(TD)DFT for noncollinear spins: orbital functionals, semilocal approximations, and xc torques

Carsten A. Ullrich
University of Missouri

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Outline

DFT for noncollinear magnetism:

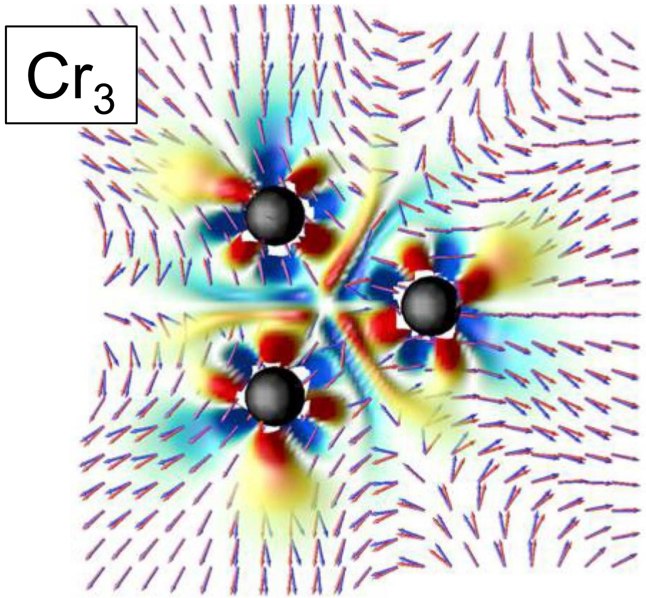
►XC orbital functionals and new meta-GGA
►application to Cr_3 and Cr_5

Significance of XC magnetic torques:

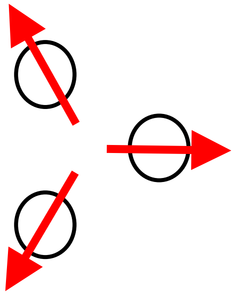
►Spin dynamics in Hubbard clusters with spin frustration

C. A. Ullrich, Phys. Rev. B **98**, 035140 (2018)
C. A. Ullrich, Phys. Rev. A **100**, 012516 (2019)
E. A. Pluhar and C. A. Ullrich, Phys. Rev. B **100**, 125135 (2019)
N. Tancogne-Dejean, A. Rubio, and C. A. Ullrich, Phys. Rev. B **107**, 165111 (2023)
D. Hill, J. Shotton, and C. A. Ullrich, Phys. Rev. B **107**, 115134 (2023)

Motivation I: noncollinear magnetism

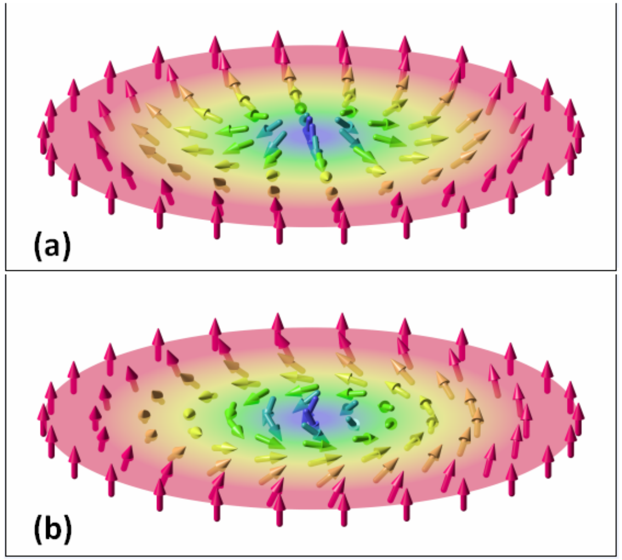


G. Scalmani and M.J. Frisch, JCTC **8**, 2193 (2012)



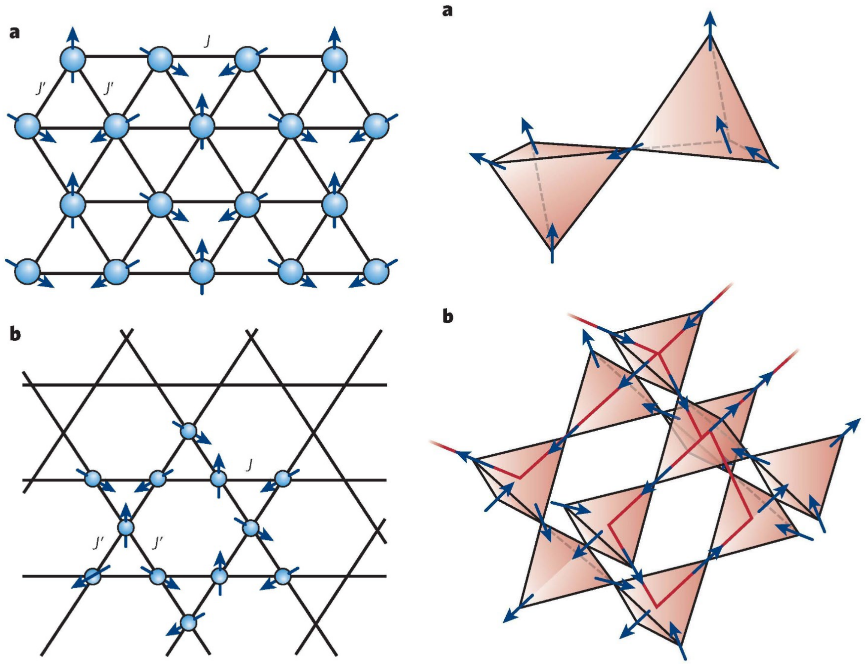
Romming et al., Science **341**, 636 (2013)

skyrmions



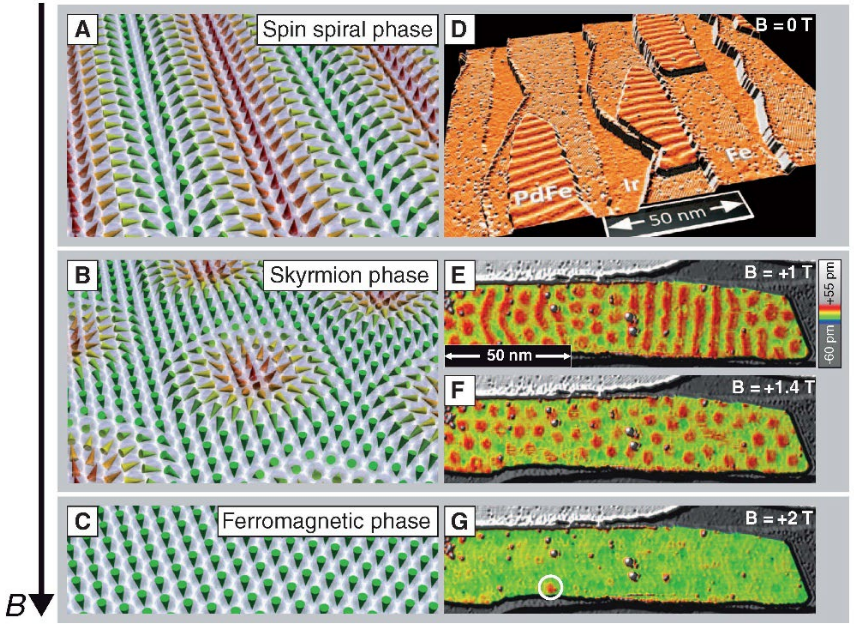
https://en.wikipedia.org/wiki/Magnetic_skyrmion

Many noncollinear magnetic materials exist in nature

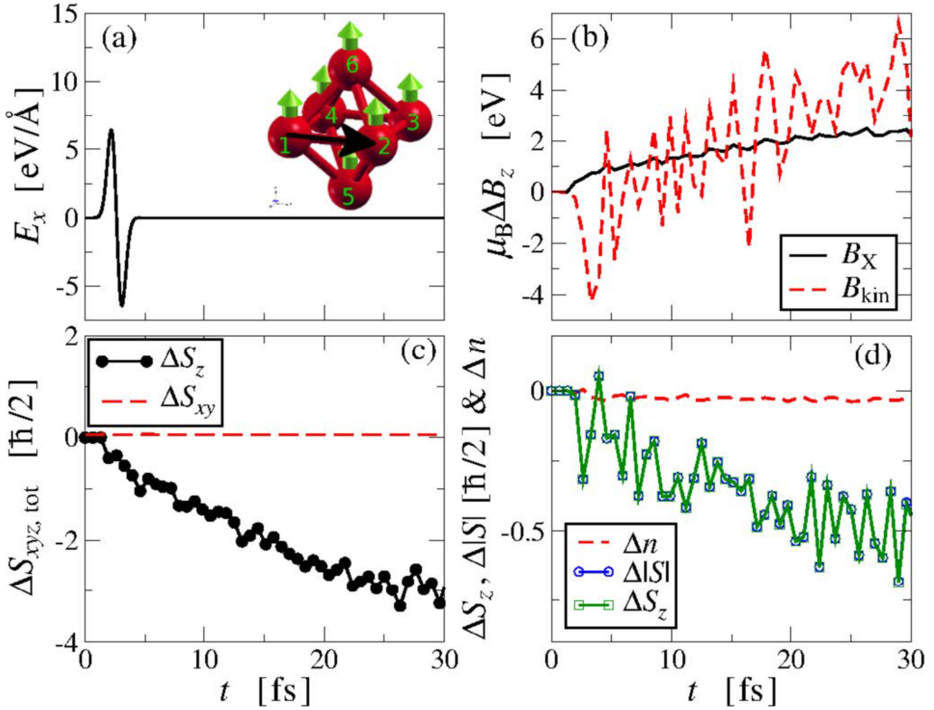


spin frustrations and quantum spin liquids

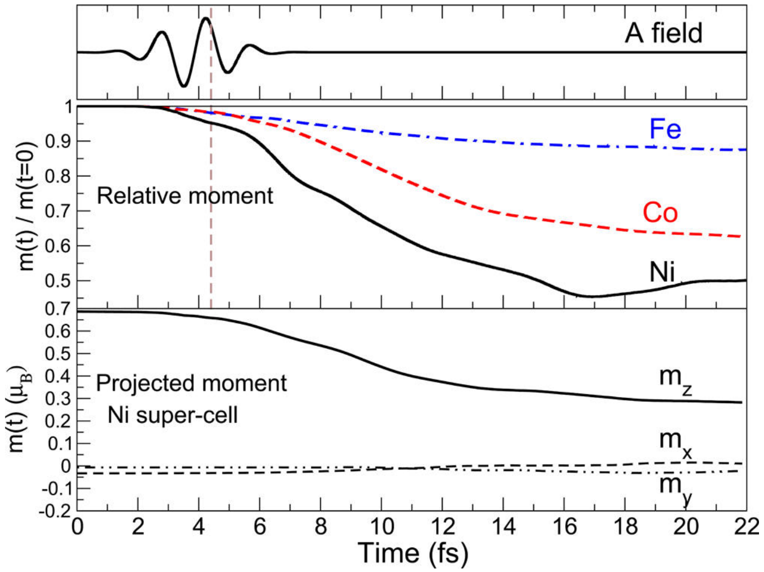
L. Balents, Nature **464**, 199 (2010)



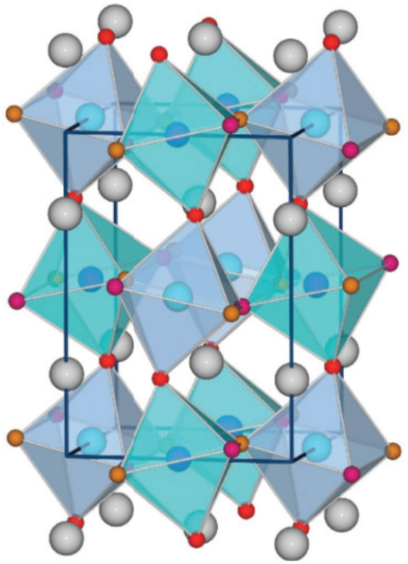
Motivation II: ultrafast spin dynamics and femtomagnetism



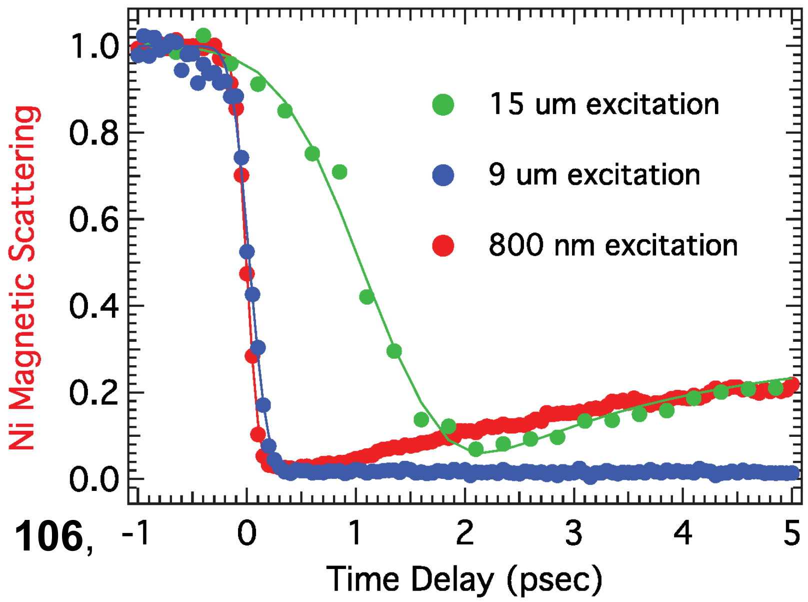
Simoni, Stamenova & Sanvito, PRB **95**, 024412 (2017)



Krieger et al., JCTC **11**, 4870 (2015)



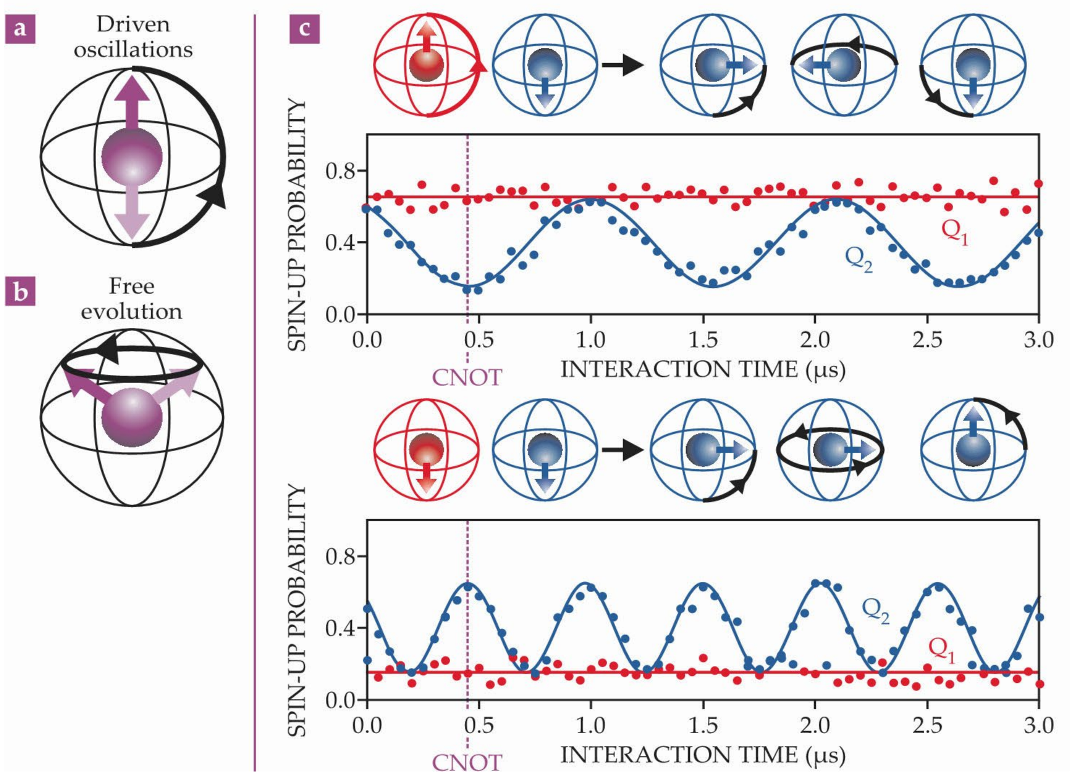
$NdNiO_3$

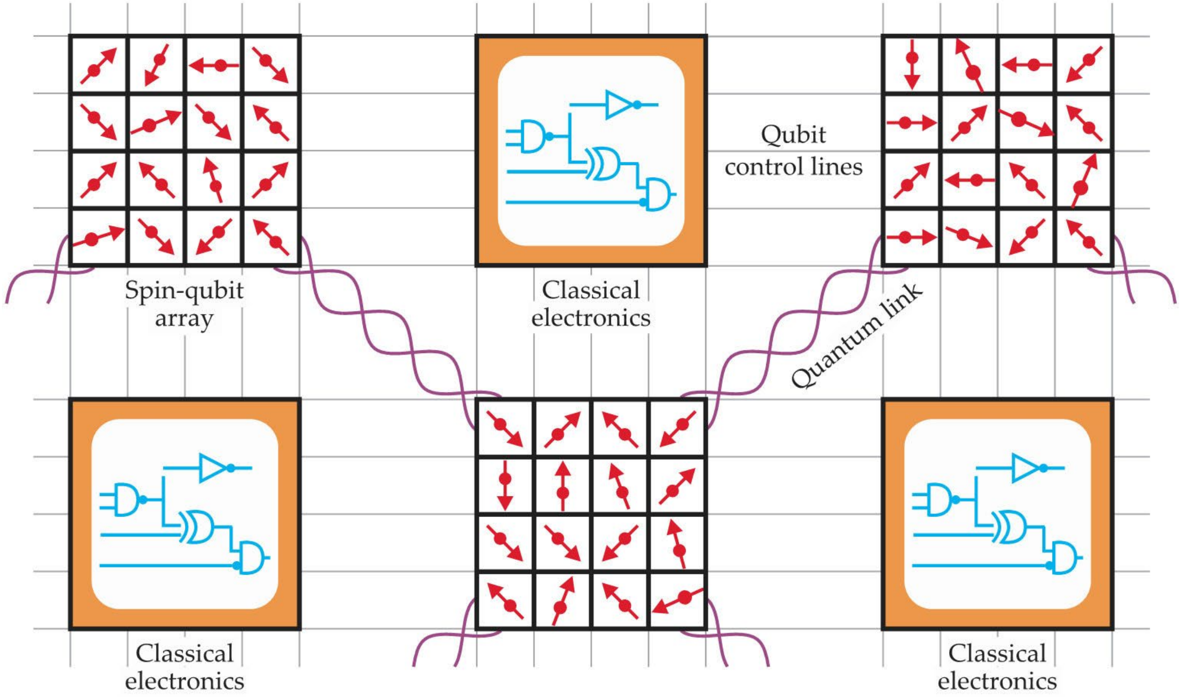


Stoica et al., PRB **106**, 165104 (2022)

Magnetic materials can be controlled by fs laser pulses

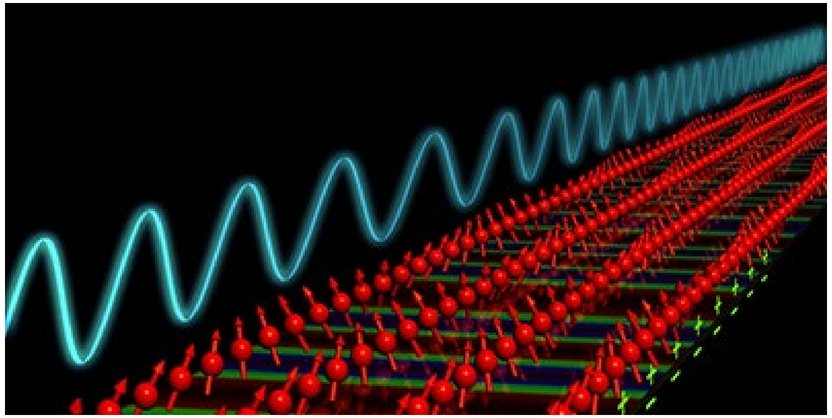
Motivation III: manipulations of spin qubits



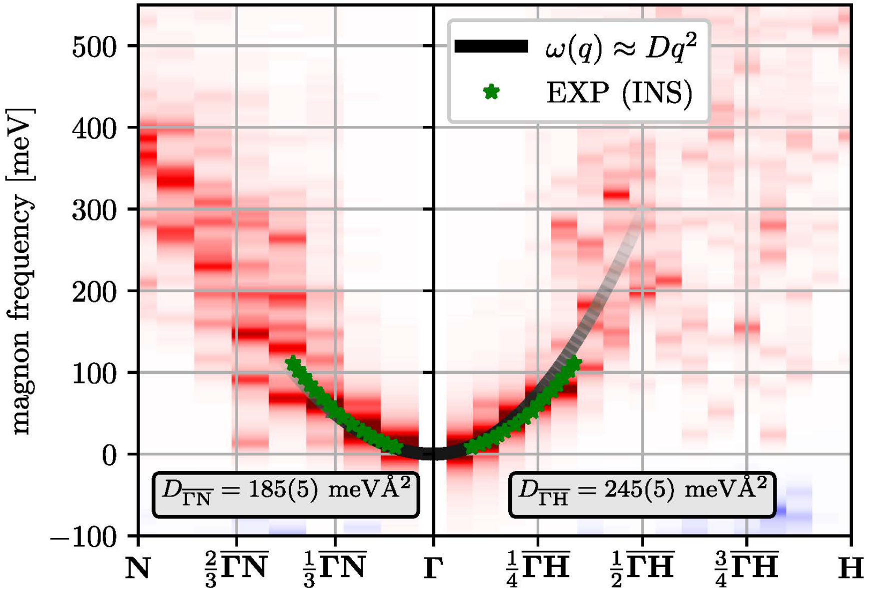


Vandersypen & Eriksson, *Physics Today* **72,** 38-45 (2019)

Motivation IV: spin waves and magnonics

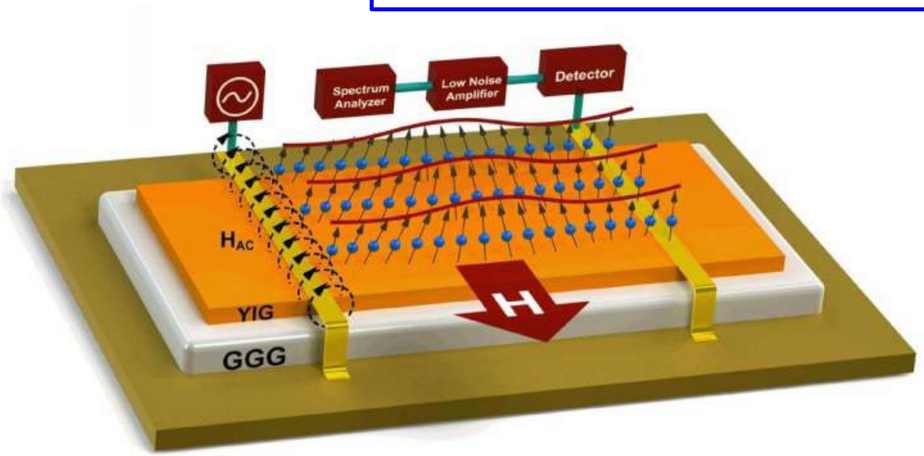


X. Zhang, T. Liu, M. E. Flatté, and H. X. Tang
Phys. Rev. Lett. **113**, 037202 (2014)

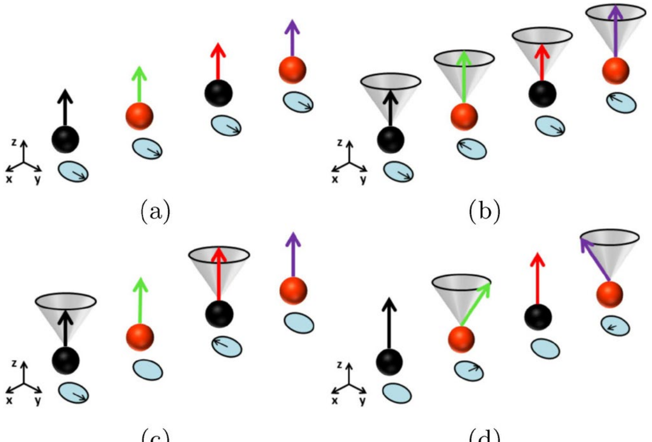


N. Tancogne-Dejean, F.G. Eich & A. Rubio,
JCTC **16**, 1007 (2020)

- ►**Spin waves as carrier of information**
- ►**Need materials with minimal losses**
- ►**LR or RT-TDDFT for magnons**



https://phys.org/news/2019-03-magnonic-devices-electronics-noise.html



N. Singh, P. Elliott, J.K. Dewhurst & S. Sharma,
PRB **103**, 134402 (2021)

DFT for noncollinear spins: interacting system

N-electron system in a magnetic field, acting on spins only:

$$\hat{H} = \sum_{j=1}^{N} \left(-\frac{\nabla_j^2}{2} + V(\mathbf{r}_j) + \boldsymbol{\sigma}_j \cdot \mathbf{B}(\mathbf{r}_j) \right) + \frac{1}{2} \sum_{j \neq k}^{N} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|}$$

($\mathbf{B}$ contains μ_B)

U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972)
O. Gunnarsson and B. I. Lundqvist, PRB **13**, 4274 (1976)
N. I. Gidopoulos, PRB **75**, 134408 (2007)

DFT for noncollinear spins: basic variables

spin-density matrix:

$$\underline{\underline{n}}(\mathbf{r}) = \langle \Psi | \hat{\psi}^\dagger_\beta(\mathbf{r}) \hat{\psi}_\alpha(\mathbf{r}) | \Psi \rangle = \begin{pmatrix} n_{\uparrow\uparrow} & n_{\uparrow\downarrow} \\ n_{\downarrow\uparrow} & n_{\downarrow\downarrow} \end{pmatrix}$$

density: $n(\mathbf{r}) = n_{\uparrow\uparrow}(\mathbf{r}) + n_{\downarrow\downarrow}(\mathbf{r})$

magnetization: $\mathbf{m}(\mathbf{r}) = \mathrm{tr}\{\boldsymbol{\sigma}\, \underline{\underline{n}}(\mathbf{r})\}$

$$\mathbf{m} = \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = \begin{pmatrix} n_{\uparrow\downarrow} + n_{\downarrow\uparrow} \\ i(n_{\uparrow\downarrow} - n_{\downarrow\uparrow}) \\ n_{\uparrow\uparrow} - n_{\downarrow\downarrow} \end{pmatrix}$$

DFT for noncollinear spins: Kohn-Sham equation

2-component spinors:

$$\Psi_i(\mathbf{r}) = \begin{pmatrix} \psi_{i\uparrow}(\mathbf{r}) \\ \psi_{i\downarrow}(\mathbf{r}) \end{pmatrix}$$

v. Barth & Hedin (1972)
Gunnarsson & Lundqvist (1976)

$$\left[\left(-\frac{\nabla^2}{2} + V_{\text{ext+H+xc}}(\mathbf{r})\right) I + \boldsymbol{\sigma}\cdot\mathbf{B}_{\text{ext+xc}}(\mathbf{r})\right]\Psi_i(\mathbf{r}) = \varepsilon_i \Psi_i(\mathbf{r})$$

$$V_{\text{xc}}(\mathbf{r}) = \frac{\delta E_{\text{xc}}[n,\mathbf{m}]}{\delta n(\mathbf{r})}$$

$$\mathbf{B}_{\text{xc}}(\mathbf{r}) = \frac{\delta E_{\text{xc}}[n,\mathbf{m}]}{\delta \mathbf{m}(\mathbf{r})}$$

local xc torque:

$$\boldsymbol{\tau}_{\text{xc}} = \mathbf{m} \times \mathbf{B}_{\text{xc}}$$

Exchange-correlation torque and spin dynamics

Capelle, Vignale & Györffy, PRL **87**, 206403 (2001)

Time evolution of magnetization in many-body system:

$$\frac{d\mathbf{m}(\mathbf{r},t)}{dt} + \nabla \cdot \mathbf{J}(\mathbf{r},t) = \mathbf{m}(\mathbf{r},t) \times \mathbf{B}_{\text{ext}}(\mathbf{r},t)$$

Formally equivalent:

$$\frac{d\mathbf{m}(\mathbf{r},t)}{dt} + \nabla \cdot \mathbf{J}_{KS}(\mathbf{r},t) = \mathbf{m}(\mathbf{r},t) \times \mathbf{B}_{\text{ext+xc}}(\mathbf{r},t)$$

Zero-torque theorem:

$$\int d\mathbf{r}\; \mathbf{m}(\mathbf{r},t) \times \mathbf{B}_{\text{xc}}(\mathbf{r},t) = 0$$

Some approximations may violate ZTT, but the ZTT can be enforced as constraint.
Pluhar and Ullrich, Phys. Rev. B **100**, 125135 (2019)

DFT for noncollinear spins: LSDA

Assume local spin quantization axis (Kübler 1988, Sandratskii 1998):

$$\mathbf{B}_{\mathrm{xc}}^{\mathrm{LSDA}}(\mathbf{r}) = \frac{\delta E_{\mathrm{xc}}^{\mathrm{LSDA}}[n,\mathbf{m}]}{\delta \mathbf{m}(\mathbf{r})}$$

$$\equiv \left.\frac{\partial e_{\mathrm{xc}}^{\mathrm{unif}}(\overline{n},\overline{m})}{\partial \overline{m}}\right|_{\substack{\overline{n}=n(\mathbf{r})\\ \overline{m}=m(\mathbf{r})}} \frac{n(\mathbf{r})\mathbf{m}(\mathbf{r})}{m(\mathbf{r})}$$

$\mathbf{B}_{\mathrm{xc}}^{\mathrm{LSDA}}(\mathbf{r})$ **is always parallel to** $\mathbf{m}(\mathbf{r})$

$$\Rightarrow \boldsymbol{\tau}_{\mathrm{xc}}^{\mathrm{LSDA}} = 0$$

Density functionals with local xc torque

►Spin-spiral reference state of homogeneous electron gas

M.I. Katsnelson and V.P. Antropov, PRB **67**, 140406 (2003)
F.G. Eich and E.K.U. Gross, PRL **111**, 156401 (2013)

►GGAs for noncollinear spin systems

Scalmani & Frisch, JCTC **8**, 2193 (2012)
Bulik, Scalmani, Frisch & Scuseria, PRB **87**, 035117 (2013)
Pu et al., Phys. Rev. Res. **5**, 013036 (2023)
} upgrade existing GGAs

Eich, Pittalis & Vignale, PRB **88**, 245102 (2013)
Pittalis, Vignale & Eich, PRB **96**, 035141 (2017)
Tancogne-Dejean, Rubio & Ullrich, PRB **107**, 165111 (2023)
} new (m)GGAs

►Source-free LSDA

Sharma, Gross, Sanna & Dewhurst, JCTC **14**, 1247 (2018)
Dewhurst, Sanna & Sharma, EPJB **91**, 218 (2018)

►Orbital functionals:

- **no reference system (electron gas) needed**
- **works for Hubbard model and real materials alike**
- **will produce xc torques**

$$E_x = -\frac{1}{2}\int\int \frac{d\mathbf{r}d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\mathrm{Tr}\left[\underline{\underline{\gamma}}(\mathbf{r},\mathbf{r}')\underline{\underline{\gamma}}(\mathbf{r}',\mathbf{r})\right]$$

Can construct local EXX potential via OEP or KLI

Krieger, Li & Iafrate, PRA **45**, 101 (1992)
Sharma et al., PRL **98**, 196405 (2007)

Noncollinear Slater potential:

$$\underline{\underline{V}}_x^S(\mathbf{r})\underline{\underline{n}}(\mathbf{r}) + \underline{\underline{n}}(\mathbf{r})\underline{\underline{V}}_x^S(\mathbf{r}) = -2\int \frac{d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\underline{\underline{\gamma}}(\mathbf{r},\mathbf{r}')\underline{\underline{\gamma}}(\mathbf{r}',\mathbf{r})$$

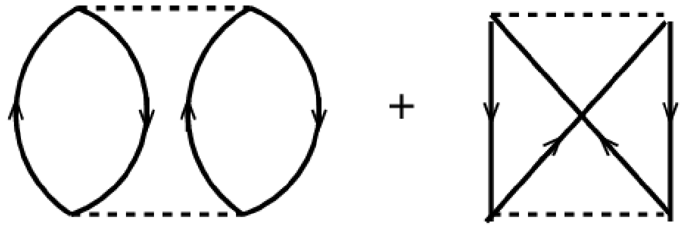
C.A. Ullrich, PRB **98**, 035140 (2018)

Orbital-dependent correlation functionals

► **Self-interaction correction (Perdew-Zunger):**

$$E_{\rm xc}^{\rm SIC}[n,\mathbf{m}] = E_{\rm xc}^{\rm approx}[n,\mathbf{m}] - \sum_j \left(E_{\rm H}[n_j] + E_{\rm xc}^{\rm approx}[n_j,\mathbf{m}_j] \right)$$

► **Many-body perturbation theory (MP2 or GL2)**



► **Functionals based on 2-body density matrix**

$$E_{\rm c} = W[\underline{\underline{\gamma}}_2] - E_{\rm H}[n] - E_{\rm x}[\underline{\underline{\gamma}}]$$

Colle & Salvetti (1975)

► **STLS: based on fluctuation-dissipation theorem**

Singwi, Sjölander, Tosi & Land, PR **176**, 589 (1968)
C. A. Ullrich, Phys. Rev. B **98**, 035140 (2018)

Noncollinear (meta)-GGAs: exchange

S. Pittalis, G. Vignale & F. G. Eich, Phys. Rev. B **96**, 035141 (2017)
N. Tancogne-Dejean, A. Rubio, and C. A. Ullrich, Phys. Rev. B **107**, 165111 (2023)

Exact U(1)xSU(2) invariant exchange energy:

$$E_{\mathrm{x}} = -\frac{1}{2}\int\int \frac{d\mathbf{r}d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\mathrm{Tr}\left[\underline{\underline{\gamma}}(\mathbf{r},\mathbf{r}')\underline{\underline{\gamma}}(\mathbf{r}',\mathbf{r})\right]$$

Rewrite this in terms of exchange hole:

$$E_{\mathrm{x}} = -\frac{1}{2}\int d\mathbf{r}n(\mathbf{r})\int d\mathbf{r}'\frac{h_x(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \qquad h_x(\mathbf{r},\mathbf{r}') = \frac{\mathrm{Tr}\left[\underline{\underline{\gamma}}(\mathbf{r},\mathbf{r}')\underline{\underline{\gamma}}(\mathbf{r}',\mathbf{r})\right]}{n(\mathbf{r})}$$

Idea:
- follow Becke and Roussel, PRA **39,** 3761 (1989)
- short-range expansion of spherical average of exchange hole
- gauge invariant, recovers collinear limit and homogeneous limit

Noncollinear (meta)-GGAs: exchange

Spherical average of effective exchange hole (s = radius):

$$h_x(s) = n\zeta_x + s^2 k_F^2 \left[\frac{2}{3} q - \frac{\gamma}{5} \alpha \right]$$

$$\zeta_x(\mathbf{r}) = \frac{1}{2}\left(1 + \frac{|\mathbf{m}(\mathbf{r})|^2}{n(\mathbf{r})^2} \right)$$

spin polarization factor

$$\alpha = (\bar{\tau} - \tau^W) \big/ \bar{\tau}^{unif}$$

iso-orbital indicator

$$q = \nabla^2 n \big/ 4k_F^2 n \zeta_x$$

reduced gradient

Gauge invariant kinetic energy density:

$$2n\bar{\tau} = \mathrm{Tr}\left[\underline{\underline{n}}\,\underline{\underline{\tau}} + \underline{\underline{\tau}}\,\underline{\underline{n}} - 2i\nabla(\underline{\underline{n}}\,\underline{\underline{j}} + \underline{\underline{j}}\,\underline{\underline{n}}) - 2\underline{\underline{\mathbf{j}}}\cdot\underline{\underline{\mathbf{j}}} \right]$$

$$+\sum_\sigma \left[n_{\sigma\sigma}\nabla^2 n_{\bar{\sigma}\bar{\sigma}} - \Re(n_{\sigma\bar{\sigma}}\nabla^2 n_{\bar{\sigma}\sigma}) - \frac{1}{2}|\nabla n_{\sigma\bar{\sigma}}|^2 + \frac{1}{2}\nabla n_{\sigma\sigma}\cdot\nabla n_{\bar{\sigma}\bar{\sigma}} \right]$$

Noncollinear (meta)-GGAs: exchange

Fitting the averaged exchange hole with a hydrogenic model:

$$E_x = -3\frac{(3\pi^2)^{1/3}}{4\pi}\int d\mathbf{r}\, n(\mathbf{r})^{4/3}\zeta_x(\mathbf{r})^{1/3}F_x(\mathbf{r})$$

$$F_x(\mathbf{r}) = \frac{4\pi^{2/3}e^{x(\mathbf{r})/3}}{3^{4/3}x(\mathbf{r})}\left[1 - e^{-x(\mathbf{r})}\left(1 - \frac{x(\mathbf{r})}{2}\right)\right]$$

enhancement factor (x comes from the hydrogenic fitting of h_x, see Becke-Roussel)

S. Pittalis, G. Vignale & F. G. Eich, Phys. Rev. B **96**, 035141 (2017)

Noncollinear (meta)-GGAs: correlation

Colle & Salvetti (1975):

$$E_c = -4a\int d\mathbf{r}\,\frac{\rho_2(\mathbf{r},\mathbf{r})}{n(\mathbf{r})}\left[\frac{1+br_s^8(\mathbf{r})[\nabla_s^2\rho_2(\mathbf{r},\mathbf{s})]_{s=0}\,e^{-cr_s(\mathbf{r})}}{1+dr_s(\mathbf{r})}\right]$$

approximate the 2-body RDM as

$$\rho_2^{HF}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{2}\left[n(\mathbf{r}_1)n(\mathbf{r}_2) - \mathrm{Tr}[\underline{\underline{\gamma}}(\mathbf{r}_1,\mathbf{r}_2)\underline{\underline{\gamma}}(\mathbf{r}_2,\mathbf{r}_2)]\right]$$

Then follow the derivation by Lee, Yang & Parr (LYP) (1988)

R. Colle and O. Salvetti, Theor. Chim. Acta **37**, 329 (1975)
C. Lee, W. Yang, and R. G. Parr, Phys. Rev. B **37**, 785 (1988)

Noncollinear (meta)-GGAs: correlation

$$E_c = -a\int d\mathbf{r}\, n\zeta_c^{\,2}\left[\frac{1+(br_s^5/2)\left[\bar{\tau}+(|\nabla\mathbf{m}|/4n)-3\tau^W\right]e^{-cr_s}}{1+dr_s}\right]$$

$$\zeta_c(\mathbf{r}) = 1-\frac{|\mathbf{m}(\mathbf{r})|^2}{n(\mathbf{r})^2}$$

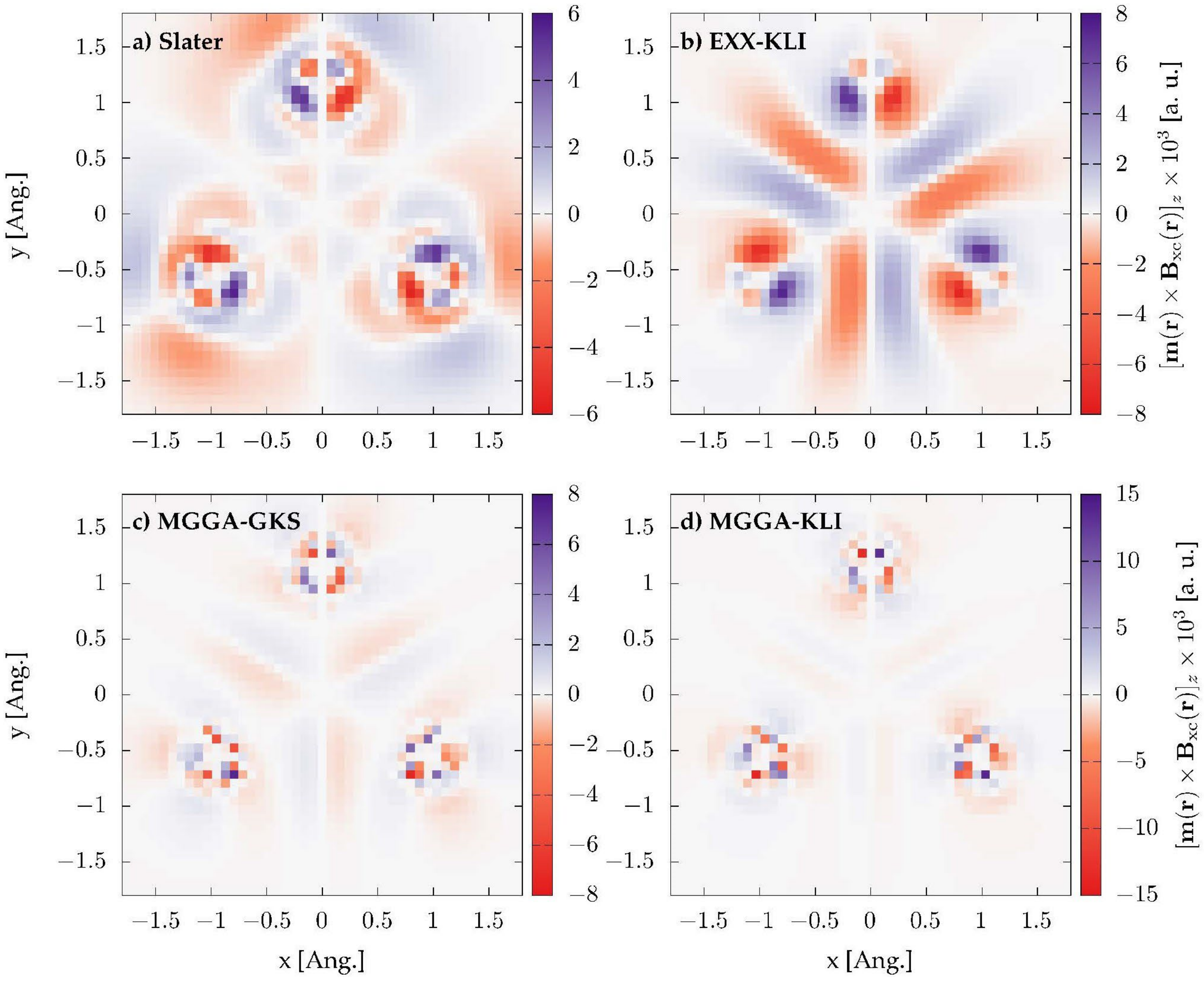
rescaled LYP parameters:

$a = 0.04918 \quad b = 0.132(4\pi/3)^{8/3}$

$c = 0.2533(4\pi/3)^{1/3} \quad d = 0.349(4\pi/3)^{1/3}$

Note: to convert this into a GGA requires 2nd order gradient expansion of $\bar{\tau}$ which must preserve gauge invariance (future work)

Exchange torque: comparison with Slater and EXX for Cr_3



Real-space calculation with Octopus

Grid spacing 0.1 Bohr

HGH fully relativistic pseudopotentials

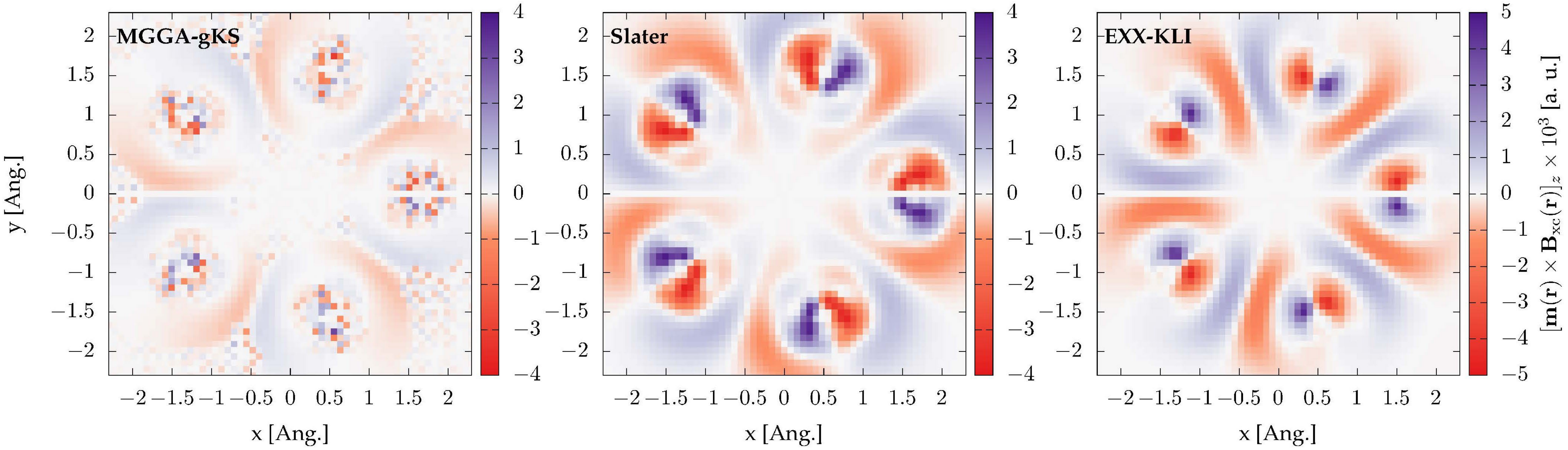
Similar magnitude as Slater and EXX
Similar shape around the atoms

Improved magnetic moments and ionization energy compared to LSDAx

Sign not correct in the interstitial region: failure of the short-range expansion
Path toward further improvements

N. Tancogne-Dejean, A. Rubio, and C. A. Ullrich, Phys. Rev. B **107**, 165111 (2023)

Exchange torque: comparison with Slater and EXX for Cr_5



Same conclusions as for Cr_3:

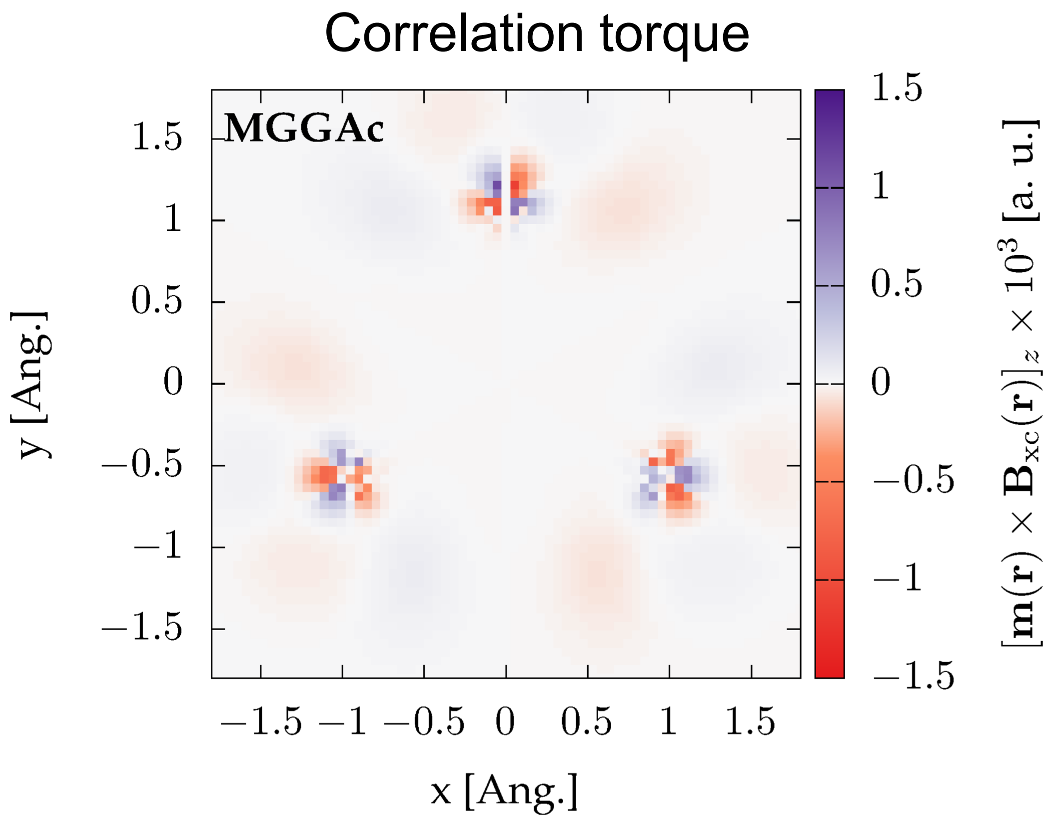
- Similar magnitude as Slater and EXX
- Similar shape around the atoms
- Improved magnetic moments and ionization energy compared to LSDAx
- Sign not correct in the interstitial region

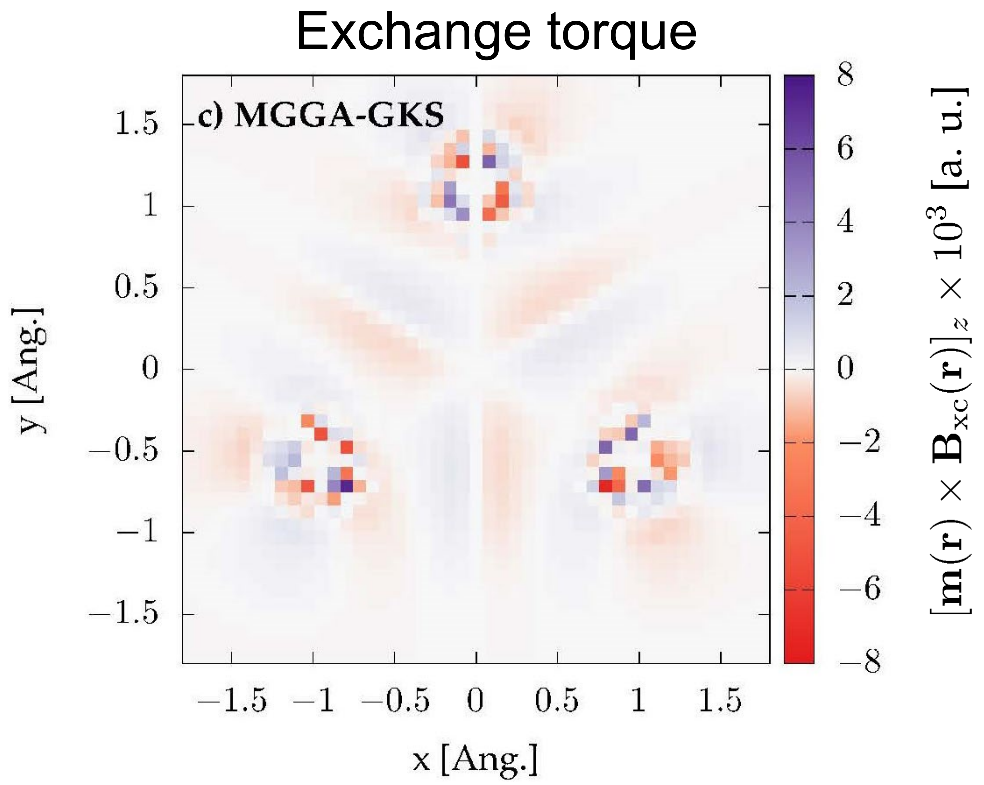
Noncollinear (meta)-GGAs: test for Cr clusters

TABLE I. Local magnetic moment $|\mathbf{m}|$, in μ_B, and ionization potential I_p, in eV, of the Cr atoms in Cr_3 obtained for different levels of theory (see text).

Functional	$\|\mathbf{m}\|$	I_p
LSDA	1.67	2.90
LSDAx	2.66	2.30
LSDAx+MGGAc-gKS	1.81	2.60
MGGAx+MGGAc-gKS ($\gamma = 0.8$)	2.30	4.61
MGGAx-gKS ($\gamma = 0.8$)	3.04	3.65
MGGAx-gKS ($\gamma = 1$)	3.07	3.53
MGGAx-KLI ($\gamma = 0.8$)	3.09	3.59
MGGAx-KLI ($\gamma = 1$)	3.14	3.47
Slater	3.48	6.52
EXX-KLI	3.81	4.68
Hartree-Fock	3.86	4.86

Correlation torque vs exchange torque for Cr_3



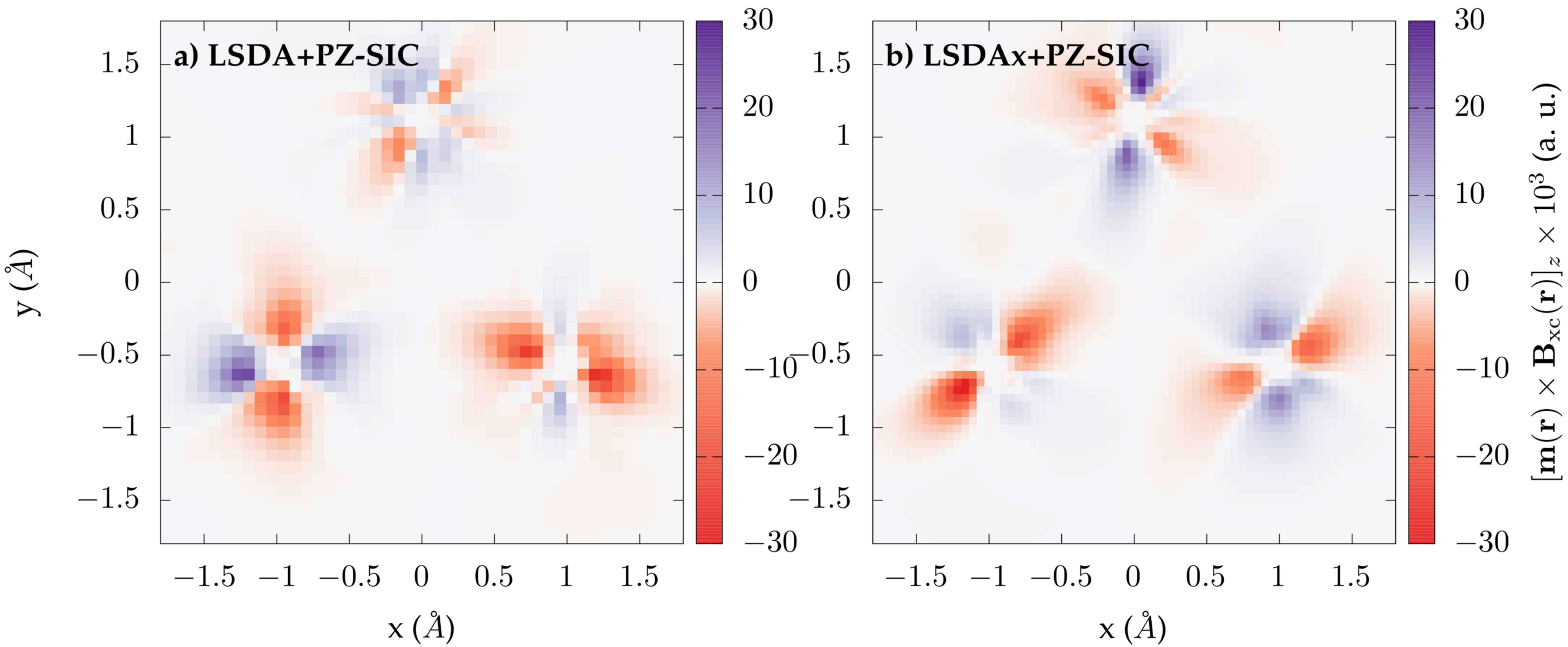


Correlation torque:
- smaller magnitude,
- more localized around nuclei
- opposite sign of exchange torque

} intricate interplay between X and C torques

N. Tancogne-Dejean, A. Rubio, and C. A. Ullrich, Phys. Rev. B **107**, 165111 (2023)

Preliminary test of noncollinear PZ-SIC



- ▶Large difference between LSDA-SIC and LSDAx-SIC
- ▶quite different from EXX (torques seem a bit high)
- ▶zero-torque theorem?

N. Tancogne-Dejean and C. A. Ullrich, unpublished

Some questions

1. How good are approximate xc functionals compared to exact benchmark solutions?

2. What is the significance of xc torques for noncollinear spins and their dynamics?

Small Hubbard clusters are ideal model systems to study this!

The extended Hubbard model

$$\hat{H} = -t \sum_{\langle k,l \rangle \sigma} [\hat{c}^{+}_{k\sigma}\hat{c}_{l\sigma} + \hat{c}^{+}_{l\sigma}\hat{c}_{k\sigma}] + U_0 \sum_{k} \hat{c}^{+}_{k\uparrow}\hat{c}_{k\uparrow}\hat{c}^{+}_{k\downarrow}c_{k\downarrow}$$

$$+U_1 \sum_{\langle k,l \rangle} (\mathbf{c}^{\dagger}_{k}\mathbf{c}_{k})(\mathbf{c}^{\dagger}_{l}\mathbf{c}_{l}) + \sum_{k} \left[V_k \mathbf{c}^{\dagger}_{k}\mathbf{c}_{k} + \mathbf{B}_k \cdot \mathbf{c}^{\dagger}_{k}\boldsymbol{\sigma}\mathbf{c}_{k} \right]$$

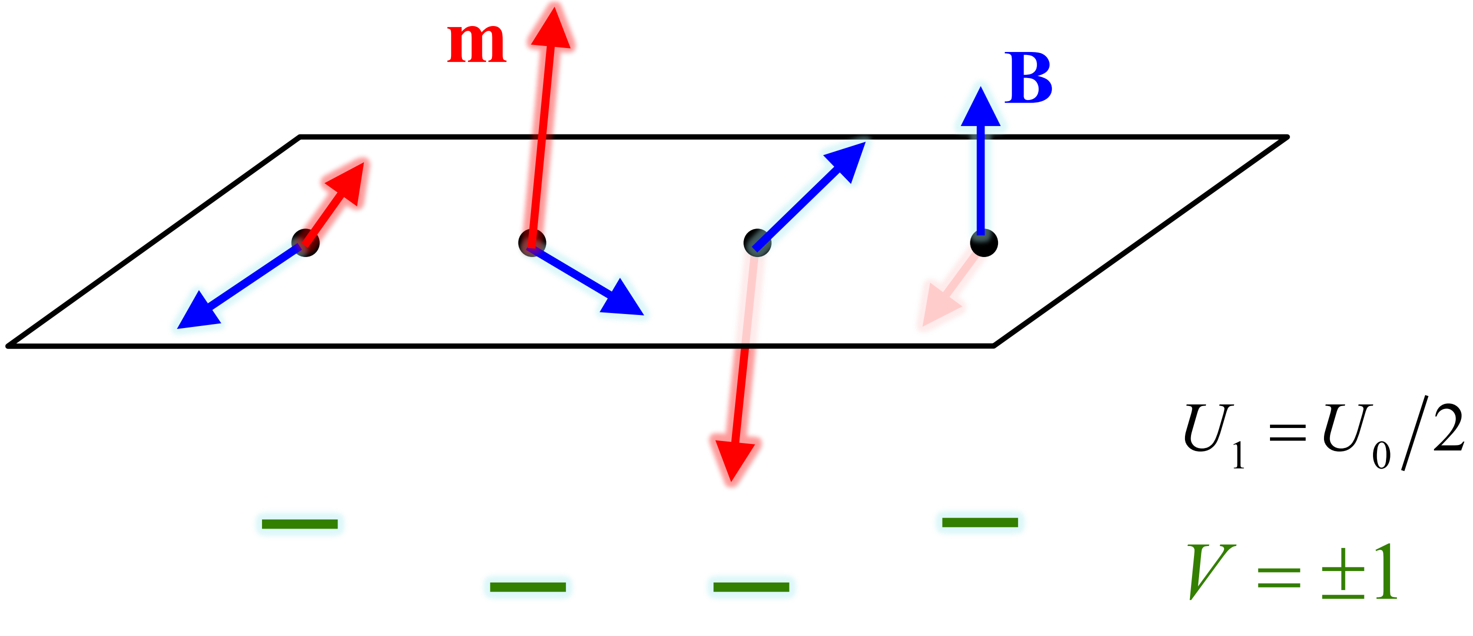
Why include nearest-neighbor interaction U_1?

Using only U_0 exchange becomes trivial:

$$V_{x,k} = -U_0 n_k$$

$$\mathbf{B}_{x,k} = -U_0 \mathbf{m}_k \quad \Rightarrow \quad \textbf{no x-torque!}$$

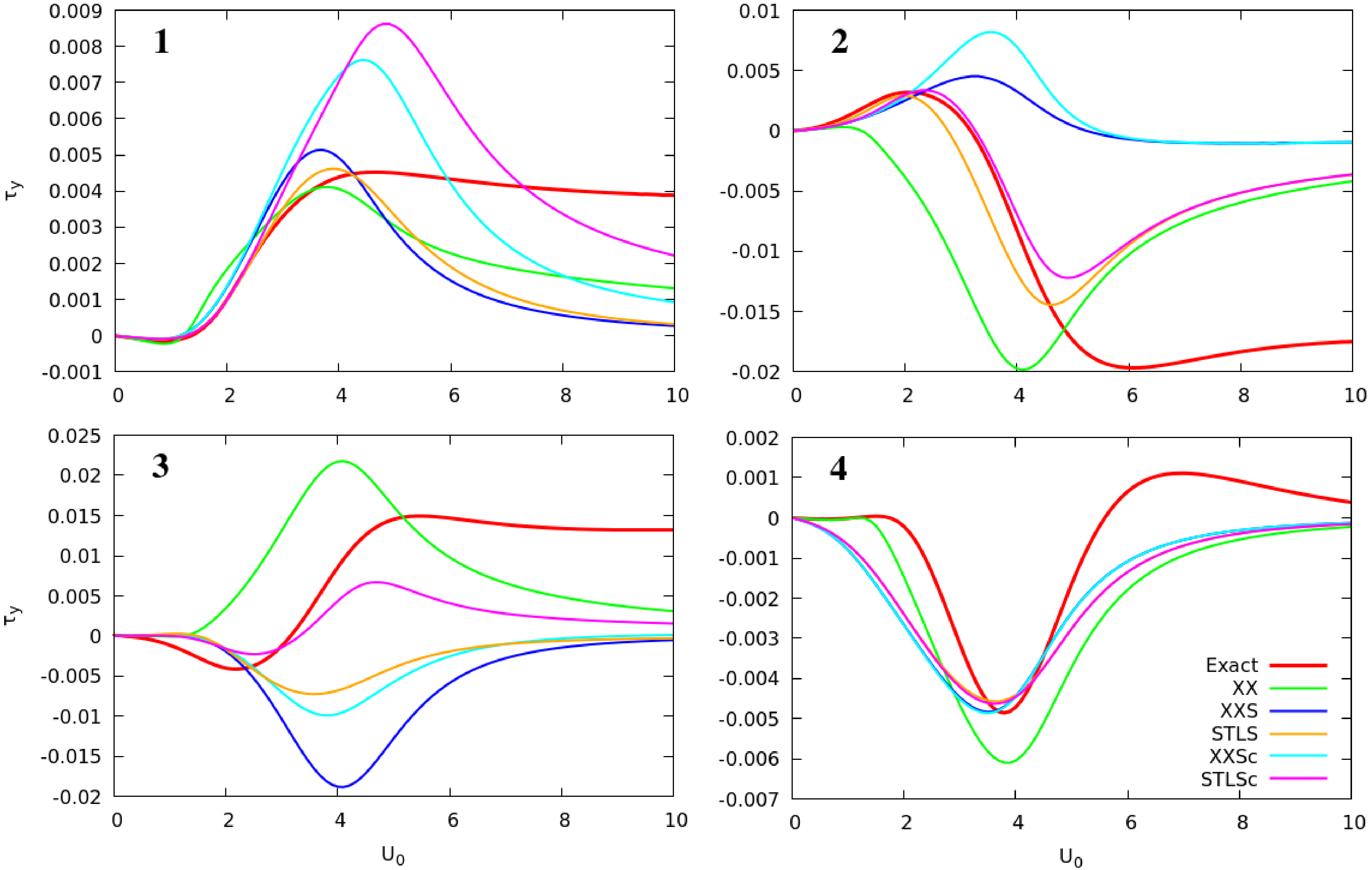
Hubbard tetramer, 2 electrons, NN interactions



►Hubbard model, only U_0: xc torque is **purely correlation**
C.A. Ullrich, PRB **98**, 035140 (2018)

►NN interaction U_1: xc torque can have **exchange contributions**
(first fully nontrivial case: tetramer)
E. A. Pluhar and C. A. Ullrich, Phys. Rev. B **100**, 125135 (2019)

Exact vs approximate xc torques



Approximations are reasonable for moderate interaction strengths.

XC torques in the ground state

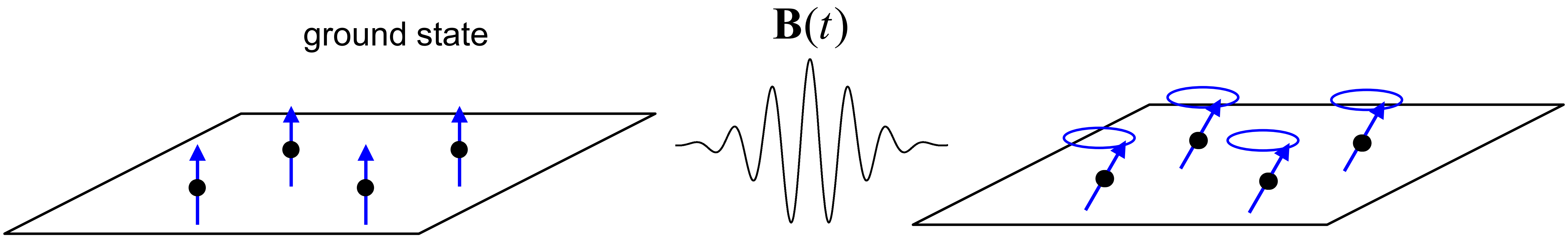
► Play a minor role for total energies
(contribute only within 2nd order perturbation theory)

► Become more important after crossover into
strongly correlated regime (symmetry!)

► The approximations considered appear reasonable
as long as the correlations remain moderate

E. A. Pluhar and C. A. Ullrich, Phys. Rev. B **100**, 125135 (2019)

Spin dynamics



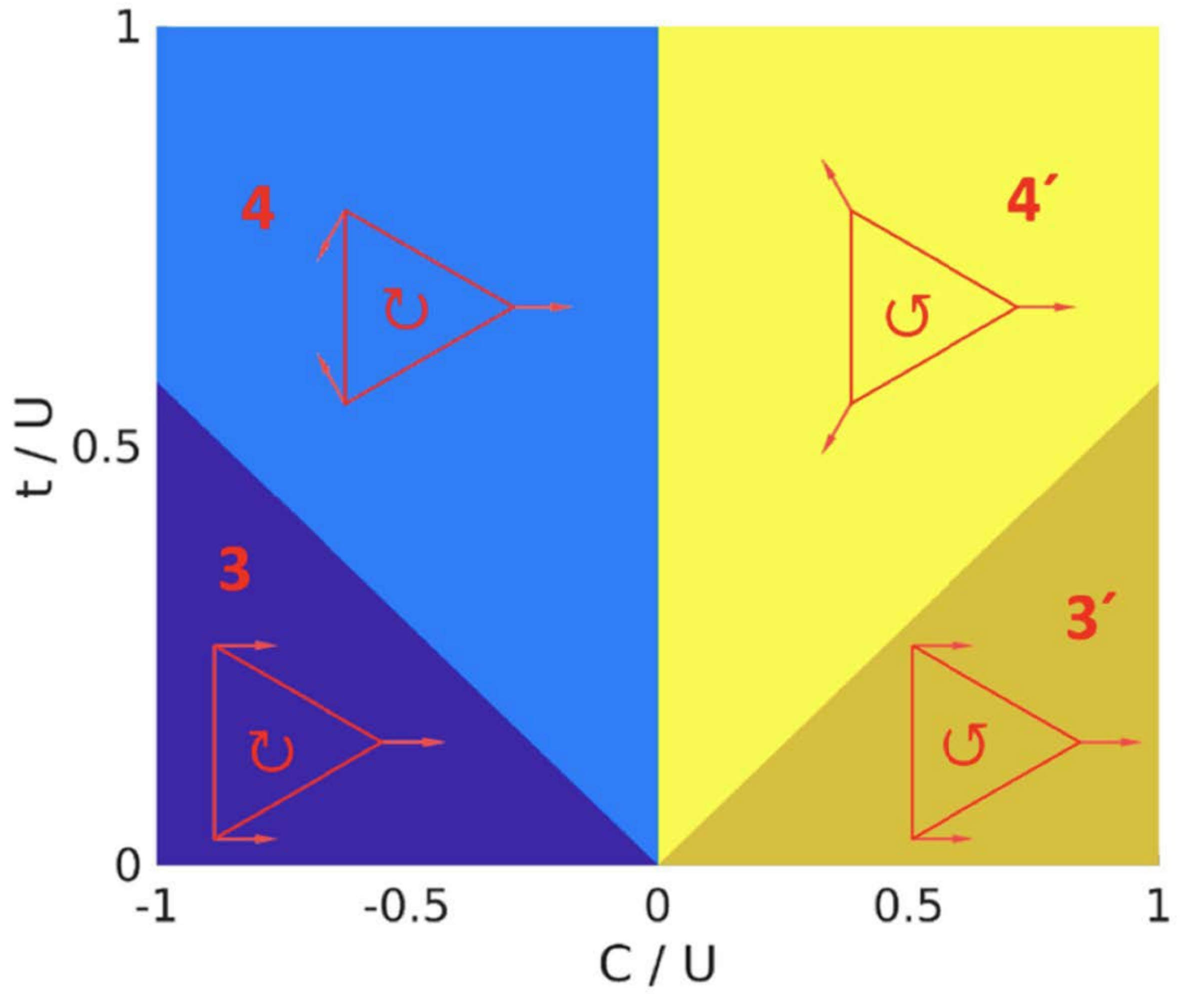
► **Consider intrinsically noncollinear systems**

► **Role of correlations and xc torques?**

► **Symmetries and symmetry breaking: extra sensitivity?**

D. Hill, J. Shotton, and C. A. Ullrich, Phys. Rev. B **107**, 115134 (2023)

Frustrated spins on half-filled Hubbard trimer



Tabrizi, Arbuznikov & Kaupp, J. Phys. Chem. A **123**, 2361 (2019)

Hopping term with spin-orbit coupling strength C:

$$-t_{SOC}\sum_{\langle k,l\rangle\sigma} e^{-i\sigma\theta}\hat{c}^{+}_{k\sigma}\hat{c}_{l\sigma} + h.c.$$

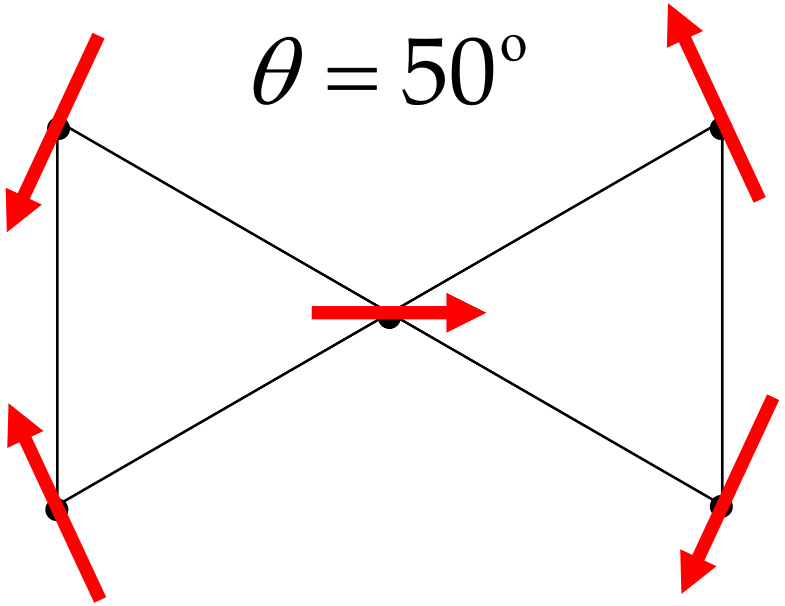
$$t_{SOC} = |t + iC|$$

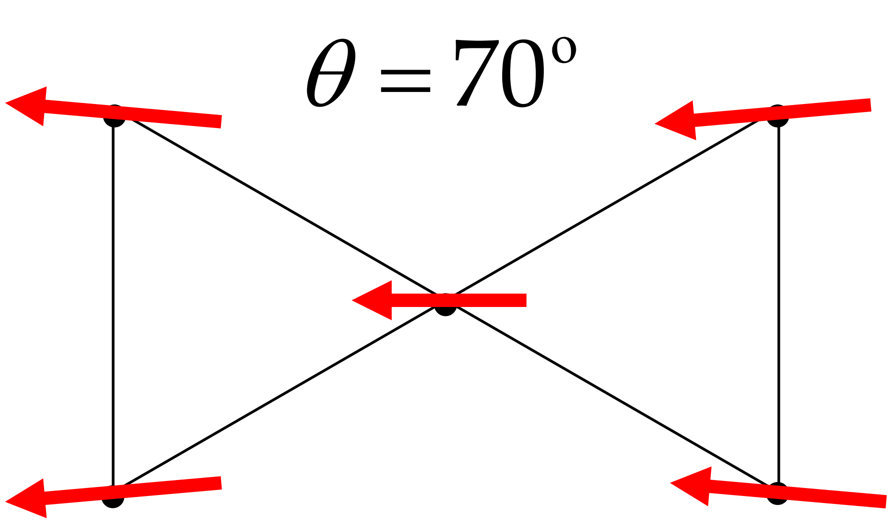
$$t = t_{SOC}\cos(\theta)$$

$$C = t_{SOC}\sin(\theta)$$

…but trimer has no X-torques.
Need something bigger.

Frustrated spins on half-filled Hubbard bowtie



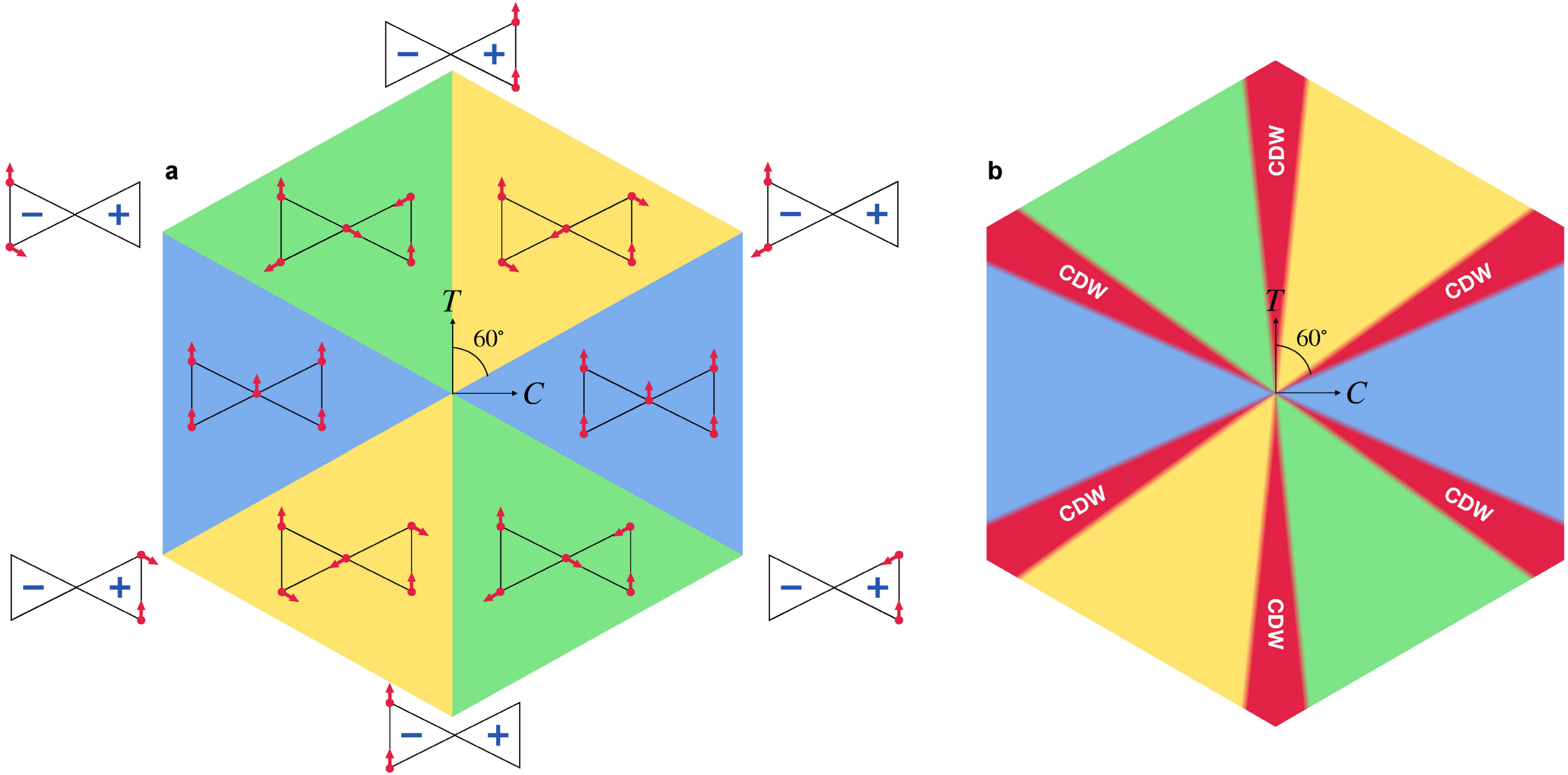


►Phase diagram boundaries at $\theta_{crit} = \frac{n\pi}{3}$ (smooth transition)

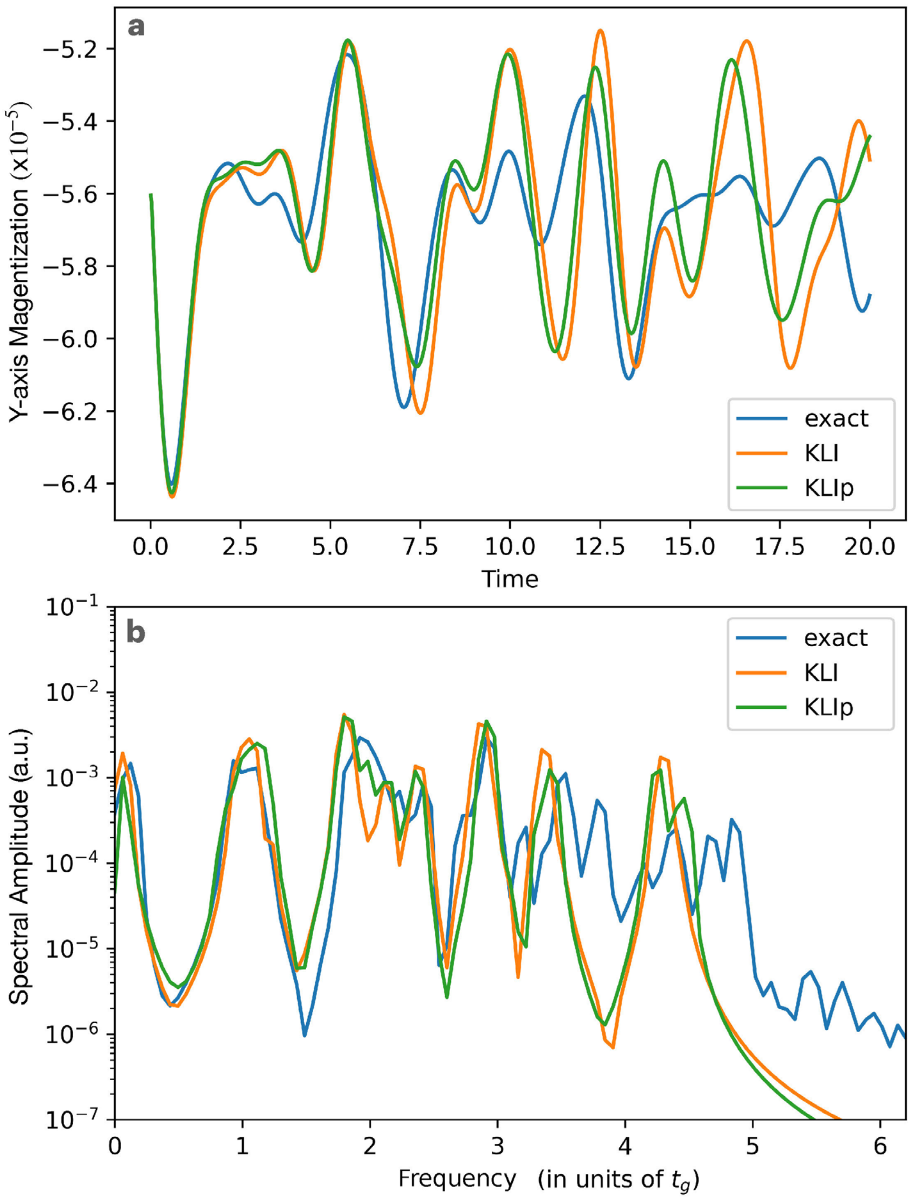
►EXX phase diagram: basic features OK, but breaks symmetry prematurely → phase transition region too broad.

Strongly correlated around phase boundaries!

Half-filled Hubbard bowtie: phase diagram



Spin dynamics on Hubbard bowtie

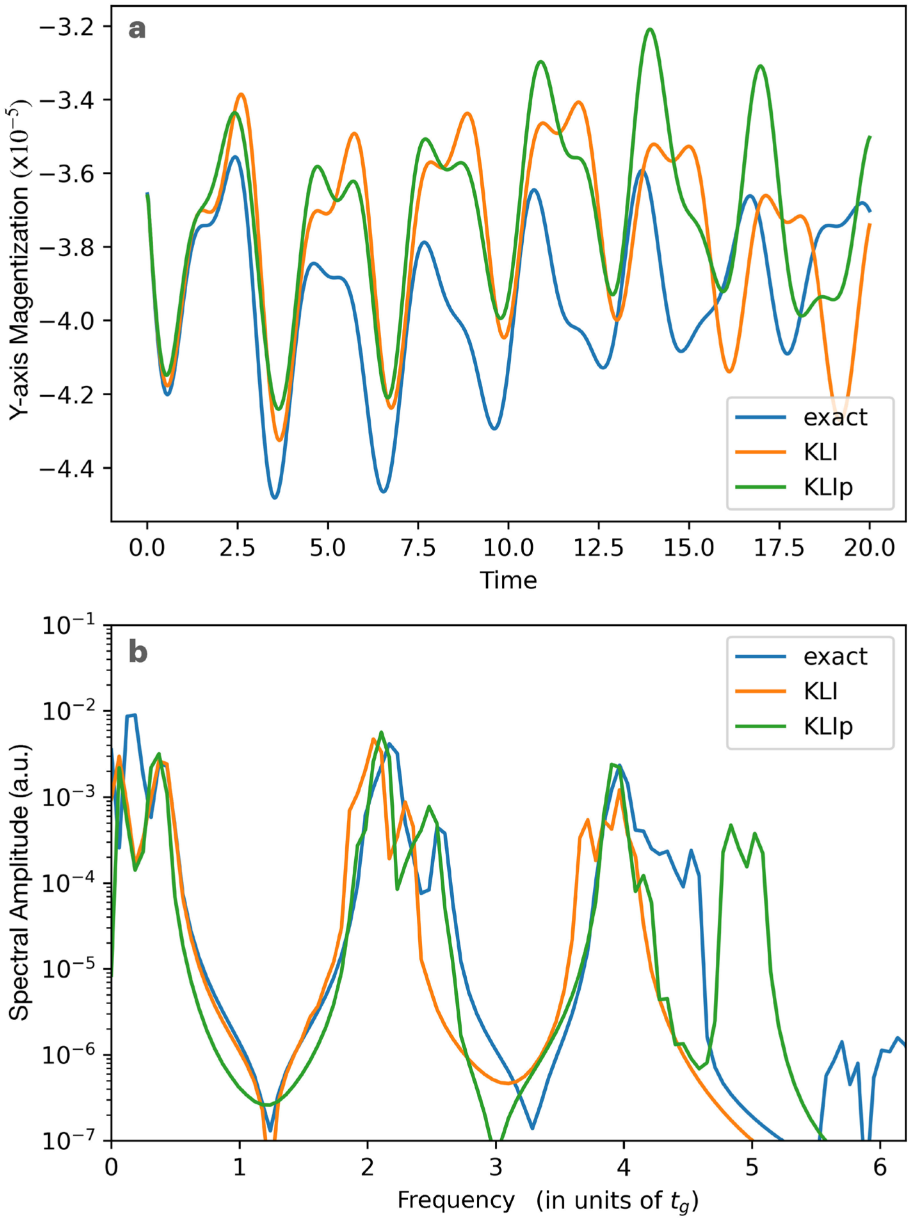


$$\theta = 30^{\circ} \qquad U_0 = 1$$

- Construct initial KS system to reproduce exact (n,**m**)
- Propagate with X-only KLI and KLI_projected (no torque)
- Free propagation after short-pulse excitation

  - Weak correlation
  - good agreement with exact solution
  - torques not very important

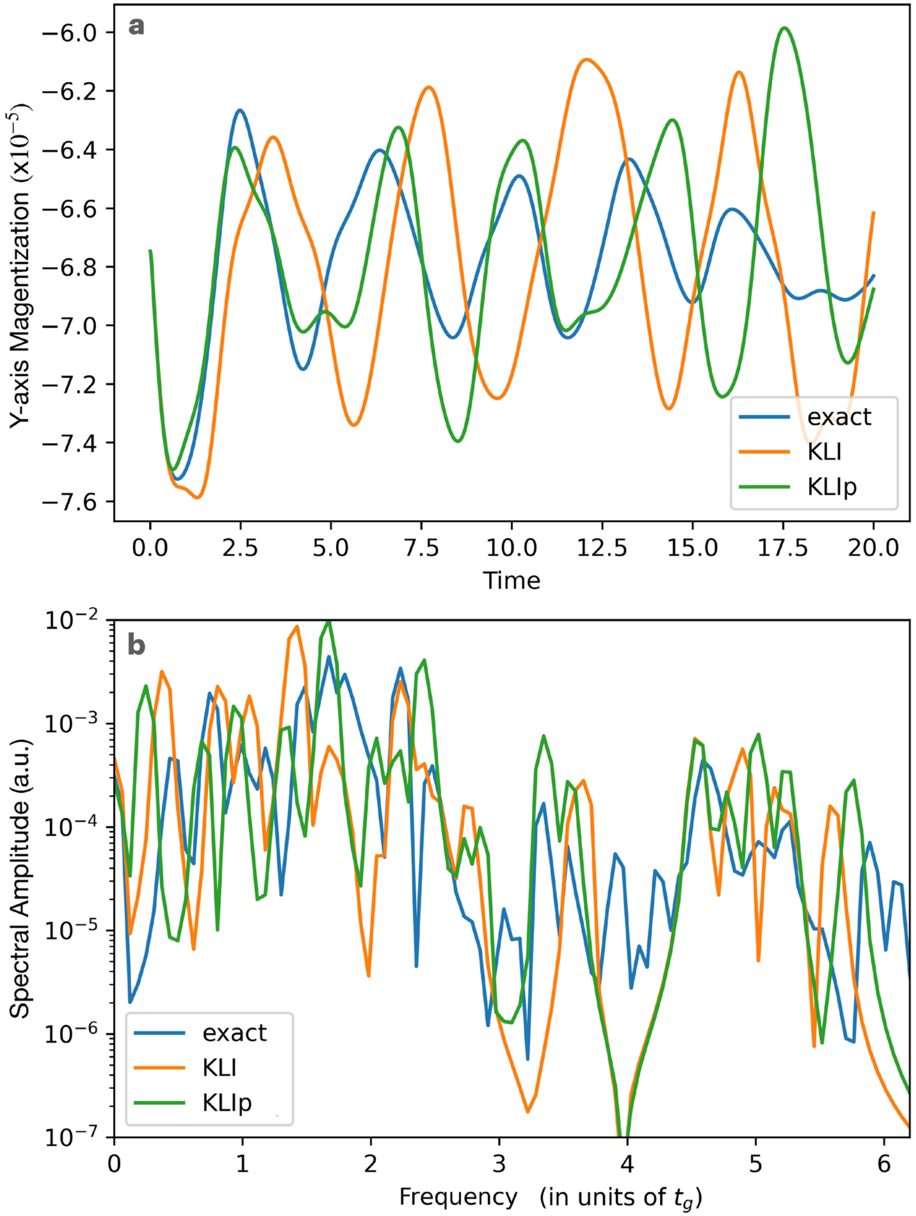
Spin dynamics on Hubbard bowtie



$$\theta = 60^{o} \qquad U_0 = 1$$

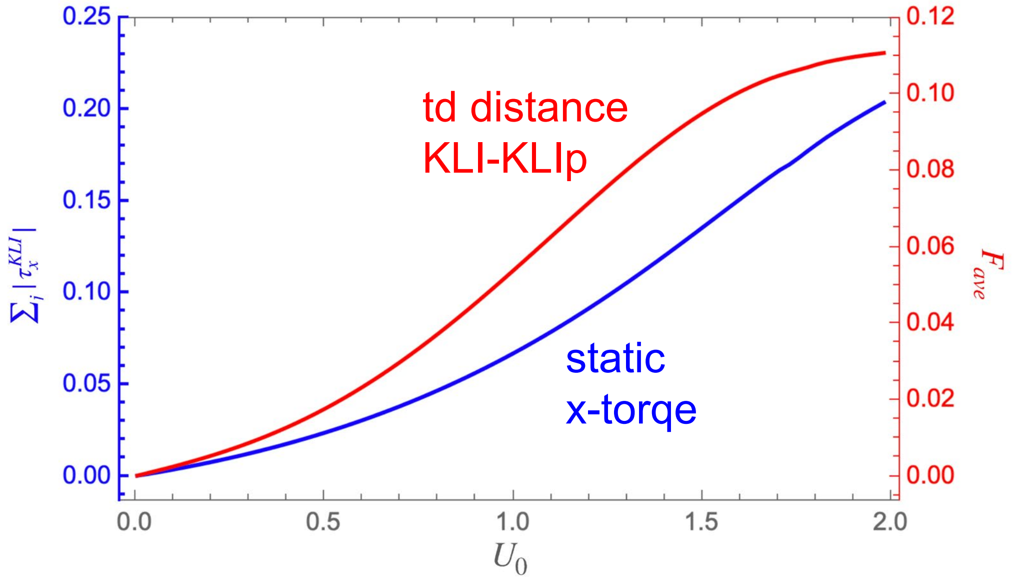
- In phase-boundary region: strongly correlated
- exchange torques relatively weak
- System dominated by symmetry-broken CDW state

Spin dynamics on Hubbard bowtie



$\theta = 30^o \qquad U_0 = 3$

- Moderate correlation
- Projected solution (no torques) agrees better!
  → X and C torques counteract.
  (recall Cr_3 example)



Summary

(TD)DFT for noncollinear magnetism

- ►**Formal framework well understood**
- ►**New XC functionals:**
  - ● *orbital based (unbiased, flexible)*
  - ● *MGGA (numerically well behaved, cheaper)*
- ►**Role of XC torques:**
  - ● *can be important for strong interactions*
  - ● *more tests needed (dynamics!)*

Many potential applications

- ►**Unconventional spin structures (e.g. skyrmions)**
- ►**Ultrafast dynamics, magnonics**

Challenges

- ►**Magnetic materials can be complex (YIG, ferrites, perovskites, heterostructures)**
- ►**May need large unit cells or supercells**
- ►**Correlations can be significant**

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Collaborators:

Irene D'Amico (University of York/UK)
Klaus Capelle (UFABC)
Giovanni Vignale (MU-Singapore)
Florent Perez (CNRS/Université Paris)
Angel Rubio (MPI Hamburg)
Nicolas Tancogne-Dejean (MPI Hamburg)

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