Proximity effects on topological surface: TI/FM heterostructures

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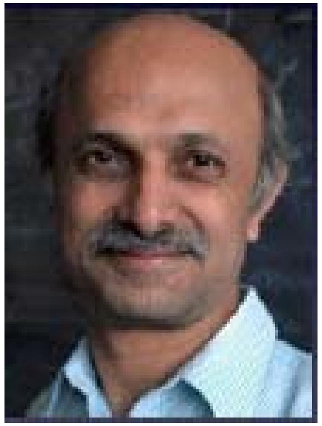
Collaborators:



Flavio S. Nogueira
IFW Dresden & RUB

Jagadeesh Moodera
MIT

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MIT

Electrodynamics of the topological insulator

In a 3d+1 Z_2 topological insulator (class AII) there is another term (θ-term)

$$S_\theta = \frac{e^2}{4\pi\hbar c^2}\int d^3r dt \theta \varepsilon^{\mu\nu\sigma\tau}\partial_\mu A_\nu \partial_\sigma A_\tau = \frac{e^2}{2\pi\hbar c^2}\int d^3r dt \theta \mathbf{E}\cdot\mathbf{B}$$

- does not depend on the metric but only on the topology of the underlying space
- serves as an alternative definition of the non-trivial topological insulator

X.-L. Qi, T. L. Hughes, and S.-C. Zhang, PRB 78, 195424 (2008)
A.M. Essin, J. E. Moore, and D. Vanderbilt, PRL 102, 146805 (2009)

Electrodynamics of the topological insulator

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- the value of θ is defined modulo 2π
- S_θ is an integral over a total derivative (no effect for θ = const.)
- matters at interfaces and surfaces, where θ changes
- for strong topological insulator $\theta=\pi$ (possibility to classify TI even in the presence of interactions)

Application of the Gauss-Theorem gives the CS term on the surface

$$S_\theta = \frac{e^2\theta}{2\pi\hbar c^2}\int d^2r dt \varepsilon^{\nu\sigma\tau} A_\nu \partial_\sigma A_\tau$$

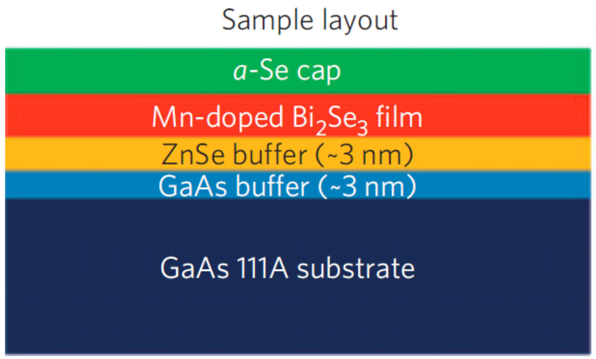
Outline

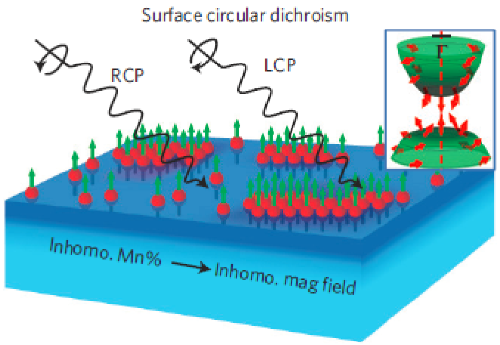
- **FM insulator/TI heterostructures**

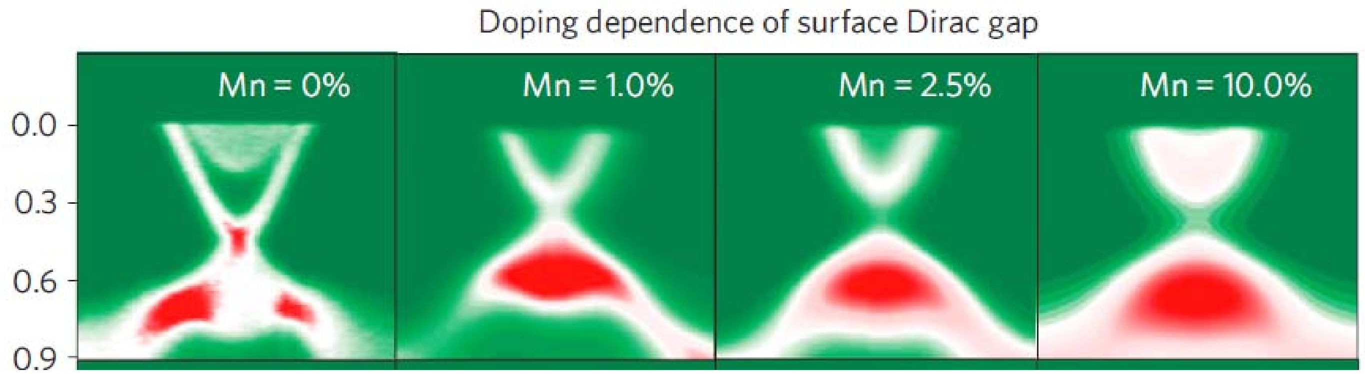
- **Interaction effects at the interface:** **spontaneous generation of the Chern-Simons term and RKKY interaction**

- **Finite temperature effects:** **shift of Curie temperature and Dzyloshinsky-Moriya interaction**

ferromagnetic order in TI by doping with specific Elements (Mn,Fe,Cr…)



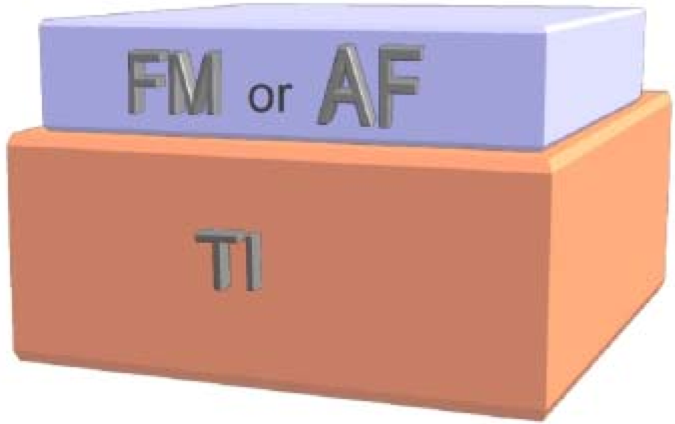




Exp.:Y. L. Chen et al., Science 329, 659 (2010); L. A. Wray et al., Nat. Phys. 7, 32 (2010); J. G. Checkelsky et al., Nat. Phys. 8, 729 (2012); S.-Y. Xu et al., Nat. Phys. 8, 616 (2012); Z. Wang et al., APL Mater.. (2015)

- hard to separate the surface and the bulk phases
- transport of a TI can be influenced by metallic overlayer or atoms
- crystal defects, magnetic scattering centers, as well as impurity states in the insulating gap

Proximity induced symmetry breaking



TI = Bi_2Se_3 or Sb_2Te_3

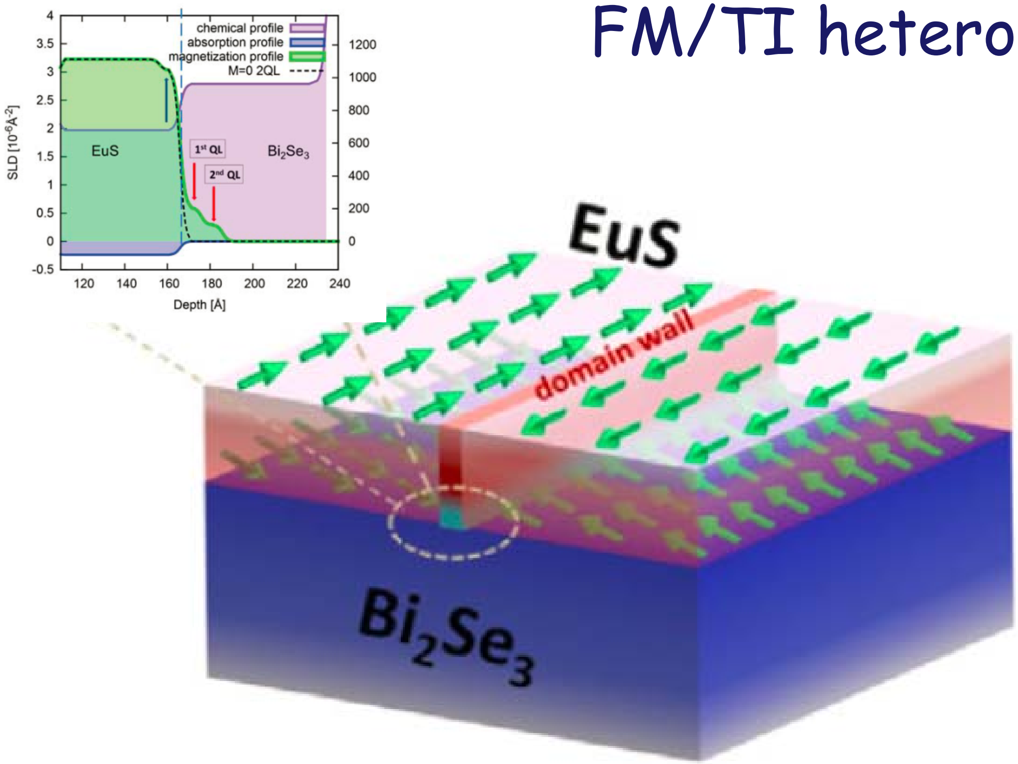
Material	Mag. order	$T_{c,N}$ (K)
EuO	FM	69.3
EuS	FM	16.6
EuSe	FM	pressure
MnSe	AF	247
MnTe	AF	307
$RbMnCl_3$	AF	99

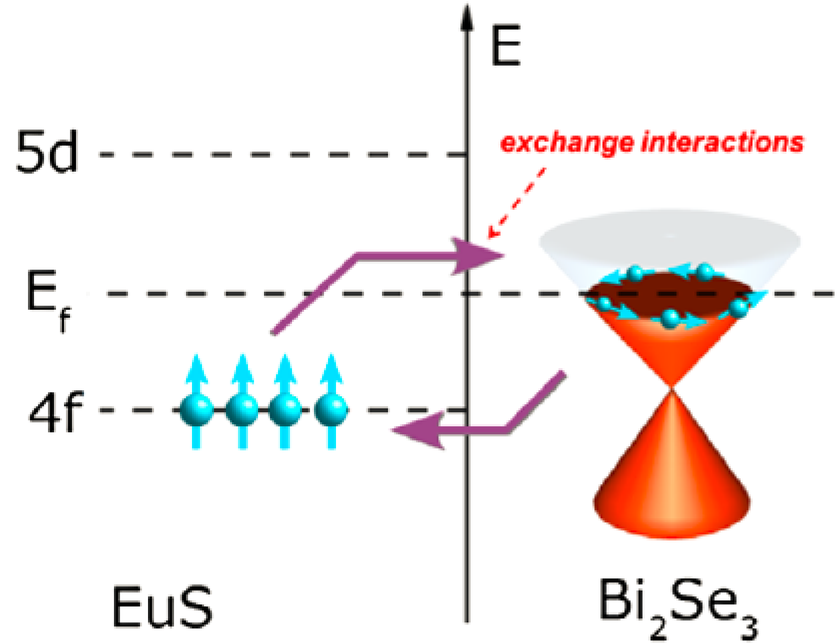
Candidate materials

- Ab initio calculations indicate that MnSe has good matching properties
  [W. Luo and X.-L. Qi, PRB **87**, 085431 (2013)]

S.V. Eremeev et al., PRB 88, 144430 (2014); JMMM 383 (2014;)Sci. Rep. 5 (2015)

Proximity induced symmetry breaking:
FM/TI heterostructure



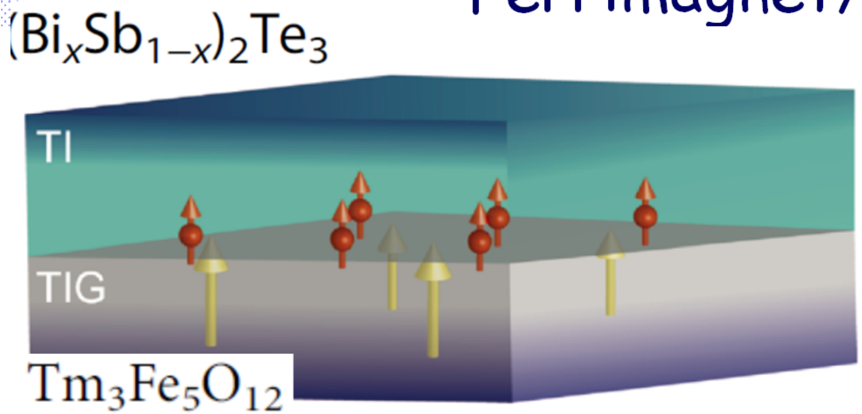


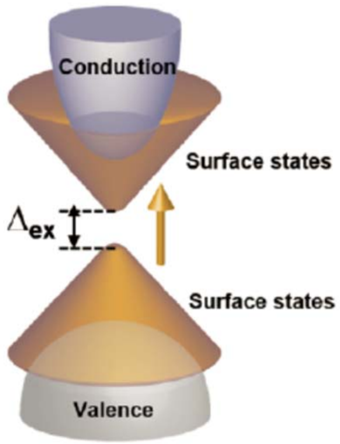
- EuS well behaved Heisenberg-like ferromagnetic insulator

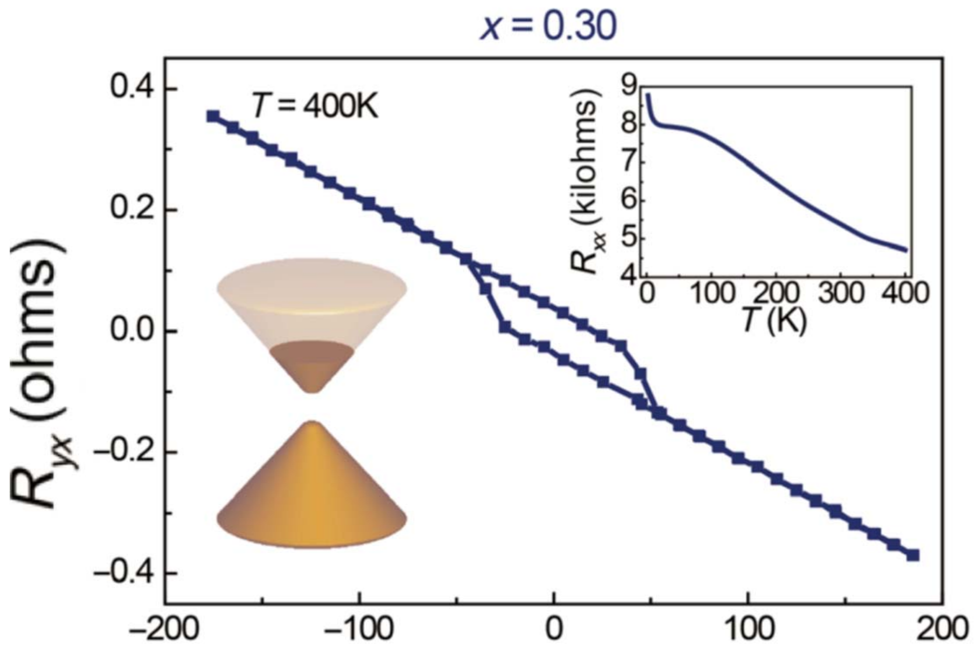
- Local time-reversal symmetry breaking at the interface

P. Wei et al. PRL 110, 186807 (2013);
Qi I. Yang et al., PRB 88, 081407(R) (2014)
L.D. Alegria et al., Appl. Phys. Lett. 105, 053512 (2014)
FMI($Y_3Fe_5O_{12}$)/TI: Lang et al., NanoLett. 14, 3459 (2014)
Bi2Se3/Permalloy A. R. Melinik et al., Nature 511, 449 (2014)

Proximity induced symmetry breaking
Ferrimagnet/TI heterostructure







- Anomalous Hall effect at room temperatures
- TI surface is spin-polarized (Andreev reflection experiments)

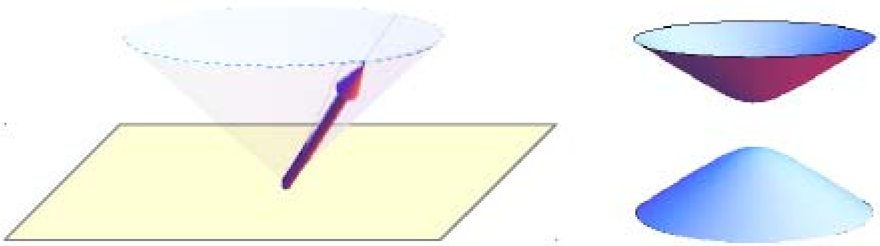
Tang et al., Sci. Adv. 2017;3: e1700307 (2017)

FI/TI Interface

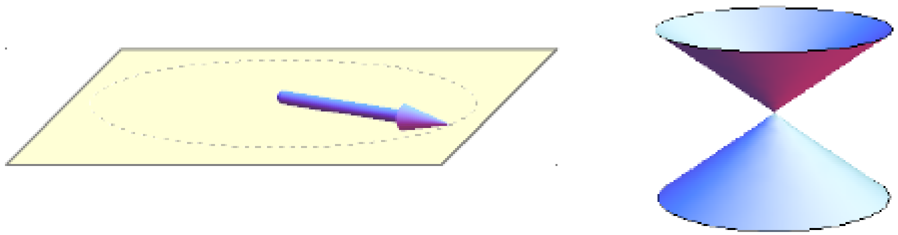
Mean-field type Hamiltonian at the interface

$$H = v_F(-i\hbar\boldsymbol{\nabla} \times \hat{\mathbf{z}}) \cdot \boldsymbol{\sigma} - J(n_x\sigma_x + n_y\sigma_y) - J_\perp n_z\sigma_z$$

$$E_\pm = \pm\sqrt{(p_x - Jn_y)^2 + (p_y + Jn_x)^2 + J_\perp^2 n_z^2} \qquad \mathbf{p} = \hbar v_F \mathbf{k}$$



Out of plane magnetization: gapped Dirac spectrum



In-plane magnetization: gapless Dirac spectrum

Dirac point at $(Jn_y, -Jn_x)$

FI/TI Interface: vanishing out-of-plane magnetization

Electronic Lagrangian at the interface:

QED-like form in $d = 2 + 1$

$$\mathcal{L}_0 = \bar{\psi}[i\gamma_0\hbar\partial_t - i\vec{\gamma}\cdot(v_F\hbar\boldsymbol{\nabla} + iJ\mathbf{a})]\psi$$

vector potential $\mathbf{a} = (n_y, -n_x)$ $\gamma^0 = \sigma_z$, $\gamma^1 = -i\sigma_x$, and $\gamma^2 = i\sigma_y$

Add screened Coulomb interaction

$$\mathcal{H}_{\text{int}} = \frac{g}{2}(\psi^\dagger\psi)^2 = \frac{g}{2}(\bar{\psi}\gamma^0\psi)^2$$

The full Lagrangian in terms of auxilary field a_0

$$\mathcal{L} = \bar{\psi}(i\partial\!\!\!/ - J a\!\!\!/)\psi - \frac{J^2}{2g}a_0^2$$

FI/TI Interface: Effective action

(a) recall the situation $J_\perp \neq 0$ $\quad m = J_\perp \langle n_z \rangle$

$$\mathcal{L} = \bar{\psi}(i\partial\!\!\!/ - J a\!\!\!/ - m)\psi - \frac{J^2}{2g} a_0^2$$

- Integrating out N fermionic degrees of freedom and expanding the action in terms of the components of the vector field

$$S_{\text{eff}} = -N \operatorname{Tr} \ln(\partial\!\!\!/ - iJ a\!\!\!/ + m) + \frac{J^2}{2g} \int d^3x a_0^2$$

- expanding the action in terms of the components of the vector field a_μ

$$S_{eff} \approx \frac{J^2}{8\pi} \int d^3x \sum_{i=1}^{N} \left[-\frac{1}{6|m_i|} f_{\mu\nu} f^{\mu\nu} + \frac{m_i}{|m_i|} \varepsilon_{\mu\nu\lambda} a^\mu \partial^\nu a^\lambda \right]$$

$$f_{\mu\nu} = \partial_\mu a_\nu - \partial_\nu a_\mu$$

FI/TI Interface: Effective action

(a) recall the situation $J_\perp \neq 0$

$$S_{eff} \approx \frac{J^2}{8\pi} \int d^3x \sum_{i=1}^{N} \left[-\frac{1}{6|m_i|} f_{\mu\nu} f^{\mu\nu} + \frac{m_i}{|m_i|} \varepsilon_{\mu\nu\lambda} a^\mu \partial^\nu a^\lambda \right]$$

- The first (Maxwell) term contains a dimensional coefficient
- the CS term is universal (depends on the sign of m), independent of the scale transformations

$$S_{CS} = \frac{J^2}{8\pi} \left(\sum_{i=1}^{N} \frac{m_i}{|m_i|} \right) \int d^3x \epsilon_{\mu\nu\lambda} a^\mu \partial^\nu a^\lambda$$

FI/TI Interface: Effective action

(a) the situation $J_\perp \neq 0$, N is odd $N = 2n+1$

$$S_{\rm CS} = \frac{J^2}{4\pi}\left(n+\frac{1}{2}\right)\frac{m}{|m|}\int d^3x\,\epsilon_{\mu\nu\lambda}a^\mu\partial^\nu a^\lambda.$$

- Two-component Dirac fermions
- the broken symmetries are **TRS** and **mirror symmetry** N=2n+1

Mirror symmetry: $(x_0,x_1,x_2)\to(x_0,-x_1,x_2)$, $\psi\to\gamma^1\psi$, $\bar\psi\to-\bar\psi\gamma^1$
TR symmetry: $(x_0,x_1,x_2)\to(-x_0,x_1,x_2)$, $\psi\to\gamma^2\psi$, $\bar\psi\to-\bar\psi\gamma^2$

$$\theta=\pi,\quad \alpha=J^2$$

FI/TI Interface: Landau-Lifshitz equations

(a) $J_\perp \neq 0$

$$S_{CS} = \frac{NJ^2\theta}{8\pi^2}\int dt \int d^2r(n_y\partial_t n_x - n_x\partial_t n_y - 2\mathbf{n}\cdot\mathbf{E})$$

$\mathbf{E} = -\boldsymbol{\nabla} a_0$ $\Rightarrow$ Electric field associated with screened Coulomb potential

$\mathbf{n} = (n_x, n_y, m/J_\perp)$

I. Garate and M. Franz, Phys. Rev. Lett. 104, 146802 (2010)
T. Yokoyama, J. Zang, and N. Nagaosa, PRB 81, 241410(R) (2010);
Ya. Tserkovnyak and D. Loss PRL 108, 187201 (2012)
F.S. Nogueira and I. Eremin PRL109 (2012)

$$\partial_t n_i = \epsilon_{ij} E_j$$ Spin-Hall response

To get the full magnetization dynamics

$$L_{FM} = \mathbf{b}\cdot\partial_t \mathbf{n} - \frac{\kappa}{2}\left[(\nabla\mathbf{n})^2 + (\partial_z \mathbf{n})^2\right] - \frac{r^2}{2}\mathbf{n}^2 - \frac{u}{4!}\left(\mathbf{n}^2\right)^2$$

the fluctuations in n_z around $\langle n_z \rangle$

FI/TI Interface: Landau-Lifshitz equations

(a) $J_\perp \neq 0$ the fluctuations in n_z around $\langle n_z \rangle$

$$S_{eff} \approx \frac{NJ^2}{8\pi}\int d^2rdt\left[-\frac{1}{6|m|}f_{\mu\nu}f^{\mu\nu}+\frac{m}{|m|}\varepsilon_{\mu\nu\lambda}a^\mu\partial^\nu a^\lambda + \frac{1}{|m|}\left[(\partial_t\tilde{n}_z)^2-(\nabla\tilde{n}_z)^2\right]\right]$$

$$\frac{\delta S_{eff}}{\delta n_i}=0$$

F.S. Nogueira and I. Eremin PRL109 (2012)

$$\partial_t \mathbf{n} = \gamma\left(\mathbf{n}\times\mathbf{H}_{eff}\right) + \frac{ZNJ^2}{2\pi\upsilon_F}\left[\mathbf{n}\times\mathbf{E}+\frac{1}{3|m|}(\mathbf{n}\cdot\mathbf{e}_z)\partial_t\mathbf{E}\right]$$

Landau-Lifshitz torque Magnetoelectric torque

- Coupled to the equation determining the scalar potential $\frac{\delta S_{eff}}{\delta\varphi}=0$

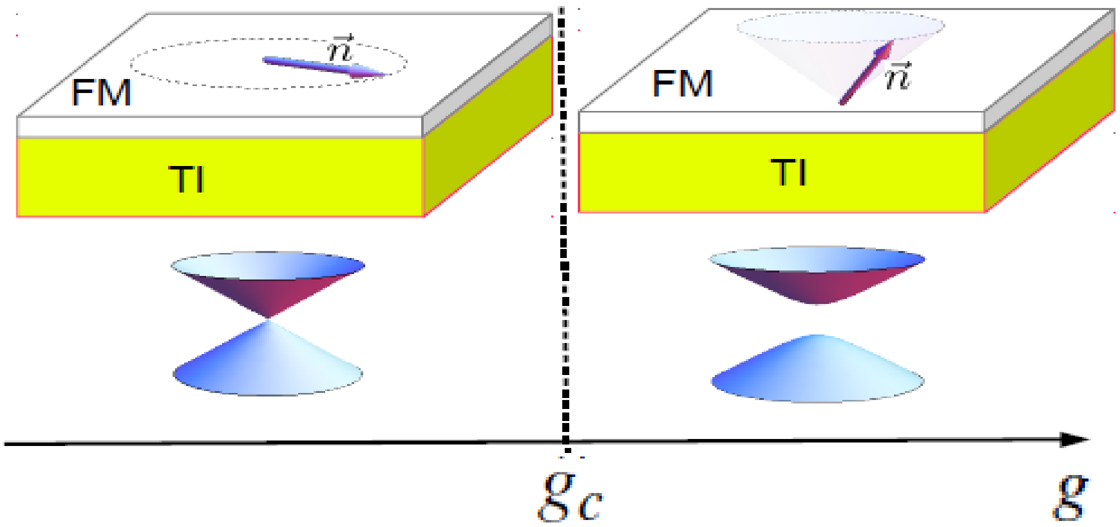
Outline

- **FM insulator/TI heterostructures**

- **Interaction effects at the interface:** spontaneous generation of the Chern-Simons term and RKKY interaction

- **Finite temperature effects: shift of Curie temperature and Dzyloshinsky-Moriya interaction**

FI/TI Interface: planar ferromagnet



$$\mathcal{L}_e = \bar{\psi}(i\partial\!\!\!/ - J a\!\!\!/)\psi - \frac{J^2}{2g} a_0^2$$

⇒ From effective action derive the propagator for the bosonic excitations (charge and spin fluctuations)

⇒ Compute the self-energy for the fermions and see what is the condition to have Σ(0)≠0

⇒ once it is non-zero it means the breaking of TRS and parity (generation of the Chern-Simons term)

Planar FM: self-consistent equation for the mass generation

- N even (graphene-like): $N/2$ fermions have $m = +|m|$, while the remaining $N/2$ ones have $m = -|m|$ with

$$\boxed{|m| = \left(\frac{\pi+1}{3\pi}\right)\frac{\hbar v_F}{a}\left(1-\frac{U}{U_c}\right)} \quad U_c = \frac{4\pi^2}{\pi+1}\left(\frac{\hbar v_F}{a}\right)\left[1-\frac{8}{\pi^2}\left(\frac{aJ}{hv_F}\right)^2\right]$$

No CS term is generated because its coefficient is proportional to $\frac{1}{N}\sum_{a=1}^{N}\frac{m_a}{|m_a|} \Longrightarrow$ mirror and TR symmetries are overall conserved

Gap vanishes continuously at U_c

- N odd (TI): $g \sim Ua/t \sim Ua/(\hbar v_F)$, $a =$ lattice spacing

All $m > 0 \Longrightarrow$ $\boxed{m = \frac{hv_F}{a}\exp\left[-\frac{(\pi+1)\pi}{128a}\left(\frac{hv_F}{J}\right)^2 (U-U_c)\right]}$

CS term is generated $\Longrightarrow$ mirror and TR symmetries are spontaneously broken [Nogueira and Eremin, PRB 88, 085126 (2013)]

Gap vanishes discontinuously at U_c

Outline

- **FM insulator/TI heterostructures**

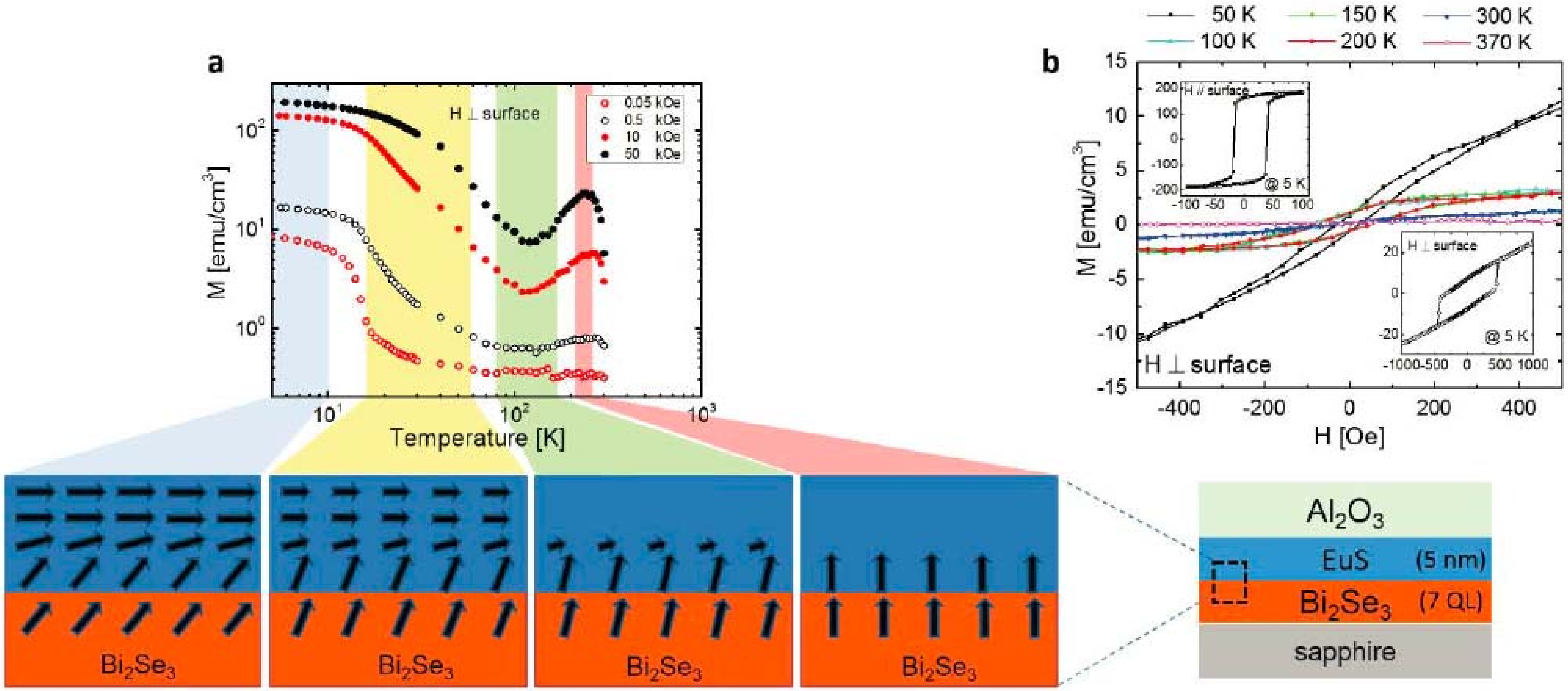
- **Interaction effects at the interface: spontaneous generation of the Chern-Simons term and RKKY interaction**

- **Finite temperature and chemical potential effects:** Tc shift and Dzyloshinsky-Moriya Interaction (DMI)

Finite temperature effects: shift of Curie temperature at the interface and out-of-plane magnetic anisotropy

⇒ FI/TI heterostructure

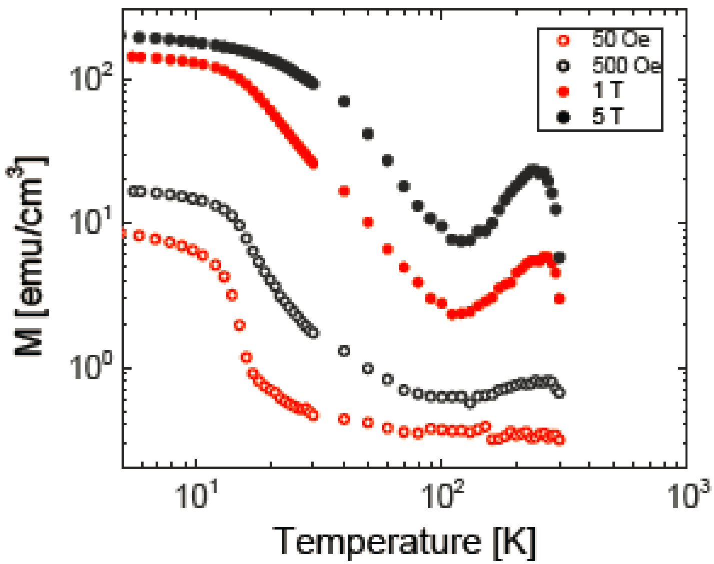
F. Katmis et al., Nature 533, 513 (2016)

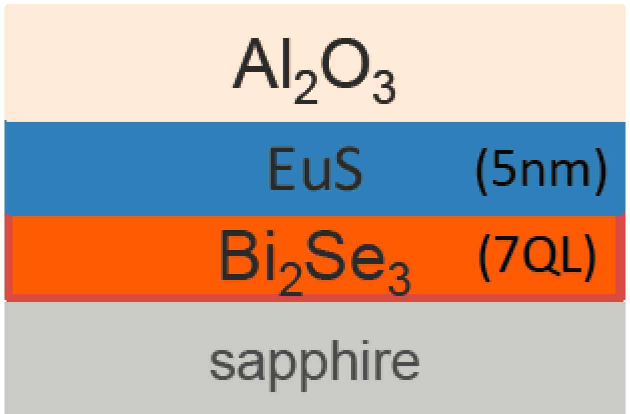


- Bulk Curie Temperature for EuS, Tc=17K
- At the interface the magnetization persists up to much higher temperatures

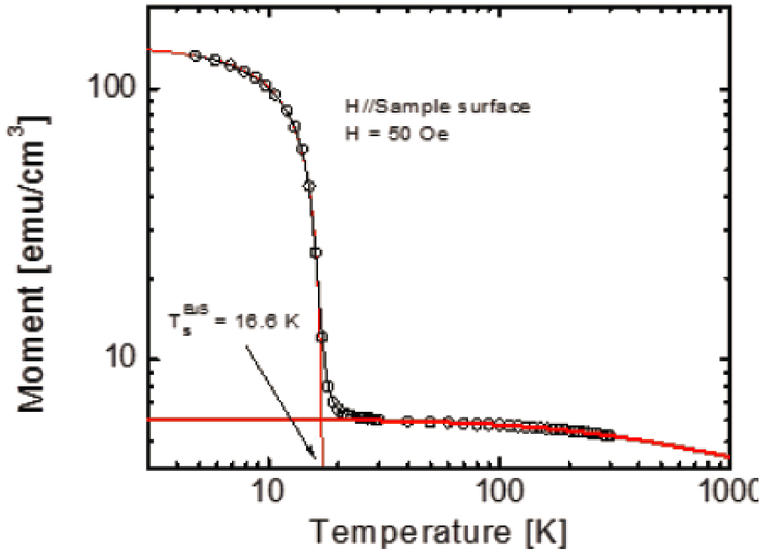
Finite temperature effects: shift of Curie temperature at the interface

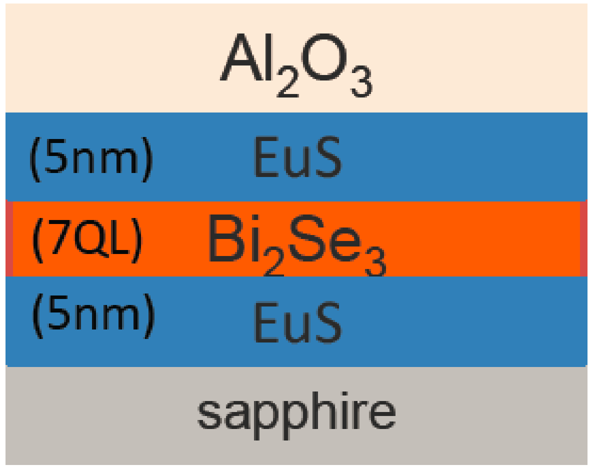
Bi-layer



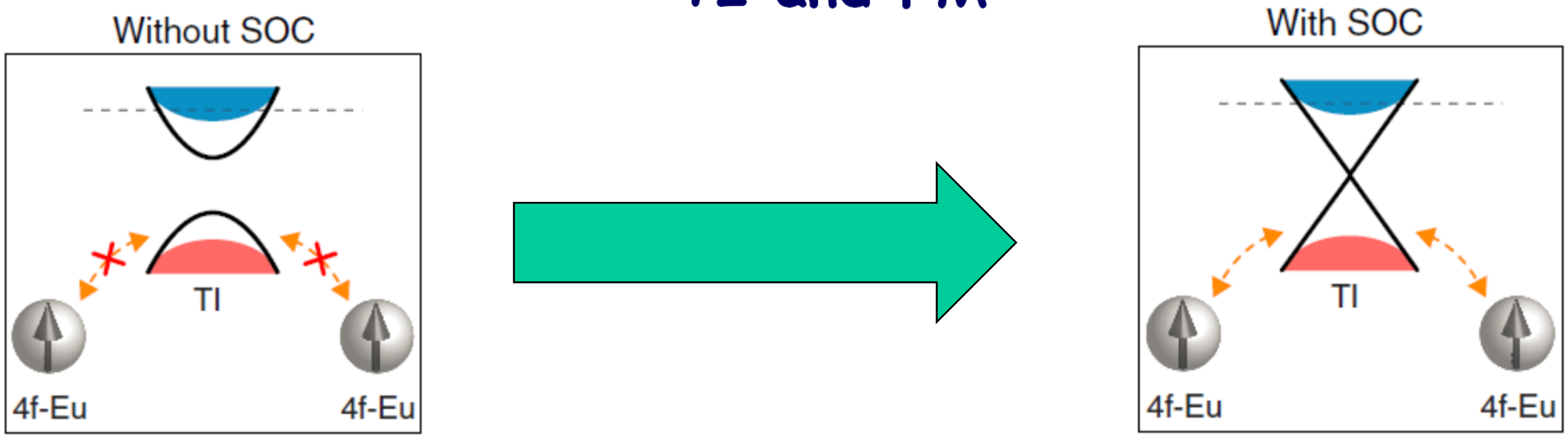


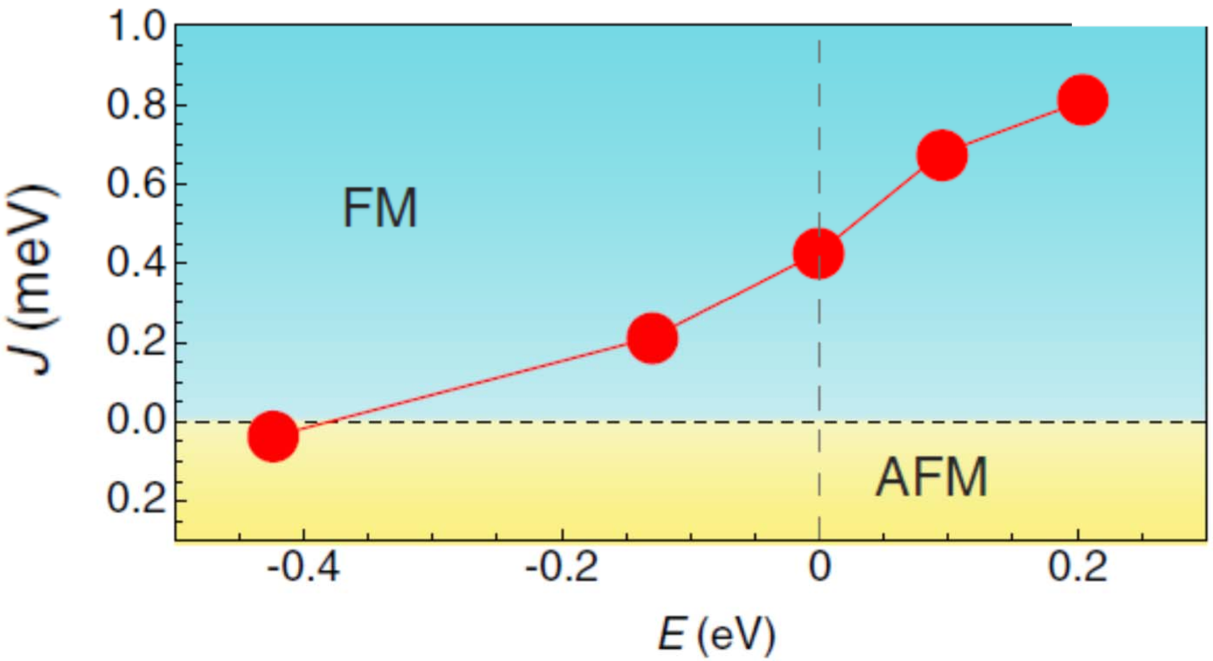
Tri-layer





Planar FM: RKKY type interaction on the interface between TI and FM





J. Kim et al., PRL 119, 027201 (2017)

Finite temperature effects: shift of Curie temperature at the interface

- Interface free energy: (z=0)

$$\mathcal{F}_{\rm Dirac} = -\int \frac{d^2k}{(2\pi)^2}\left[\mu + E(\mathbf{k},\mathbf{M}_0)\right] - \frac{1}{\beta}\sum_{\sigma=\pm}\int \frac{d^2k}{(2\pi)^2}\ln\left\{1 + e^{-\beta[E(\mathbf{k},\mathbf{M}_0)-\sigma\mu]}\right\}$$

$$E(\mathbf{k},\mathbf{M}_0) = \sqrt{(\hbar v_F k_x - \gamma\mu_B M_{0y})^2 + (\hbar v_F k_y + \gamma\mu_B M_{0x})^2 + (\gamma\mu_B M_{0z})^2}$$

- Free energy of FM insulator:

$$\mathcal{F}_{FM} = \frac{\rho_s}{2M_S^2}(\nabla\mathbf{M})^2 + \frac{a(T)}{2}\mathbf{M}^2 + \frac{1}{4}\left[(u+2K)(\mathbf{M}^2)^2 - 2K\sum_\alpha M_\alpha^4\right]$$

$$a(T) = a_0(T/T_c - 1) \qquad K < 0 \qquad u + 2K > 0$$

Finite temperature effects: shift of Curie temperature at the interface

- Boundary conditions:

$$\mathbf{M}(z=0)=\mathbf{M}_0$$

$$\frac{\rho_s}{M_S^2}\left.\frac{d\mathbf{M}}{dz}\right|_{z=0}=-\frac{\mathcal{F}_{\rm Dirac}}{\partial \mathbf{M}_0}$$

$$\frac{T_{ci}}{T_c}-1\approx\frac{1}{\epsilon_0^2}\left[\frac{4\ln(1+\sqrt{2})}{\sqrt{\pi}}\hbar v_F\sqrt{n_{2D}}-\epsilon_F\right]^2,$$

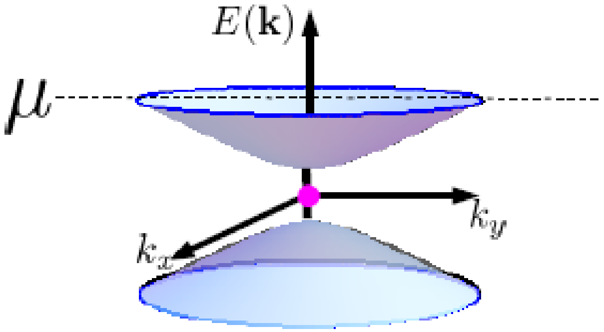
Magnetization at the interface is exponentially decaying in the bulk

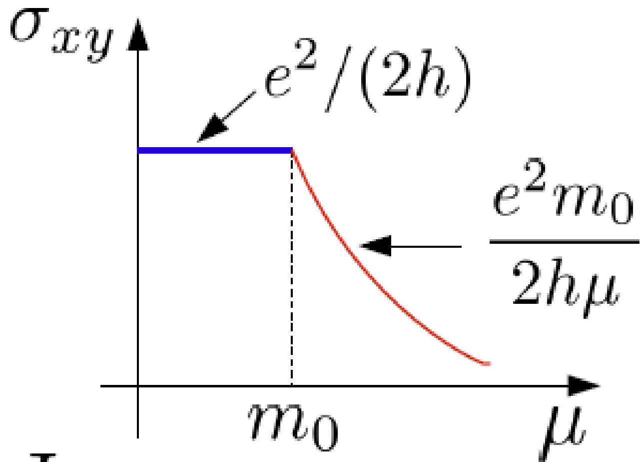
Effect of the temperatures on Chern Simons term

$$\boxed{\mathcal{S}_{\text{CS}} \approx \frac{\sigma(T,m)}{2}\int dt \int d^2 r \epsilon_{\mu\nu\lambda} a^{\mu}\partial^{\nu} a^{\lambda}}$$

Set $\sigma(T,m) = N J^2 \tilde{\sigma}(T,m)/(v_F^2 e^2)$

- $T = \mu = 0$: $\tilde{\sigma} = \sigma_{xy} = \frac{e^2}{2h}$
- $T = 0$ and $\mu \neq 0$:
  $\sigma_{xy}(0, m_0) = \frac{e^2}{2h}\left[\left(\text{sgn}(m_0) - \frac{m_0}{\mu}\right)\theta(|m_0| - \mu) + \frac{m_0}{\mu}\right]$





$$m_0 = J_{\perp} n_z$$

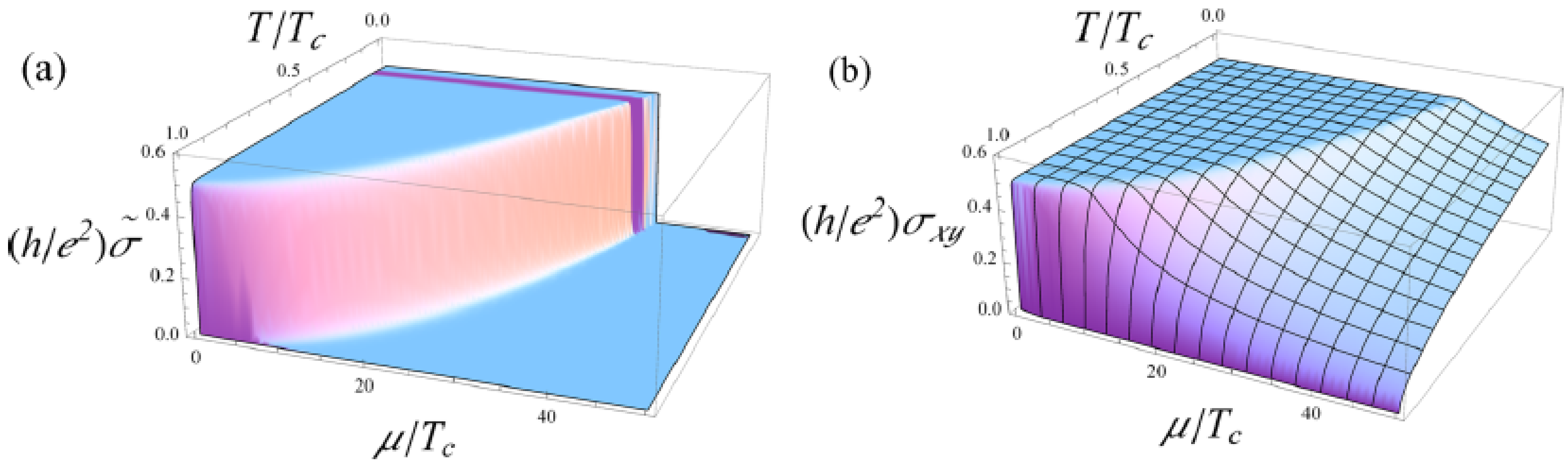
- Hall conductivity non-quantized and non-universal for $|m_0| < \mu$

Effect of the temperatures on Chern Simons term

$$\boxed{\mathcal{S}_{\rm CS} \approx \frac{\sigma(T,m)}{2}\int dt \int d^2 r \epsilon_{\mu\nu\lambda} a^\mu \partial^\nu a^\lambda}$$

- $T \neq 0$ and $\mu < |m|$:

$$\boxed{\tilde{\sigma}(T,m) = \frac{e^2 \mathrm{sgn}(m) \sinh(|m|/T)}{2h[\cosh(|m|/T) + \cosh(\mu/T)]}}$$



F.S. Nogueira and I. Eremin, PRB 90, 014431 (2014); RRB 92, 224507 (2015)

What happens above Curie temperature:
generation of Dzyloshinsky-Moriya interaction

Hamiltonian for Eu compounds:

$$\mathcal{H}_{\mathrm{FMI}} = \frac{\rho_s}{2} \sum_{i=x,y,z} [(\nabla n_i)^2 + (\partial_z n_i)^2] + U_{\mathrm{anis}}(\mathbf{n})$$

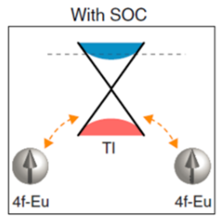
$$U_{\mathrm{anis}} = K_1(n_x^2 n_y^2 + n_x^2 n_z^2 + n_y^2 n_z^2) + K_2 n_x^2 n_y^2 n_z^2$$

$$K_1(T_c) = K_2(T_c) = 0$$

$$\mathbf{n} = \mathbf{M}/M$$

For $T \geq T_c$ fermionic gap and K_1 and K_2 must vanish

What happens above Curie temperature:
generation of Dzyloshinsky-Moriya interaction
(chemical potential is finite)



$$H_{\text{Dirac}} = \left[-i\hbar v_F \nabla - \frac{J_0 S}{2} \mathbf{n}(\mathbf{r}, z=0) \right] \cdot \vec{\sigma}$$

Partition function: $Z = \int \mathcal{D}\mathbf{n}\mathcal{D}\lambda e^{-\beta H_{\text{eff}}}$

$$H_{\text{eff}} = \int d^3 r \left[\mathcal{H}_{\text{FMI}} + \frac{i\lambda}{2}(\mathbf{n}^2 - 1) \right] + F_{\text{Dirac}}$$

$$F_{\text{Dirac}} = -\frac{1}{\beta} \ln \left[\text{tr} \left(e^{-\beta H_{\text{Dirac}}(\mathbf{n}(\mathbf{r}))} \right) \right]$$

What happens above Curie temperature:
generation of Dzyloshinsky-Moriya interaction

$$F = F_{\mathrm{FMI}} + F_{\mathrm{Dirac}} \qquad \vec{M} = S\mathbf{n} \qquad F_{\mathrm{Dirac}} = \int d^2 r \mathcal{F}_{\mathrm{Dirac}}(\mathbf{n}(\mathbf{r}))$$

$$F_{\mathrm{Dirac}} = F_{\mathrm{Dirac}}(0) + \delta F_{\mathrm{Dirac}}$$

$$\delta F_{\mathrm{Dirac}} = \frac{J_0^2}{2\beta} \sum_{n=-\infty}^{\infty} \int \frac{d^2 k}{(2\pi)^2} \int \frac{d^2 q}{(2\pi)^2} \mathrm{tr}[\sigma_a G(\omega_n, \mathbf{q}) \sigma_b G(\omega_n, \mathbf{q} + \mathbf{k})] n_a(\mathbf{k}) n_b(-\mathbf{k})$$

$$G(\omega_n, \mathbf{k}) = \frac{i\omega_n + \mu - \hbar v_F \mathbf{k} \cdot \vec{\sigma}}{(i\omega_n + \mu)^2 - (\hbar v_F)^2 k^2}$$

$$\Longrightarrow \delta F_{\mathrm{Dirac}} = \frac{J_0^2}{2} \int \frac{d^2 k}{(2\pi)^2} [S_{ab}(\mathbf{k}) + A_c(\mathbf{k}) \epsilon_{abc}] n_a(\mathbf{k}) n_b(-\mathbf{k})$$

What happens above Curie temperature:
generation of Dzyloshinsky-Moriya interaction

$$\mathcal{F}_{\mathrm{Dirac}} = \frac{s}{2}\left\{[\nabla \mathbf{n}(\mathbf{r})]^2 + [\nabla \cdot \mathbf{n}(\mathbf{r})]^2\right\} - \frac{a}{2}\mathbf{n}(\mathbf{r}) \cdot [\nabla \times \mathbf{n}(\mathbf{r})]$$

This term doesn't usually arise in DM materials

$$s = J_0^2 \mathcal{S}(\beta, \mu) \qquad a = J_0^2 \mathcal{A}(\beta, \mu)$$

$$\mathcal{S}(\beta, \mu) = \frac{\beta}{48\pi \cosh^2(\beta\mu/2)} \qquad \mathcal{A}(\beta\mu) = \frac{1}{8\pi\hbar v_F} \tanh\left(\frac{\beta\mu}{2}\right)$$

What happens above Curie temperature: generation of Dzyloshinsky-Moriya interaction

$$\boxed{\mathcal{F}_{\text{Dirac}} = \frac{s}{2}\left\{[\nabla \mathbf{n}(\mathbf{r})]^2 + [\nabla \cdot \mathbf{n}(\mathbf{r})]^2\right\} - \frac{a}{2}\mathbf{n}(\mathbf{r}) \cdot [\nabla \times \mathbf{n}(\mathbf{r})]}$$

- Cutoff term shifts Lagrange multiplier field λ
- At saddle-point, $\lambda \sim \xi^{-2} \implies \tilde{\lambda} = \lambda - \Lambda J_0^2/(4\pi\hbar v_F)$
- $\lambda = d\left(\frac{4\pi}{3}\right)^2 \rho_s^3(\beta_c - \beta)^2 \implies T_c$ shifts upwards

Field equation at the interface:

$$\begin{aligned} &- \quad s\nabla^2\mathbf{n}(\mathbf{r}) - s\nabla(\nabla \cdot \mathbf{n}(\mathbf{r})) \\ &+ \quad a(\nabla \times \mathbf{n}(\mathbf{r})) + \tilde{\lambda}\mathbf{n}(\mathbf{r}) = \rho_s \partial_z \mathbf{n}(\mathbf{r}, z)|_{z=0} \end{aligned}$$

Conclusions:

TI/FI heterostructure:

- For interacting Dirac fermions coupled to an in-plane exchange field there is a spontaneous breaking of parity and TRS due to a dynamical gap generation

$$\boxed{m = \frac{hv_F}{a} \exp\left[-\frac{(\pi+1)\pi}{128a} \left(\frac{hv_F}{J}\right)^2 (U - U_c) \right]}$$

- Upward shift of the Curie temperature at the interface due to RKKY and negative interface energy of Dirac fermions

- Dynamical generation of the Dzyaloshinsky-Moriya Interaction at the interface above Tc