Workshop on Strong Electron Correlations in Quantum Materials: Inhomogeneities Frustration, and Topology

Nonlinear Hall effect induced by a quantum metric dipole in antiferromagnetic heterostructures

Thaís Victa Trevisan (trevisan@berkeley.edu)

Lawrence Berkeley National Laboratory and UC Berkeley

Gao, Liu, Qiu, Gosh, Trevisan et al., Science (2023) - DOI: 10.1126/science.adf1506

ICTP, São Paulo, Brazil – June 19th 2023







Professor Eduardo Miranda taught me:









UNIVERSITY OF CAMPINAS









Thank you, Eduardo!



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Yihua Qiang,^{1,2} Victor L. Quito,^{1,2} Thaís V. Trevisan,^{1,2} and Peter P. Orth^{1,2,3}

¹Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA ²Ames National Laboratory, Ames, Iowa 50011, USA ³Department of Physics, Saarland University, 66123 Saarbrücken, Germany (Dated: January 26, 2023)



(Victor Quito talk on Wednesday)

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Multi-institute collaboration through the Center for the Advancement of Topological Semimetals

Theory collaborators:

- Peter P. Orth (Iowa State University)
- Liang Fu (MIT)
- Arun Bansil (Northeastern University)
- David C. Bell (Harvard)
- Bahadur Singh (Tata Institute of Fundamental Research)
- Tay-Rong Chang (National Cheng Kung University)

Experiment collaborators:

- Su-Yang Xu (Harvard)
- Qiong Ma (Boston College)
- Chunhui Rita Du (UC San Diego)
- Ni Ni (UCLA)
- Takashi Taniguchi (National Institute for Materials Science)



Introduction

- Generalities of the Hall effects
- Quantum metric: what it is and where it appears
- Theory of the intrinsic quantum metric anomalous Hall effect
- The quantum metric Hall effect in MnBi₂Te₄ and BP heterostructure
 - An ideal platform for the quantum metric Hall effect
 - Minimal model
- Summary

Linear Hall effect:

• External $B \Rightarrow$ normal Hall [E. Hall, Am. J. Math. (1879)]



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$$J_x(\omega) = \sigma_{xy}(\omega) E_y(\omega)$$

Hall conductivity

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[N. Nagaosa et al., Rev. Mod. Phys. 82 (2010)]

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Require break of time-reversal symmetryDifferent microscopic mechanism

The Hall effect family grows



[Adapted from C. Chang et al. J. Phys. Cond. Matt. (2016), R. Samajdar et al. PRB (2019) and Z.Z. Du et al. Nat. Phys. (2021)]

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The non-linear anomalous Hall effects

• Hall current oscillates at a different frequency than the electric field

This talk: second-order anomalous Hall effect



$$\begin{split} J_y(\Sigma) &= \sigma_{yxx}(\omega_1,\omega_2)E_x(\omega_1)E_x(\omega_2)\\ \hline \\ \Sigma &= \omega_1 + \omega_2 \end{split} \text{ antisymmetric in y and x} \end{split}$$

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Two possibilities:

b)
$$\omega_2 = -\omega_1 \Rightarrow \Sigma = 0$$

a) $\omega_1 = \omega_2 \Rightarrow \Sigma = 2\omega$

- Can happen even in the presence of time-reversal symmetry
- Require inversion symmetry breaking

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What is the microscopic mechanism?





(Linear) anomalous Hall

<u>Extrinsic</u>: disorder \rightarrow depend on electron lifetime τ

Intrinsic: anomalous velocity \rightarrow independent of τ



Cannot be explained by band structure alone!

(Linear) anomalous Hall

Intrinsic: anomalous velocity \rightarrow independent of τ

$$\mathbf{v}_{\rm an} = \frac{e}{\hbar} \mathbf{E} \times \Omega_n(\mathbf{k})$$



(Linear) anomalous Hall

Intrinsic: anomalous velocity \rightarrow independent of τ

$$\mathbf{v}_{\mathrm{an}} = \frac{e}{\hbar} \mathbf{E} \times \Omega_n(\mathbf{k}) - \mathbf{Berry\ curvature!}$$



Electrons in solids:

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{r} | u_{n,\mathbf{k}} \rangle$$

 $\boldsymbol{\Omega}_{n}(\mathbf{k}) = \boldsymbol{\nabla}_{\mathbf{k}} \times \left\langle u_{n,\mathbf{k}} \right| \boldsymbol{\nabla}_{\mathbf{k}} u_{n,\mathbf{k}} \right\rangle$

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Electrons in solids:

_cell periodic

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Electrons in solids:

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$$\boldsymbol{\Omega}_{n}(\mathbf{k}) = \boldsymbol{\nabla}_{\mathbf{k}} \times \left\langle \left. u_{n,\mathbf{k}} \right| \boldsymbol{\nabla}_{\mathbf{k}} u_{n,\mathbf{k}} \right\rangle$$

Electric current:

$$\mathbf{J} = -e \int_{\mathbf{k}} f_0(\mathbf{k}) \mathbf{v}_{an} \quad \Longrightarrow \quad \sigma_{yx} = \frac{e^2}{\hbar} \sum_{n \in \text{occ}} \int \frac{d^d k}{(2\pi)^d} f_0(\mathbf{k}) \Omega_n^z(\mathbf{k})$$



Non-linear Hall: beyond the Berry curvature

• Extrinsic contributions to the non-linear Hall effect also involves the Berry curvature



[Sodemann, Fu (2014; Ma et al. (2018); Kang et al. (2018)]

Non-linear Hall: beyond the Berry curvature

• Extrinsic contributions to the non-linear Hall effect also involves the Berry curvature



[Sodemann, Fu (2014; Ma et al. (2018); Kang et al. (2018)]

• Intrinsic second-order Hall effect is generated by dipoles of the quantum metric

The quantum geometry of the electrons

• <u>Quantum geometric tensor: geometric properties of the electron wave functions</u>

$$\mathcal{Q}_{\mu\nu}^{(n)}(\mathbf{k}) = \langle \partial_{\mu} u_{n} | \partial_{\nu} u_{n} \rangle - \langle \partial_{\mu} u_{n} | u_{n} \rangle \langle u_{n} | \partial_{\nu} u_{n} \rangle = -\sum_{m \neq n} \mathcal{A}_{mn}^{(\mu)}(\mathbf{k}) \mathcal{A}_{nm}^{(\nu)}(\mathbf{k})$$
$$\mathcal{A}_{mn}^{(\mu)} = i \langle u_{m,\mathbf{k}} | \partial_{\mu} u_{n,\mathbf{k}} \rangle$$

Non-Abelian Berry connection

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Non-Abelian Berry connection

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[J. P. Provost and G. Valle et al. Communications in Mathematical Physics (1980)]

• Semiclassical description (second order in E, with B = 0) [Y. Gao et al. PRL 112 (2014)]

$$\begin{cases} \dot{\mathbf{r}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \tilde{\varepsilon}_{n,\mathbf{k}} - \dot{\mathbf{k}} \times \Omega_n(\mathbf{k}) - \dot{\mathbf{k}} \times \left(\nabla_{\mathbf{k}} \times \overset{\leftrightarrow}{G}_n \mathbf{E} \right) \\ \dot{\mathbf{k}} = -\frac{e}{\hbar} \mathbf{E} \\ \text{field correction to the} \\ \text{anomalous velocity } (\tilde{v}_{an}) \end{cases}$$

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For $E \hat{\mathbf{x}}$: $\tilde{v}_{an,y} = \frac{e}{\hbar} \left(\partial_{x} G_{yx} - \partial_{y} G_{xx} \right) \\ G_{n,\mu\nu}(\mathbf{k}) = 2 \operatorname{Re} \sum_{m \neq n} \frac{\mathcal{A}_{mn}^{(\mu)}(\mathbf{k}) \mathcal{A}_{nm}^{(\nu)}(\mathbf{k})}{\varepsilon_{n}(\mathbf{k}) - \varepsilon_{m}(\mathbf{k})} \quad \longleftarrow \text{Berry curvature polarizability}$

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Theory of the intrinsic non-linear Hall effect

• From the field correction to the anomalous velocity:

$$\sigma_{yxx} = 2e^3 \sum_{n} \int \frac{d^d k}{(2\pi)^d} \frac{v_y^n g_{xx}^{(n)}(\mathbf{k}) - v_x^n g_{yx}^{(n)}(\mathbf{k})}{\varepsilon_{n,\mathbf{k}} - \varepsilon_{\bar{n},\mathbf{k}}} \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_F) + \text{AIC}$$

Antisymmetric:

$$\sigma_{yxx} = -\sigma_{xyx}$$

[Y. Gao et al. PRL 112 (2014), C. Wang et al. PRL 127 (2021) Gao, Liu, Qiu, Gosh, <u>Trevisan</u> et al., Science (2023)]

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Quantum metric dipole: $D_{yxx}(\mathbf{k})$

$$\int_{0}^{0} \frac{\partial A}{\partial z} \int_{0}^{0} \frac{\partial A}{$$

[Y. Gao et al. PRL 112 (2014), C. Wang et al. PRL 127 (2021) Gao, Liu, Qiu, Gosh, <u>Trevisan</u> et al., Science (2023)] al. PRL 127 (2021)]

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$$\int \text{Quantum metric dipole: } D_{yxx}(\mathbf{k})$$

Antisymmetric:

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Additional interband contributions

[Adapted from Liu et al. PRL 127 (2021)]

[Y. Gao et al. PRL 112 (2014), C. Wang et al. PRL 127 (2021) Gao, Liu, Qiu, Gosh, <u>Trevisan</u> et al., Science (2023)] • What about the original anomalous velocity contribution?

$$\dot{\mathbf{r}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \tilde{\varepsilon}_{n,\mathbf{k}} - \dot{\mathbf{k}} \times \Omega_n(\mathbf{k}) - \dot{\mathbf{k}} \times \left(\nabla_{\mathbf{k}} \times \overset{\leftrightarrow}{G}_n \mathbf{E} \right)$$

• Quantum metric Hall effect dominates in \mathcal{PT} symmetric materials

Time-reversal (
$$\mathcal{T}$$
): $\Omega_n(\mathbf{k}) \xrightarrow{\mathcal{T}} -\Omega_n(-\mathbf{k})$
Inversion (\mathcal{P}): $\Omega_n(\mathbf{k}) \xrightarrow{\mathcal{P}} \Omega_n(-\mathbf{k})$

$$\Omega_n(\mathbf{k}) \stackrel{\mathcal{PT}}{=} 0$$

[Y. Gao et al. PRL 112 (2014), C. Wang et al. PRL 127 (2021)

First observation in a heterostructure of MnBi₂Te₄ and BP

Experimentally measured anomalous Hall effect

• Material: heterostructure composed by MnBi₂Te₄ (MBT) and black phosphorus (BP)

SETUP: $V_{\rm TG}$ BP MR ZBG

<u>Suyang Xu</u> Harvard



[Gao, Liu, Qiu, Gosh, <u>Trevisan</u> et al., Science (2023)] **16**

Experimentally measured anomalous Hall effect

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[Gao, Liu, Qiu, Gosh, Trevisan et al., Science (2023)] 16



CRYSTAL STRUCTURE



• Crystal space group:
$$R\overline{3}m \implies \begin{cases} C_{3z} \checkmark \\ \mathcal{P} \checkmark \end{cases}$$
 (spatial inversion)

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- Mn moments ferromagnetically in each SL below ~25K
- Ground state is AFM

CRYSTAL STRUCTURE



• Crystal space group: $R\overline{3}m \implies \begin{cases} C_{3z} \checkmark \\ \mathcal{P} \checkmark$ (spatial inversion)

Mn moments ferromagnetically in each SL below ~ 25 K

 $\mathcal{PT} \square$



• Low energy physics dominated by p_z orbitals of Bi and Te atoms

Each SL: k.p model around the center of BZ [B. Lian et al. PRL 124 (2020)]

$$\hat{h}_{\varsigma}(\mathbf{k}) = \hat{h}_{N}(\mathbf{k}) + (-1)^{\varsigma} \gamma_{af} \hat{h}_{M}(\mathbf{k})$$



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Normal state
Ferromagnetic
(consistent with $R\overline{3}m$)
ordering in each SL



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Inter-SL hopping: $T_0(\mathbf{k})$



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ordering in each SL

Inter-SL hopping: $T_0(\mathbf{k})$

Large quantum metric!







Black phosphorus (BP) promotes the needed C_{3z} breaking



• Low energy physics: tight-biding dominated by p_z orbitals of P atoms

[Ezawa et al. NJP (2014) Rudenko et al. PRB (2015)]

[Gao, Liu, Qiu, Gosh, Trevisan et al., Science (2023)]

Black phosphorus (BP) promotes the needed C_{3z} breaking



• Low energy physics: tight-biding dominated by p_z orbitals of P atoms

[Ezawa et al. NJP (2014) Rudenko et al. PRB (2015)]

• BP tetragonal lattice breaks C_{3z}

Sources of C_{3z} breaking:

[Gao, Liu, Qiu, Gosh, <u>Trevisan</u> et al., Science (2023)]

a) Hybridization of BP and MBT bands

Next-neighbor interlayer hoping: \widehat{U}_b and \widehat{U}_t

b) Lattice mismatch \Rightarrow strain

The BP/MBT/BP heterostructure: results from theoretical modeling





Large quantum metric at small band gaps

The BP/MBT/BP heterostructure: results from theoretical modeling







Quantum metric dipole:

For $\mu = -50$ meV:



$$\int_{\mathrm{FS}} d\mathbf{k} \left[v_y g_{xx} - v_x g_{yx} \right] \neq 0$$

Large quantum metric at small band gaps

 \hat{U}_t









 \hat{U}_t



 \hat{U}_t

Strain alone cannot capture the features of the observed Hall signal

- Large mismatch between MBT and BP lattice induces strain
- New terms in the MBT minimal model

$$\hat{h}(\mathbf{k}) = \hat{h}_N(\mathbf{k}) + (-1)^{\zeta} \gamma_{\mathrm{af}} \hat{h}_{\mathrm{AFM}}(\mathbf{k}) + \gamma_s \hat{h}_s(\mathbf{k})$$



Strain and MBT-BP hybridization







[Gao, Liu, Qiu, Gosh, Trevisan et al., Science (2023)] 22

 \hat{U}_t



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3)Hall signal changes sign under time-reversal 4) Symmetry constraint rule out Berry curvature dipole

Summary

- Second-order anomalous Hall effect
 - Extrinsic: disorder, Berry curvature multipoles
 - Intrinsic: dipoles of quantum metric
- Intrinsic component dominates in PT-symmetric materials with large quantum metric
 - BP/MBT/BP is an ideal platform
 - Main features captured by a minimal model
 - Hybridization between MBT and BP bands is essential to account for sign change of the Hall signal
- Future direction: what about multipoles of quantum metric?







Thank you!

Extra Slides

Frequency dependence of the quantum metric anomalous Hall conductivity



Fig. S23. Measured frequency dependence of the nonlinear Hall effect. (A) $\sigma_{yxx}^{2\omega} - n_e$ at discrete frequency ω values. (B-E) $\sigma_{yxx}^{2\omega} - \omega$ at four charge density n_e values (noted by the black arrows in panel A).

Dominant contribution of the quantum metric term



Fig. S42. Quantum metric dipole dominated nonlinear Hall conductivity. Two-band model (quantum metric dipole D_{Metric} contribution) and multiband model (D_{Metric} + additional inter band contributions AIC) calculated nonlinear Hall conductivity as a function of carrier density. The nonlinear Hall signals are dominated by the quantum metric dipole contribution.