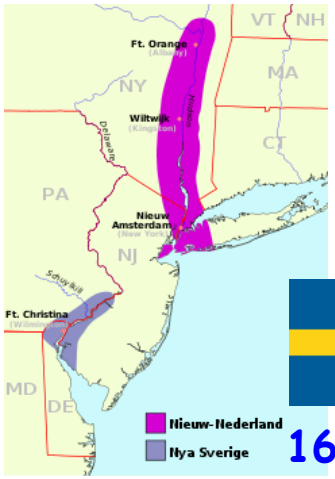
Spin and Charge Pumping in the Presence of Spin-Orbit Coupling in THz Spintronics with Antiferromagnets

Branislav K. Nikolić

Department of Physics & Astronomy, University of Delaware, Newark, DE 19716, U.S.A.



1638–1655

CENTER FOR HYBRID, ACTIVE, AND RESPONSIVE MATERIALS

CHARM

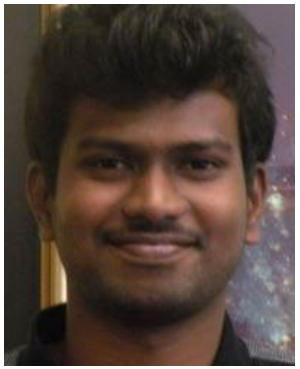
at the UNIVERSITY OF DELAWARE

https://mrsec.udel.edu/

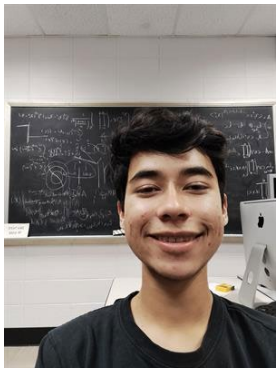
https://wiki.physics.udel.edu/qttg

QTTG

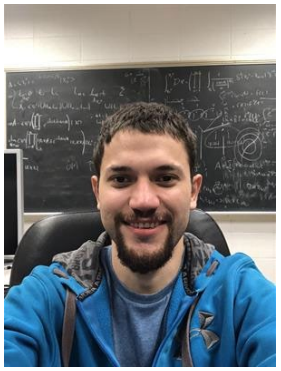
Collaborators



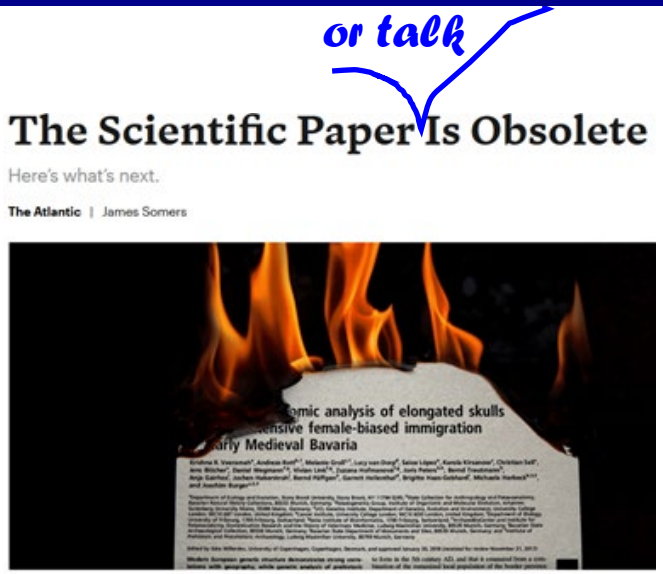
Abhin Suresh



Federico Garcia-Gaitan



Jalil Varela-Manjarres



Dr. Kapildeb Dolui

Dr. Marko D. Petrović

Prof. Adrian Feiguin

Prof. Benjamin Jungfleisch

Ultrafast-Light-Driven Demagnetization and THz Radiation in a Nutshell

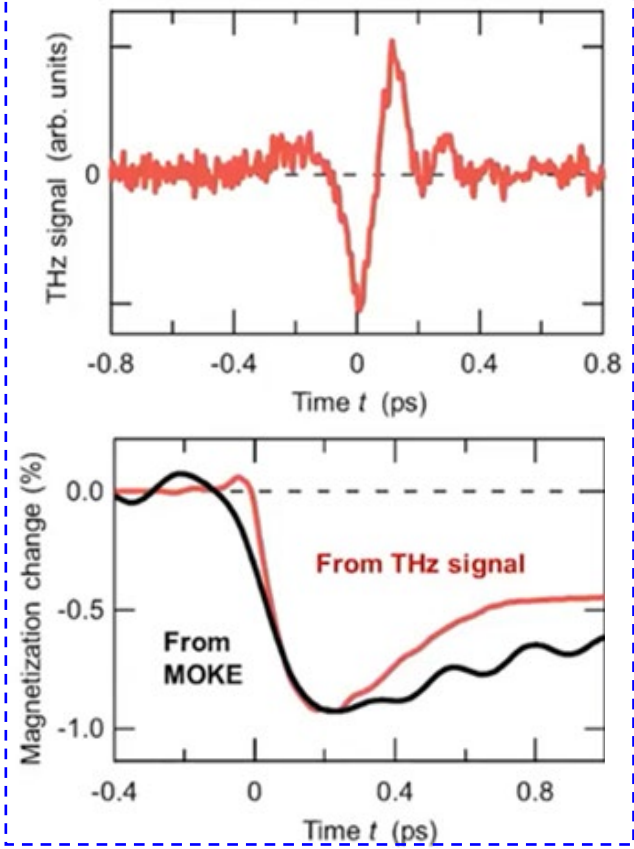
PHYSICAL REVIEW B **106**, 144427 (2022)

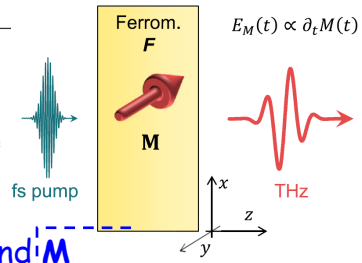
Editors' Suggestion

Laser-induced terahertz spin transport in magnetic nanostructures arises from the same force as ultrafast demagnetization

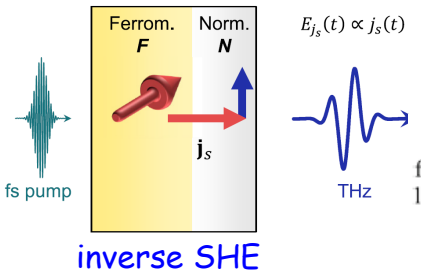
Reza Rouzegar,[1,2,*] Liane Brandt,[3] Lukáš Nádvorník,[1,2,4] David A. Reiss,[1] Alexander L. Chekhov,[1,2] Oliver Gueckstock,[1,2] Chihun In,[1,2] Martin Wolf,[2] Tom S. Seifert,[1] Piet W. Brouwer,[1] Georg Woltersdorf,[3] and Tobias Kampfrath[1,2,†]

- ~100 times smaller than THz from F/N_{SO}
- invariant under sample turning by 180° around **M**

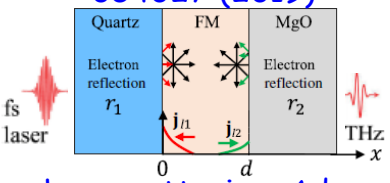




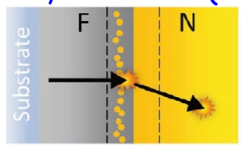
inverse SHE
Edelstein effect:
PRL **120**, 207207 (2018)



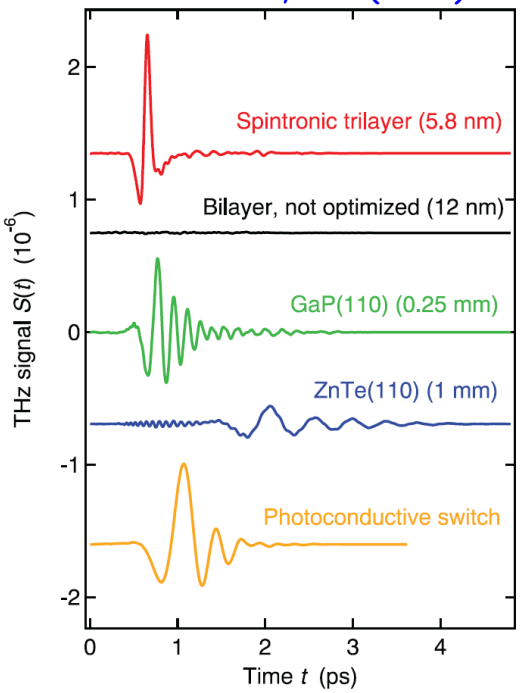
AHE: PR Appl. **12**, 054027 (2019)

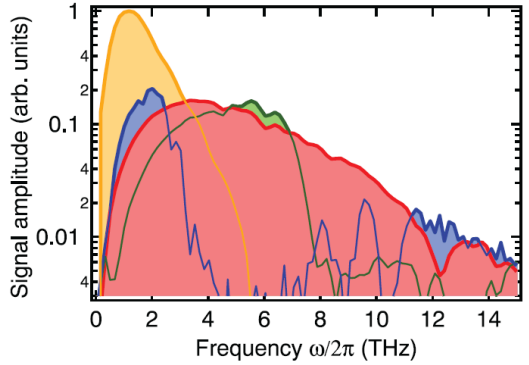


skew-scattering: Adv. Mater. **33**, 2006281 (2021)

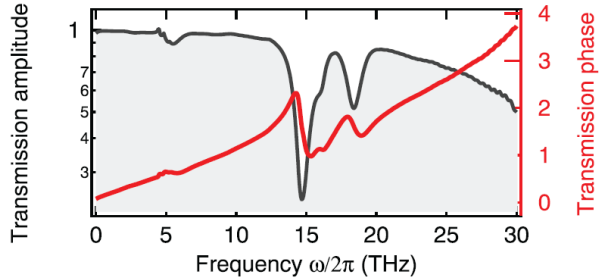


Nat. Phot. **10**, 483 (2016)





(c)



THz Driven Antiferromagnets

SPINTRONICS

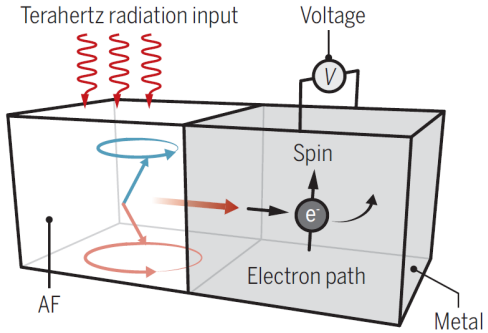
Spin pumping gathers speed

Coherent spin pumping from an antiferromagnet into a metal occurs at ~400 gigahertz

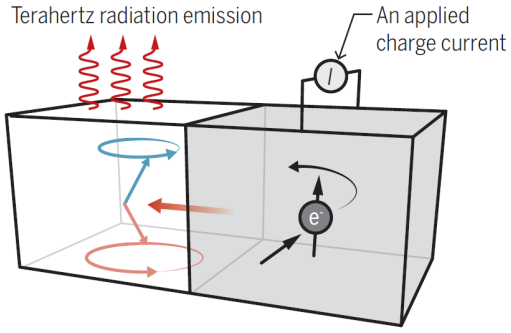
By **Axel Hoffmann**

Spin pumping with antiferromagnets

In an antiferromagnet (AF), terahertz irradiation excites magnetization dynamics at high frequencies because of additional exchange energy involved with the relative canting between the two spin directions.



Spin pumping
Terahertz radiation pumps spin currents into adjacent metals, which get converted into charge currents and concomitant charge voltages through spin Hall effects.



Spin torque driven magnetization dynamics
Charge currents are converted to spin current through spin Hall effects. Injection into antiferromagents can excite magnetization dynamics that can drive terahertz emission.

Nature **578**, 70 (2020)
Science **368**, 160 (2020)

Science **368**, 160 (2020)

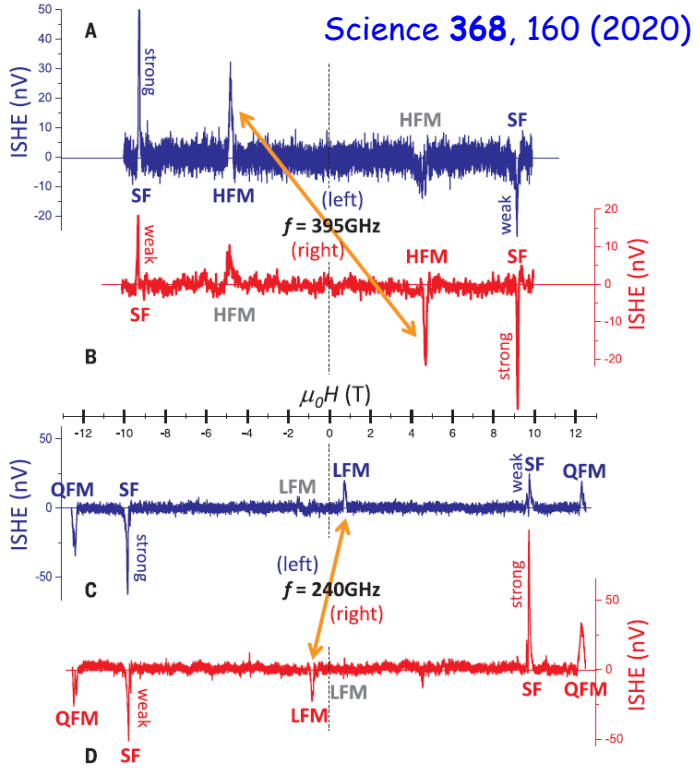


Fig. 2. Inverse spin Hall effect in MnF_2/Pt. ISHE signal obtained in MnF_2/Pt for sample 3 at f = 395 GHz (**A**) left- and (**B**) right-handed circularly polarized microwaves and for sample 2 at f = 240 GHz microwaves with both (**C**) left- and (**D**) right-handed circular polarization. A monotonous signal background has been subtracted from all spectra (*26*). Three distinct features are observed at 240 GHz: The LFM at $\mu_0 H = \pm 0.8$ T, the SF transition resonance at $\mu_0 H = \pm 9.73$ T, and the QFM resonance at $\mu_0 H = \pm 12.37$ T. Only the HFM and the SF resonances are observable for 395 GHz at $\mu_0 H = \pm 4.70$ and ± 9.15 T, respectively, within the available field range.

Theories of Laser-Driven Magnets Rarely Calculate Emitted Radiation that is Measured

PHENOMENOLOGICAL

IOP Publishing
J. Phys.: Condens. Matter **30** (2018) 115801 (10pp)
Journal of Physics: Condensed Matter
https://doi.org/10.1088/1361-648X/aaad95

Transport theory for femtosecond laser-induced spin-transfer torques

Superdiffusion+LLG equations

Pavel Baláž[1,3], Martin Žonda[1], Karel Carva[1], Pablo Maldonado[2] and Peter M Oppeneer[2]

PHYSICAL REVIEW APPLIED **11,** 054083 (2019)

Boltzmann+Helmholtz equations

Simulation of Hot-Carrier Dynamics and Terahertz Emission in Laser-Excited Metallic Bilayers

Dennis M. Nenno,[1,2] Rolf Binder,[2] and Hans Christian Schneider[1,*]

PHYSICAL REVIEW B **97**, 014424 (2018)

Vlasov+LLG equations

Spin current generation by ultrafast laser pulses in ferromagnetic nickel films

Jérôme Hurst, Paul-Antoine Hervieux, and Giovanni Manfredi*

MICROSCOPIC ⟺ HAMILTONIAN-BASED

PRL **115,** 217204 (2015) PHYSICAL REVIEW LETTERS week ending 20 NOVEMBER 2015

Many-Body Theory of Ultrafast Demagnetization and Angular Momentum Transfer in Ferromagnetic Transition Metals

W. Töws and G. M. Pastor

New J. Phys. **23** (2021) 033042 https://doi.org/10.1088/1367-2630/abe72b

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PAPER

Ultrafast spin dynamics in inhomogeneous systems: a density-matrix approach applied to Co/Cu interfaces

F Töpler*, J Henk and I Mertig

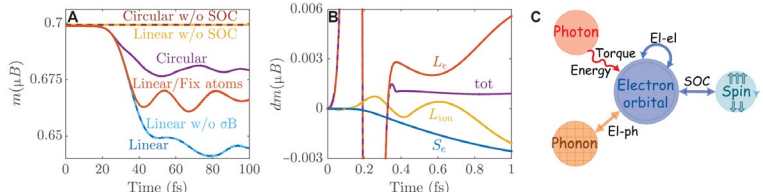
FIRST-PRINCIPLES ⟺ TDDFT

SCIENCE ADVANCES | RESEARCH ARTICLE

CONDENSED MATTER PHYSICS

Role of initial magnetic disorder: A time-dependent ab initio study of ultrafast demagnetization mechanisms

Zhanghui Chen and Lin-Wang Wang*



JCTC Journal of Chemical Theory and Computation Article
pubs.acs.org/JCTC

Laser-Induced Demagnetization at Ultrashort Time Scales: Predictions of TDDFT

K. Krieger,[†] J. K. Dewhurst,[†] P. Elliott,[†] S. Sharma,[*,†,‡] and E. K. U. Gross[†]

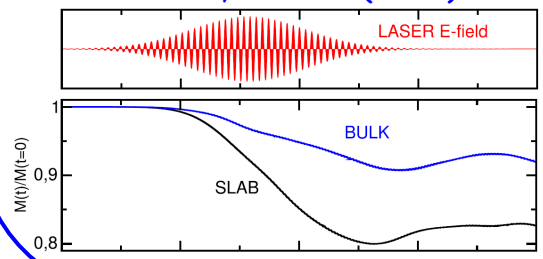
NANO LETTERS Letter
Cite This: *Nano Lett.* 2018, 18, 1842−1848
pubs.acs.org/NanoLett

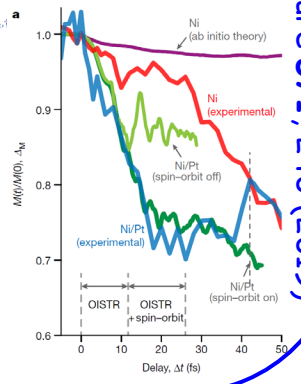
arXiv:2307.11736

Laser-Induced Intersite Spin Transfer

John Kay Dewhurst,[†] Peter Elliott,[†] Sam Shallcross,[‡] Eberhard K. U. Gross,[†] and Sangeeta Sharma[*,†]

JPCM **29**, 224001 (2017)

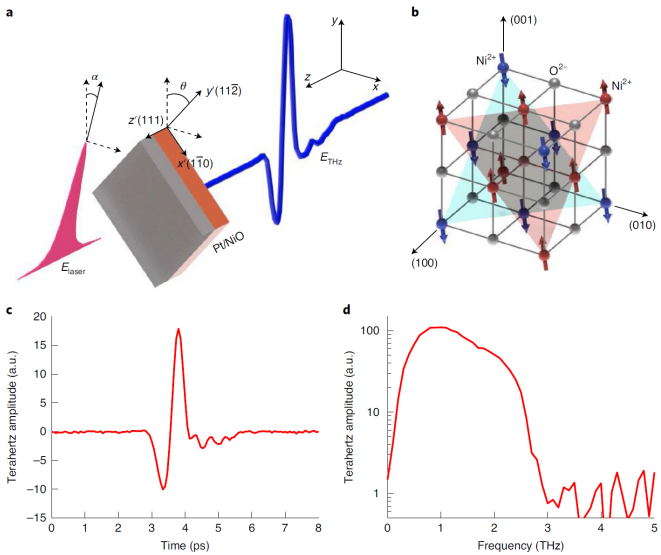




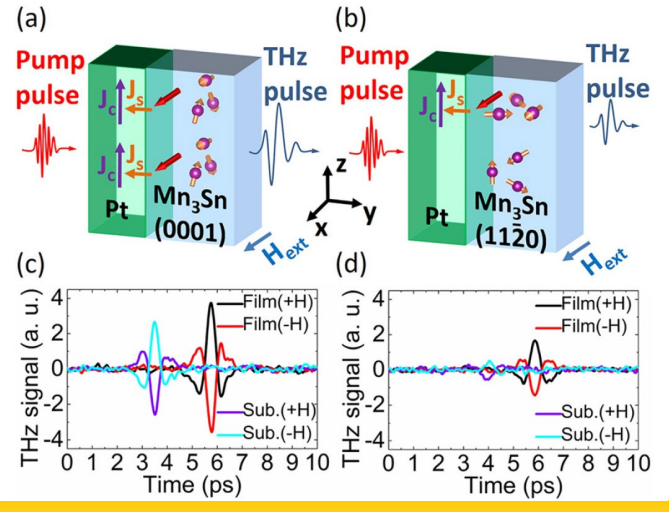
Nature **571**, 240 (2019)

Ultrafast-Light-Driven Antiferromagnets: Experiments and Movies from QME+LLG+Jefimenko

Nat. Phys. **17**, 389 (2021)

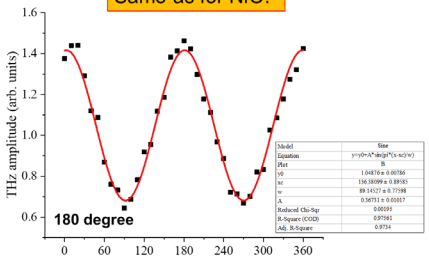


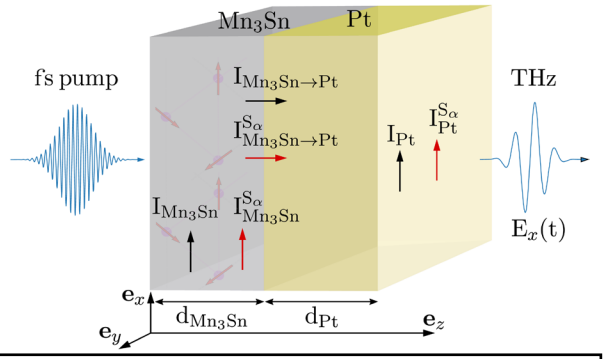
APL **115**, 182402 (2019)



Jungfleisch Lab unpublished

Same as for NiO!

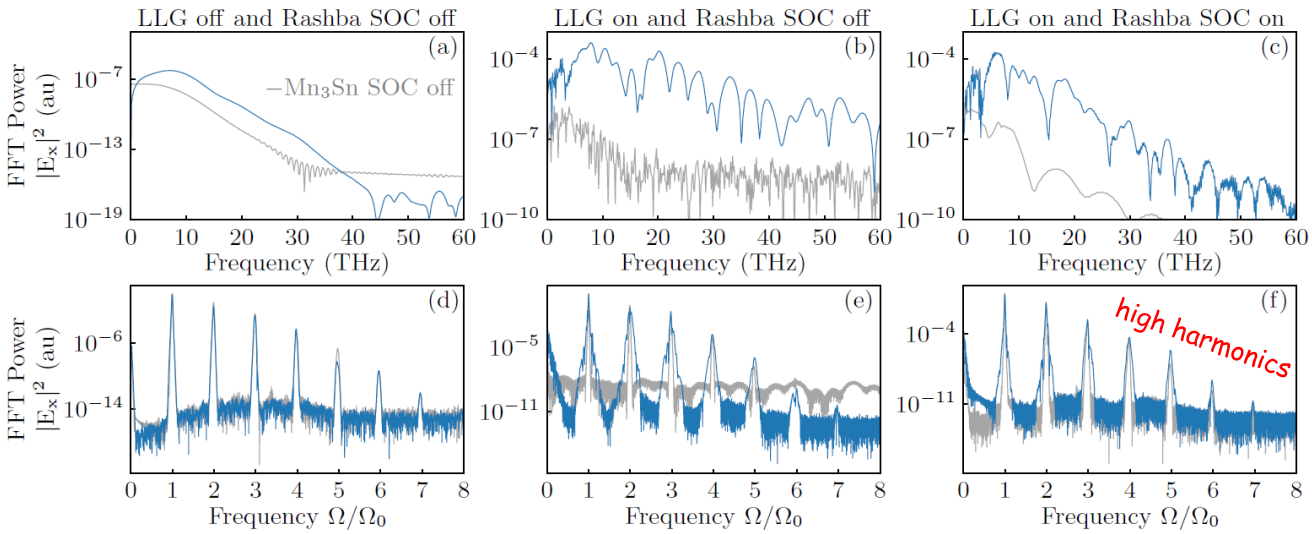


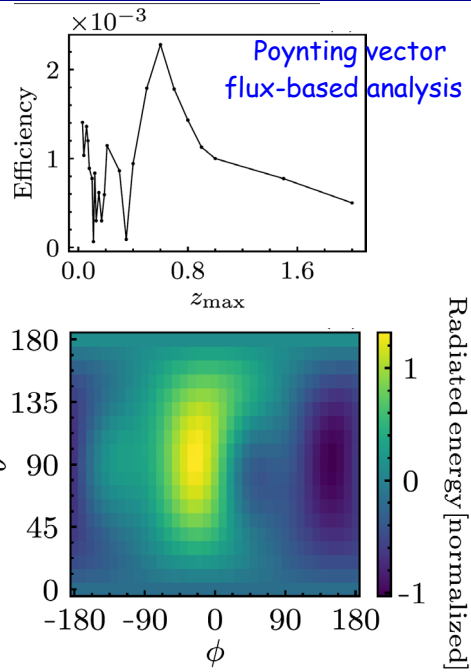


This is a movie → it will play in, e.g., Xodo if you click on arrow

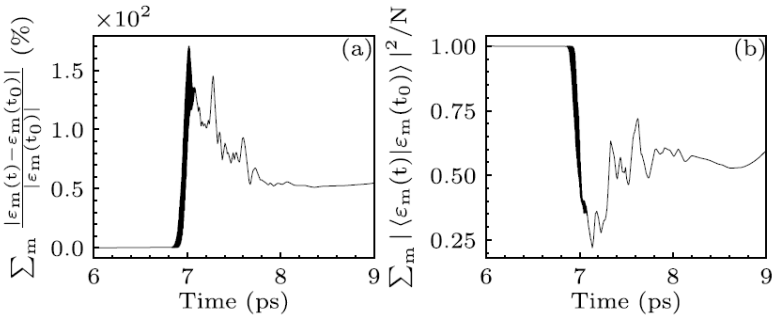
Ultrafast-Light-Driven Mn_3Sn: Pumped Spin and Charge Currents and Emitted Radiation

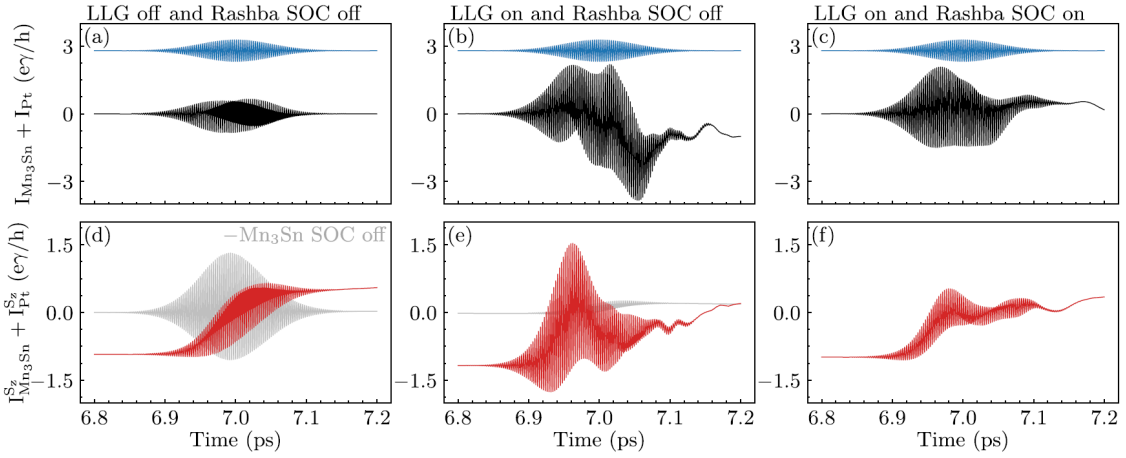
PRB **107**, 174421 (2023)





far-from-equilibrium Mn_3Sn: eigenenergies and eigenstates are far away from their equilibrium counterparts, so the Lindblad operators **must be** defined in instantaneous eigenbasis to bring current to zero in the long-time limit





Spin and Charge Pumping and Radiation from Lindblad QME + LLG + Jefimenko Equations

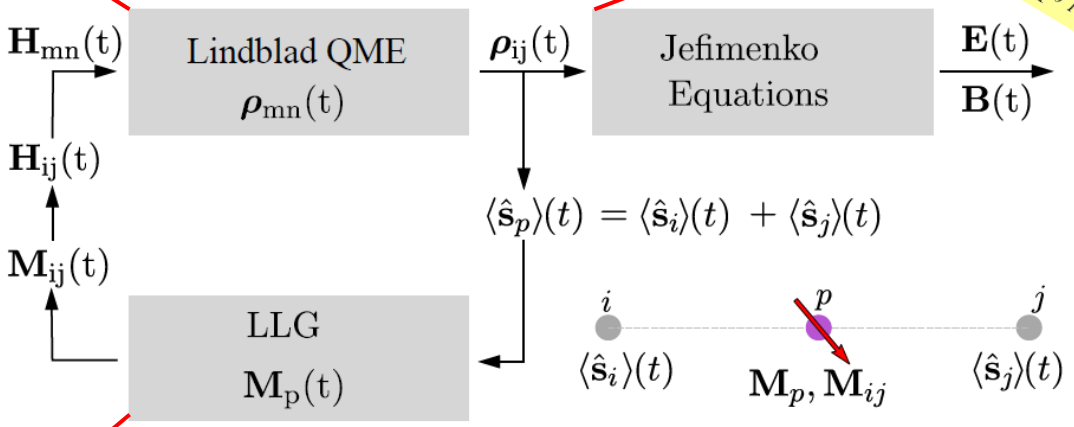
$$\hat{H}_{\mathrm{Mn_3Sn}}(t) = \sum_{\langle i,j\rangle_{xy}} \gamma_{ij}^{xy}(t)\hat{\mathbf{c}}_i^\dagger\hat{\mathbf{c}}_j + \sum_{\langle i,j\rangle_{z}} \gamma_{ij}^{z}(t)\hat{\mathbf{c}}_i^\dagger\hat{\mathbf{c}}_j - J_{sd}\sum_{\langle i,j\rangle_{xy}} \hat{\mathbf{c}}_i^\dagger\hat{\boldsymbol{\sigma}}\hat{\mathbf{c}}_j\cdot\mathbf{M}_{ij}(t) + i\lambda_z\sum_{\langle i,j\rangle_{xy}}(-1)^{\xi_{i,j}}\hat{\mathbf{c}}_i^\dagger\hat{\sigma}_z\hat{\mathbf{c}}_j$$

$$\frac{\partial\hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}(t),\hat{\rho}] + \mathcal{L}[\hat{F}](\hat{\rho})$$

$$\mathcal{L}[\hat{F}](\hat{\rho}) = \hat{F}\hat{\rho}\hat{F}^\dagger - \frac{1}{2}(\hat{F}^\dagger\hat{F}\hat{\rho} + \hat{\rho}\hat{F}^\dagger\hat{F})$$

$$\mathbf{E}(\mathbf{r},t) = \frac{1}{4\pi\epsilon_0}\left\{\sum_{i=1}^{N}\left[e\rho_{ii}(t_r)\frac{\mathbf{r}-\mathbf{r}_i}{|\mathbf{r}-\mathbf{r}_i|^3} + \frac{1}{c}\frac{\partial e\rho_{ii}(t_r)}{\partial t}\frac{\mathbf{r}-\mathbf{r}_i}{|\mathbf{r}-\mathbf{r}_i|^2}\right] - \sum_{P_{i\to j}=1}^{N_b}\int_{P_{i\to j}}\frac{1}{c^2}\frac{\partial\, I_{i\to j}(t_r)}{\partial t}\frac{}{|\mathbf{r}-\mathbf{l}|}d\mathbf{l}\right\}$$

$$\mathbf{B}(\mathbf{r},t) = \frac{\mu_0}{4\pi}\sum_{P_{i\to j}=1}^{N_b}\int_{P_{i\to j}}\left[\frac{I_{i\to j}(t_r)}{|\mathbf{r}-\mathbf{l}|^3} + \frac{1}{c}\frac{\partial\, I_{i\to j}(t_r)}{\partial t}\frac{}{|\mathbf{r}-\mathbf{l}|^2}\right]d\mathbf{l}\times(\mathbf{r}-\mathbf{l})$$



PRB **107**, 174421 (2023)

$$\mathcal{H}(t) = J_1\sum_{\langle p,q\rangle_{xy}}\mathbf{M}_p\cdot\mathbf{M}_q + J_2\sum_{\langle p,q\rangle_{z}}\mathbf{M}_p\cdot\mathbf{M}_q + \sum_{\langle p,q\rangle_{xy}}\mathbf{D}_{pq}\cdot(\mathbf{M}_p\times\mathbf{M}_q) - K\sum_p(\hat{\mathbf{n}}_p\cdot\mathbf{M}_p)^2 - J_{sd}\sum_p\langle\hat{\mathbf{s}}_p\rangle\cdot\mathbf{M}_p(t)$$

$$\frac{\partial\mathbf{M}_p}{\partial t} = -\frac{g}{1+\lambda^2}\left[\mathbf{M}_p\times\mathbf{B}_p^{\mathrm{eff}} + \lambda\mathbf{M}_p\times\left(\mathbf{M}_p\times\mathbf{B}_p^{\mathrm{eff}}\right)\right]$$

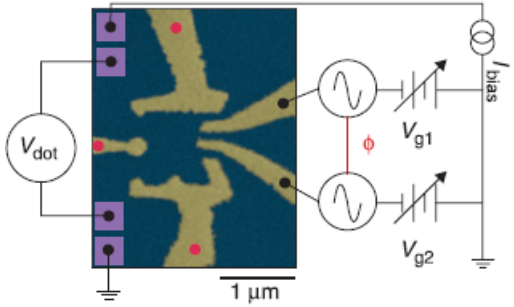
Crash Course on Spin Pumping

Charge Pumping

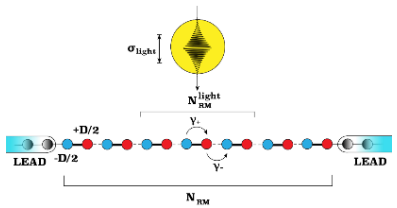
An Adiabatic Quantum Electron Pump

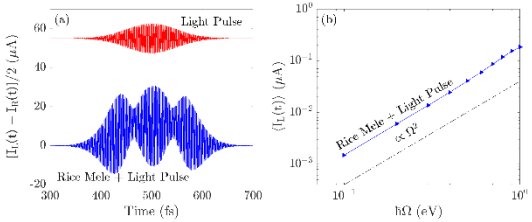
M. Switkes,[1] C. M. Marcus,[1]* K. Campman,[2] A. C. Gossard[2]

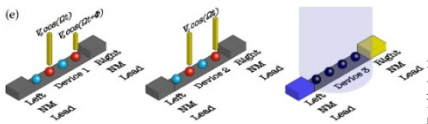
Science **283**, 1905 (1999)

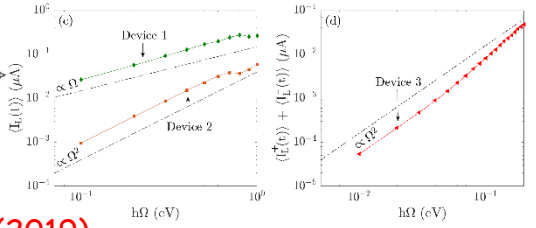


requires quantum-coherence and low temperatures + very difficult to disentangle from other competing effects









J. Phys. Mater. **2**, 025004 (2019)

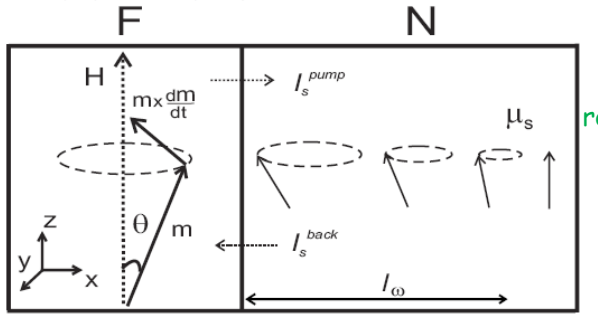
Spin Pumping

REVIEWS OF MODERN PHYSICS, VOLUME 77, OCTOBER 2005

Nonlocal magnetization dynamics in ferromagnetic heterostructures

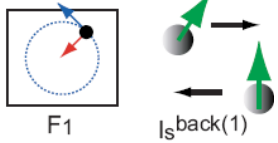
Yaroslav Tserkovnyak
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138, USA
Arne Brataas
Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway
Gerrit E. W. Bauer
Kavli Institute of NanoScience, Delft University of Technology, 2628 CJ Delft, The Netherlands
Bertrand I. Halperin
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

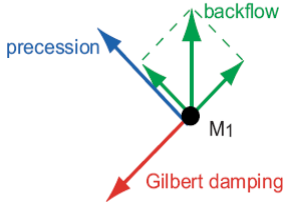
diffuse-transport regime only. Strong spin-orbit coupling immediately at interfaces, for example, requires generalization of spin-pumping and circuit theories beyond the scope of this review.

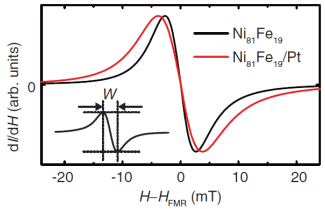


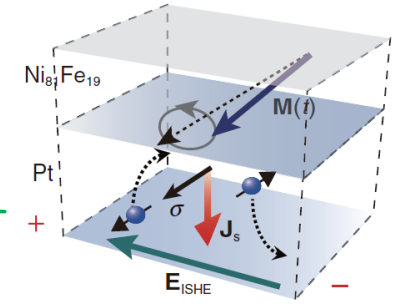
robust and ubiquitous effect in magnetic heterostructures, even at room temperature

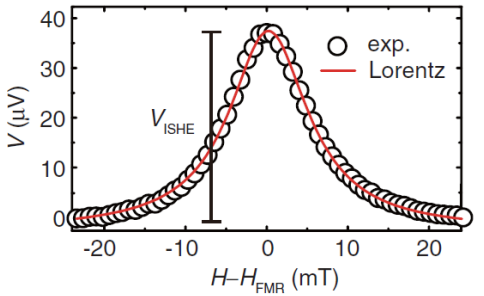
Experimental manifestations







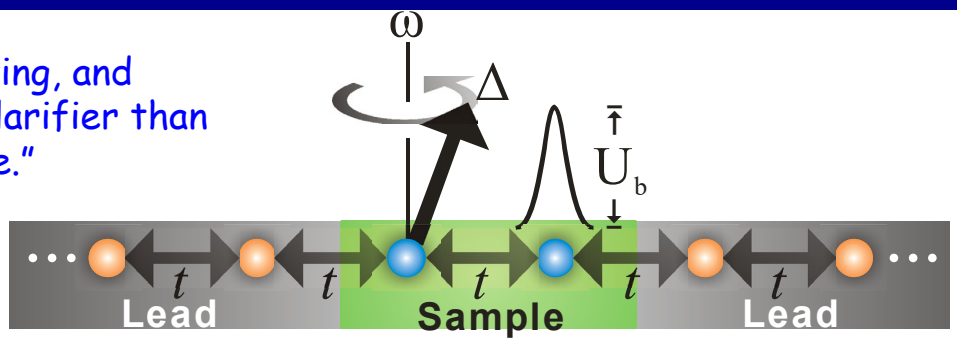




Simplest Example of Spin Pumping: 1D Tight-Binding Chain with a Single Precessing Classical Spin

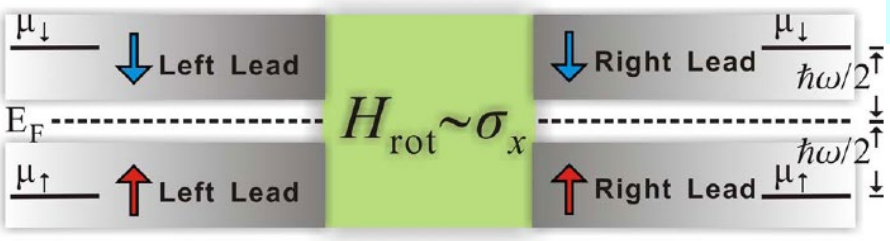
PRB **79**, 054424 (2009)

MOTTO: "In teaching, writing, and research, there is no greater clarifier than a well-chosen example."



$$\hat{H}_{\rm lab}(t) = \sum_{\mathbf{r},\sigma,\sigma'} \left(\varepsilon_{\mathbf{r}} \delta_{\sigma\sigma'} - \frac{\Delta_{\mathbf{r}}}{2} \mathbf{m}_{\mathbf{r}}(t) \cdot \hat{\boldsymbol{\sigma}}^{\sigma\sigma'} \right) \hat{c}^{\dagger}_{\mathbf{r}\sigma} \hat{c}_{\mathbf{r}\sigma'} - \gamma \sum_{\langle \mathbf{r}\mathbf{r}' \rangle \sigma} \hat{c}^{\dagger}_{\mathbf{r}\sigma} \hat{c}_{\mathbf{r}'\sigma}$$

$$\hat{H}_{\rm rot} = \hat{U} \hat{H}_{\rm lab}(t) \hat{U}^{\dagger} - i\hbar \hat{U} \frac{\partial}{\partial t} \hat{U}^{\dagger} = \hat{H}_{\rm lab}(0) - \frac{\hbar\omega}{2} \hat{\sigma}_z$$



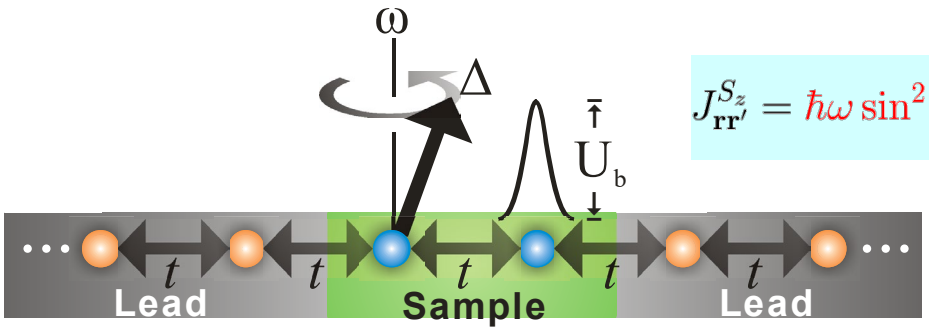
$$I_L^S = \frac{e\omega}{2\pi} \int_{\rm BZ} d\mathbf{k}_{||} \left(T_{LR}^{\uparrow\downarrow} + T_{RL}^{\uparrow\downarrow} + 2T_{LL}^{\uparrow\downarrow} \right)$$

$$I = \frac{e\omega}{2\pi} \int_{\rm BZ} d\mathbf{k}_{||} \left(T_{RL}^{\uparrow\downarrow} - T_{LR}^{\uparrow\downarrow} \right)$$

$$V_{\rm pump} = IG(\theta)^{-1}$$

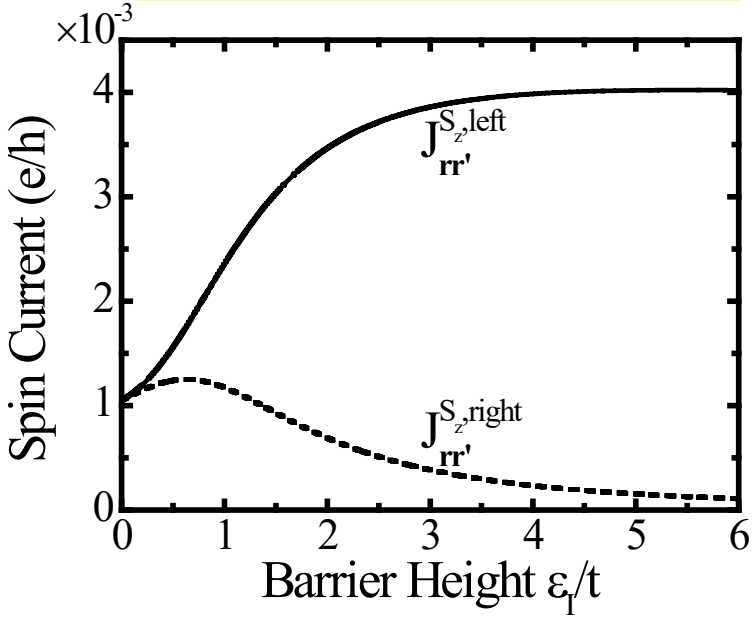
Exact Solution for Pumped Spin and Charge Currents in the Rotating Frame

PRB **79**, 054424 (2009)

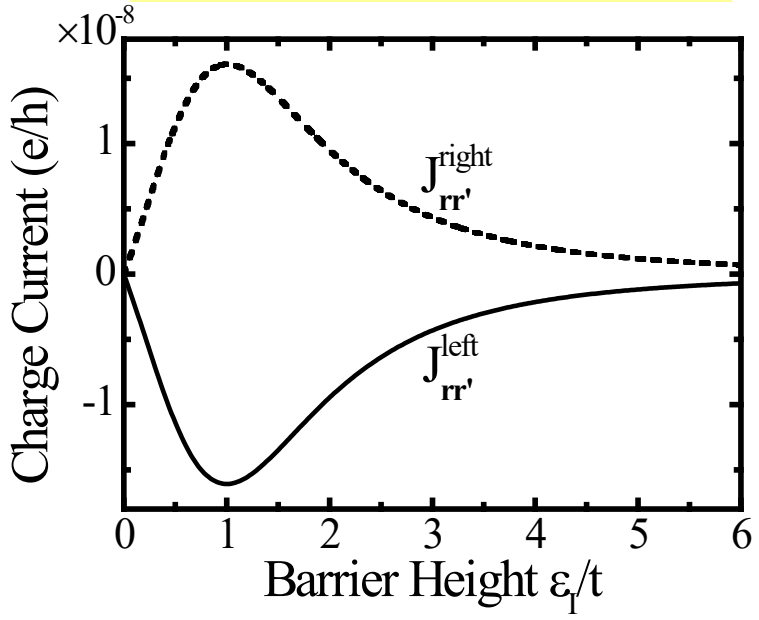


$$J^{S_z}_{\mathbf{rr'}} = \hbar\omega \sin^2\theta \Delta^2 \frac{\gamma^2 (\mathrm{Im}\,\Sigma_{1D})^2}{8\pi |R|^2} \left[4\left(\gamma^2 + \varepsilon_I^2\right) + 4|\Sigma_{1D}|^2 - 8\varepsilon_I \mathrm{Re}\,\Sigma_{1D}\right]$$

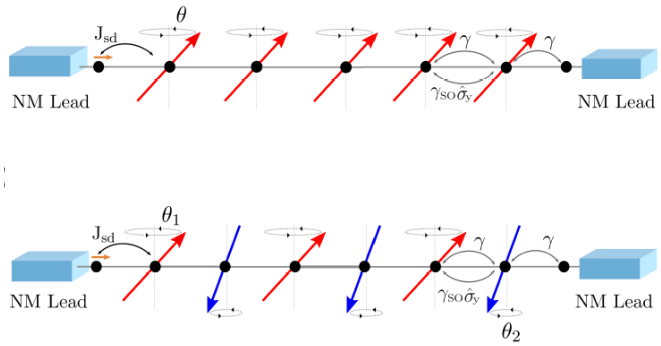
Spin current pumping from a single precesing spin



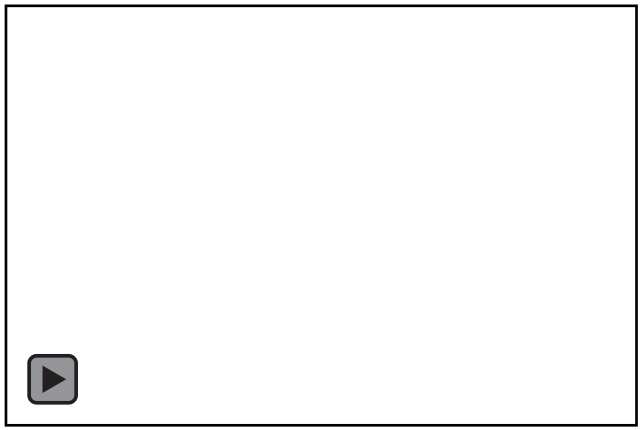
Charge current pumping from a single precessing spin

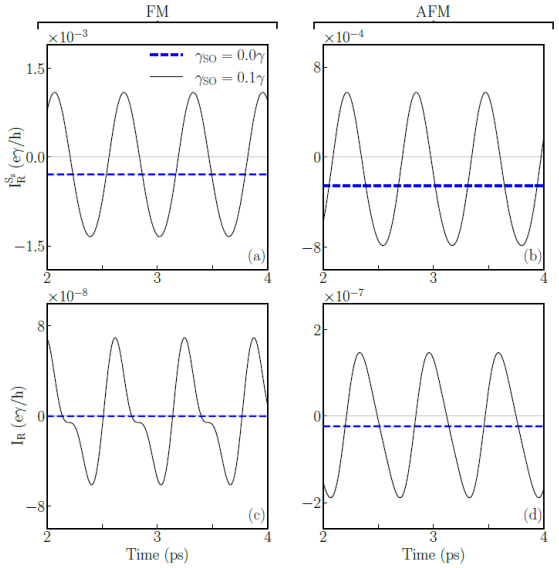


High Harmonics in Spin Pumping from Ferromagnets or Antiferromagnets with Spin-Orbit Coupling



J. Phys. Mater. **6**, 045001 (2023)





Floquet-Keldysh Green's functions

$$G^r(t,t') \xrightarrow{\text{double FT}} G^r(E,E') \xrightarrow{\text{restricted to}} G^r_n(E) = G^r(E, E+n\hbar\omega)$$

$$\check{\mathbf{H}}_F = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \iddots \\ \cdots & \mathbf{H}_0 & \mathbf{V} & 0 & \cdots \\ \cdots & \mathbf{V}^\dagger & \mathbf{H}_0 & \mathbf{V} & \cdots \\ \cdots & 0 & \mathbf{V} & \mathbf{H}_0 & \cdots \\ \iddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad \check{\Omega} = \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \iddots \\ \cdots & -\hbar\omega\mathbf{1} & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & \hbar\omega\mathbf{1} & \cdots \\ \iddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

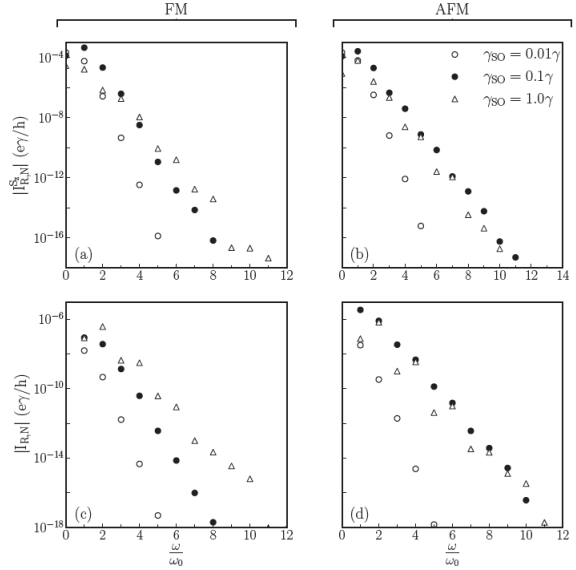
$$[(E+\check{\Omega})\check{\mathbf{S}} - \check{\mathbf{H}}_F - \check{\Sigma}^r(E)]\check{\mathbf{G}}^r(E) = \check{\mathbf{1}}$$

PRB **85**, 054406 (2012)

$$I^{S_\alpha}_{p,N} = \frac{e}{\gamma}\hbar\omega_0 \sum_{p'=L,R}\sum_{n=-\infty}^{\infty} n\mathrm{Tr}\left[\hat{\sigma}_\alpha \mathbf{S}^\dagger_{pp'}(E_F + n\hbar\omega_0, E_F)\mathbf{S}_{pp'}(E_F + (n+N)\hbar\omega_0, E_F)\right]$$

$$\mathbf{S}_{pp'}(E_F + n\hbar\omega_0, E_F) = \delta_{pp'}\delta_{E_F+n\hbar\omega_0,E_F} - i\sqrt{\mathbf{\Gamma}_p(E_F+n\hbar\omega_0)}\mathbf{G}^r_{pp'}(E_F+n\hbar\omega_0, E_F)\sqrt{\mathbf{\Gamma}_{p'}(E_F)}$$

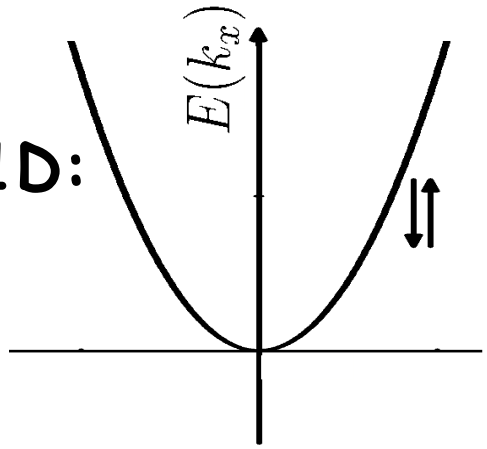
J. Phys. Mater. **6**, 045001 (2023)

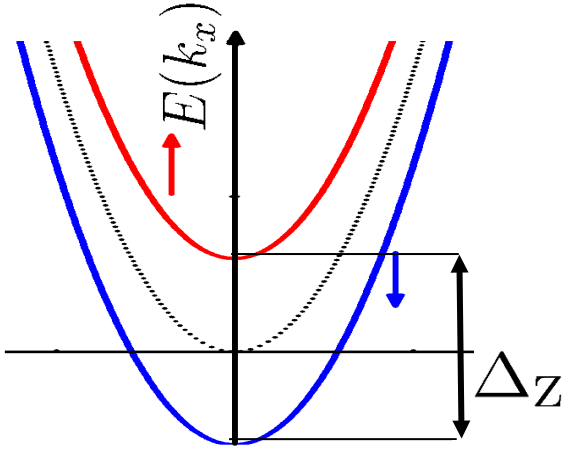


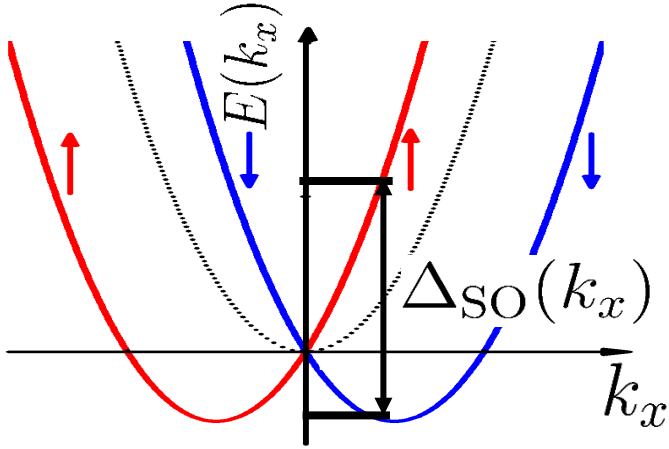
Crash Course on Rashba SOC in Solids

$$\hat{H}_{\mathrm{SO}}^{\mathrm{R}} = \frac{\alpha}{\hbar}(\hat{\boldsymbol{\sigma}} \times \hat{\mathbf{p}}) \cdot \mathbf{e}_z \equiv -\frac{g\mu_B}{2}\hat{\boldsymbol{\sigma}} \cdot \mathbf{B}_{\mathrm{R}}(\hat{\mathbf{p}})$$

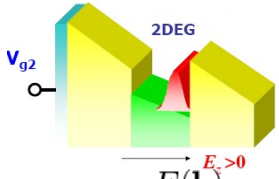
1D:

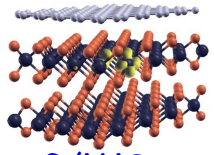


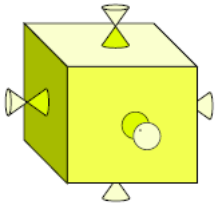




2D:



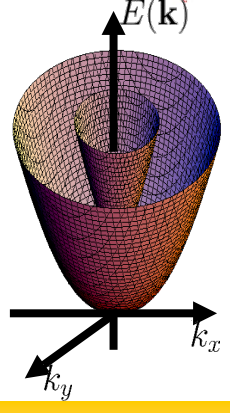


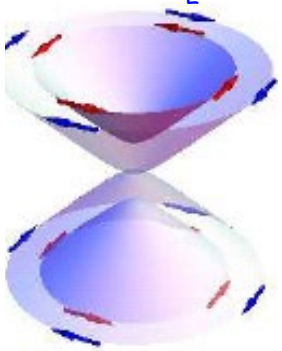


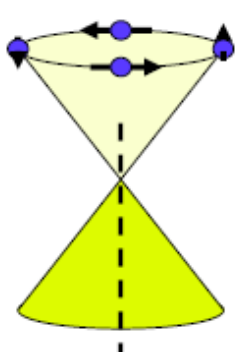
$$\varepsilon(\mathbf{k},\uparrow) = \varepsilon(-\mathbf{k},\downarrow)$$

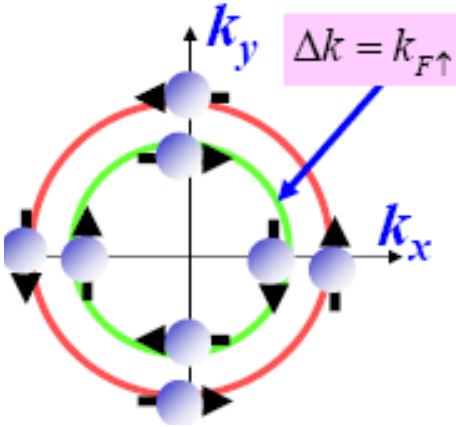
$$\varepsilon(\mathbf{k},\uparrow) \neq \varepsilon(-\mathbf{k},\uparrow)$$

$$\varepsilon(\mathbf{k},\uparrow) \neq \varepsilon(\mathbf{k},\downarrow)$$



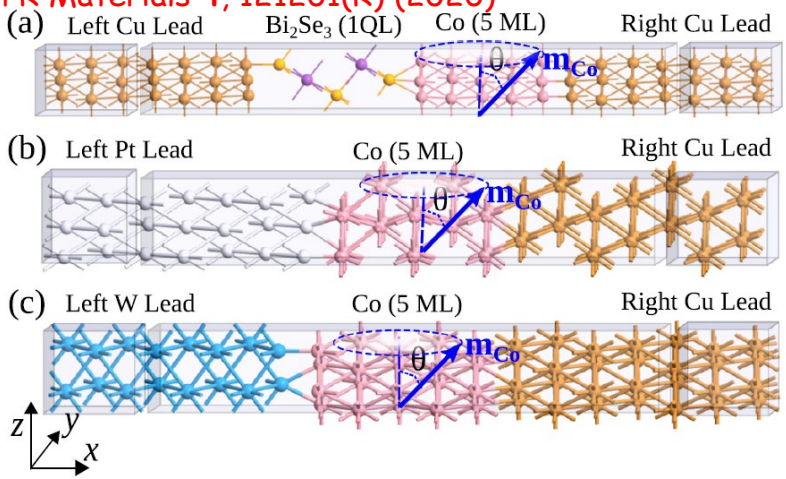






Spin Pumping from Co/Bi_2Se_3 Interface via First-Principles Floquet-Keldysh Green Functions

PR Materials **4**, 121201(R) (2020)



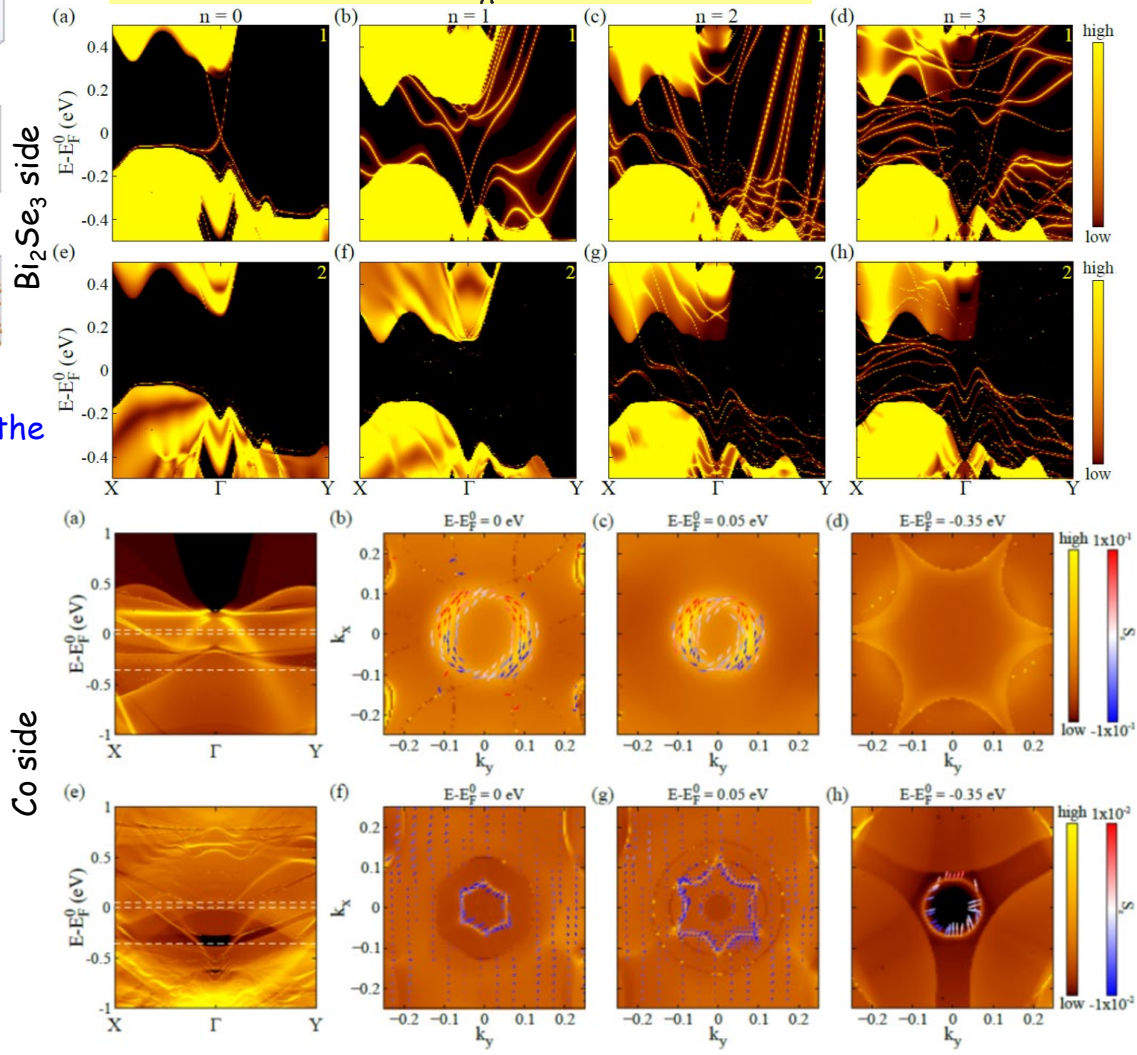
D. Ralph talk 2016: "Theorists – Can you calculate the effective spin mixing conductance for a ferromagnet/TI interface?"

TABLE I. The effective SMC $g^{\text{eff}}_{\uparrow\downarrow}$, extracted from pumped spin currents $I^{S_z}_{\text{L}}$ in Fig. 2 via Eq. (4), in the units of 10^{20} m^{-2}.

Heterostructure	$g^{\text{eff}}_{\uparrow\downarrow}$ (w/o SOC)	$g^{\text{eff}}_{\uparrow\downarrow}$ (SOC)
Cu/Co/Cu	0.7721	0.7721
Pt/Co/Cu	1.4142	0.3866
W/Co/Cu	0.4191	0.2476
Cu/1QL-Bi_2Se_3/Co/Cu	0.4721	0.1716
Cu/6QL-Bi_2Se_3/Co/Cu	0.0002	0.0074

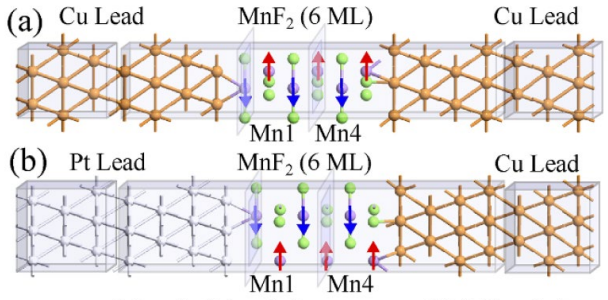
Nano Lett. **17**, 5626 (2017)

$$A(E;k_x,k_y,z) = -\frac{1}{\pi}\mathrm{Im}\left[G_{\mathbf{k}_\parallel}(E;z,z)\right]$$



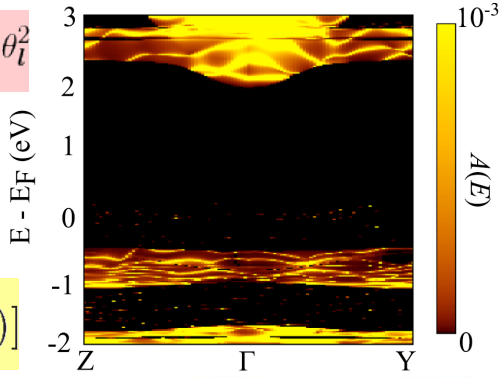
Spin Pumping from Antiferromagnetic Insulator MnF_2 via First-Principles Floquet-Keldysh Green Functions

motivated by exp: Science **368**, 160 (2020)

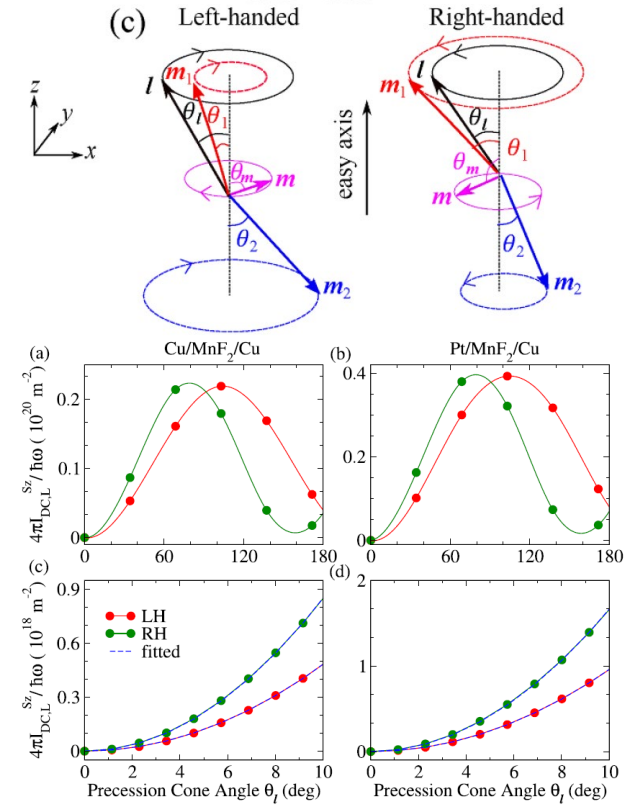


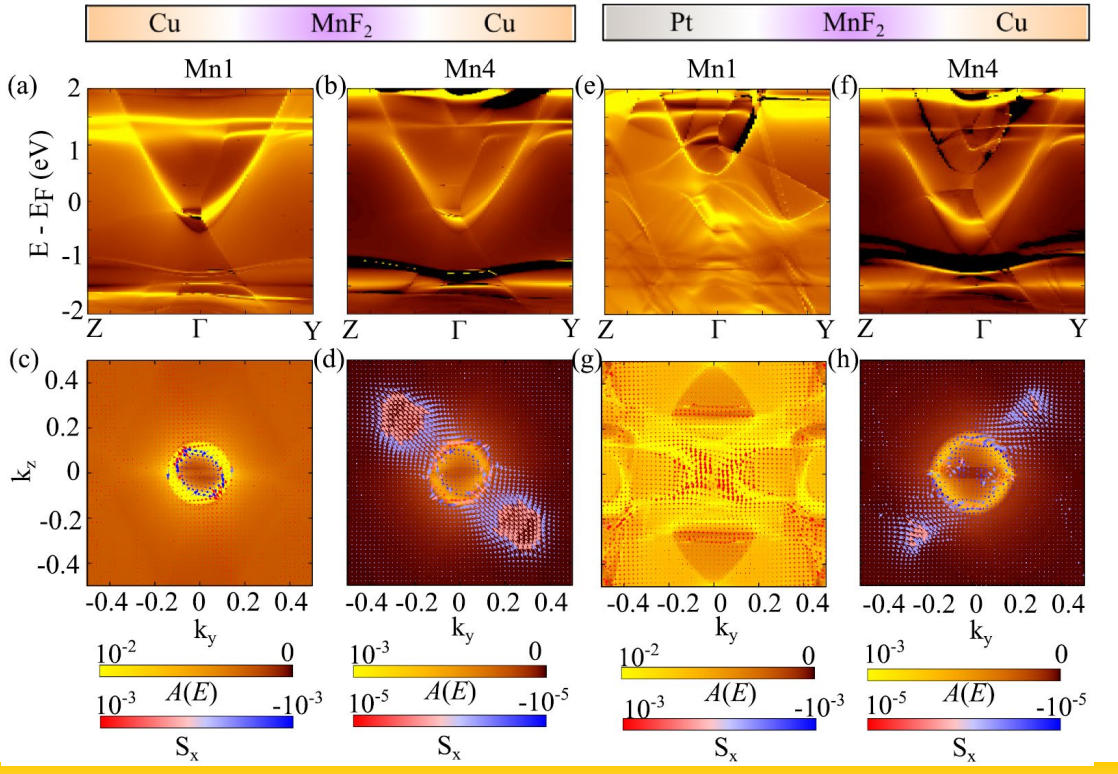
$$g = \sum_{nm}[\delta_{nm} - (r^{\uparrow\uparrow}_{nm})(r^{\downarrow\downarrow}_{nm})^*] \mapsto I^{S_z}_{\mathrm{DC},L}(\theta_l) = \frac{\hbar\omega}{4\pi} g_r^{\mathrm{eff}} \theta_l^2$$

System	$g_r^{\mathrm{eff,LH}}$	$g_r^{\mathrm{eff,RH}}$
$Cu/MnF_2/Cu$	15.82	27.89
$Pt/MnF_2/Cu$	31.42	54.52



$$A(E;k_x,k_y,z) = -\frac{1}{\pi}\mathrm{Im}\left[G_{\mathbf{k}_\parallel}(E;z,z)\right]$$





J. Phys. Mater. **5**, 034002 (2022)

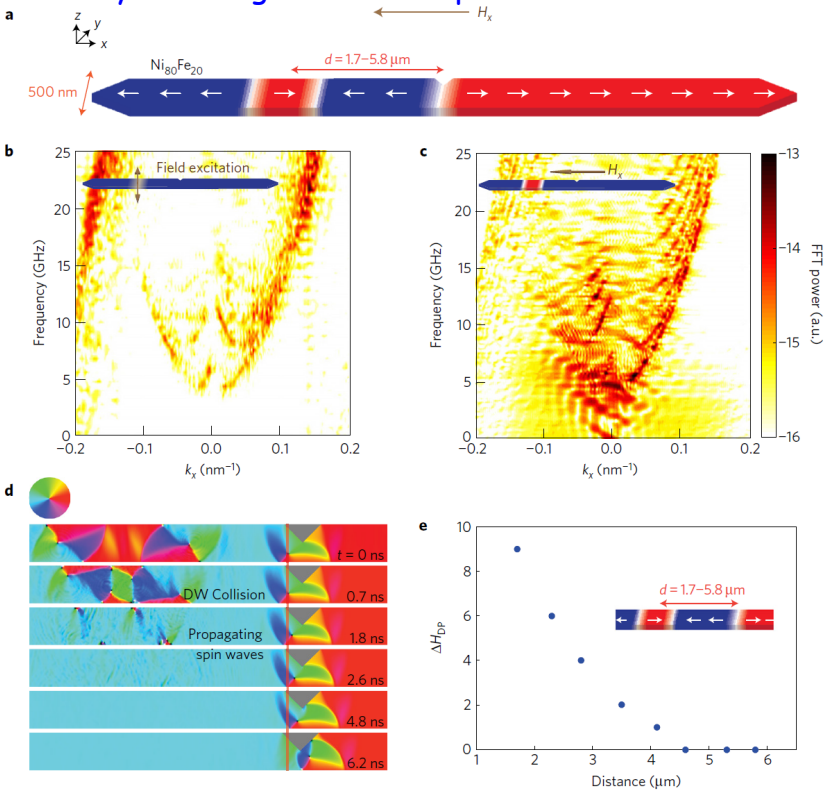
Magnonics with Annihilation of Magnetic DWs in Experiment and LLG Simulations

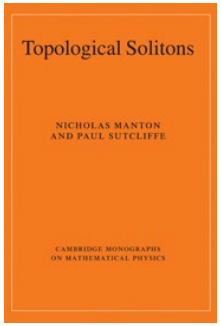
LETTERS
PUBLISHED ONLINE: 30 JANUARY 2017 | DOI: 10.1038/NPHYS4022
nature physics

Magnetic domain wall depinning assisted by spin wave bursts

Seonghoon Woo[1,2], Tristan Delaney[1] and Geoffrey S. D. Beach[1]*

Short-wavelength exchange-dominated SW burst after two DW annihilates drives motion of a third DW by exerting a force comparable to H~10 Oe

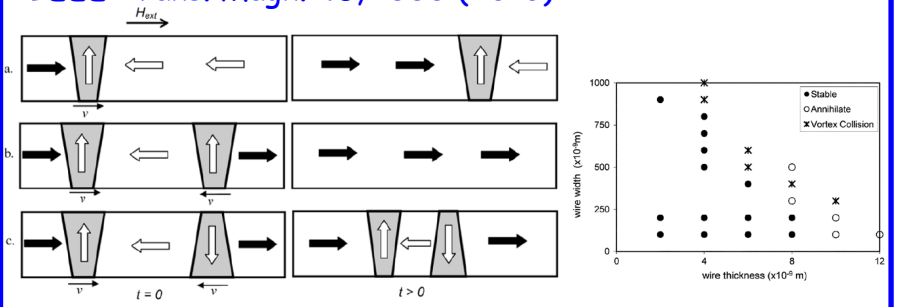




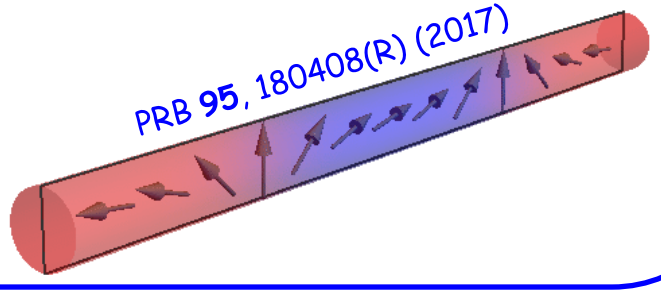
The treatment of solitons as point-like objects breaks down when the solitons come close together. If solitons collide at high speed, then the scattering behavior can be very complicated, the only certainty being the conservation of topological charge. Thus if a soliton and antisoliton collide, they may annihilate and the energy emerge as wave-like radiation - **the field pattern is generally complicated and can only be found numerically**

prior simulations of DW annihilation are based solely on classical micromagnetics

IEEE Trans. Magn. **46**, 1556 (2010)

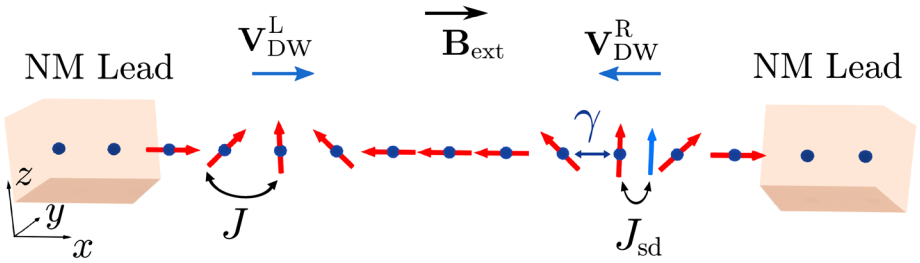


PRB **95**, 180408(R) (2017)

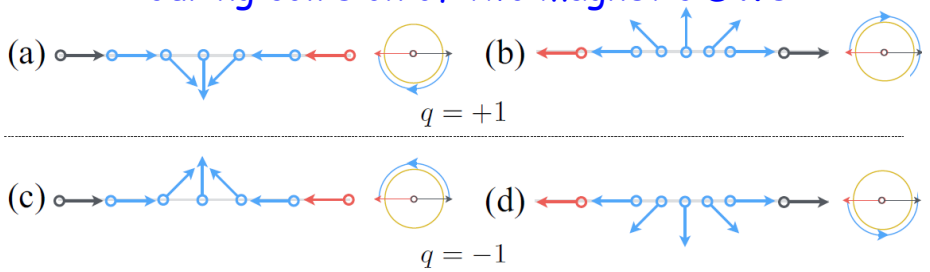


DW Annihilation Induces Burst of Spin Waves: Movie from TDNEGF+LLG

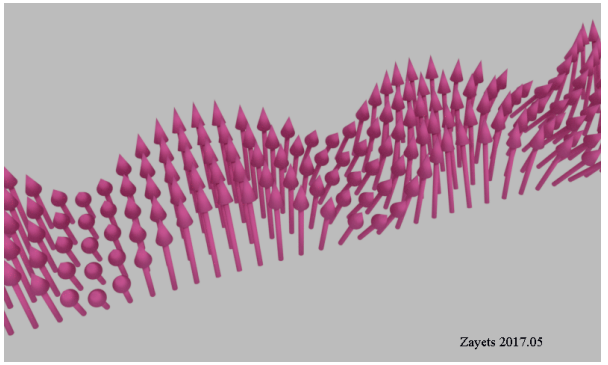
PRB **104**, L020407 (2021)



Total topological charge
(i.e., chirality or winding number) is conserved
during collision of two magnetic DWs



Spin waves in LLG classical picture



Spin Pumping and Torque for Arbitrary $\mathbf{M}_i(t)$ from Time-Dependent Nonequilibrium Green's Function (TDNEGF)

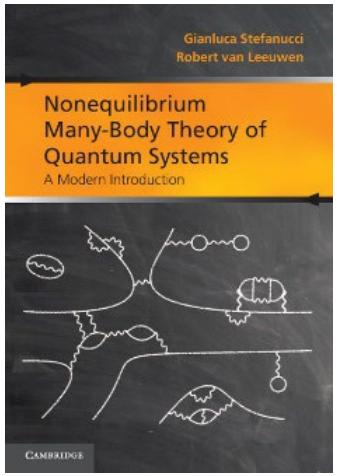
❑Fundamental quantities of NEGF formalism:

density of available quantum states:

$$G^r_{\sigma\sigma'}(t,t') = -\frac{i}{\hbar}\Theta(t-t')\langle\{\hat{c}_{\mathbf{r}\sigma}(t), \hat{c}^\dagger_{\mathbf{r}'\sigma'}(t')\}\rangle$$

how are those states occupied:

$$G^<_{\sigma\sigma'}(t,t') = \frac{i}{\hbar}\langle\hat{c}^\dagger_{\mathbf{r}'\sigma'}(t')\hat{c}_{\mathbf{r}\sigma}(t)\rangle$$



❑Equilibrium DM:

$$\boldsymbol{\rho}_{\rm eq} = -\frac{1}{\pi}\int_{-\infty}^{+\infty} dE\, \mathrm{Im}\,\mathbf{G}^r(E) f(E-E_F)$$

❑Steady-State nonequilibrium DM:

$$\boldsymbol{\rho}_{\rm neq} = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} dE\, \mathbf{G}^<(E)$$

❑Time-dependent nonequilibrium DM:

$$\boldsymbol{\rho}_{\rm neq}(t) = \frac{\hbar}{i}\mathbf{G}^<(t,t')\Big|_{t=t'}$$

$$i\hbar\frac{d\boldsymbol{\rho}_{\rm neq}}{dt} = [\mathbf{H}_{\rm TB}, \boldsymbol{\rho}_{\rm neq}] + i\sum_{p=\rm L,R}[\boldsymbol{\Pi}_p(t) + \boldsymbol{\Pi}_p^\dagger(t)] \qquad \boldsymbol{\Pi}_p(t) = \int_{t_0}^{t} dt_2\,[\mathbf{G}^>(t,t_2)\boldsymbol{\Sigma}_p^<(t_2,t) - \mathbf{G}^<(t,t_2)\boldsymbol{\Sigma}_p^>(t_2,t)]$$

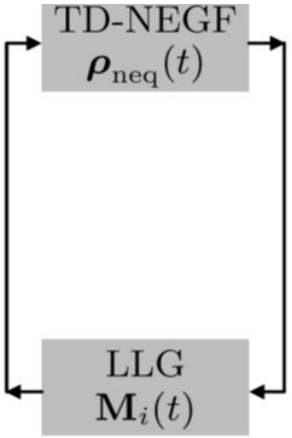
❑Nonequilibrium spin density and spin torque:

$$\langle\hat{\mathbf{s}}_i\rangle_{\rm CD}(t) = \mathrm{Tr}\big[\boldsymbol{\rho}_{\rm neq}(t)|i\rangle\langle i|\otimes\boldsymbol{\sigma}\big] - \mathrm{Tr}\big[\boldsymbol{\rho}^t_{\rm eq}|i\rangle\langle i|\otimes\boldsymbol{\sigma}\big] \qquad \mathbf{T}_i(t) \propto \langle\hat{\mathbf{s}}_i\rangle_{\rm CD}(t)\times\mathbf{M}_i(t)$$

❑Spin and charge currents:

$$I_p^{S_\alpha}(t) = \frac{e}{\hbar}\mathrm{Tr}\,[\hat{\sigma}_\alpha\boldsymbol{\Pi}_p(t)] \qquad I_p(t) = \frac{e}{\hbar}\mathrm{Tr}\,[\boldsymbol{\Pi}_p(t)]$$

TDNEGF+LLG Unravels Time-Retarded Damping Because Electron Spin is Always "Somewhat Behind"



$\Longrightarrow$

arXiv:2303.17596: Schwinger-Keldysh field theory can mimic extended LLG equation with analytical formulas

$$\frac{\partial \mathbf{M}_i(t)}{\partial t} = -g\Big[\mathbf{M}_i(t)\times \mathbf{B}_i^{0,\rm eff}(t) + \frac{J_{sd}^2}{\mu_M}\sum_{p=\rm L,R}\mathbf{M}_i(t)\times\int_{-\infty}^{+\infty} dt''\mathbf{M}_i(t'')\{\mathrm{K}_i^{p}(t'',t)+\mathrm{K}_i^{p*}(t'',t)\}\Big]$$

$\Longrightarrow$

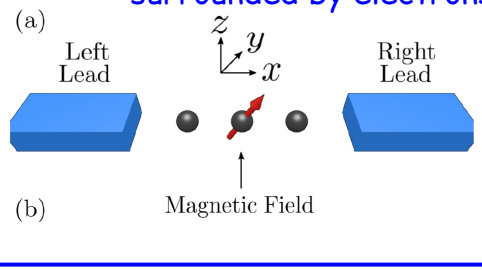
small sd exchange interaction between electron spin and localized spins

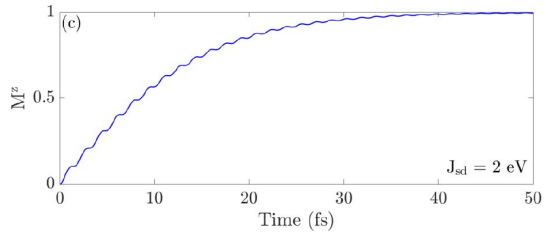
$$\frac{\partial \mathbf{M}_i(t)}{\partial t} = -g\Big[\mathbf{M}_i(t)\times \mathbf{B}_i^{0,\rm eff}(t) + \frac{J_{sd}^2}{\mu_M}\Big\{\sum_{p=\rm L,R}\lambda_{p,n}^{\rm D}(t)\Big\}\mathbf{M}_i(t)\times\frac{\partial \mathbf{M}_i(t)}{\partial t} + \frac{J_{sd}^2}{\mu_M}\Big\{\sum_{p=\rm L,R} I_{p,i}^{\rm D}(t)\Big\}\mathbf{M}_i(t)\times\frac{\partial^2 \mathbf{M}_i(t)}{\partial t^2}\Big].$$

PRB **99**, 134409 (2019)

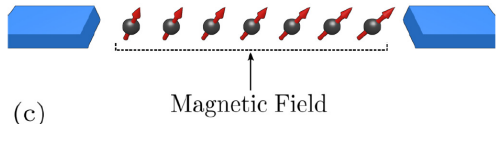
it always takes a finite time for flowing spin of conduction electron to react to the motion of

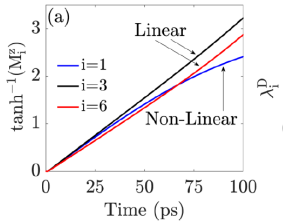
nutation due to magnetic inertia for a single classical spin surrounded by electrons with no spin-orbit coupling

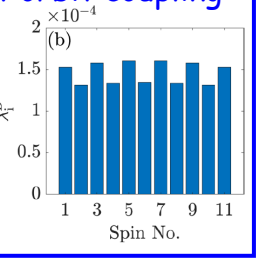




spatially and time-dependent Gilbert damping for many collinear classical spin surrounded by electrons with no spin-orbit coupling



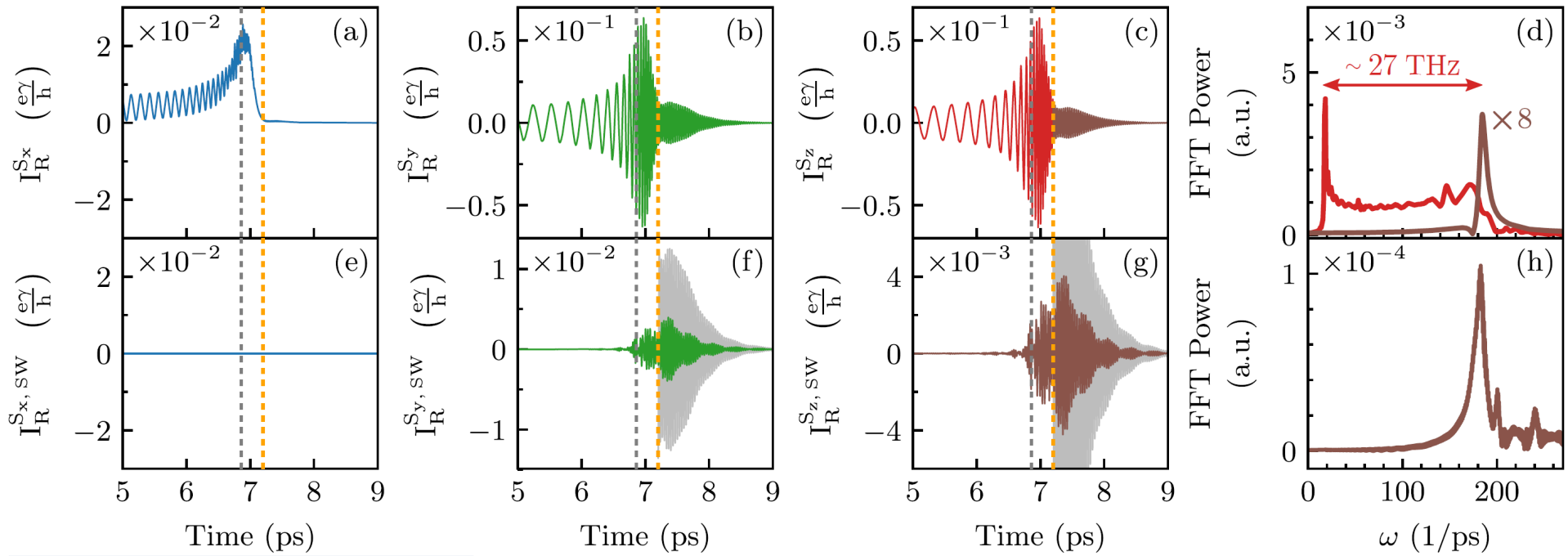




DW Annihilation Also Induces Burst of Electronic Spin Pumping over Ultrabroadband Frequencies

- Additional burst of electronic spin pumping does not exist in classical micromagnetics, but is captured by TDNEGF+LLG -> it could also be converted into time-dependent charge current and the corresponding ultrabroadband THz radiation

PRB **104**, L020407 (2021)

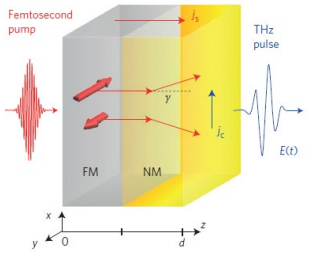


nature photonics
ARTICLES
PUBLISHED ONLINE: 23 MAY 2016 | DOI: 10.1038/NPHOTON.2016.91

Efficient metallic spintronic emitters of ultrabroadband terahertz radiation

T. Seifert[1], S. Jaiswal[2,3], U. Martens[4], J. Hannegan[5], L. Braun[1], P. Maldonado[6], F. Freimuth[7], A. Kronenberg[2], J. Henrizi[2], I. Radu[8], E. Beaurepaire[9], Y. Mokrousov[7], P. M. Oppeneer[6], M. Jourdan[2], G. Jakob[2], D. Turchinovich[10], L. M. Hayden[5], M. Wolf[1], M. Münzenberg[4], M. Kläui[2] and T. Kampfrath[1]*

Terahertz electromagnetic radiation is extremely useful for numerous applications, including imaging and spectroscopy. It is thus highly desirable to have an efficient table-top emitter covering the 1–30 THz window that is driven by a low-cost, low-power femtosecond laser oscillator. So far, all solid-state emitters solely exploit physics related to the electron charge and deliver emission spectra with substantial gaps. Here, we take advantage of the electron spin to realize a conceptually



alternative to using

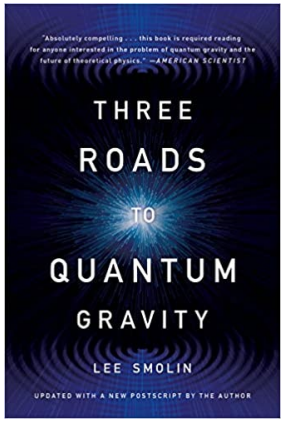
ARTICLE
Received 6 Nov 2013 | Accepted 31 Mar 2014 | Published 30 Apr 2014
DOI: 10.1038/ncomms4768
OPEN

Spin Hall voltages from a.c. and d.c. spin currents

Dahai Wei[1,*], Martin Obstbaum[1,*], Mirko Ribow[1,2], Christian H. Back[1] & Georg Woltersdorf[1,2]

Three Roads to Electron—Localized-Spin Nonequilibrium Many-Body Problem in Spintronics

THIS TALK: quantum electrons + classical spins



PHYSICAL REVIEW B **99**, 134409 (2019)

Time-retarded damping and magnetic inertia in the Landau-Lifshitz-Gilbert equation self-consistently coupled to electronic time-dependent nonequilibrium Green functions

Utkarsh Bajpai and Branislav K. Nikolić*

arXiv:2306.13013

Gilbert damping in metallic ferromagnets from Schwinger-Keldysh field theory: Intrinsically nonlocal and nonuniform, and made anisotropic by spin-orbit coupling

Felipe Reyes-Osorio and Branislav K. Nikolić*

Landau-Lifshitz-Gilbert (LLG) equation:

$$\frac{d\mathbf{M}_i}{dt} = -\gamma \mathbf{M}_i \times \mathbf{B}_i^{\text{eff}} + \lambda_i \mathbf{m}_i \times \frac{d\mathbf{m}_i}{dt} + \frac{\gamma}{\mu_M}\mathbf{T}_i$$

Requirements for validity of LLG equation:

$$S \to \infty, \ \hbar \to 0 \ (S \times \hbar \to 1)$$

$$|S_1\rangle(t) \otimes |S_2\rangle(t) \otimes \cdots \otimes |S_N\rangle(t)$$

so, nature (i.e., decoherence and dissipation) must kill many-body entangled spin states

Fate of entanglement in magnetism under Lindbladian or non-Markovian dynamics and conditions for transition to Landau-Lifshitz-Gilbert classical dynamics

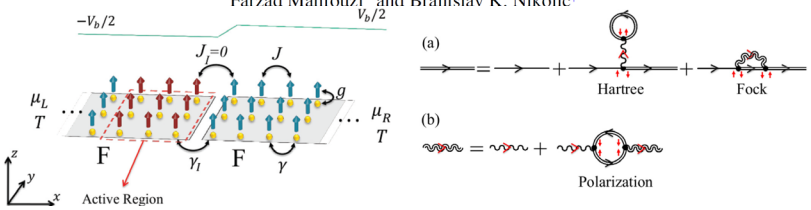
arXiv:2303.17596 Federico Garcia-Gaitan and Branislav K. Nikolić*

quantum electrons + quantum localized spins mapped to bosons

PHYSICAL REVIEW B **90**, 045115 (2014)

Signatures of electron-magnon interaction in charge and spin currents through magnetic tunnel junctions: A nonequilibrium many-body perturbation theory approach

Farzad Mahfouzi* and Branislav K. Nikolić†



PHYSICAL REVIEW B **104**, 184425 (2021)

Editors' Suggestion

Quantum many-body states and Green's functions of nonequilibrium electron-magnon systems: Localized spin operators versus their mapping to Holstein-Primakoff bosons

Utkarsh Bajpai,[1,2] Abhin Suresh,[1] and Branislav K. Nikolić[1,*]

quantum electrons + quantum localized spins

PHYSICAL REVIEW X **11**, 021062 (2021)

Spintronics Meets Density Matrix Renormalization Group: Quantum Spin-Torque-Driven Nonclassical Magnetization Reversal and Dynamical Buildup of Long-Range Entanglement

Marko D. Petrović,[1] Priyanka Mondal,[1] Adrian E. Feiguin,[2] Petr Plecháč,[3] and Branislav K. Nikolić[1,*]

PHYSICAL REVIEW LETTERS **126**, 197202 (2021)

Quantum Spin Torque Driven Transmutation of an Antiferromagnetic Mott Insulator

Marko D. Petrović,[1] Priyanka Mondal,[1] Adrian E. Feiguin,[2] and Branislav K. Nikolić[1,*]

$$\binom{2N}{N_e} 2^{N_{\text{FM}}} \Rightarrow |\Psi\rangle = \sum_{\{s\}} A[s_1]_{\alpha_1} A[s_2]_{\alpha_1,\alpha_2} \ldots A[s_{N-1}]_{\alpha_{N-1}\alpha_N} A[s_N]_{\alpha_N} |s_1 \ldots s_N\rangle$$

$$e^{-i\hat{H}\delta t/\hbar} \approx e^{-i\hat{H}_1\delta t/2\hbar} \cdots e^{-i\hat{H}_{N-1}\delta t/2\hbar} \times e^{-i\hat{H}_{N-1}\delta t/2\hbar} \cdots e^{-i\hat{H}_1\delta t/2\hbar}$$

Unreasonable Effectiveness of LLG Equation is Broken by S=1/2 or S=1 Antiferromagnets

Néel state is not the true ground state

https://wiki.physics.udel.edu/phys813/Lectures:

$|\uparrow\downarrow\uparrow\downarrow\cdots\uparrow\downarrow\rangle$ classical (Néel) GS

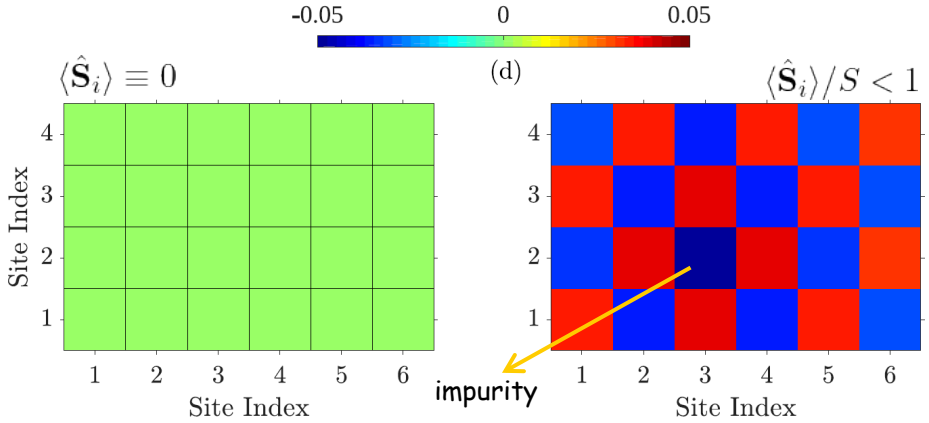
$|GS\rangle \neq |\uparrow\downarrow\uparrow\downarrow\cdots\uparrow\downarrow\rangle$ due to "quantum spin fluctuations" or "zero point motion"

what does this mean RIGOROUSLY?

⇒ diagonalize Hamiltonian of a simple 1D chain of 4 spins: → true GS has lower energy

$\langle\uparrow\downarrow\uparrow\downarrow|\hat{H}|\uparrow\downarrow\uparrow\downarrow\rangle = -|J| > \langle GS|\hat{H}|GS\rangle = -2|J|$

$|GS\rangle = \frac{1}{\sqrt{12}}\left(2|\uparrow\downarrow\uparrow\downarrow\rangle + 2|\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle\right)$



LLG is unreasonably effective in spintronics and magnonics, but **it does not apply to S=1/2 and S=1 antiferromagnets**

PHYSICAL REVIEW B **103**, 224434 (2021)

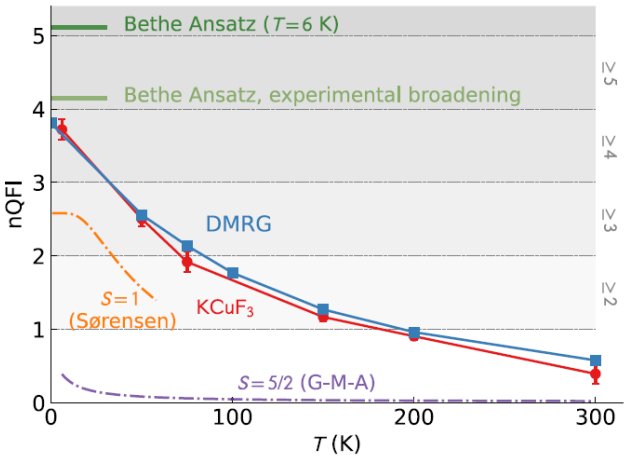
Editors' Suggestion

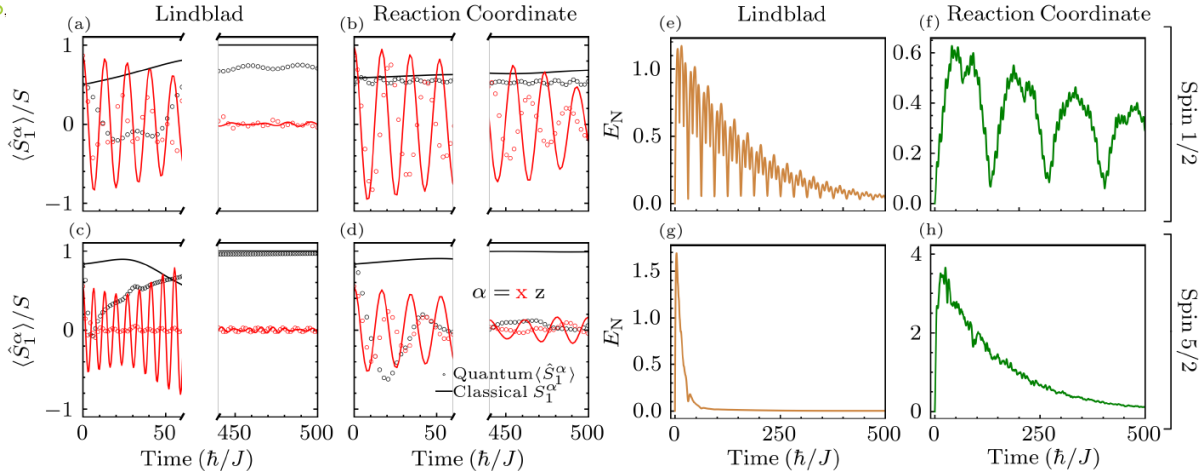
Witnessing entanglement in quantum magnets using neutron scattering

A. Scheie, Pontus Laurell, A. M. Samarakoon, B. Lake, S. E. Nagler, G. E. Granroth, S. Okamoto, G. Alvarez, and D. A. Tennant

log negativity — entangled mixed state

$$E_N > 0 \Rightarrow \hat{\rho} \neq \sum_i w_i \hat{\rho}_i^{(1)} \otimes \cdots \hat{\rho}_i^{(N)}$$

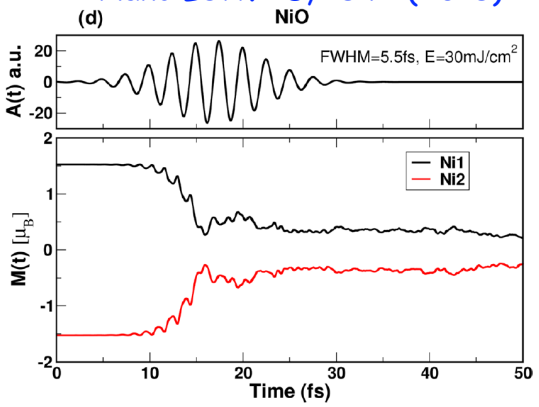




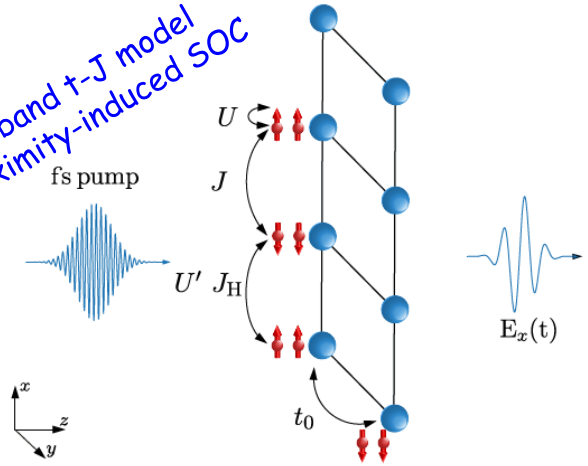
arXiv:2303.17596

Ultrafast-Light-Driven NiO: **Nonclassical** Magnetization Dynamics, Spin and Charge Pumping, and Ensuing Radiation

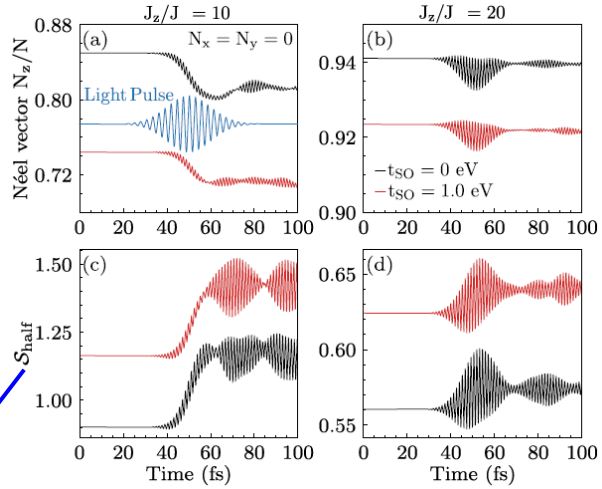
NiO is a challenge for TDDFT:
Nano Lett. **18**, 1842 (2018)



two band t-J model
+ proximity-induced SOC



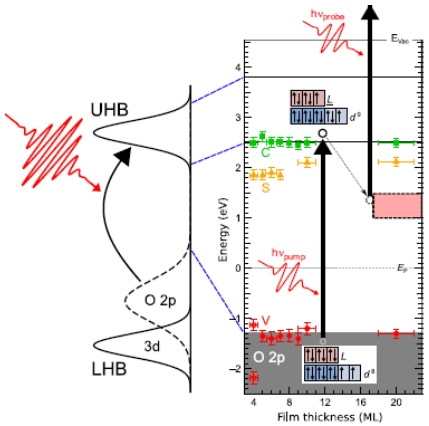
entanglement nonzero in equilibrium and grows out of equilibrium



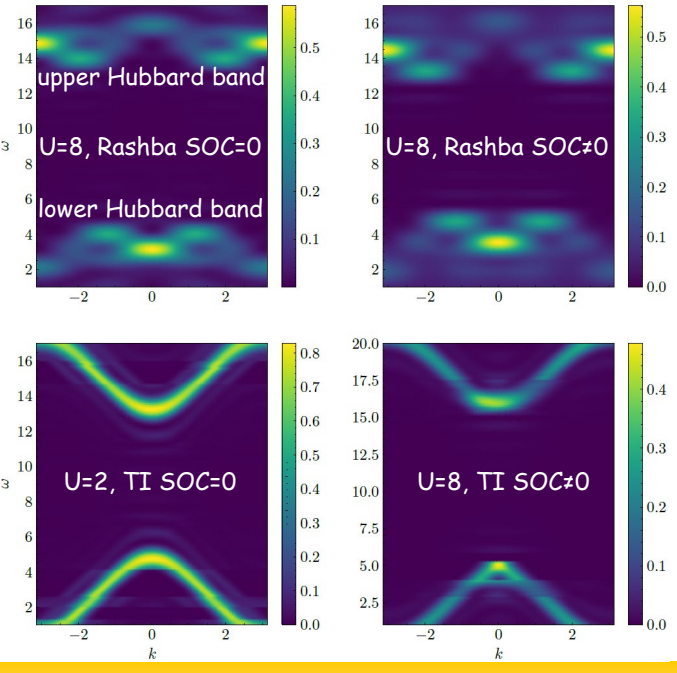
https://doi.org/10.1038/s41467-020-17925-8 OPEN

Ultrafast coupled charge and spin dynamics in strongly correlated NiO

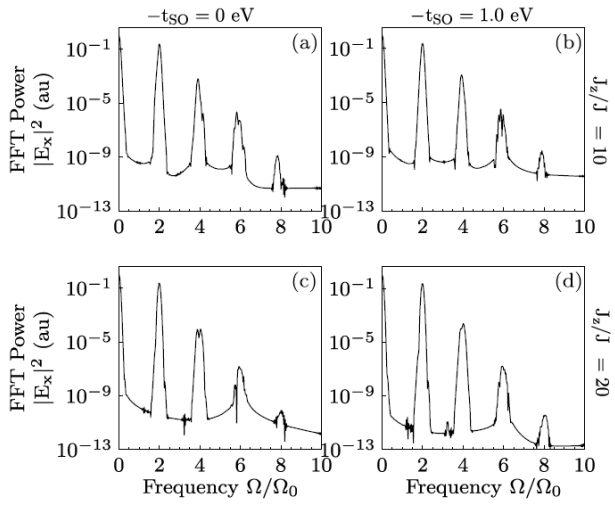
Konrad Gillmeister[1], Denis Golež[2,3], Cheng-Tien Chiang[1], Nikolaj Bittner[3], Yaroslav Pavlyukh[4], Jamal Berakdar[1], Philipp Werner[3]✉ & Wolf Widdra[1,5]✉



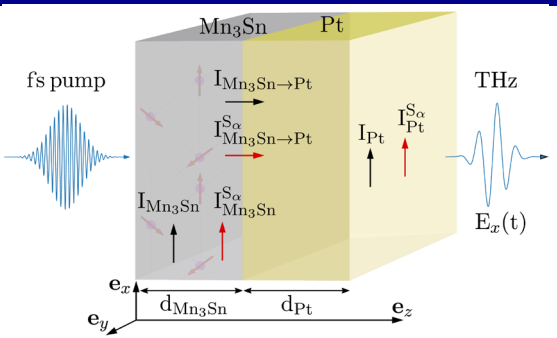
spectral function from tDMRG

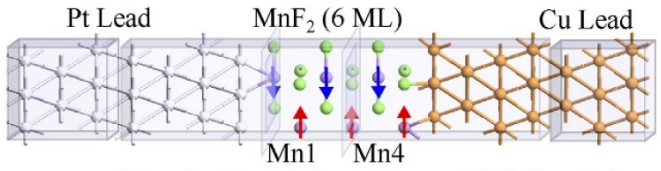


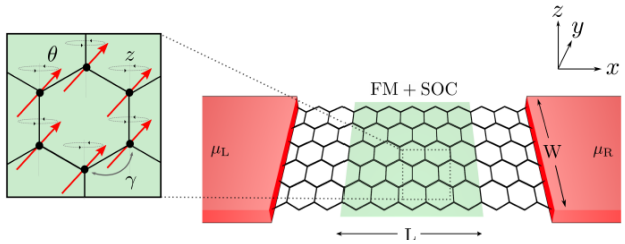
unpublished



Conclusions







- Electronic spin current pumping by dynamical localized magnetic moments (LMMs) surrounded by conduction electrons is ubiquitous phenomenon, even at room temperature.

- If conduction electrons are exposed to intrinsic or proximity spin-orbit coupling, concurrent charge pumping is also generated, while spin pumping cannot be captured anymore by the standard spin-mixing conductance → instead, use Floquet-NEGF (for single frequency) or time-dependent NEGF (for arbitrary motion of LMMs) formalisms.

REVIEWS OF MODERN PHYSICS, VOLUME 77, OCTOBER 2005

Nonlocal magnetization dynamics in ferromagnetic heterostructures

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diffuse-transport regime only. Strong spin-orbit coupling immediately at interfaces, for example, requires generalization of spin-pumping and circuit theories beyond the scope of this review.

- Spin pumping is also operative in ultrafast-light-driven magnets, where laser light generates charge photocurrents which get spin-polarized and exert torque on LMMs, that in turn pumped additional spin currents.
- In the case of Mn3Sn, charge pumping is generated without the need for spin-to-charge conversion by additional normal layer.