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Dissipative dynamics of an impurity in the presence of the spin-orbit coupling

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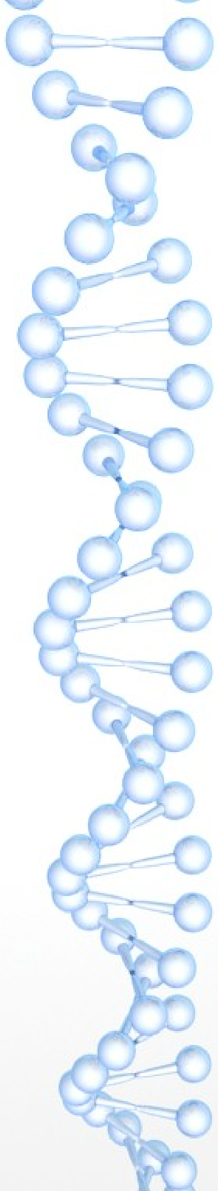
Overview

- Motivation
  - Introduction to CISS effect
  - Theoretical puzzle
- Theoretical approaches for CISS effect
  - Scattering approaches
  - Transport calculations
  - Role of the substrate
  - Many-body perspective
- Connection to impurity problem in a dissipative bath
  - One dimesnional toy model
  - Possible experimental signatures
  - Caldeira-Legett type model

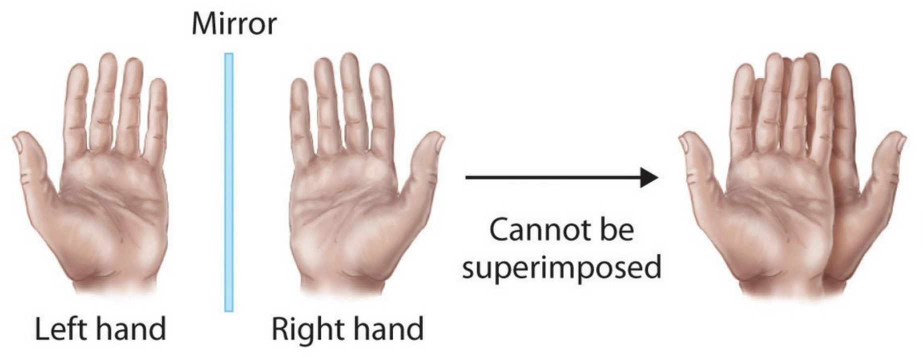


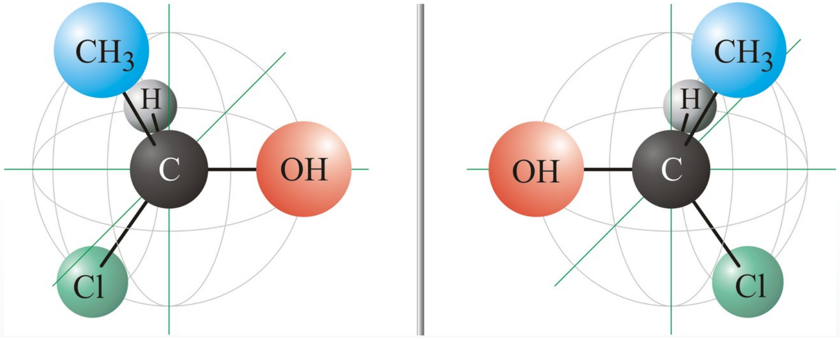
Motivation

Introduction to CISS effect

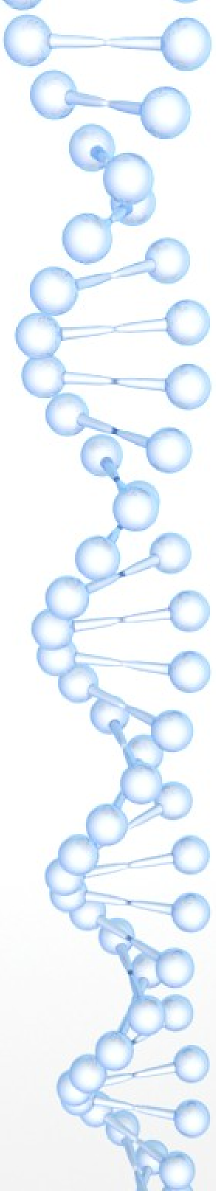
Chirality/ Chiral Molecules

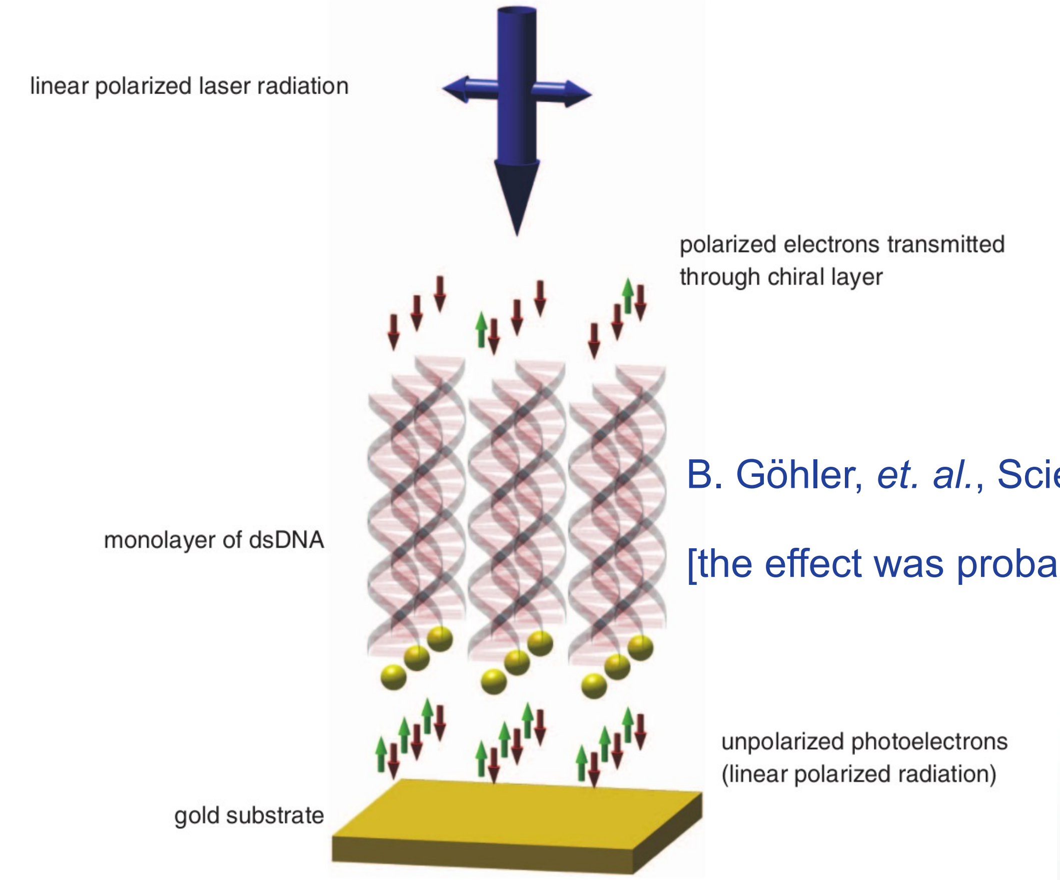
- Lacks inversion symmetry
- Mirror symmetry transforms different enantiomers into each others
- It cannot be superimposed upon its mirror image





Chiral Induced Spin Selectivity Effect

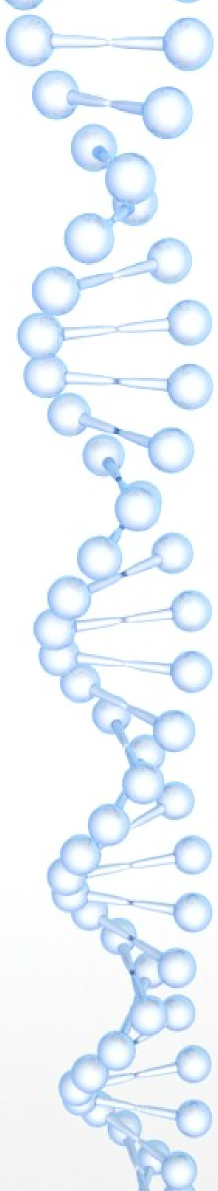




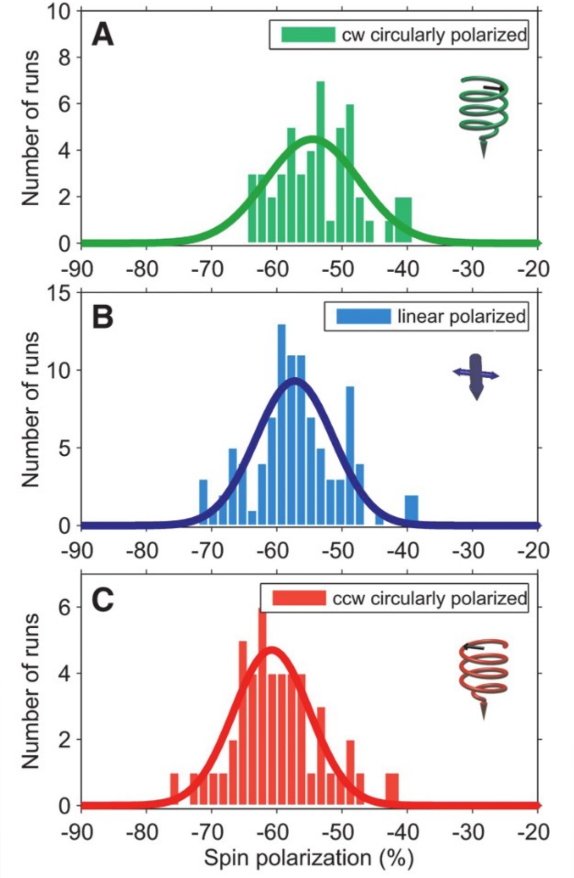
B. Göhler, *et. al.*, Science **331**, 894 (2011)

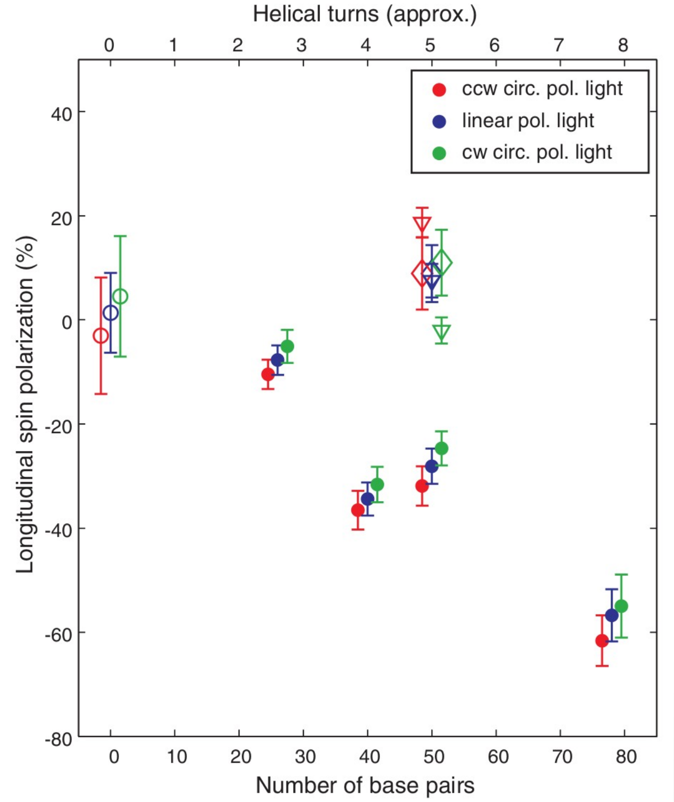
[the effect was probably seen already in 1999]

CISS effect: Interaction between Spins and Chirality (Helicity)



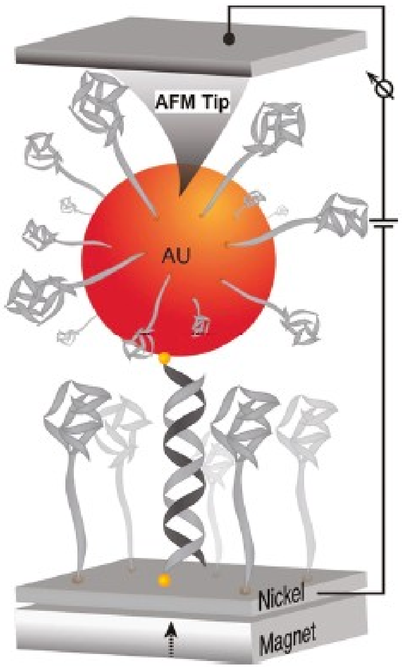
Results from the experiment

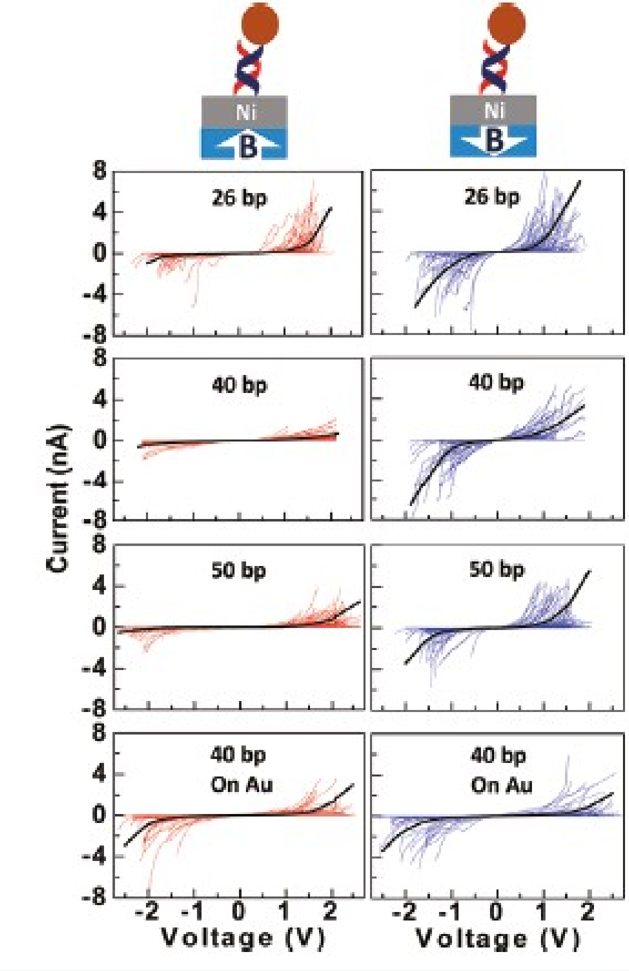




B. Göhler, *et. al.*, Science **331**, 894 (2011)

Transport measurement of CISS with DNA

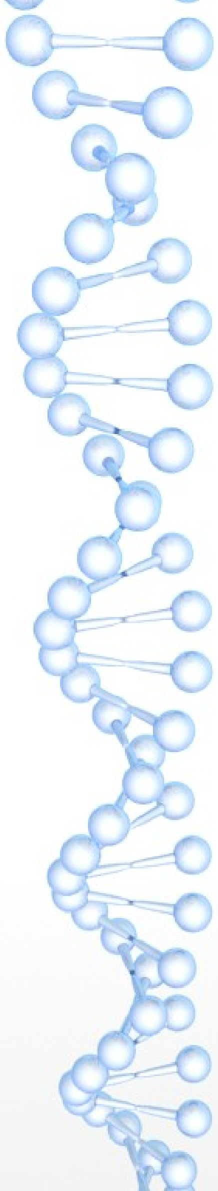


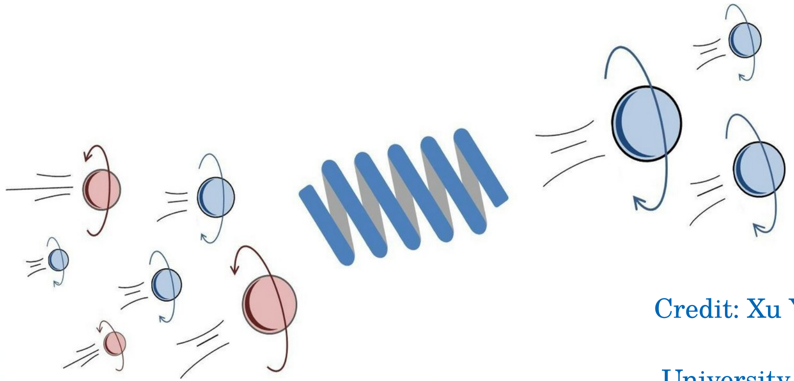


Z. Xie, et. al., Nano Lett. 11, 4652 (2011)

Universality of the CISS effect

Since 2011 experiments (Weizmann, Jerusalem, Münster, Pittsburgh, Caltech, ...) observed the CISS effect using other molecules, substrates, tools.





Credit: Xu Yang,

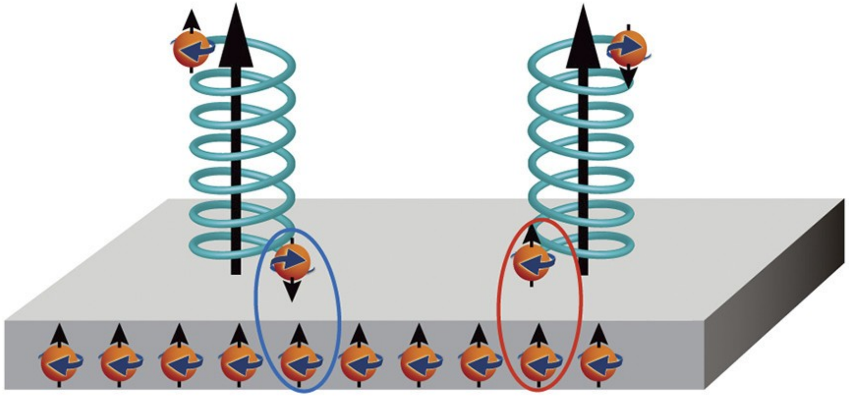
University of Groningen

Current of Electrons + Chiral Molecule = Spin-Polarized Current

(Reverse Spin) (Reverse Chirality) = (Spin) (Chirality)

Why to study the CISS

1. Selection of Enantiomers (needed in pharmacy)



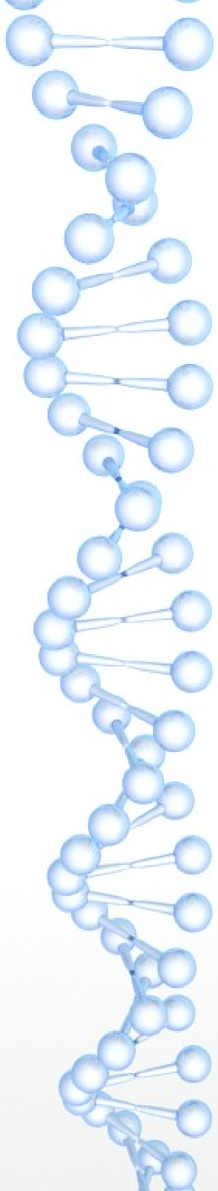
K. Banerjee-Ghosh et al.,

Science **360**, 1331 (2018)

2. Spin Filters in Spin Electronics

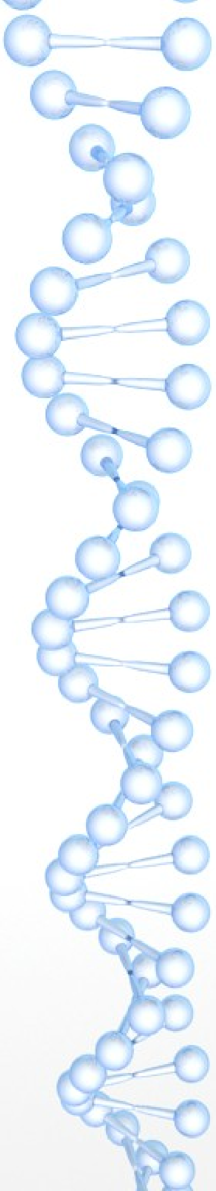
3. Better Theory of Current through Organic Molecules

□□□



Theoretical Puzzles

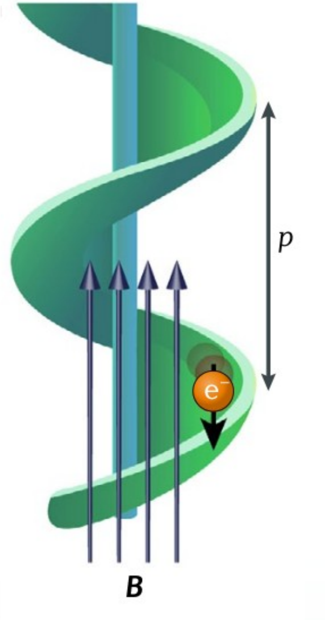
- What causes the effect? **Spin-orbit coupling?**
- Why the CISS effect is so strong [light atoms, room temperature]? **Collective quantum effect? Surface? Dissipation?**
- Is it a transient or static effect?

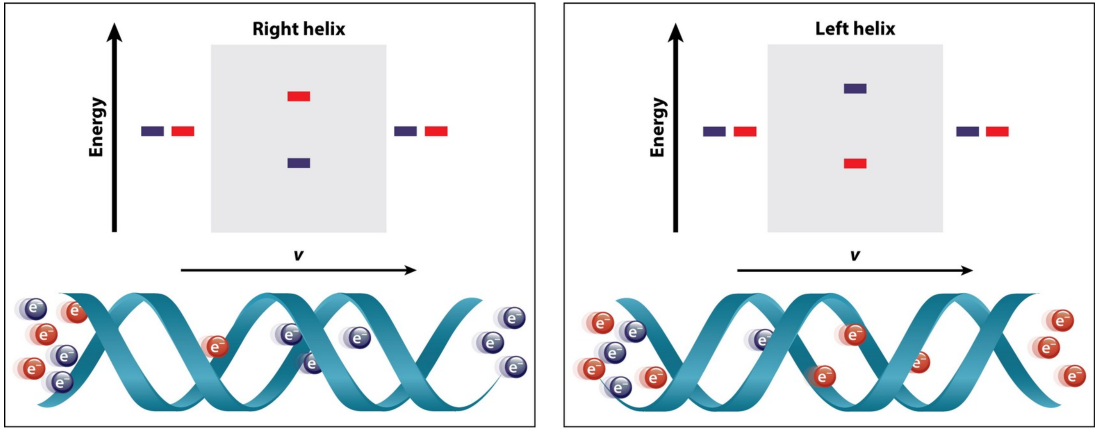


Theoretical approaches for CISS effect

Phenomenological theory of the CISS

There is no ab-initio theory that explains the CISS.





Naaman R, Waldeck DH. 2015.
Annu. Rev. Phys. Chem. 66:263–81

Effective magnetic field due to centripetal force

$$\mathrm{B}_{\mathrm{eff}} = -\frac{(\mathbf{v} \times \mathbf{E}_{\mathrm{chiral}})}{(2c)^2}$$

Scattering approaches

List of some of the relevant papers

1. S. Yeganeh, et. al., J. Chem. Phys. 131, 014707 (2009).

2. E. Medina, et. al., EPL 99, 17006 (2012).

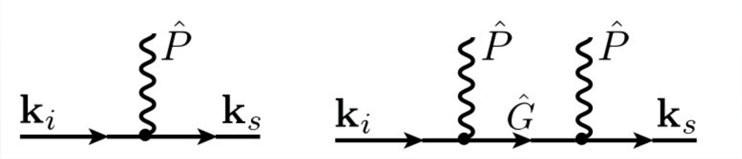
3. S. Varela, et. al., J. Phys. Cond. Mat. 26 015008 (2014).

4. A. A. Eremko and V. M. Loktev, PRB 88, 165409 (2013).

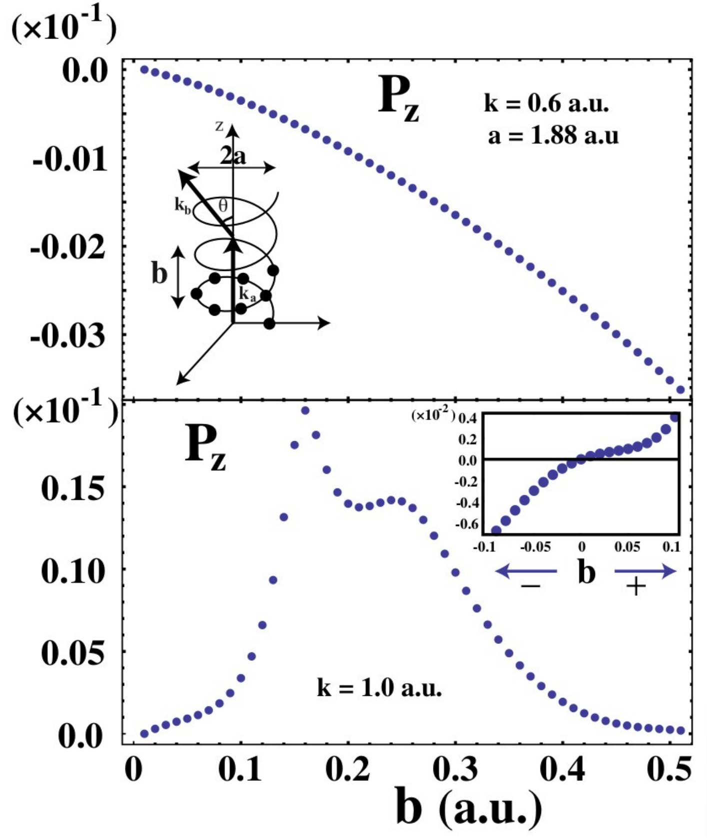
Standard scattering problem on the potential of the molecule

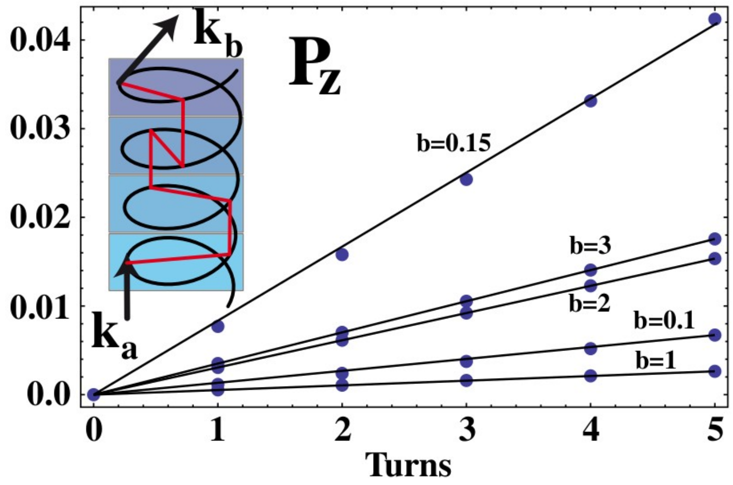
$$\psi(\mathbf{r}, s) = \left[\psi_0(\mathbf{r}) + \frac{e^{ikr}}{r}\hat{f}(\mathbf{k}_i, \mathbf{k}_s)\right]\chi_{m_s}$$

$$|\psi\rangle = |\psi_0\rangle + \hat{G}\hat{P}|\psi_0\rangle + \hat{G}\hat{P}\hat{G}\hat{P}|\psi_0\rangle$$



Results for helical molecule





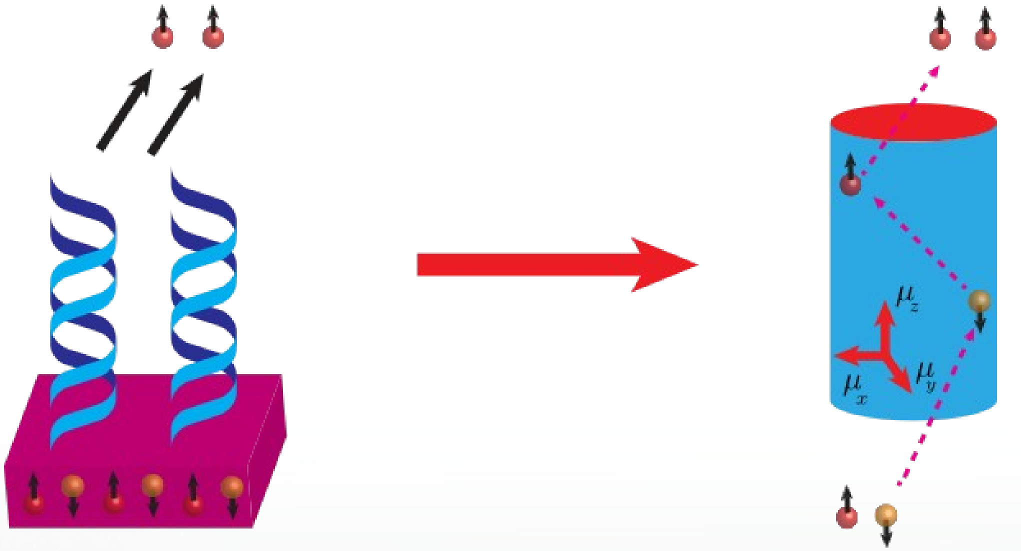
E. Medina, et. al., EPL 99, 17006 (2012).

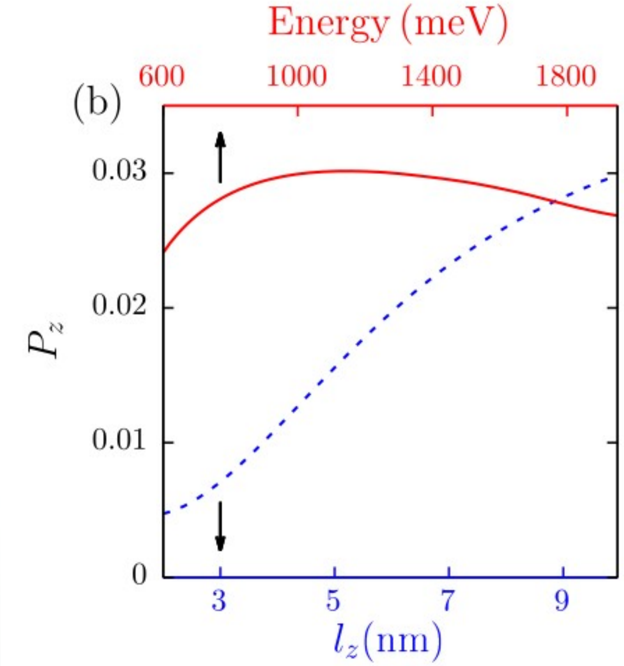
The polarization is too small compared to the experment

Helicity vs Chirality

CISS is there for any chiral molecule

The effect is stronger for helical ones

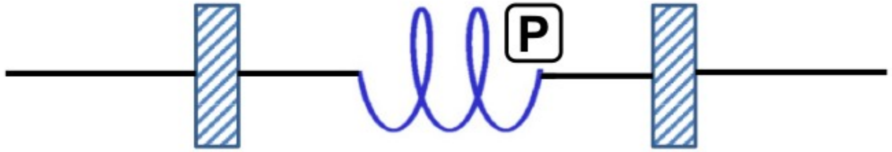




A. Ghazaryan, et. al., J. Phys. Chem. C 124, 11716 (2020).

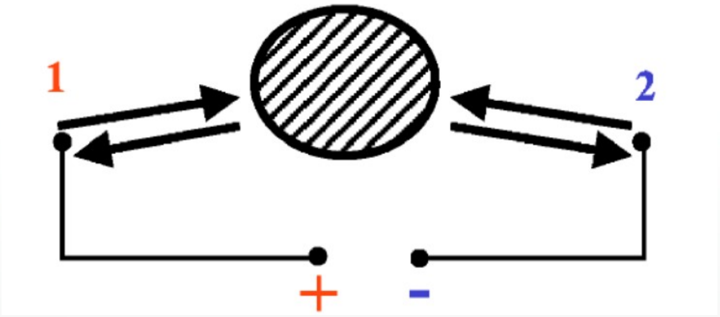
Transport calculations

Why 1D models does not work?



In 1D SOC is SU(2) gauge field can be gauged: No spin-polarization

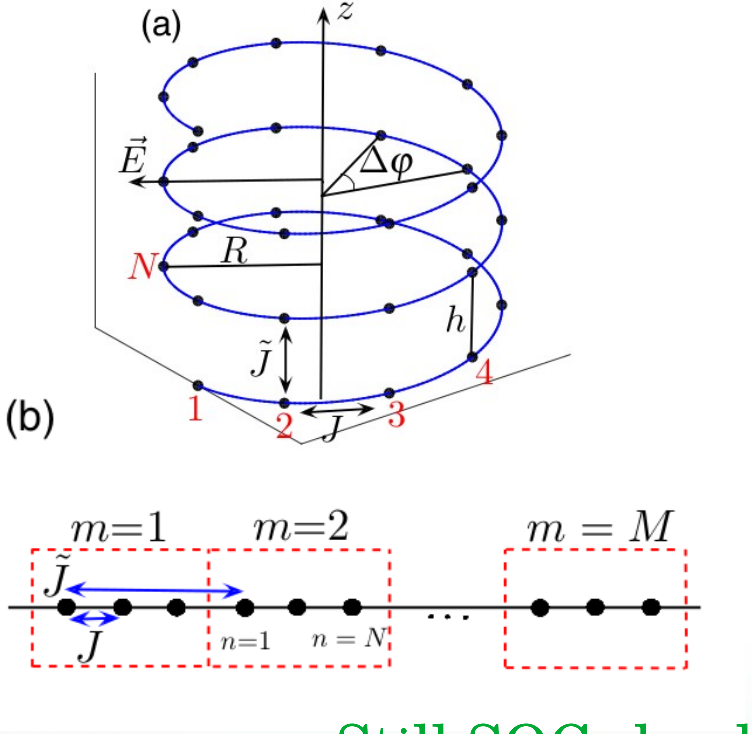
Remains true if only has two terminals with single channel and TRS

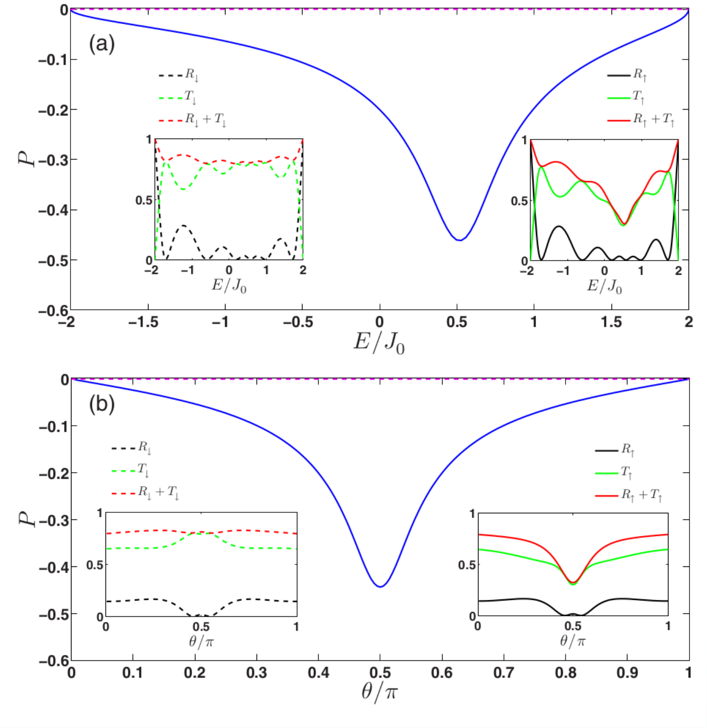


J. Bardarson, J. Phys. A 41 405203 (2008)

A.A. Kiselev and K.W. Kim, PRB 71 153315 (2005)

Effective 2D system with leakage





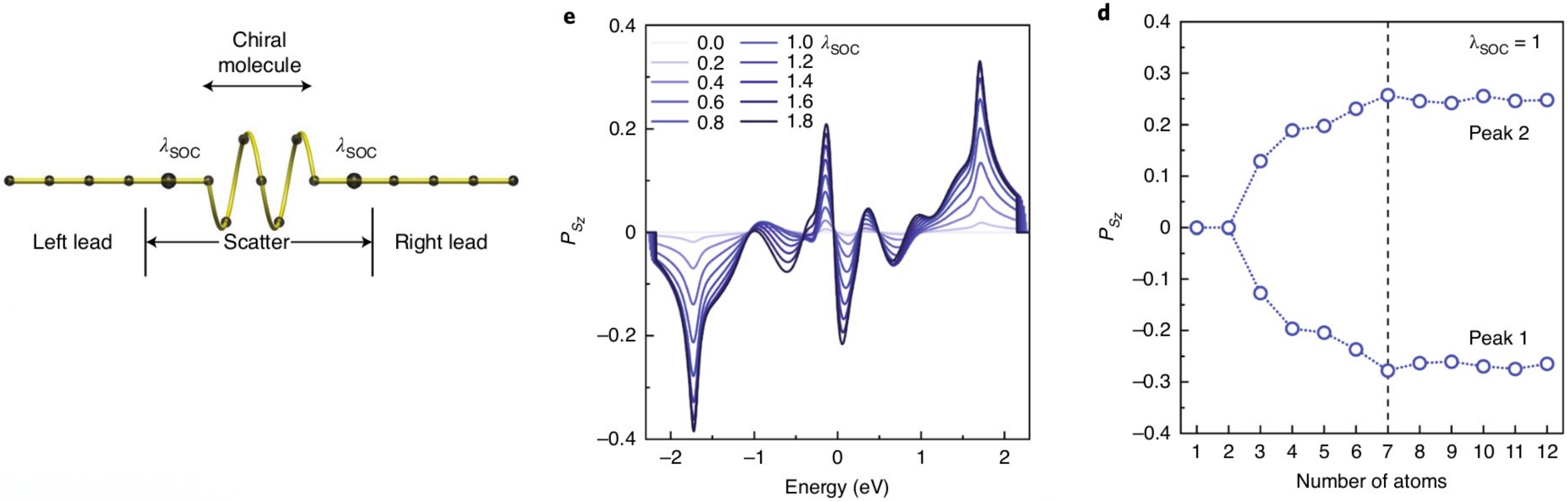
Still SOC should be taken orders of magnitude larger than for carbon atoms

S. Matityahu, et. al. PRB 93 075407 (2016)

Role of the substrate

SOC is strong in the substrate

Molecule acts as an orbital filter



CISS was observed with substrates with small SOC

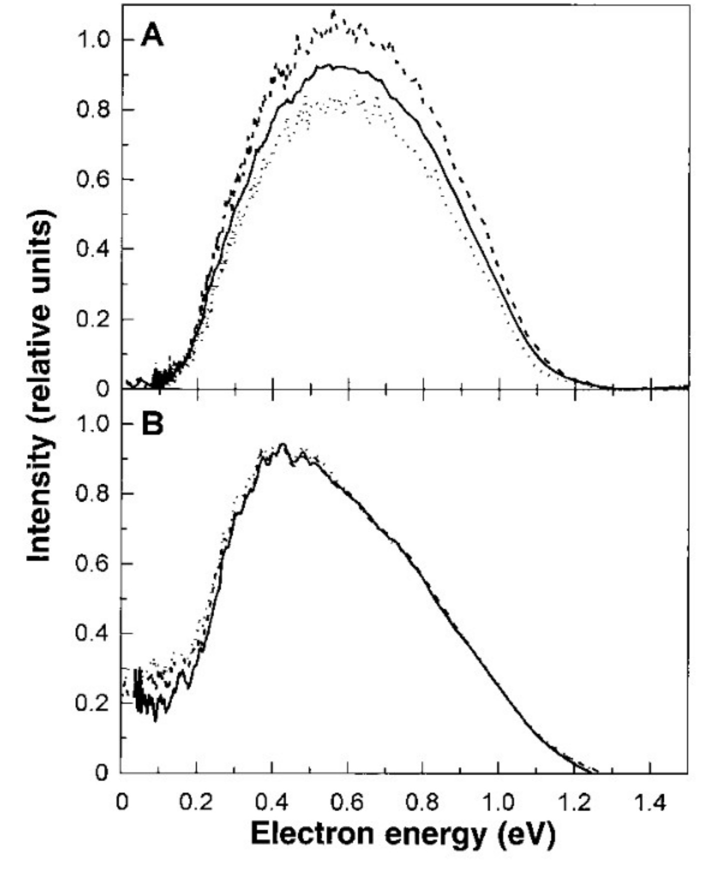
J. Gersten, et. al. J. Chem. Phys. 138, 114111 (2013).

Y. Liu, et. al., Nature Materials 20, 638 (2021).

CISS Strong → Quantum Many-Body Effect

Pure L-stearoyl lysine

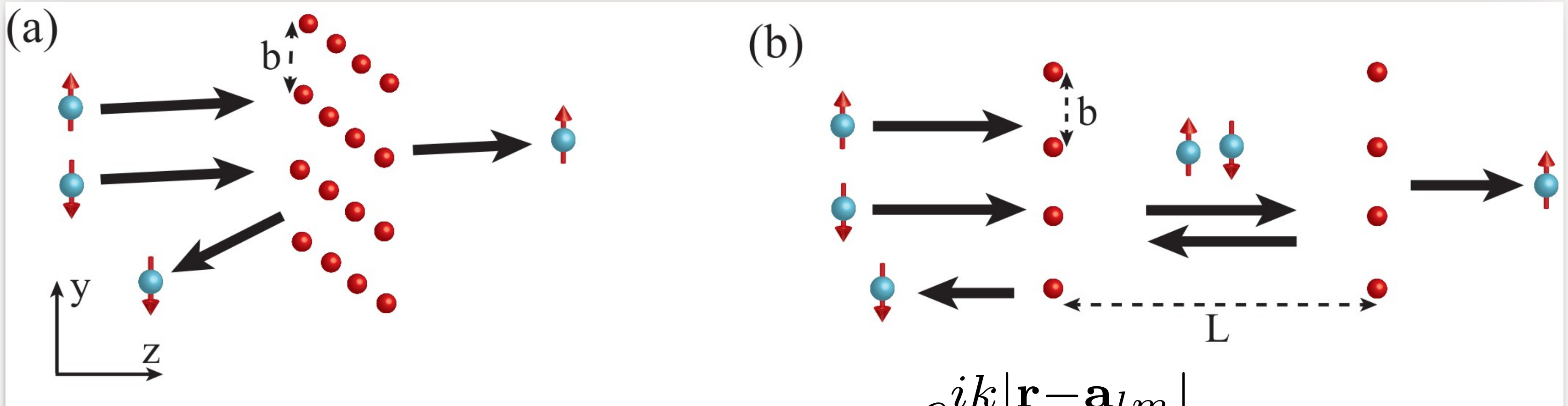
99% L-stearoyl lysine with 1% D - stearoyl



K. Ray, et. al., Science 283, 814 (1999)

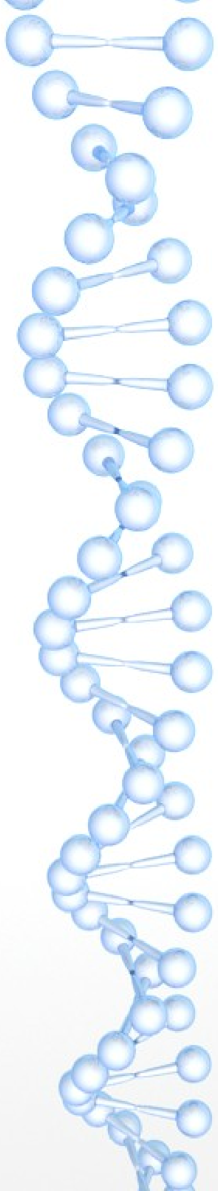
Modeling many-body effect

Electron scattering of 2D zero range magnets



$$\Psi(\mathbf{r}) = e^{ikz} + A \sum_{lm} \frac{e^{ik|\mathbf{r}-\mathbf{a}_{lm}|}}{|\mathbf{r}-\mathbf{a}_{lm}|}$$

A. Ghazaryan, et. al., Communications Physics 3, 1-7 (2020).



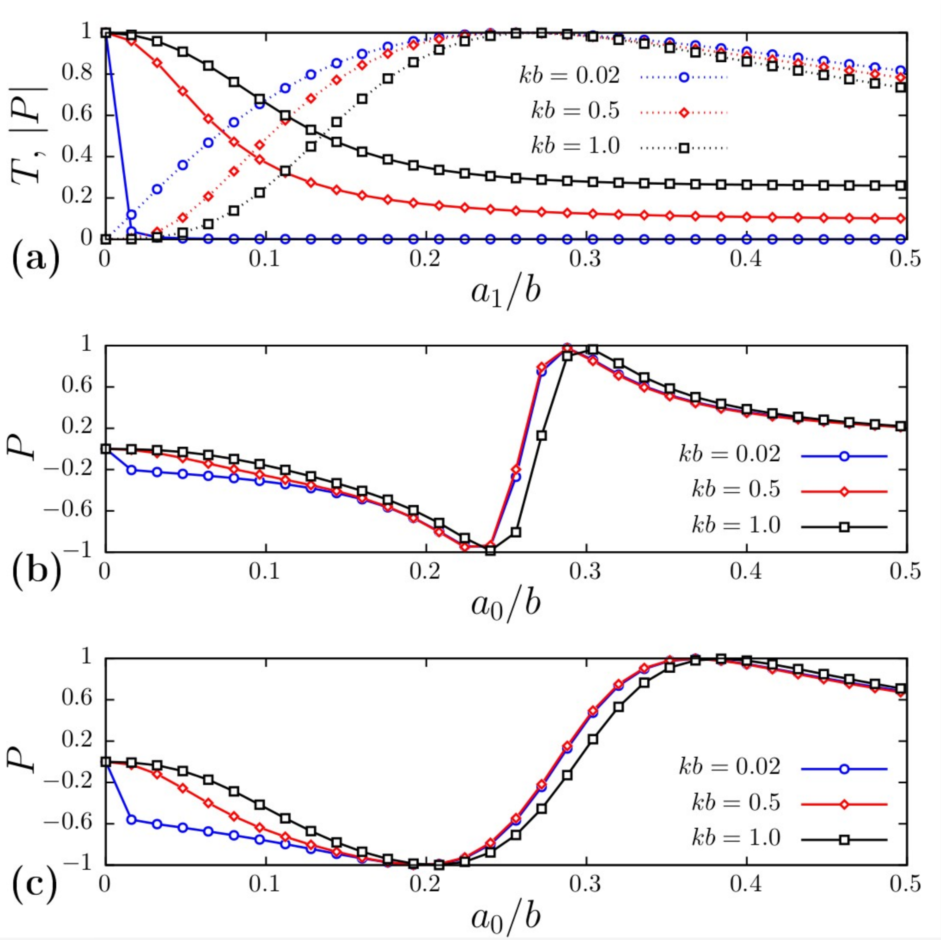
One layer case

Many-body effects are important only at magic point

$$a_0 = 0$$

$$a_1/a_0 = 0.1$$

$$a_1/a_0 = 0.3$$



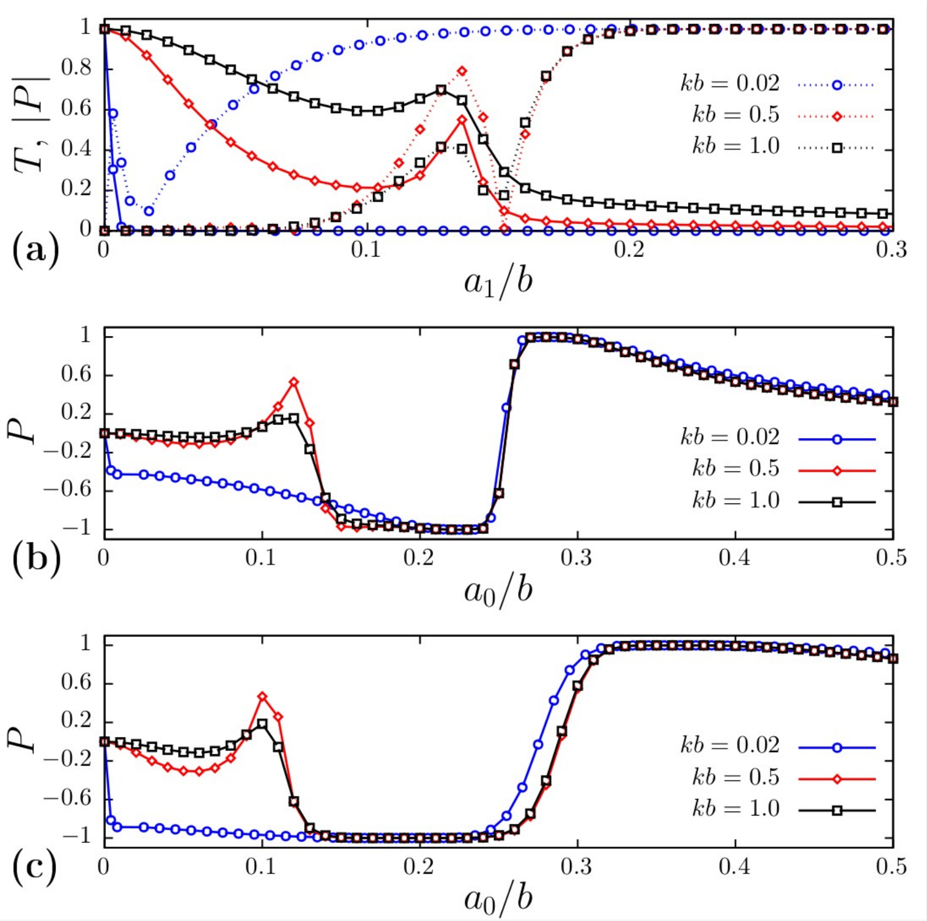
Two layer case

Two layers can act as a spin filter

$$a_0 = 0$$

$$a_1/a_0 = 0.1$$

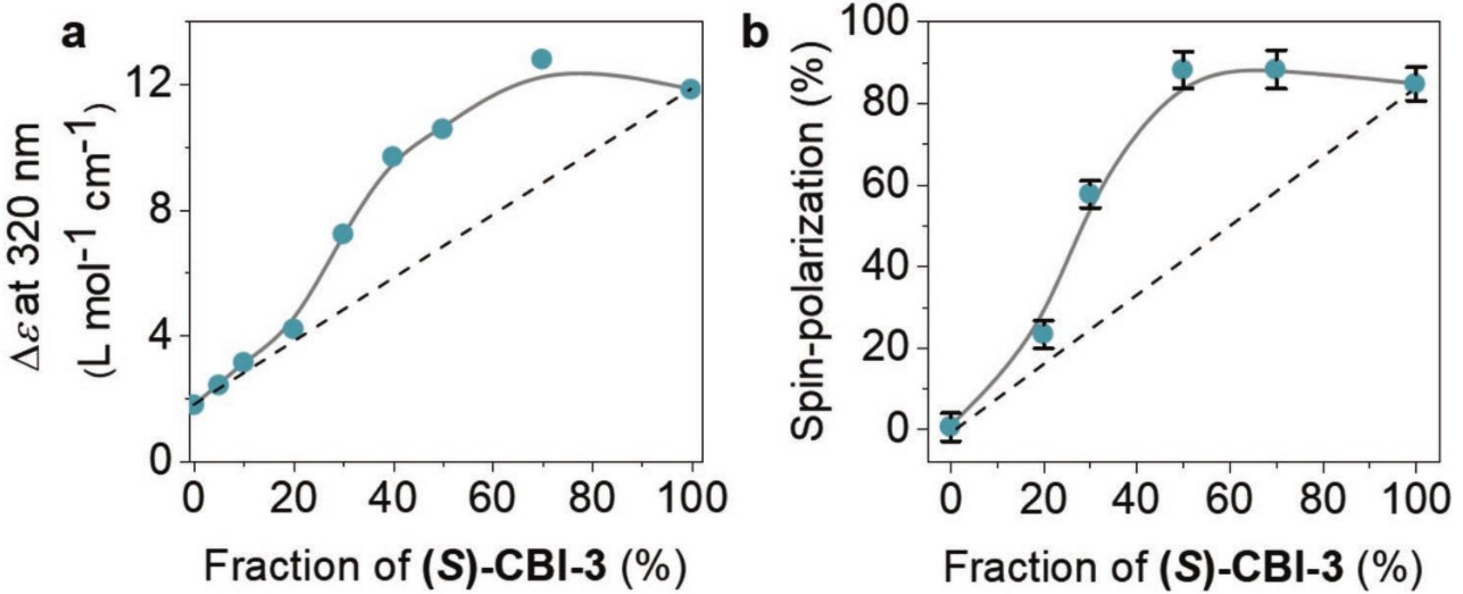
$$a_1/a_0 = 0.3$$



Seargant and Soldier effect

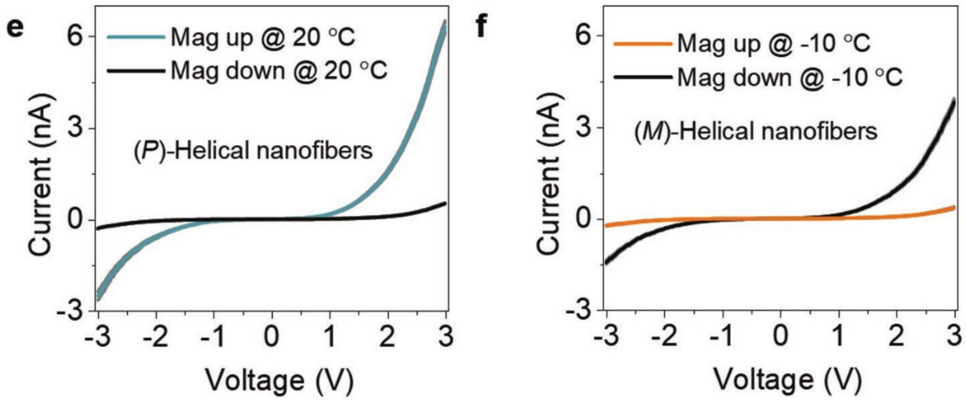
Shows non-linear dependence on chiral fraction for coronene bisimide

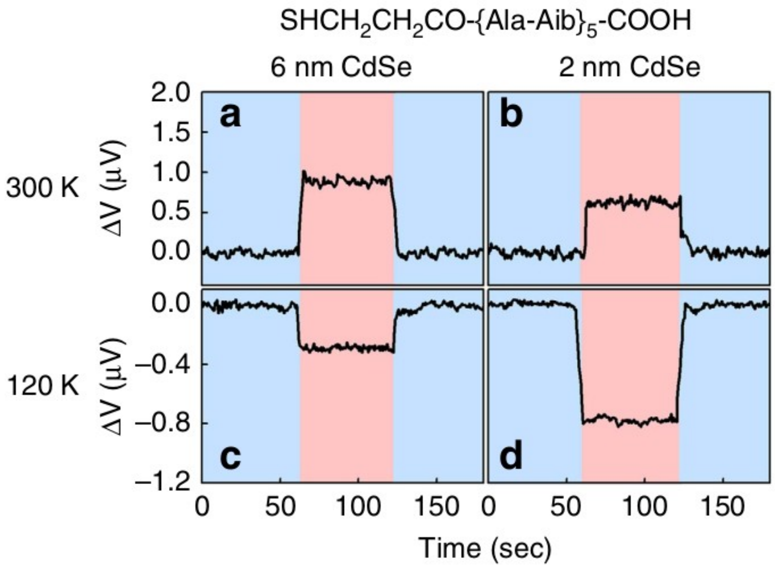
Many-Body effects are still important



C. Kulkarni, et. al., Adv. Materials 32, 1904965 (2020).

Flipping the chiral response with temperature





C. Kulkarni, et. al., Adv. Materials 32, 1904965 (2020).

M. Eckshtain-Levi, et. al., Nature Comm. 7, 10744 (2016)

Does the molecule break time-reversal symmetry

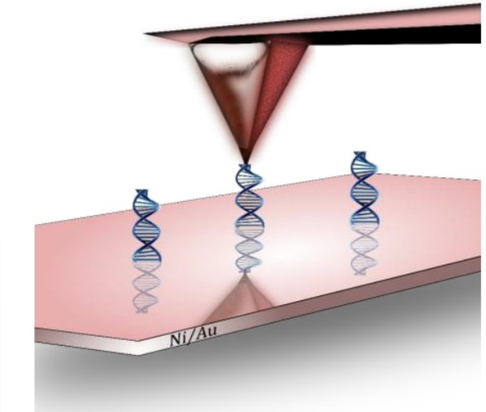
Onsager reciprocal relation

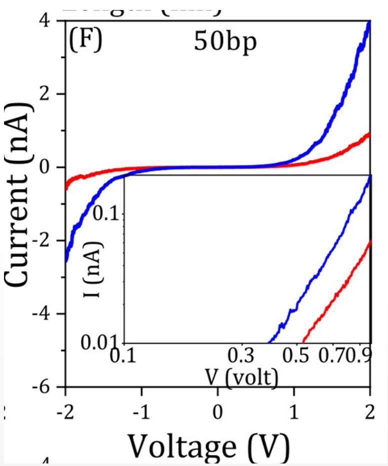
$$G_{L\to R}(M,H) = G_{R\to L}(-M,-H)$$

Linear regime

$$G_{L\to R}(M,H) = G_{L\to R}(-M,-H)$$

Both symmetry arguments fail

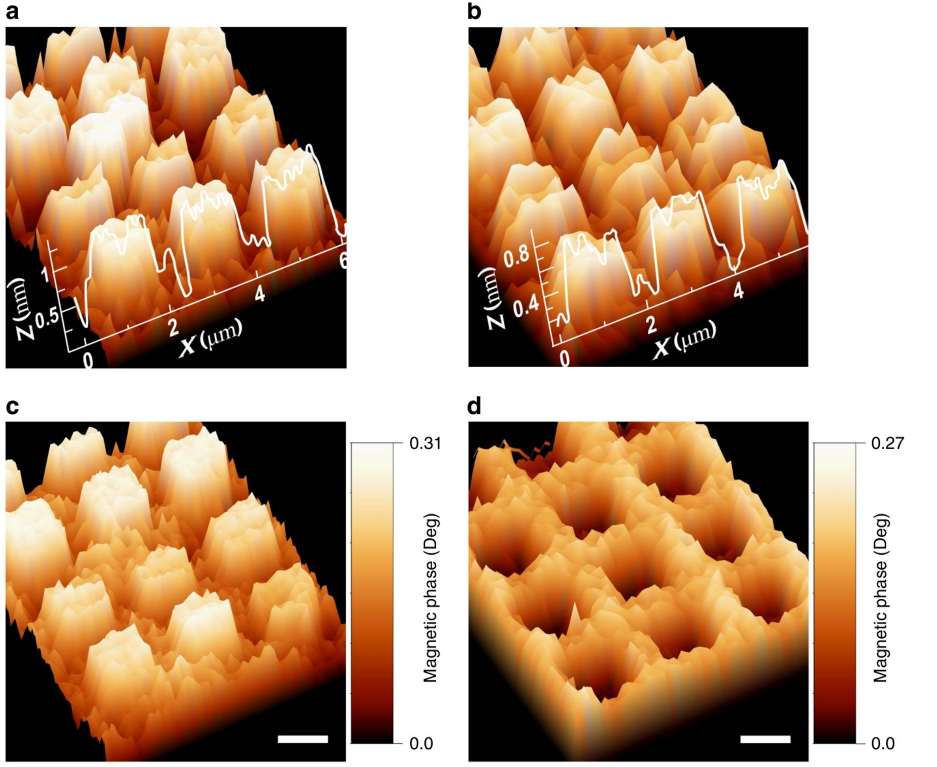


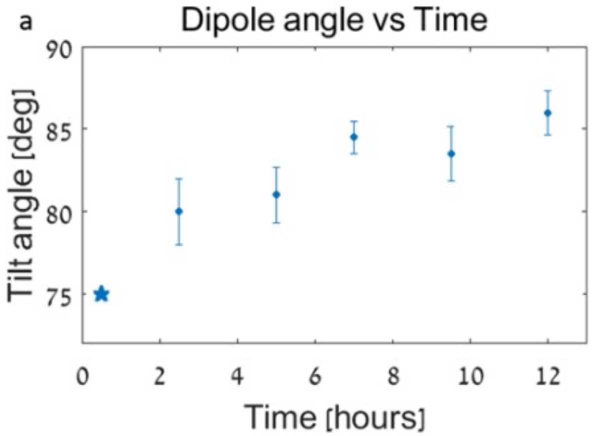


S. Mishra, et. al., J. Phys. Chem. C 124, 10776–10782 (2020).

Magnetization switching

Transient or static effect: Persistent over hours

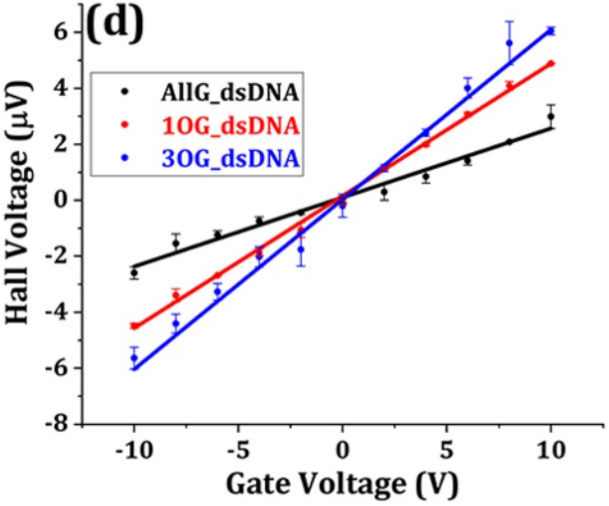


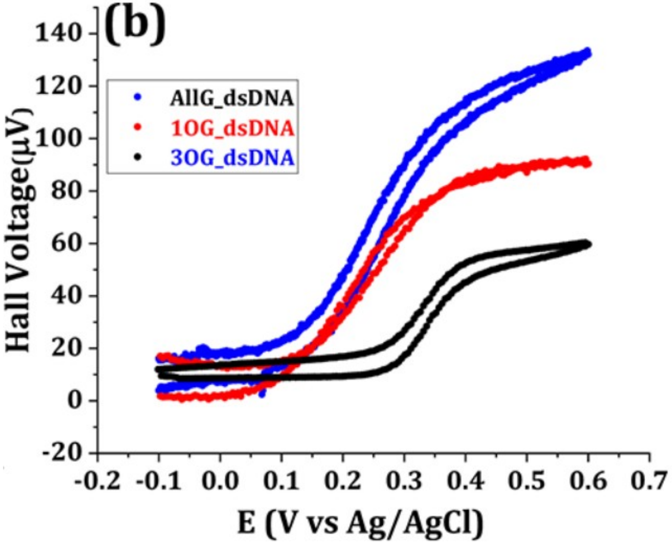


O. Ben-Dor, et. al., Nature Comm. 8, 1 (2017).

I. Meirzada, et.al, ACS Nano 15, 5574 (2021).

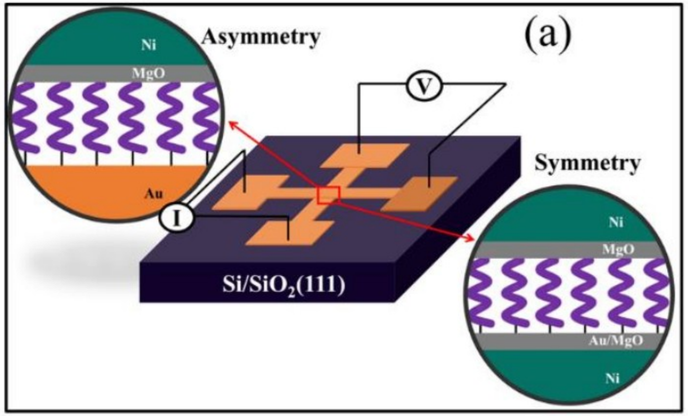
CISS effect gets stronger for DNA with damaged sites

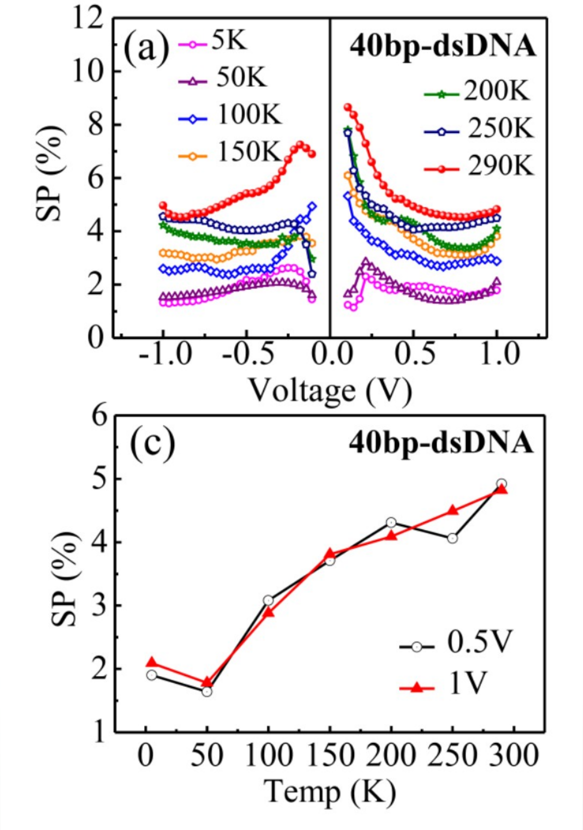




S. Mishra, et. al., J. Am. Chem. Soc. 141, 123–126 (2019)

CISS dependence on temperature





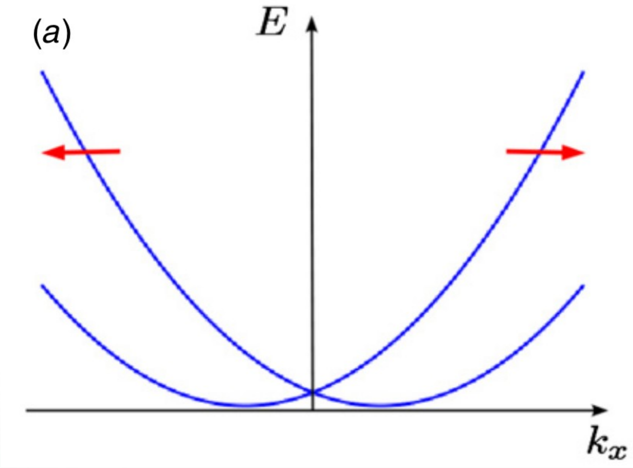
CISS effect gets stronger with temperature

T. Das, et. al., arXiv:2108.08037

Dissipation (quantum friction) Model

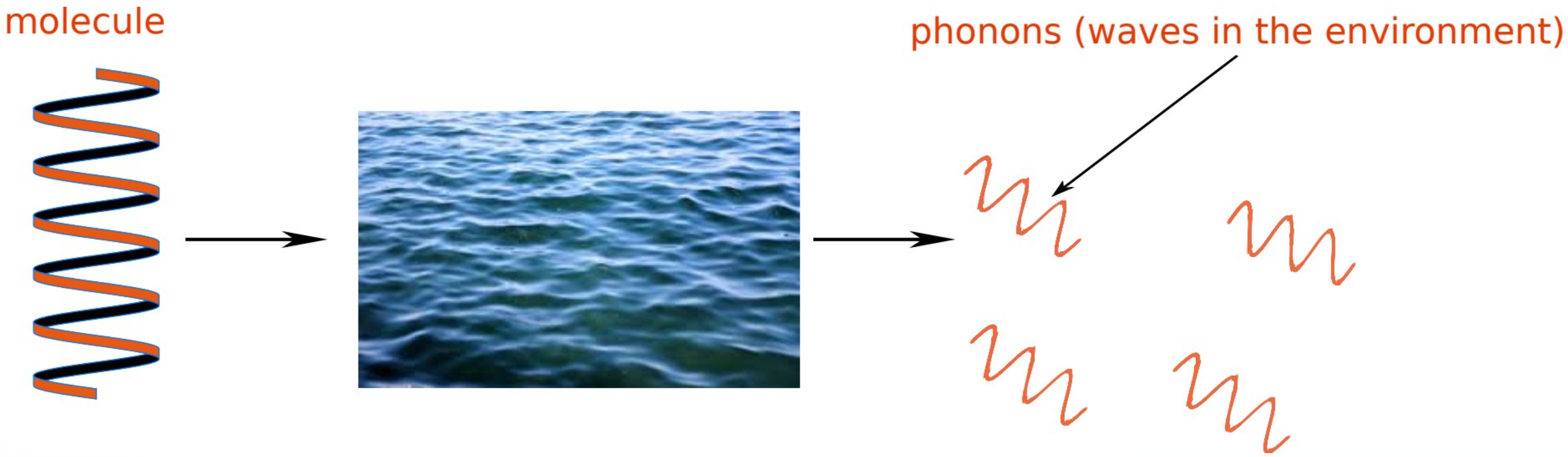
Spin-orbit coupling

Spin-momentum locking



How do we see a molecule

Molecule is a bath of phonons (excitations)



CISS → a spin-orbit coupled particle in a bath of phonons

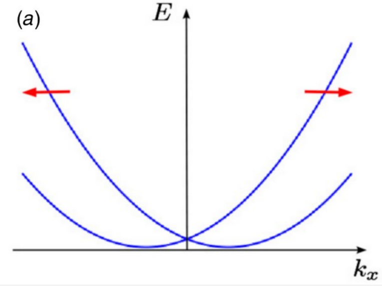
Our Model: Impurity in a dissipative medium

Phenomenological Schrodinger Equation – analogue of Master Equation with dissipation

$$i\hbar\frac{\partial\Psi_s}{\partial t} = H_s\Psi_s; \quad H_s = \frac{p^2}{2m} + \alpha ps + V(x) + \gamma W,$$

$$W = \langle p\rangle_s \left(x - \langle x\rangle_s\right)$$

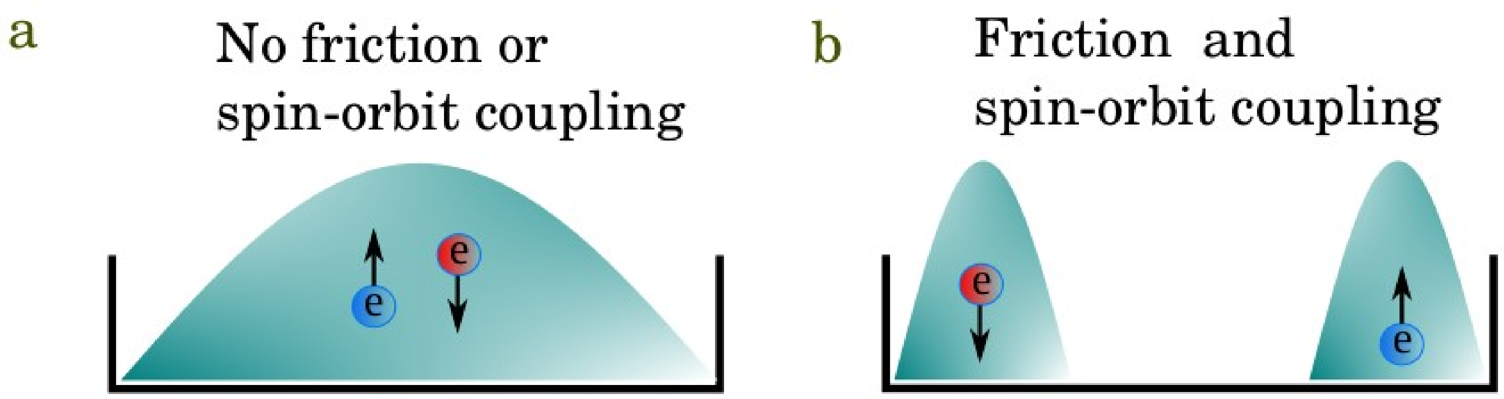
Average momentum is determined by spin-orbit coupling



A.G. Volosniev, et. al., Phys. Rev. B 104, 024430 (2021)

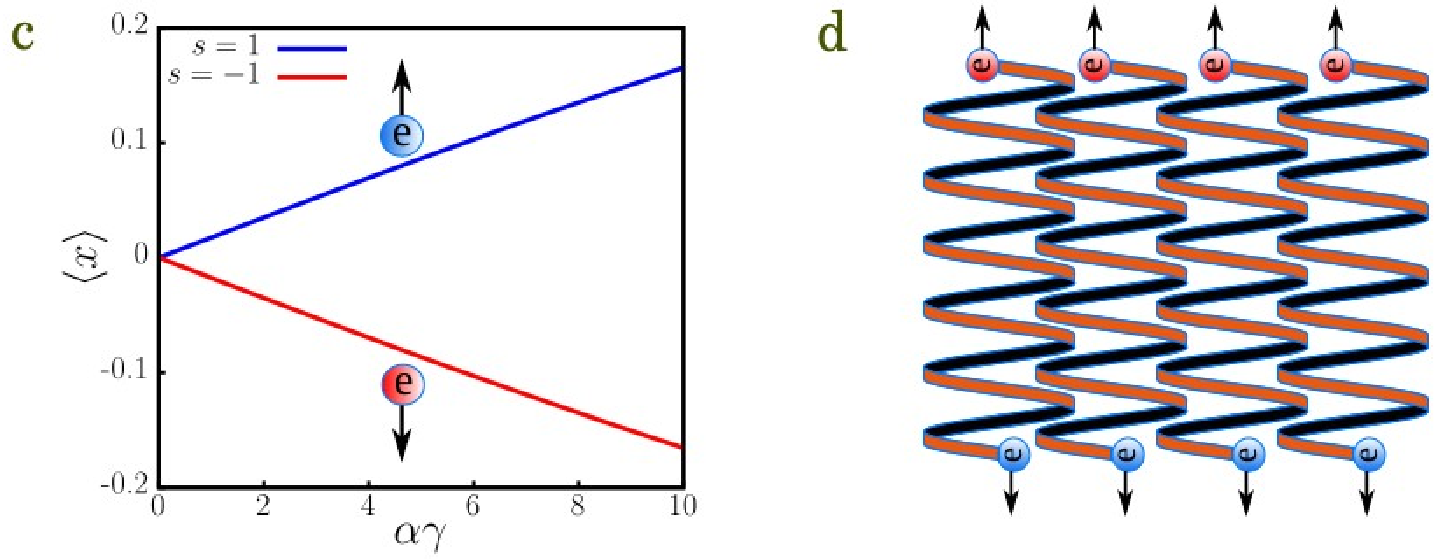
Steady-state solution

Due to spin-orbit coupling and dissipation, different spins occupy different regions



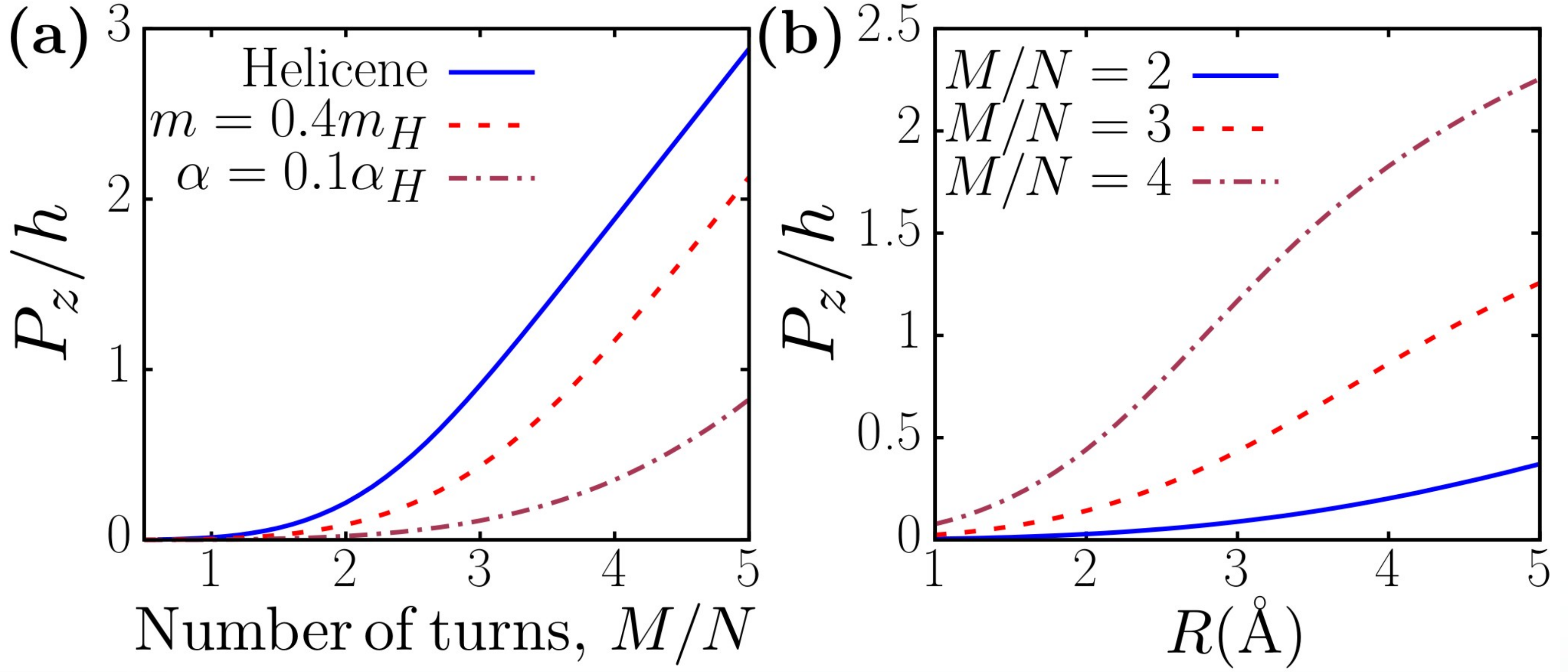
Steady-state solution

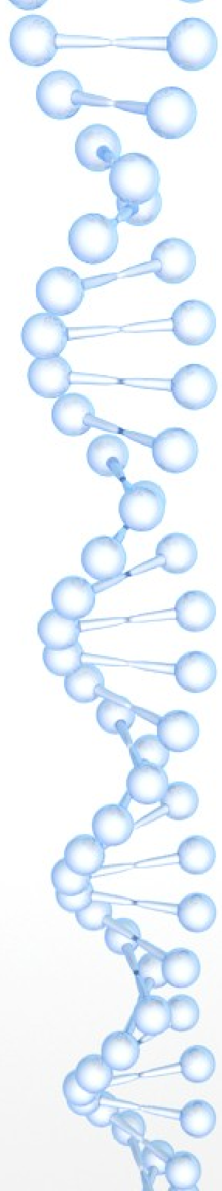
Results from the actual calculation



Friction and spin-orbit coupling come together

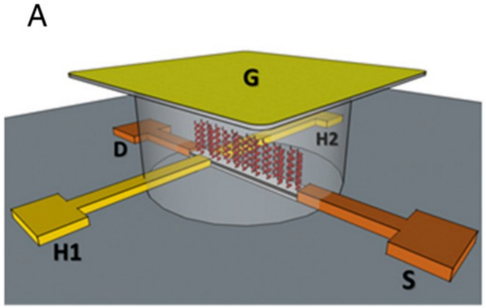
Applying the theory to Helicene

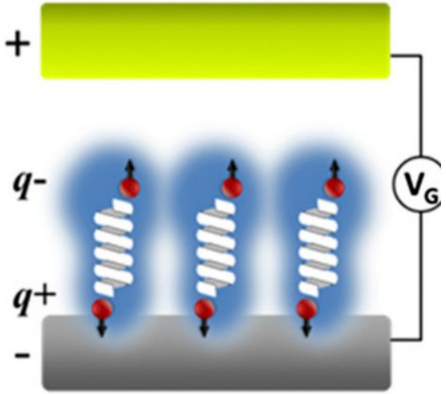


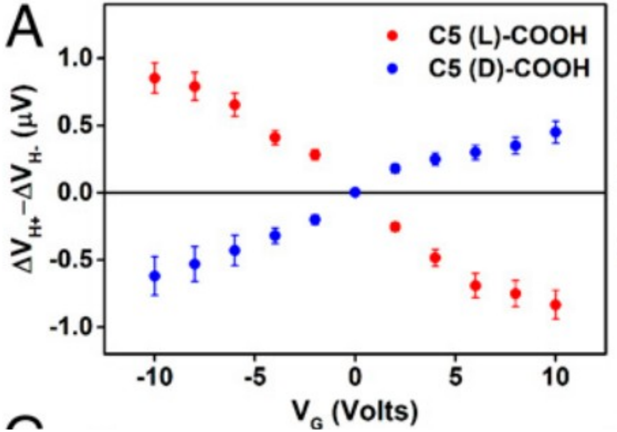


Experimental indications

Hall device measurement





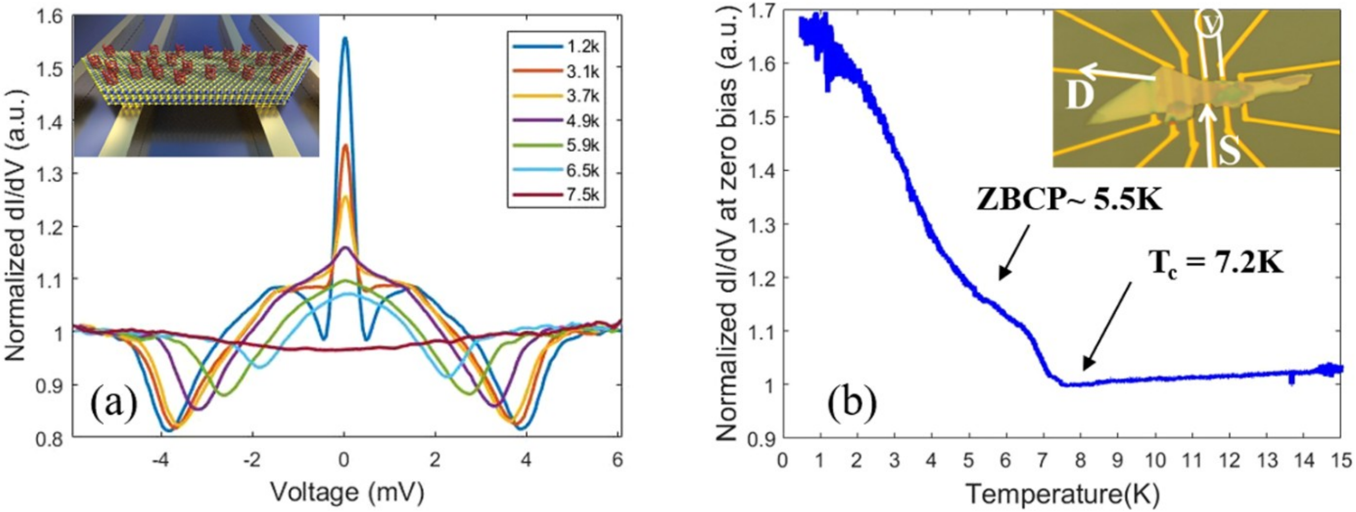


Charge redistribution is accompanied by spin polarization

A. Kumar, et. al., Proc. Natl. Acad. Sci. USA 114, 2474 (2017)

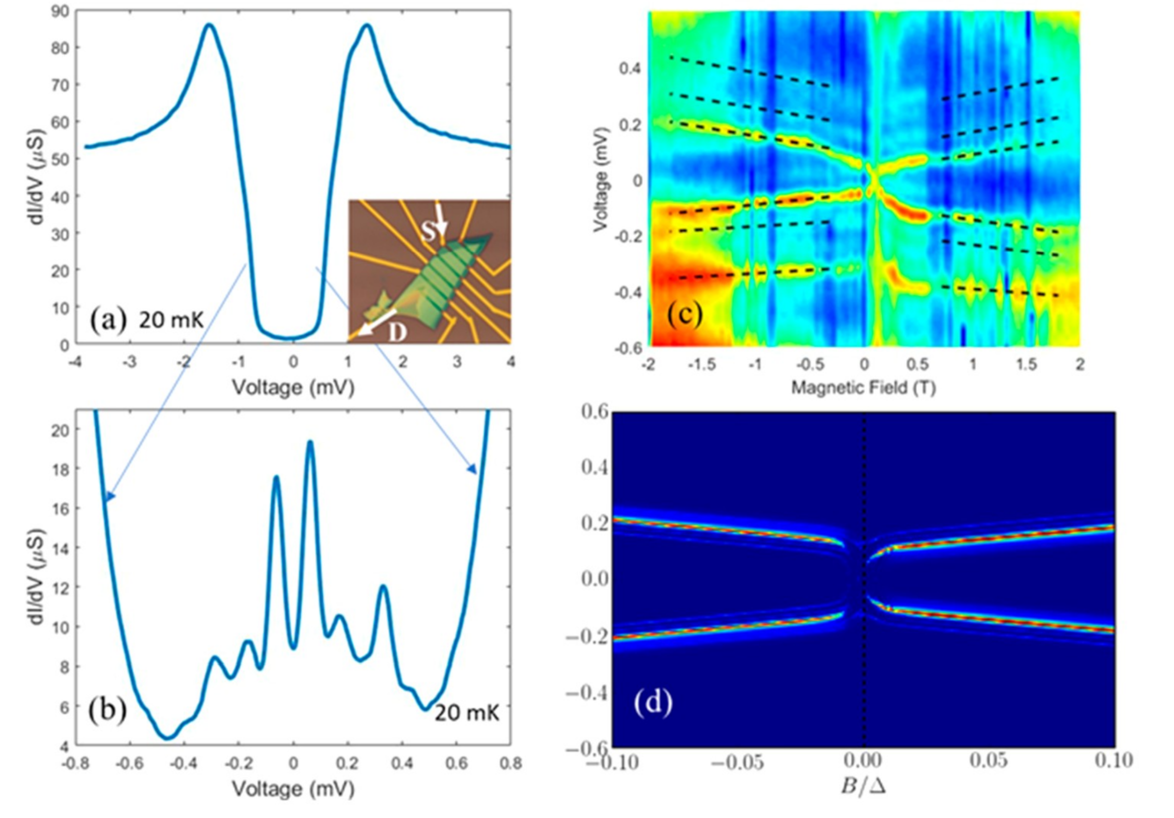
Chiral molecules on superconductor

Observation of the zero bias peak



H. Alpern, et. al., Nano Lett. 19, 5167–5175 (2019)

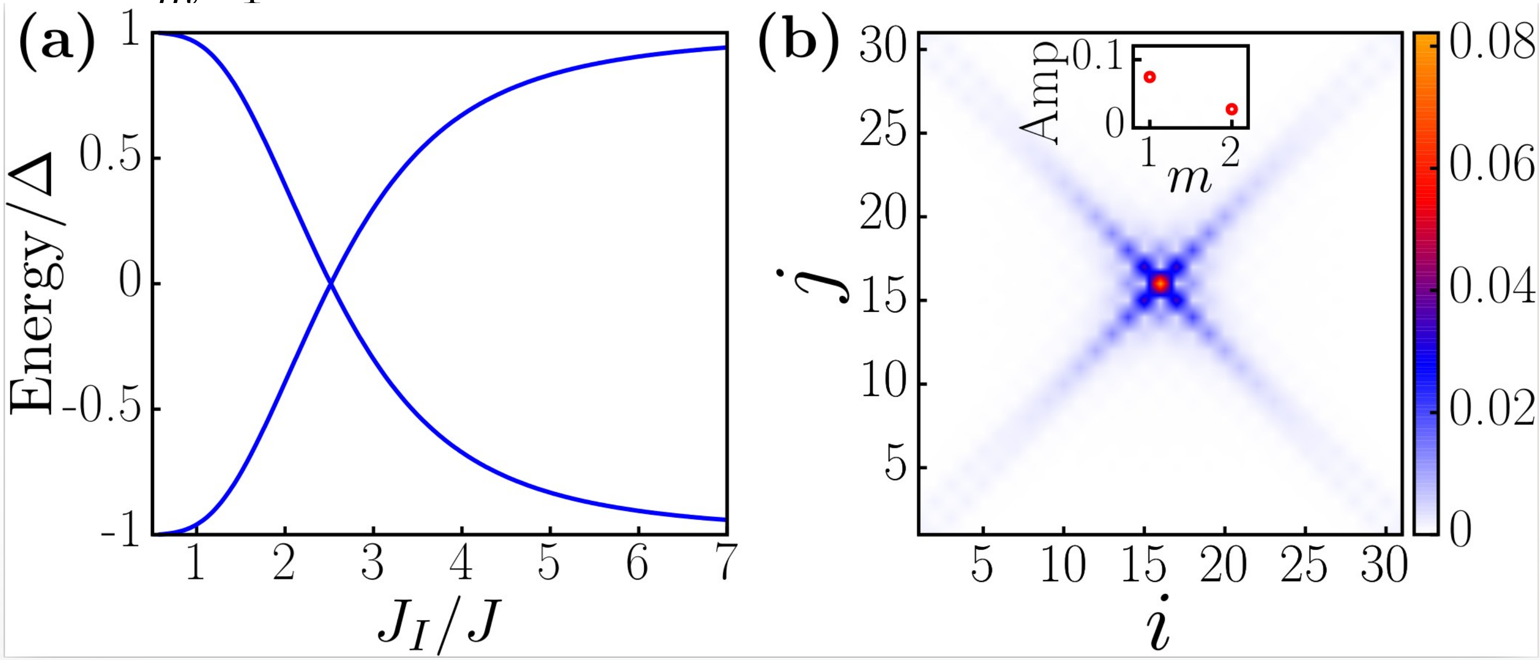
Shiba states in the experiment

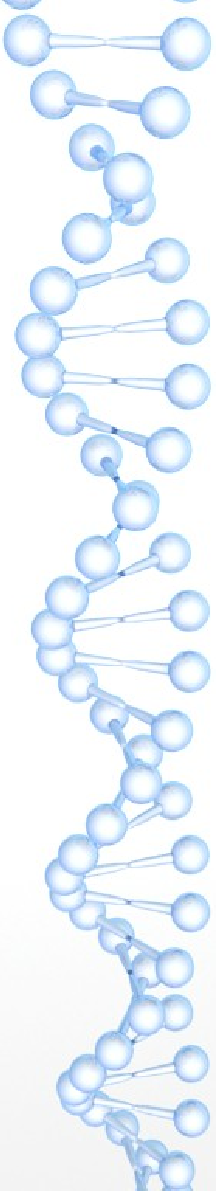


H. Alpern, et. al., Nano Lett. 19, 5167–5175 (2019)

Shiba states in theory

$$H_2 = \epsilon_0 \sum_{m=1}^{2} c_m^\dagger c_m - J\left[c_2^\dagger v c_1 + c_1^\dagger v^\dagger c_2\right] + \gamma\alpha\sigma_z\left(c_2^\dagger c_2 - c_1^\dagger c_1\right)$$





Is that the end of the story?
Caldeira-Legett model with SOC in 2D

$$\frac{d\rho_S}{dt} = -\frac{i}{\hbar}[\hat{H}_s, \rho_S] - \frac{i\gamma}{\hbar}\left[\mathbf{q}, \{\mathbf{p}, \rho_S\}\right] - \frac{2m\gamma}{\beta\hbar^2}\left[\mathbf{q}, [\mathbf{q}, \rho_S]\right]$$

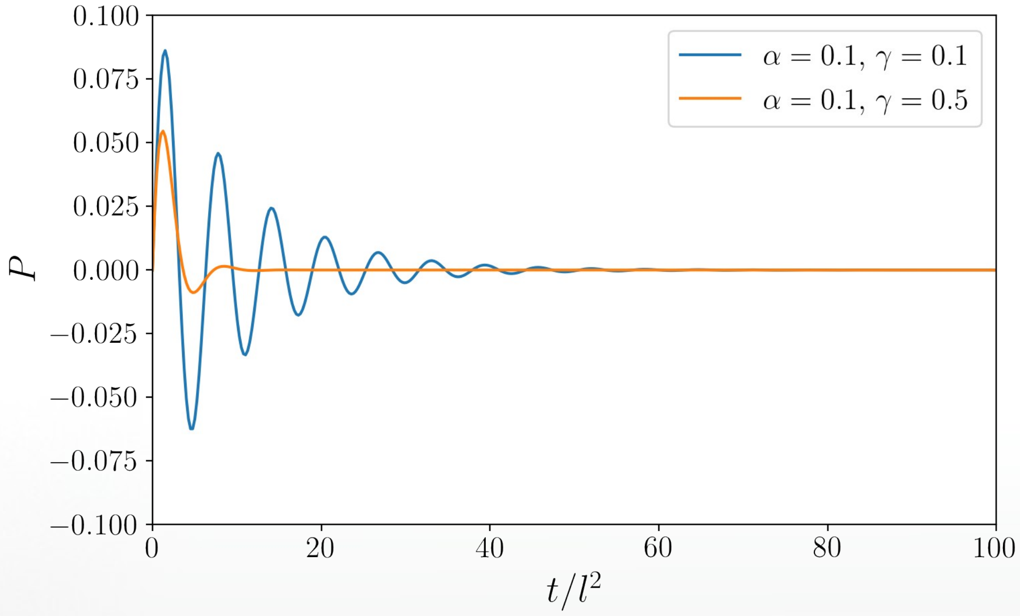
Dissipation (second term) — Decoherence (third term)

$$+\frac{i\alpha m\gamma}{\hbar}\left[\mathbf{q}, \{\sigma_y \mathbf{e}_x - \sigma_x \mathbf{e}_y, \rho_S\}\right]$$

New additional term

In 1D SOC can be gauged out and only affects initial condition

$$\tilde{\rho}_S(R, r, 0) = e^{-\frac{im\alpha\sigma_x r}{\hbar}} \rho_S(R, r, 0)$$



$$P \propto \frac{\alpha}{\gamma} e^{-\frac{t}{2\gamma}}$$

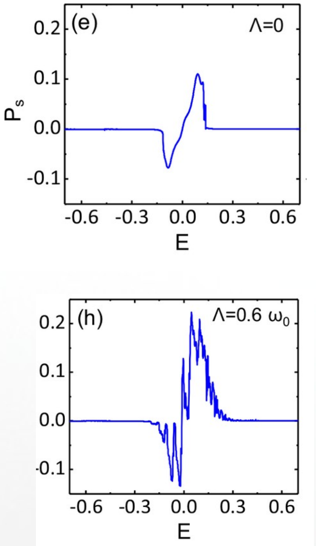
$$\gamma \gg 1$$

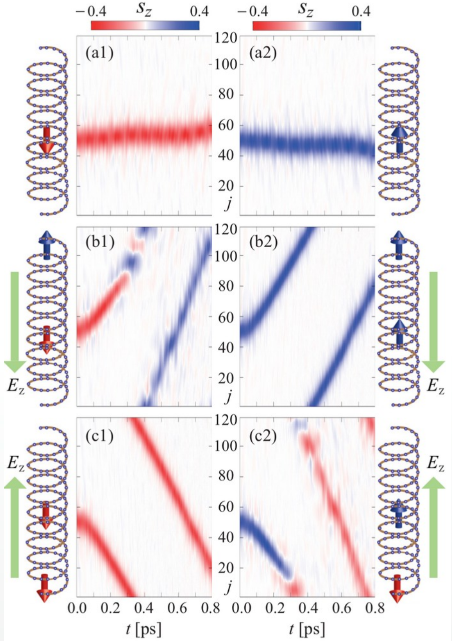
Possible solutions

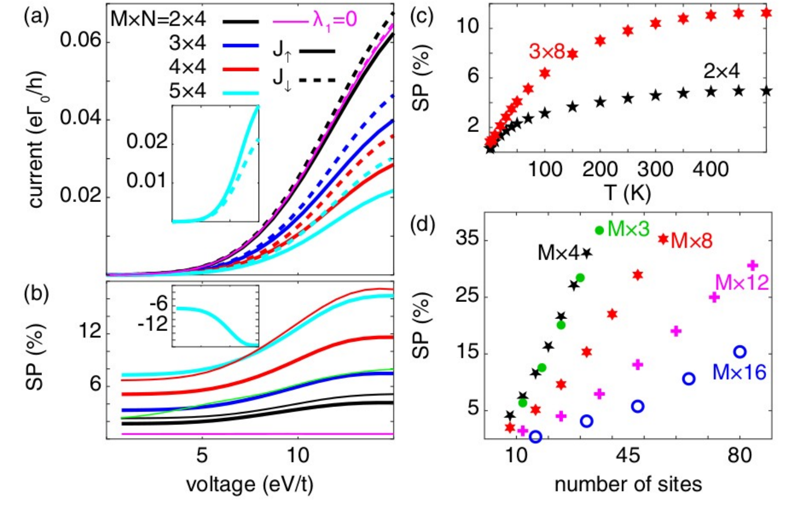
- Quasi 1D system
- Beyond Caldeira-Legett model
- Spatial dependence of SOC
- ...

Other works exploring polaron model coupled to the bath for CISS

- G.F. Du, et. al. PRB 102, 035431 (2020)
- L. Zhang, et. al., PRB 102, 214303 (2020)
- J. Fransson, et. al., PRB 102, 235416 (2020)

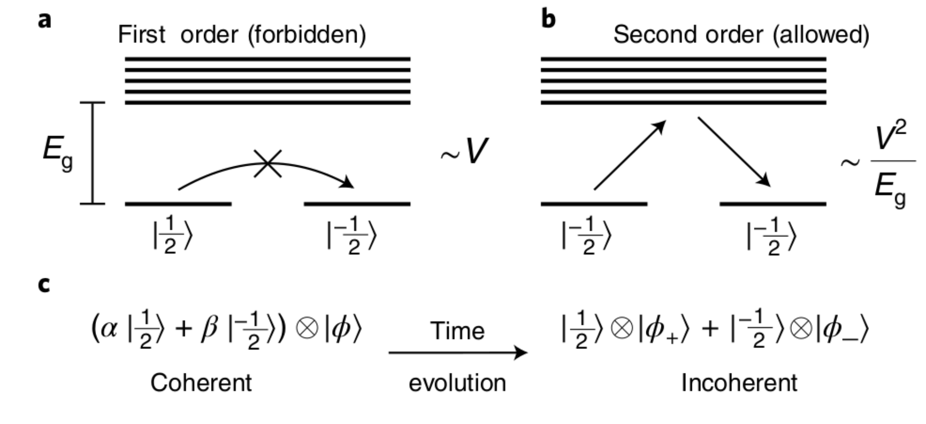






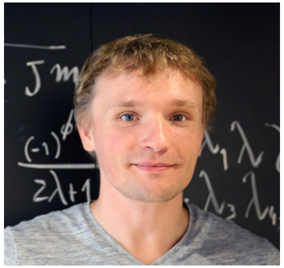
Recent interesting developments on breaking Kramer’s degeneracy with coupling to the bath

- M. McGinley and N. R. Cooper, Nat. Phys. 16, 1181 (2020)
- S. Lieu, et. al., arXiv:2105.02888
- P. Zhang and Y. Chen, arXiv:2108.05493
- T. Hata, et. al., arXiv:2108.06465



My collaborators

IST Austria



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Thank you