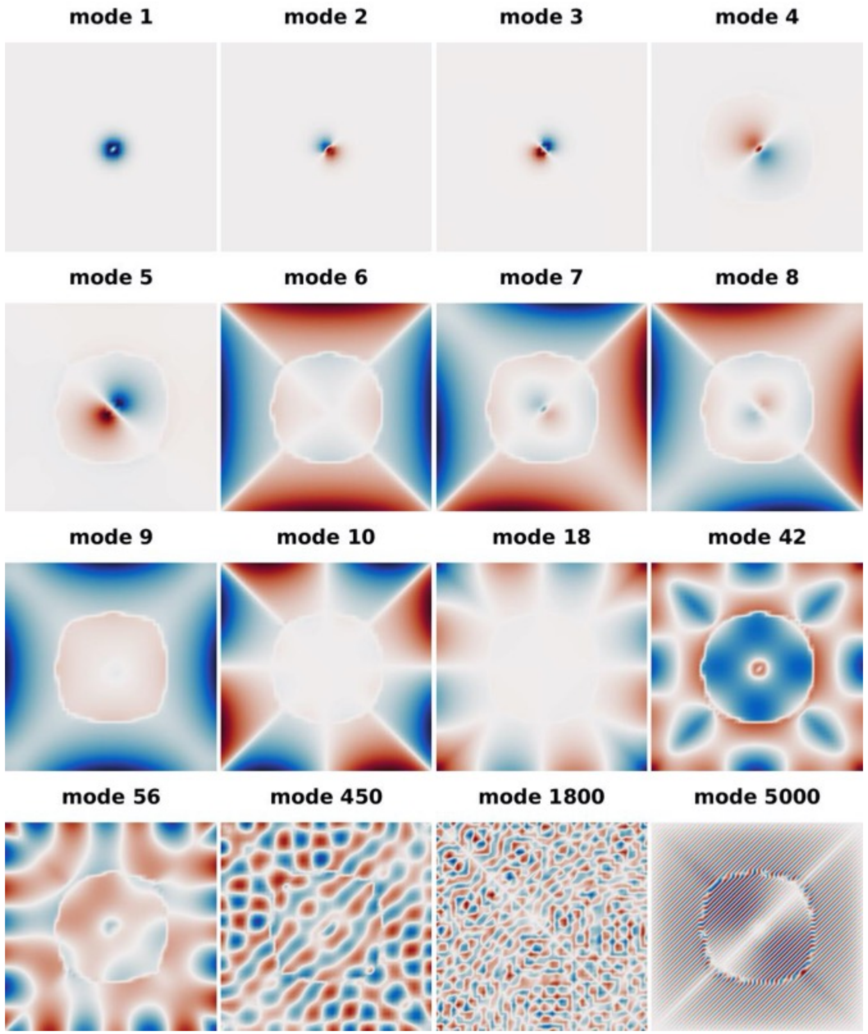


Desplat *et al.* *PRB* **98**, 134407 (2018)

Metastable skyrmion

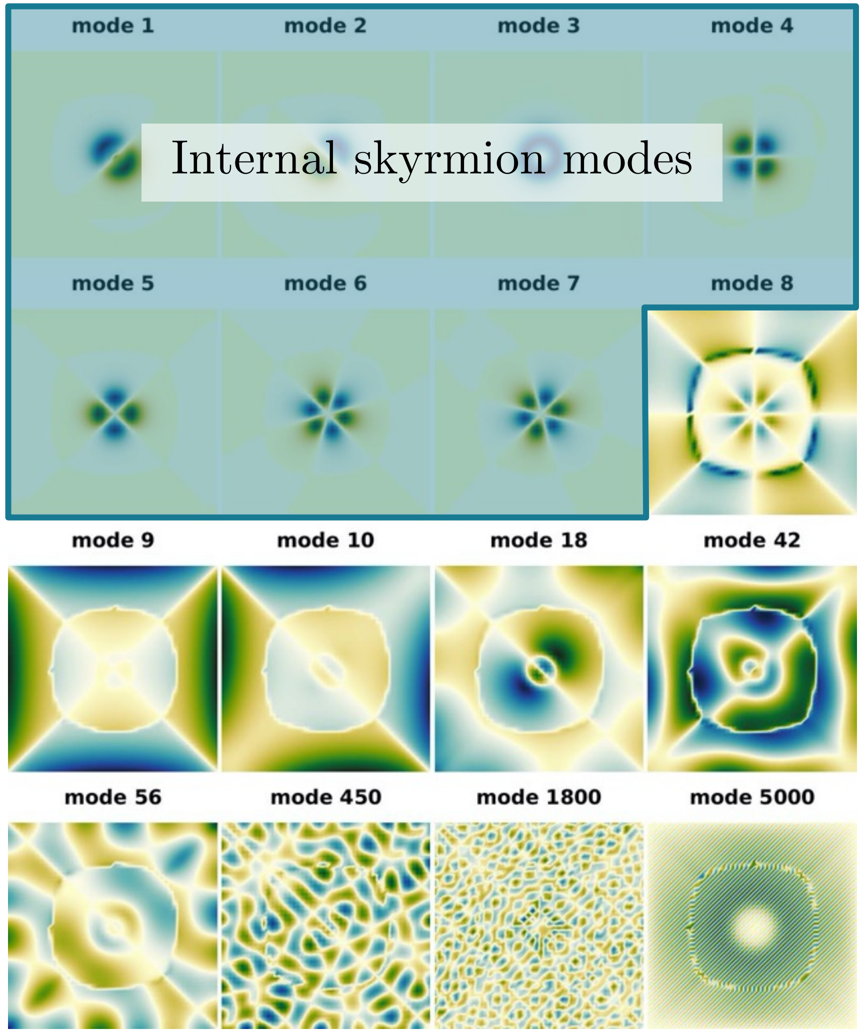


Saddle point

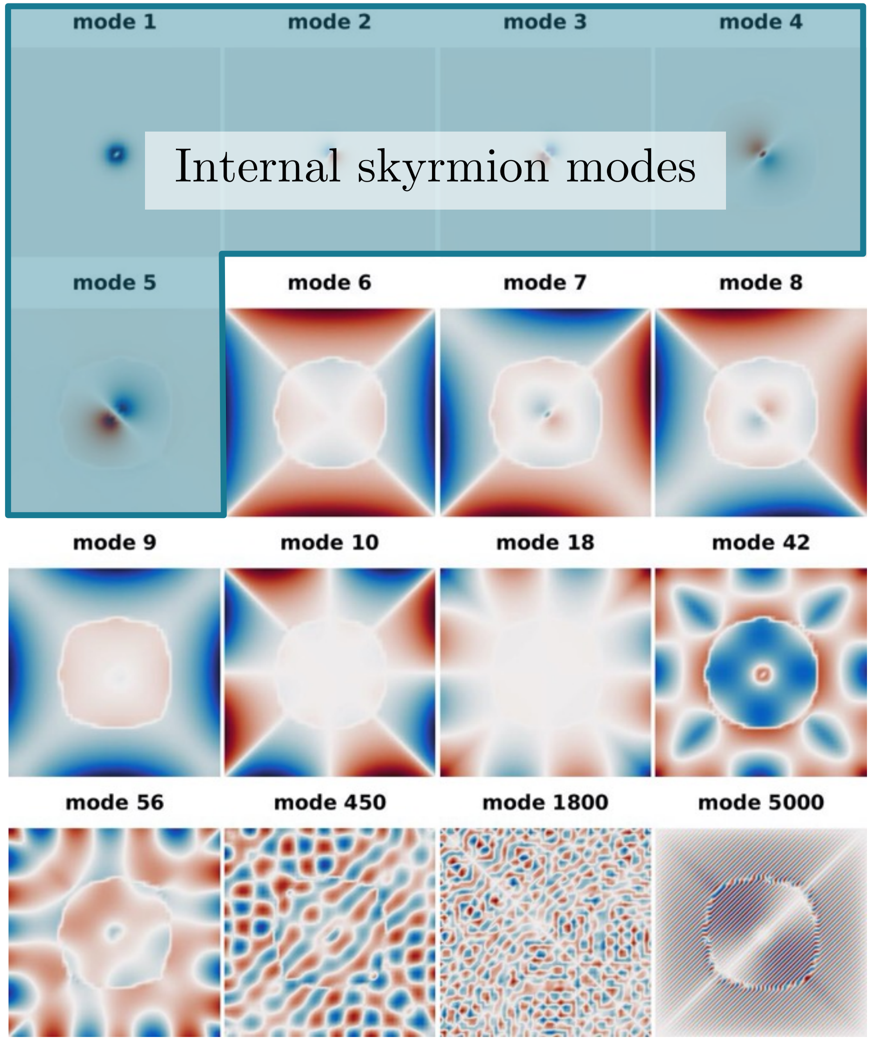


Desplat *et al.* *PRB* **98**, 134407 (2018)

Metastable skyrmion

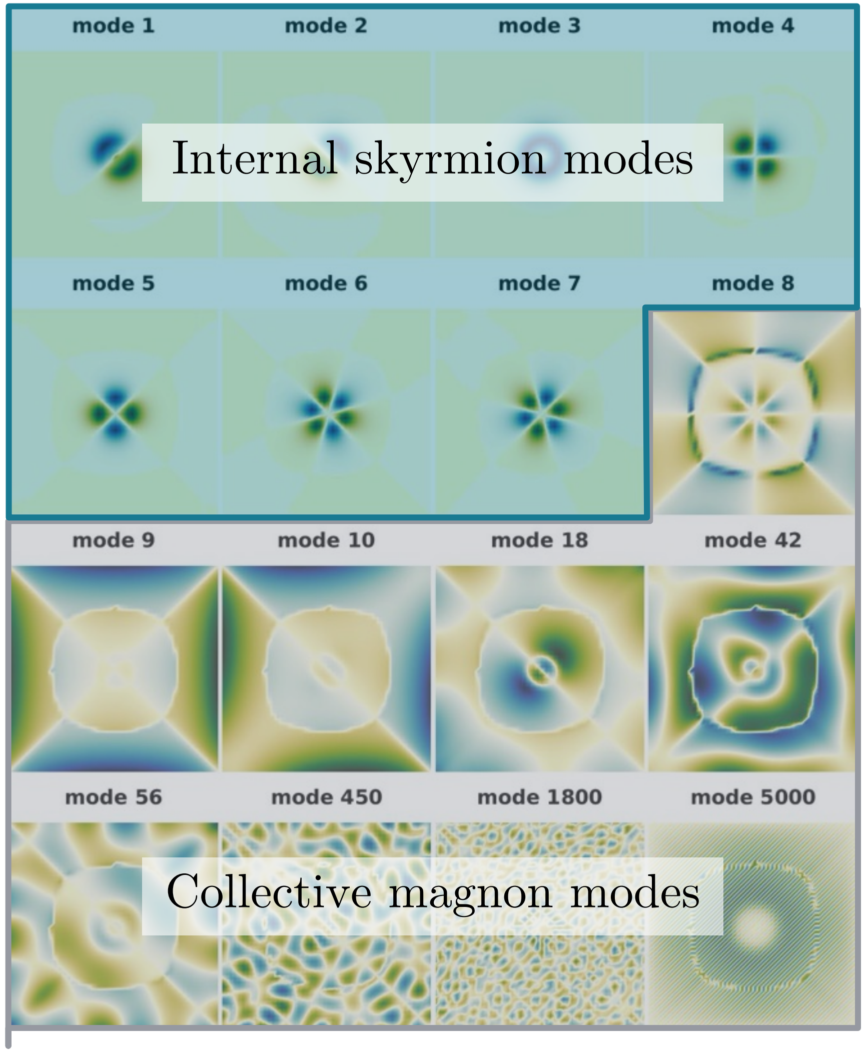


Saddle point

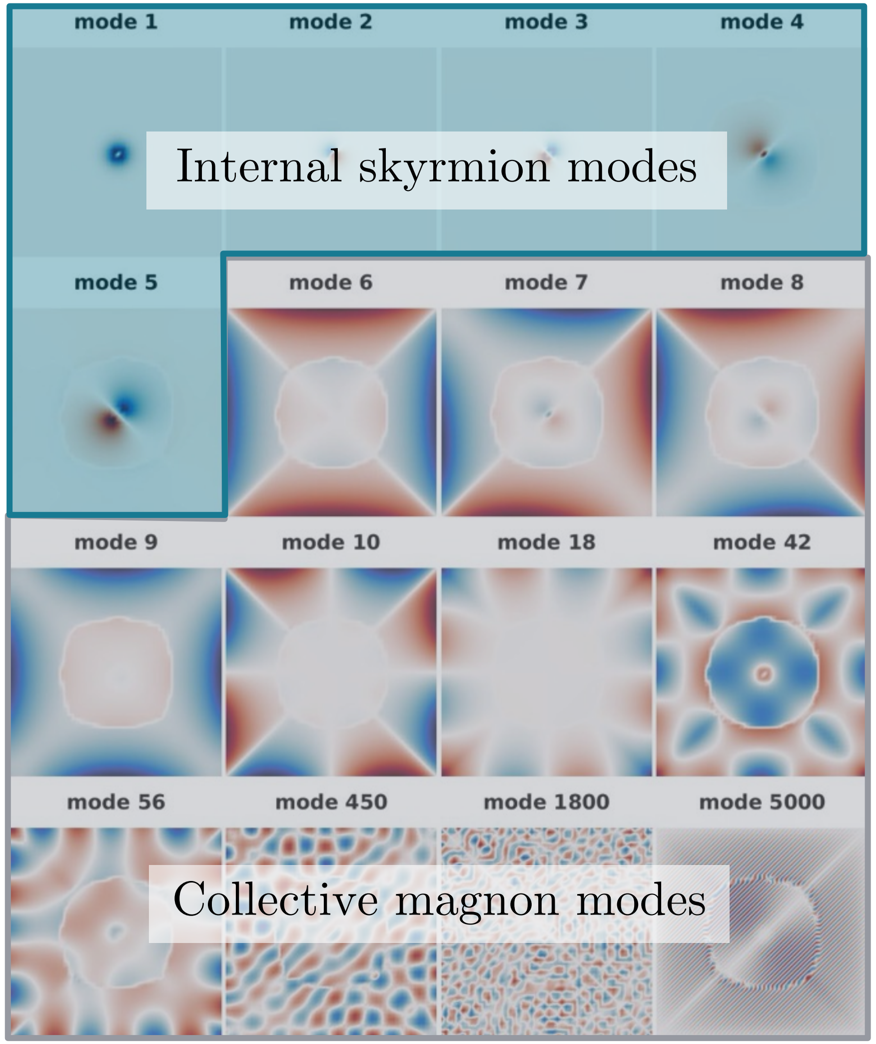


Desplat *et al.* *PRB* **98**, 134407 (2018)

Metastable skyrmion



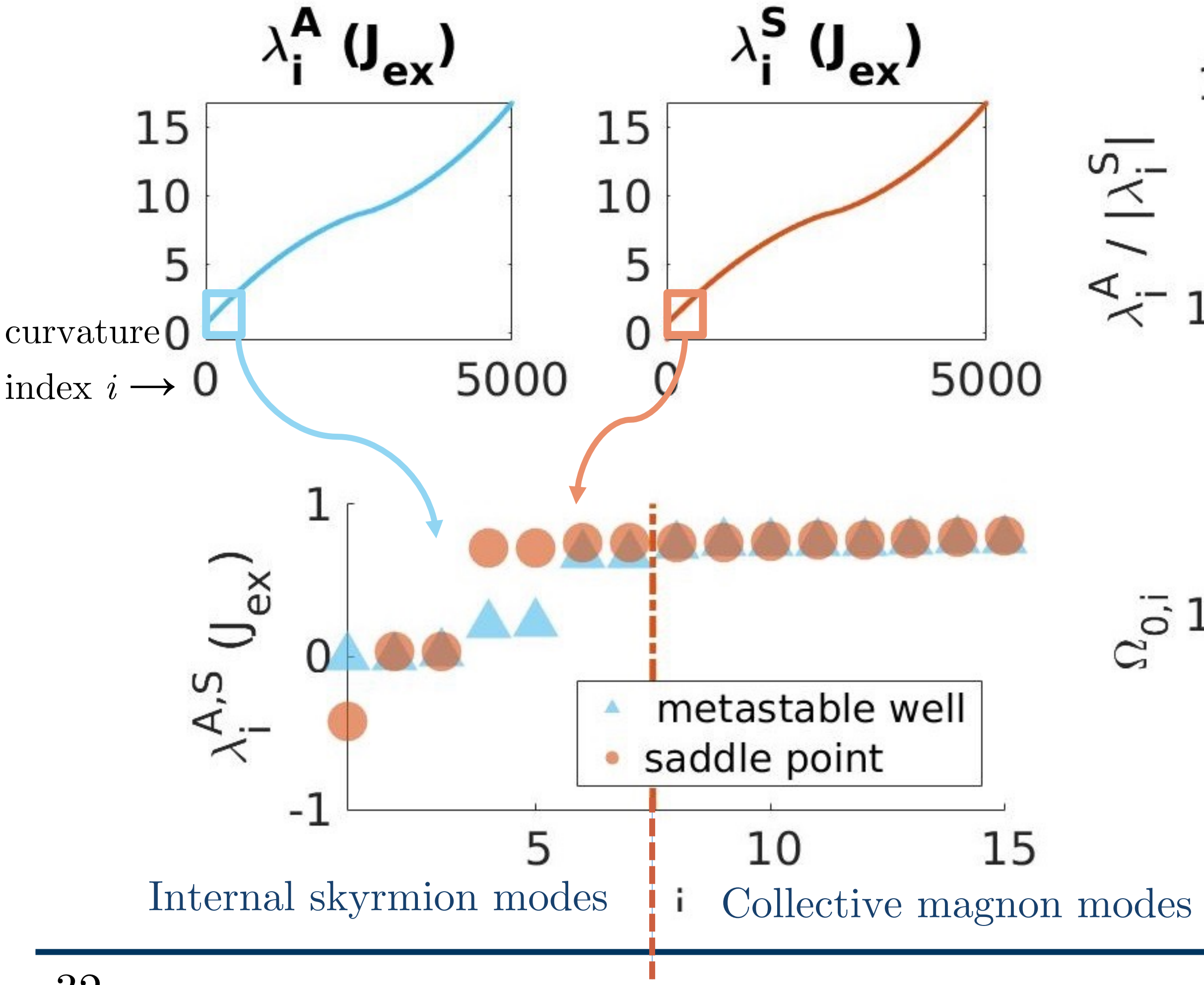
Saddle point



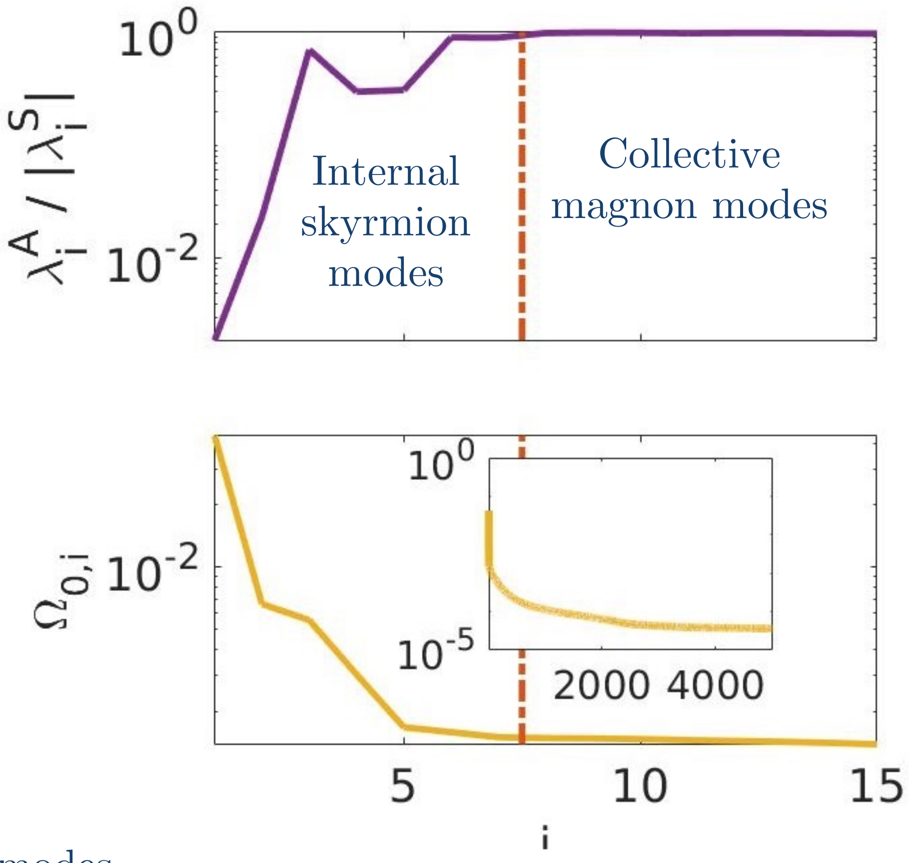
Desplat *et al.* *PRB* **98**, 134407 (2018)

Entropic contribution: $\Omega_0 = \sqrt{\frac{\Pi_i \lambda_i^A}{\Pi_j |\lambda_j^S|}} \propto e^{\Delta S/k_B}$

Energy curvatures at A and S:



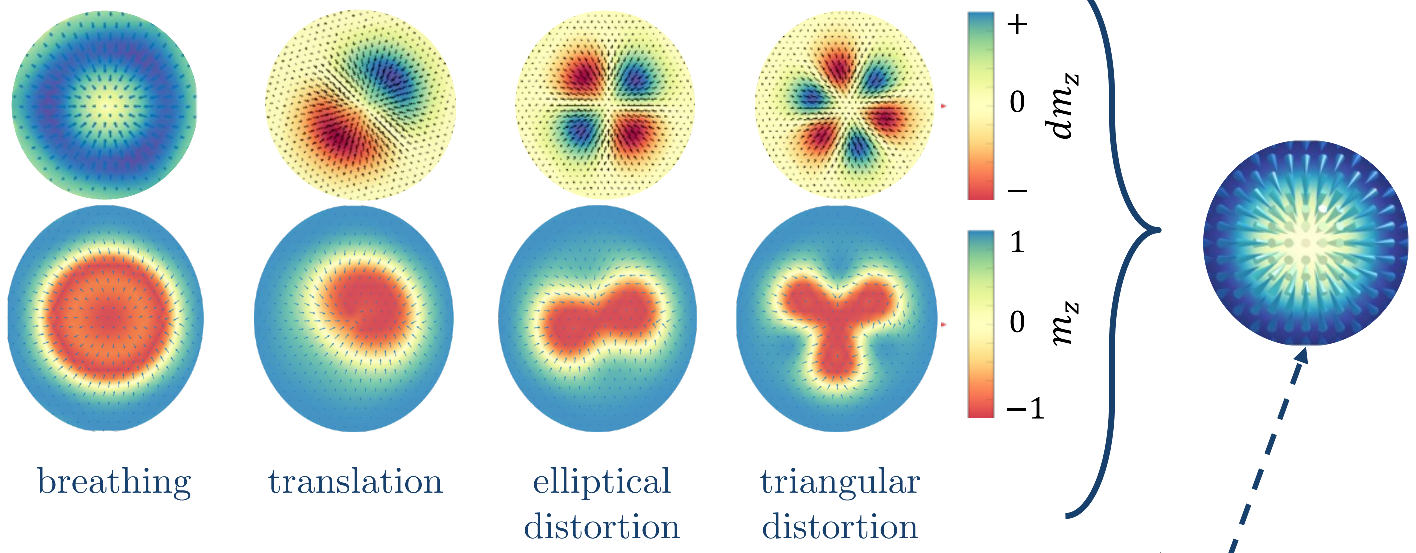
Ratio of curvatures



- **Internal skyrmion modes contribute the most to the prefactor**

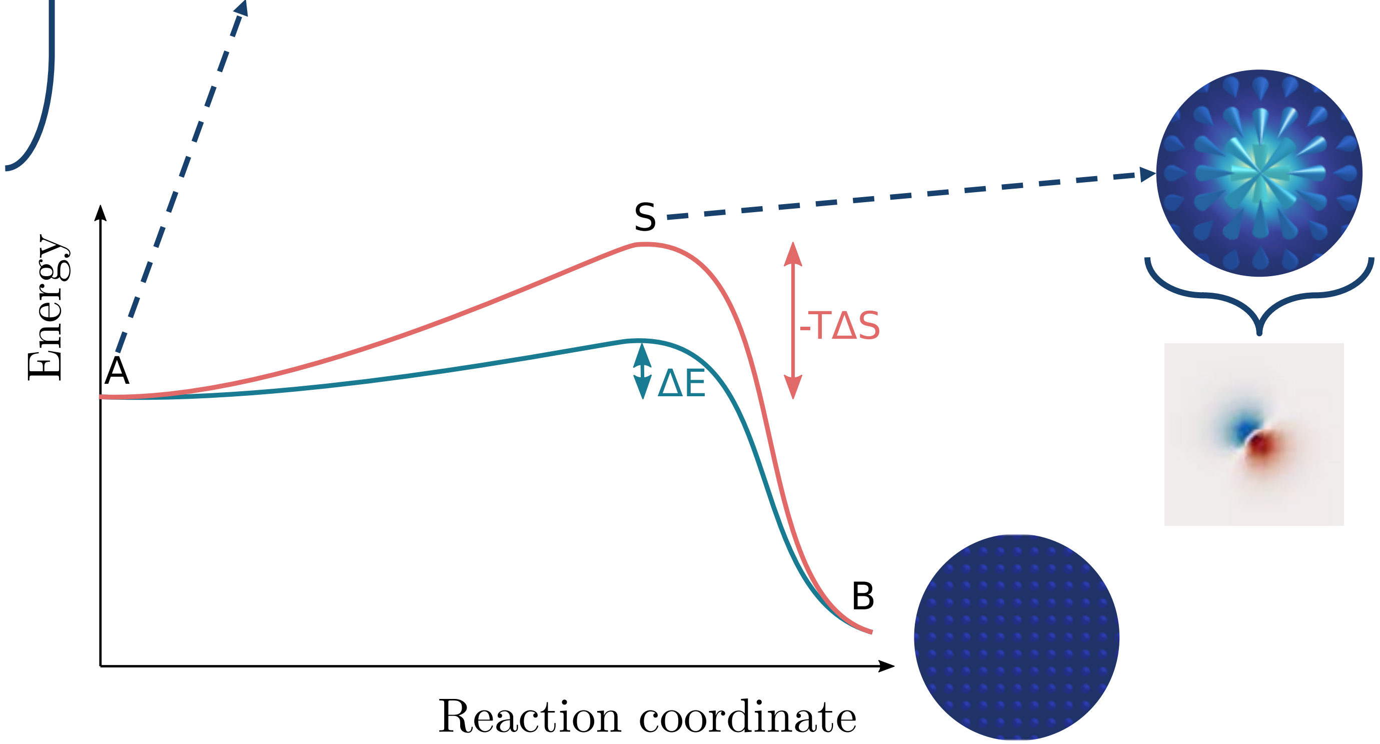
Desplat *et al.* *PRB* **98**, 134407 (2018)

Internal modes of deformation

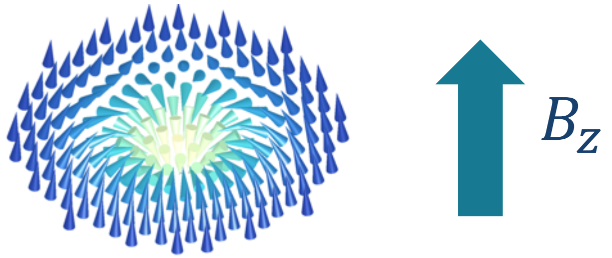


$$\Omega_0 \propto e^{\frac{\Delta S}{k_B}} < 1 \rightarrow \Delta S < 0$$

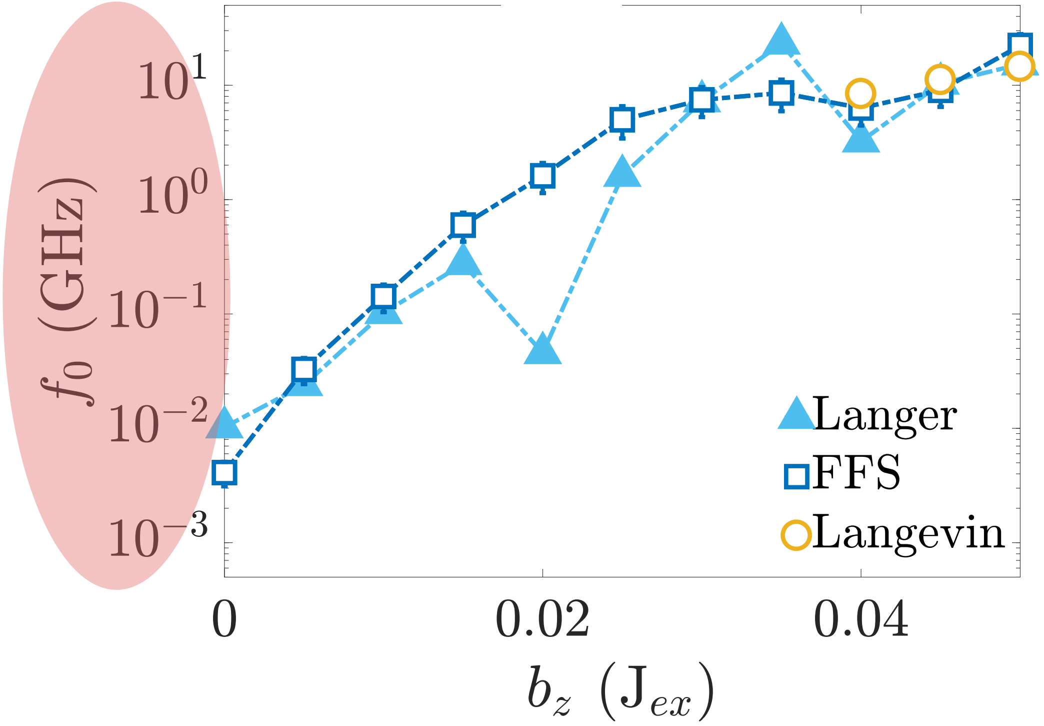
Entropic stabilization



Desplat *et al.* *PRB*, **98**, 134407 (2018)



Arrhenius prefactor

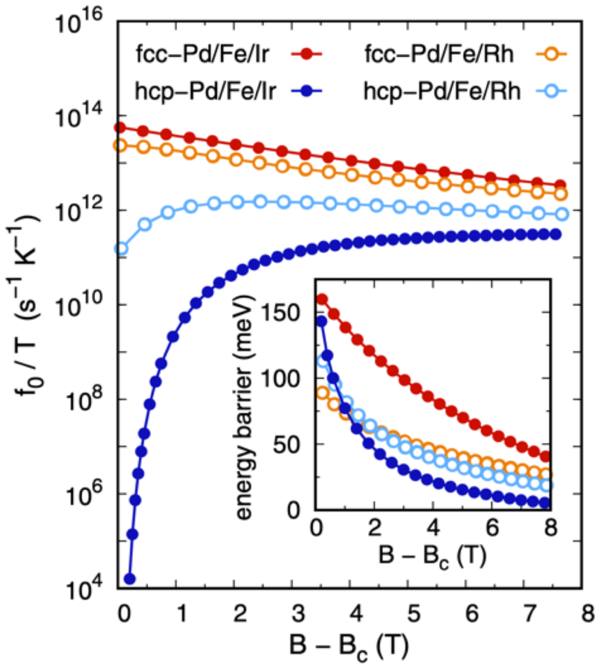


➢ **Good agreement of the methods**

Desplat *et al.* *PRB* **101**, 0604039(R) (2020)

➢ **Variation of f_0 over several orders of magnitude**
- important entropic contribution
- ΔE is not enough to estimate sk stability

❖ **Also predicted in** Pd/Fe on Ir and Rh from first principles

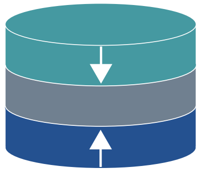


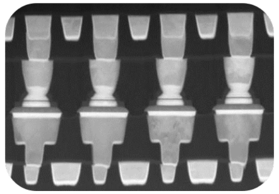
Von Malottki *et al.* *PRB* ***99***, 0604099(R) (2019)

Retention times in magnetic tunnel junctions

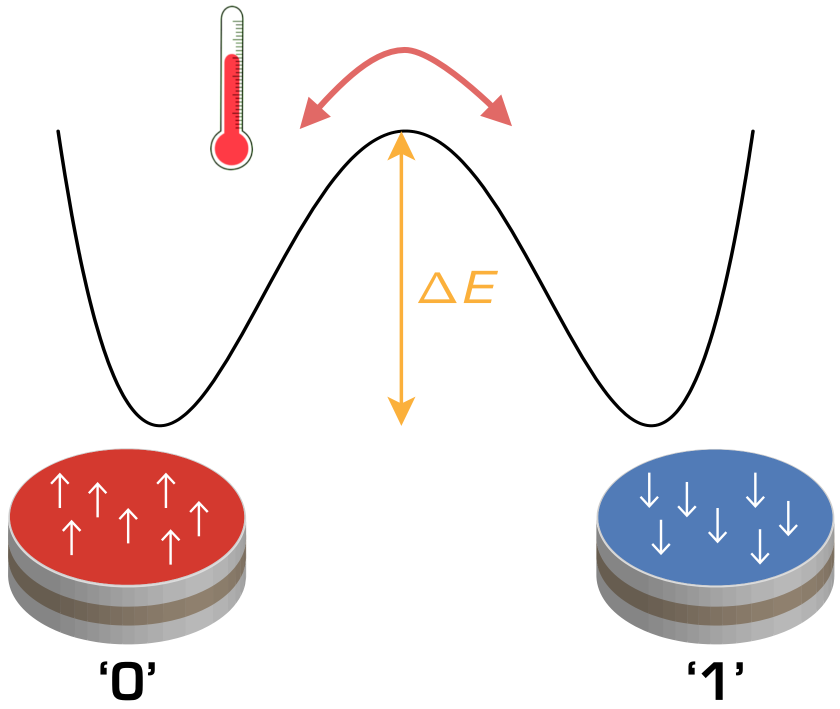
Entropy-Enthalpy Compensation

Perpendicular magnetic tunnel junctions used in STT-MRAM





(Intel)



- Information encoded by collinear magnetization state of the free layer
- Magnetization can reverse under **thermal fluctuations** → information loss
- **Information retention time:** mean waiting time between reversals $\tau = k^{-1} = f_0^{-1}\, e^{\beta \Delta E}$
- **Typical metric: stability factor** $\Delta = \beta_{300} \Delta E \gtrsim 50 \rightarrow$ 10 year stability **assuming f_0 ~GHz** ⚠

Is this valid?

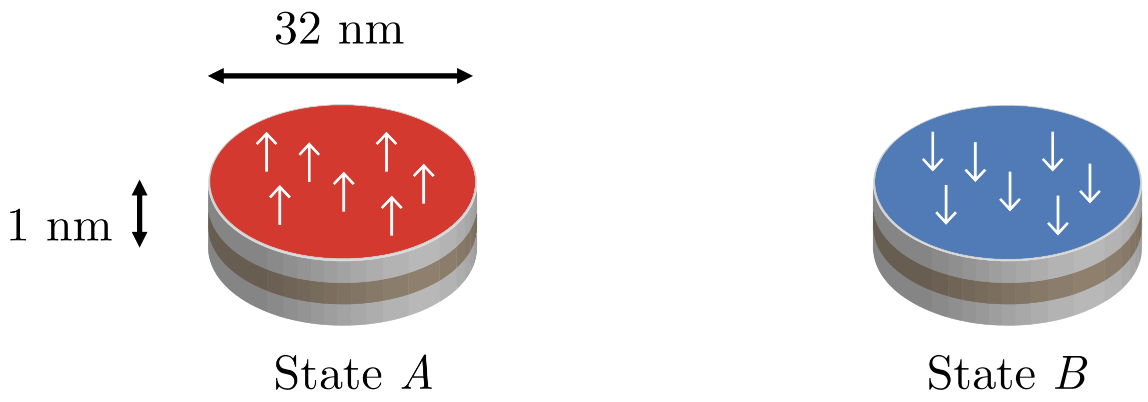
- **Perpendicularly magnetized CoFeB nanodisc**

- **Micromagnetic energy density:**

$$\varepsilon = A\left[\, \partial_x m^2 + \partial_y m^2\right] - K\, m_z^2 + D\left[m_z \partial_x m_x - m_x \partial_z m_z + id.(x \to y)\right]$$

Exchange — Anisotropy — DMI

- In some cases a full dipole-dipole (DDI) treatment was done (MuMax3)



A=10 pJ/m

M_s=1.03 MA/m

K=187 kJ/m^3

D=0.5 mJ/m^2

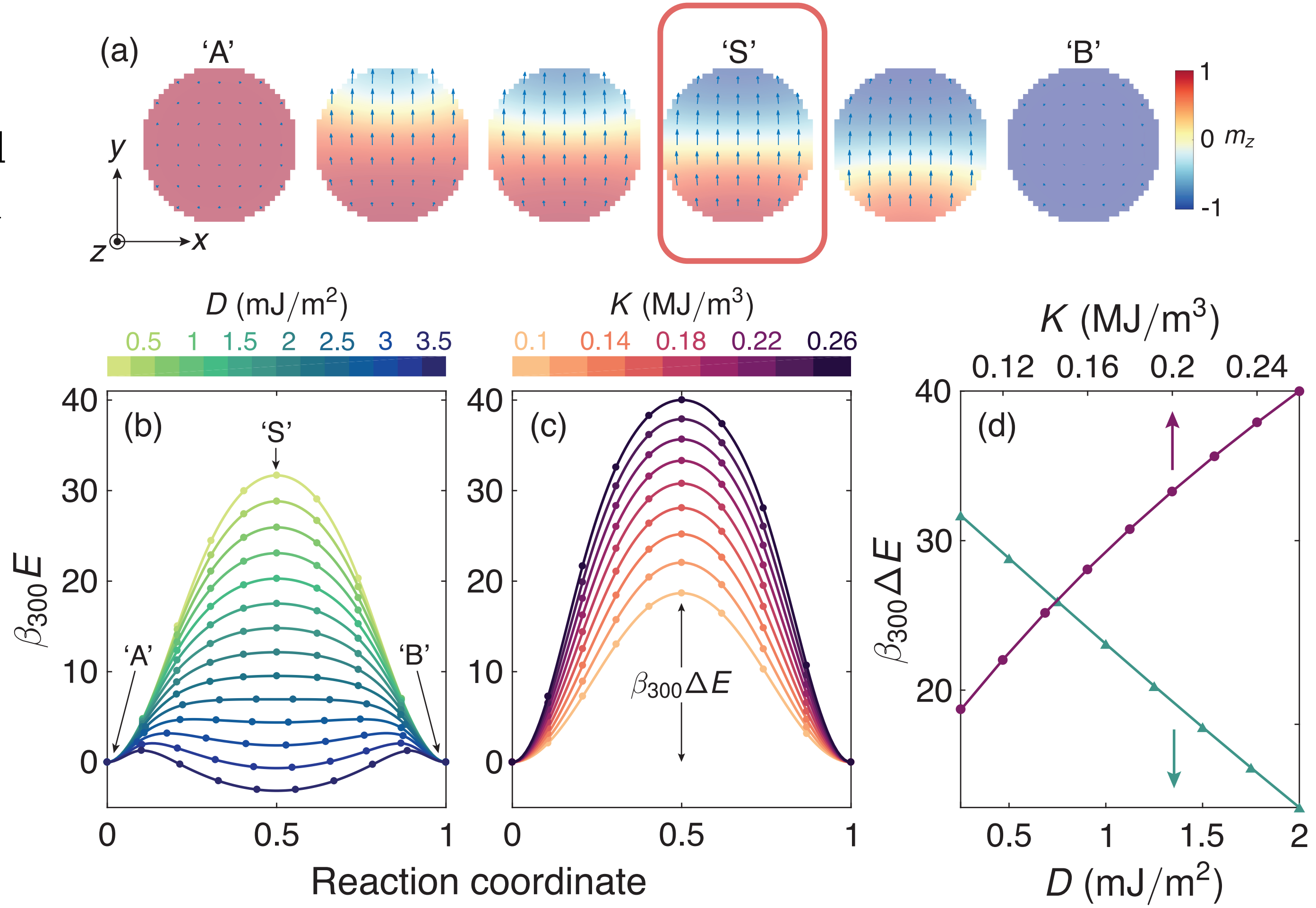
Parameters: Sampaio *et al.* Appl. Phys. Lett., **108**, 112403 (2016)

❖ Reversal pathway

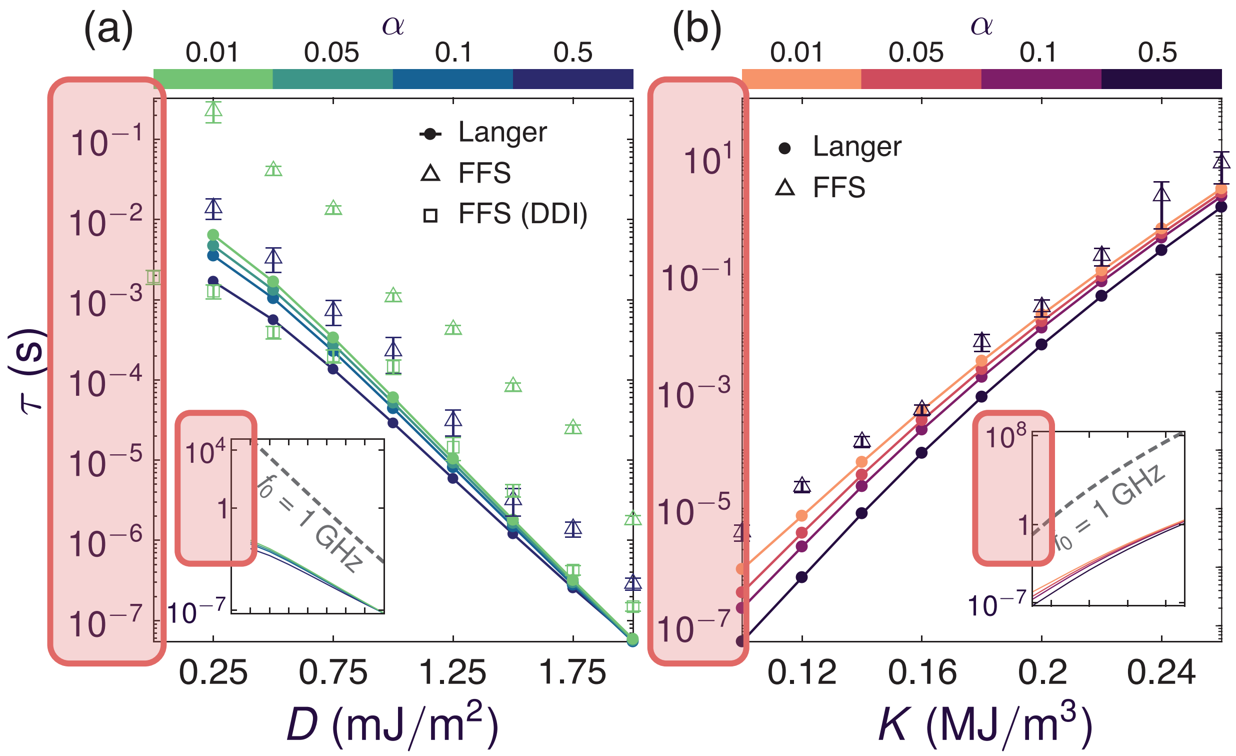
- Nucleation and propagation of a **domain wall**
- **Saddle point** S: wall in the centre of the disk

❖ Energy barriers:

- Varying DMI: $\Delta E \sim D$
- Varying anisotropy: $\Delta E \sim \sqrt{K}$



Desplat & Kim, PRL **125**, 107201 (2020)
Desplat & Kim, *PR Applied* **14**, 064064 (2020)

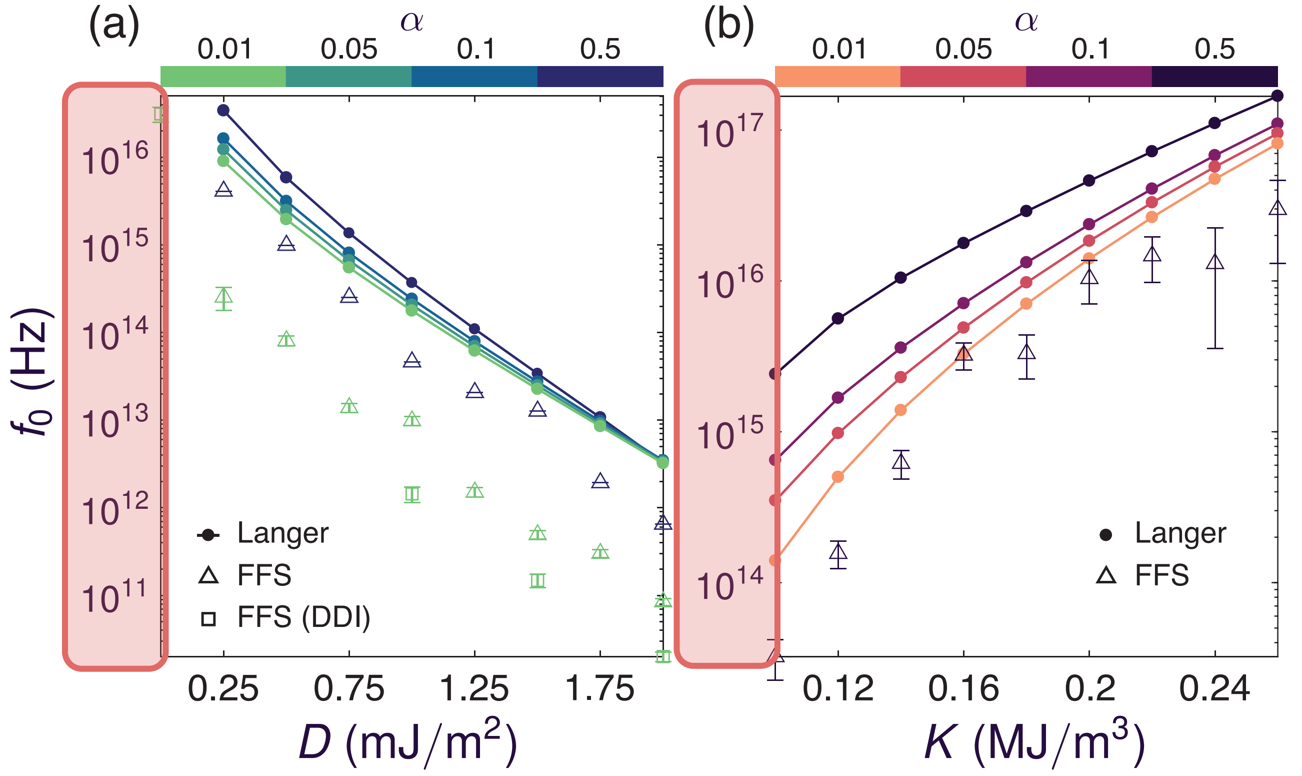


❖ Retention times:

- Qualitative agreement between Langer and FFS
- **Much shorter times than for f_0 ~GHz**

❖ Prefactor:

- **Very large values** (10^{17} s^{-1})
- **Varies over several orders of magnitude** with material parameters



Desplat & Kim, PRL **125**, 107201 (2020)
Desplat & Kim, *PR Applied* **14**, 064064 (2020)

- **Many processes in science:** transport in semiconductors, chemical reactions, biological death rates, etc
- Processes with **large energy barriers** compared to typical excitations in the system
- A family of transitions follows the MN rule if

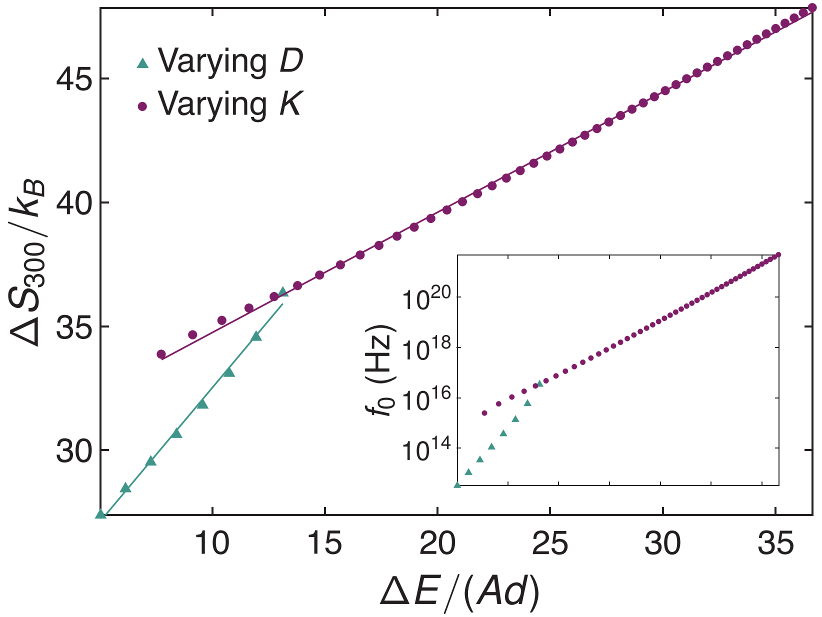
$$f_0 \propto e^{\frac{\Delta E}{E_0}}$$

- Since $\Delta F = \Delta E - T\Delta S$, $\longrightarrow$ $k = f_{00} e^{\frac{\Delta S}{k_B}} e^{-\beta \Delta E}$

and the MN rule follows if

$$\frac{\Delta S}{k_B} \propto \frac{\Delta E}{E_0}$$

ΔF - change in total free energy
ΔS - activation entropy
E_0 - characteristic Meyer-Neldel energy
d - width of the disk
Ad - energy scale of magnons

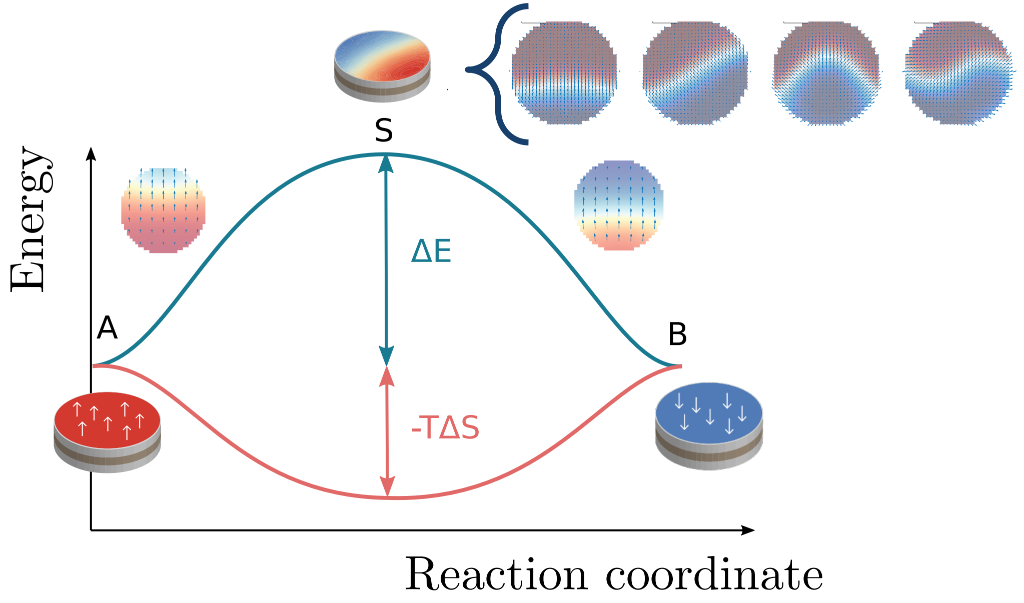


➢ **DW-mediated reversal obeys MN rule**
➢ $f_0 \propto e^{\Delta E}$

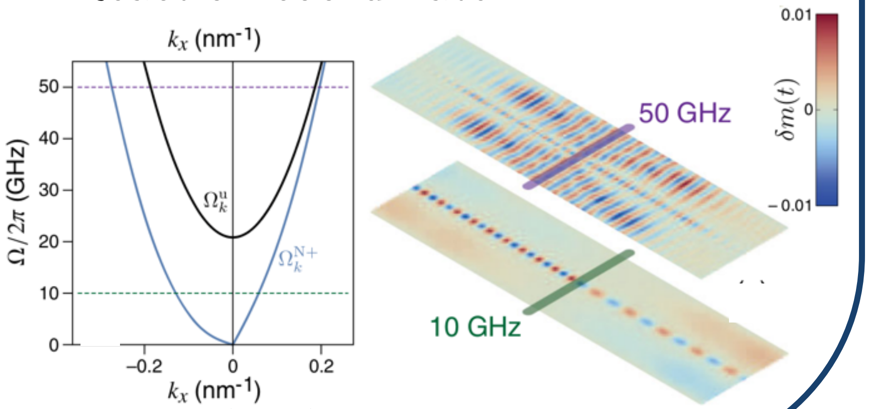
Yelon & Movaghar, *PRL* **65**, 818 (1990)
Yelon *et al.*, *PRB* **46**, 12244 (1992)

Desplat & Kim, *PRL* **125**, 107201 (2020)
Desplat & Kim, *PR Applied* **14**, 064064 (2020)

Large volume available to thermal fluctuations around the saddle point: $\Delta S > 0$

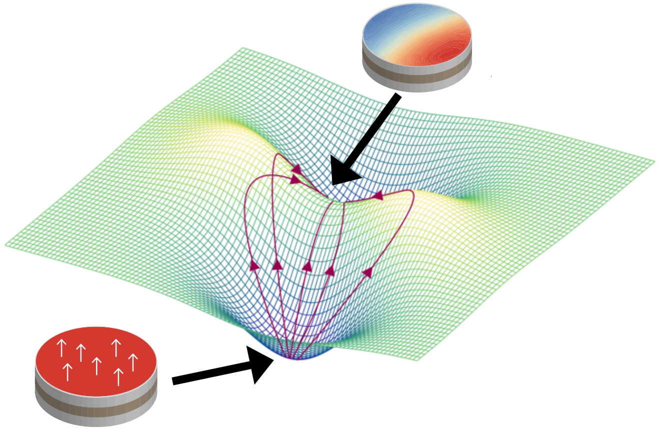


Existence of low-energy magnons propagating along domain walls



Garcia-Sanchez *et al.*, *PRL* **114**, 247206 (2015)

Overcoming a large barrier: **multi-excitation process**



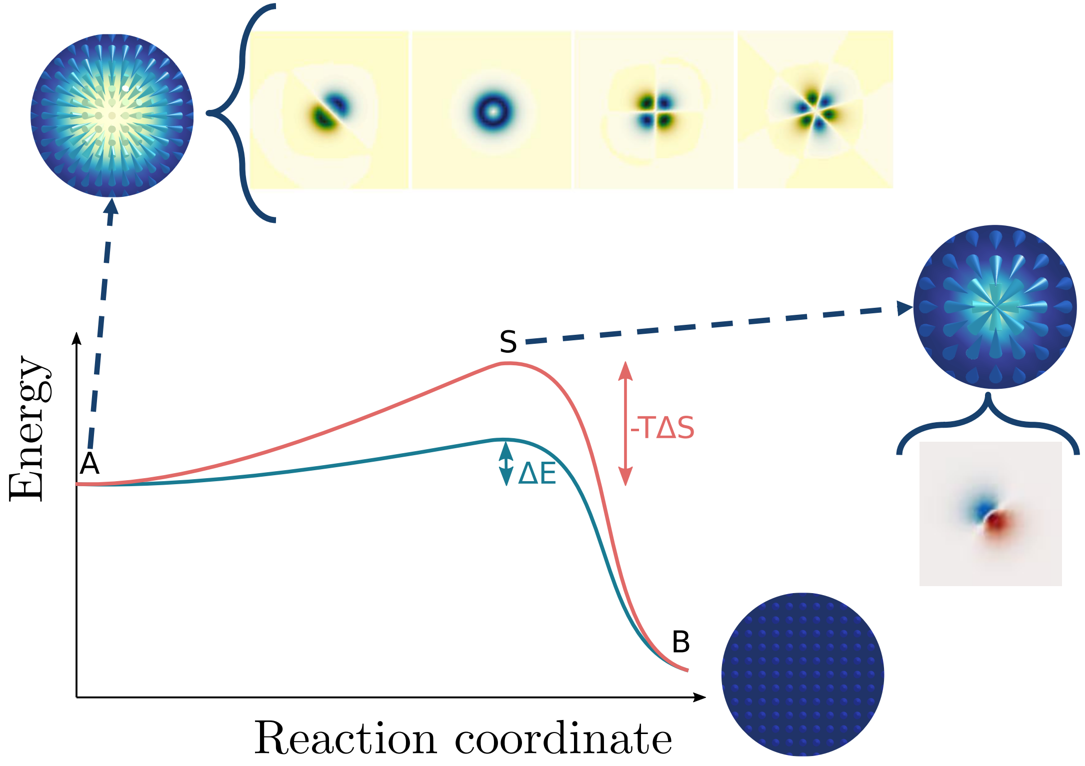
- **Existence of many pathways to the barrier top**
- **Excitation of many magnon modes**

Peacock-Lopez and Suhl, *PRB* **26**, 3774 (1982)
Yelon and Movaghar, *PRL* **65**, 818 (1990)
Yelon *et al.*, *PRB* **46**, 12244 (1992)
Desplat and Kim, *PRL* **125**, 107201 (2020)
Desplat and Kim, *PR Applied* **14**, 064064 (2020)

Conclusion

❖ Skyrmions tend to be stablized by entropy

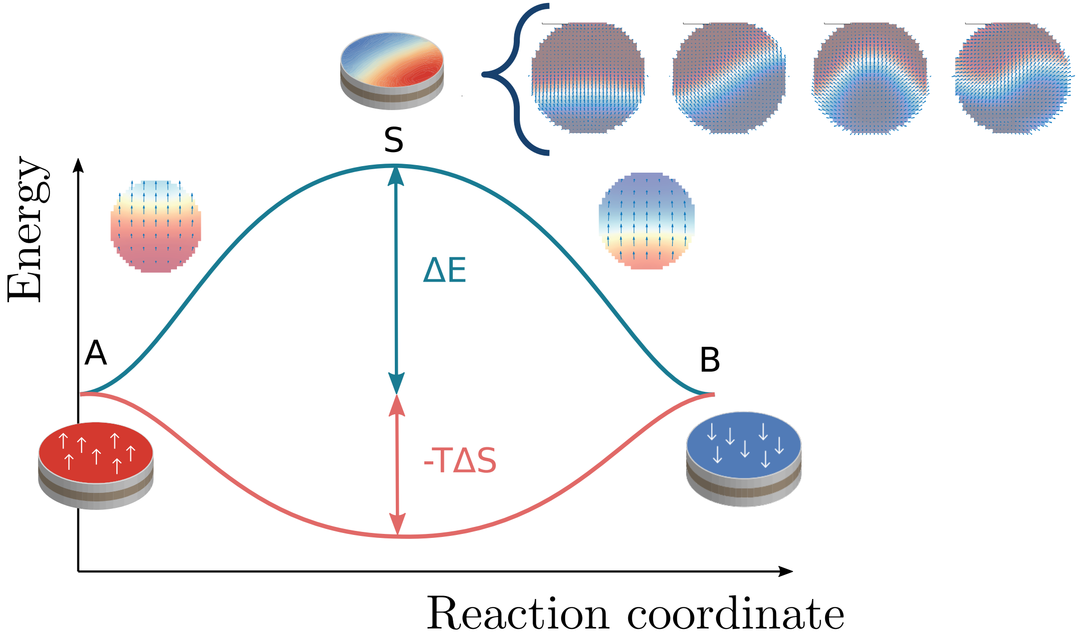
- ➢ Entropic narrowing $\Delta S < 0$



Desplat *et al.* *PRB* **98**, 134407 (2018)
Desplat *et al.* *PRB* **101**, 0604039(R) (2020)

❖ Uniformly magnetized nanodiscs tend to be destabilized by entropy

- ➢ Compensation $\Delta S \propto \Delta E > 0$



Desplat & Kim, *PRL* **125**, 107201 (2020)
Desplat & Kim, *PR Applied* **14**, 064064 (2020)

❖ In both cases: **soliton state is a high entropy state** due to **internal degrees of freedom**