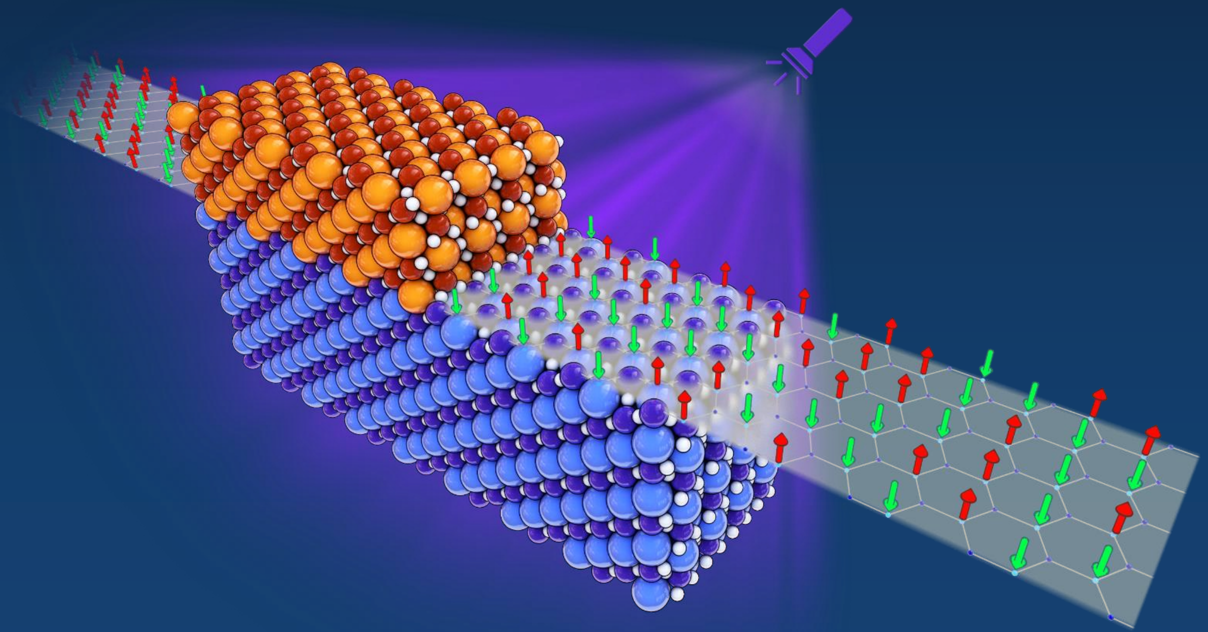
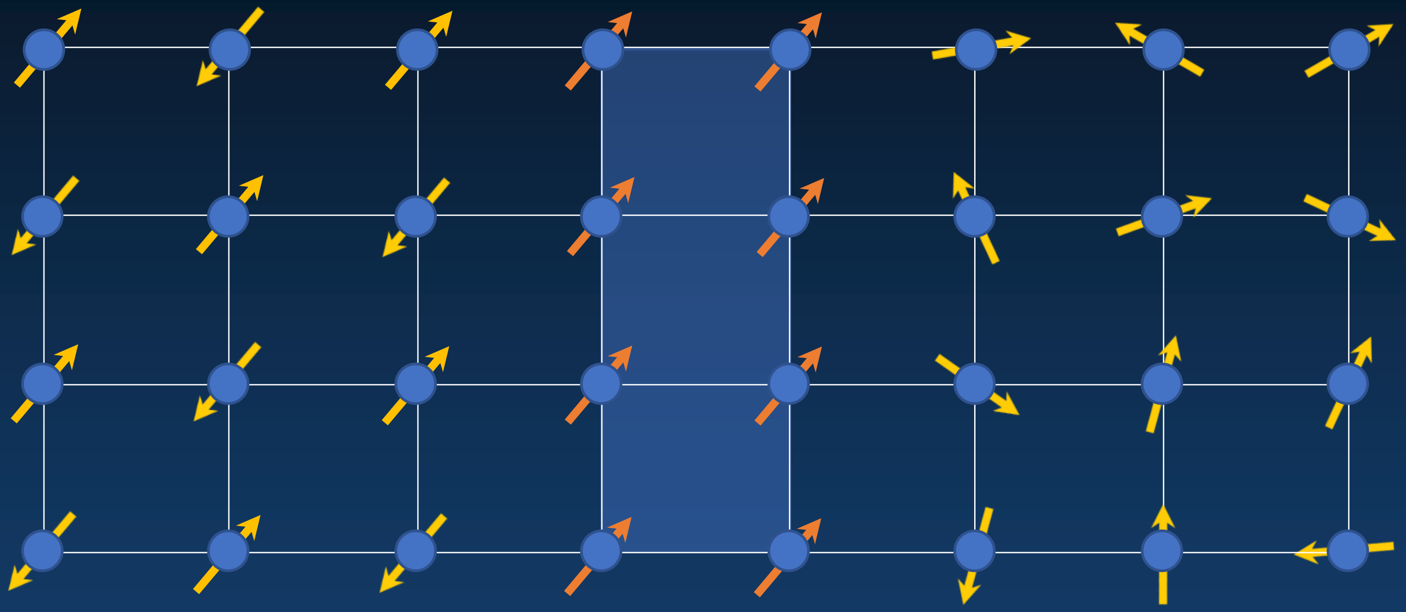
Introduction to quantum geometry

Caviglia Lab
Department of Quantum Matter Physics
University of Geneva



UNIVERSITÉ DE GENÈVE

Interfaces of quantum materials:
A laboratory for many-body physics in and out of equilibrium



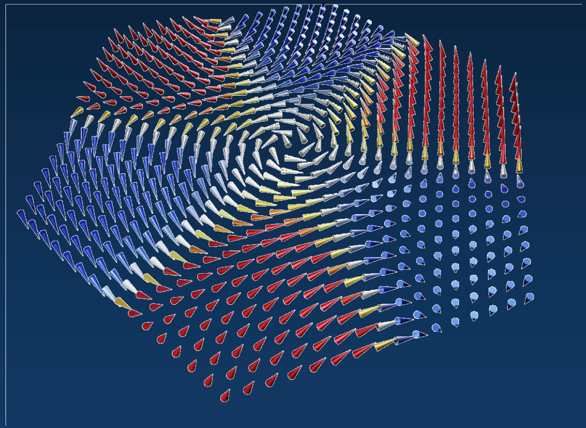
Interactions	U_1, t_1, J_1, λ_1,	**U, t, J, λ,**	U_2, t_2, J_2, λ_2,	Symmetry breaking
Geometric phases	$A_{k\ 1}$	$\mathbf{A_k}$	$A_{k\ 2}$	Quantum geometry

Why quantum geometry?

Controlling dynamics of charges orbitals and spins through purely quantum effects (no Lorentz force).

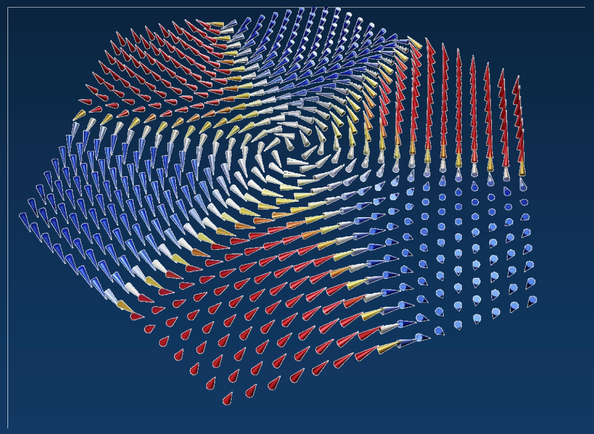
Engineering strong electromagnetic responses originating from low-energy physics, THz electrodynamics.

Large non-linear responses.



Lecture plan

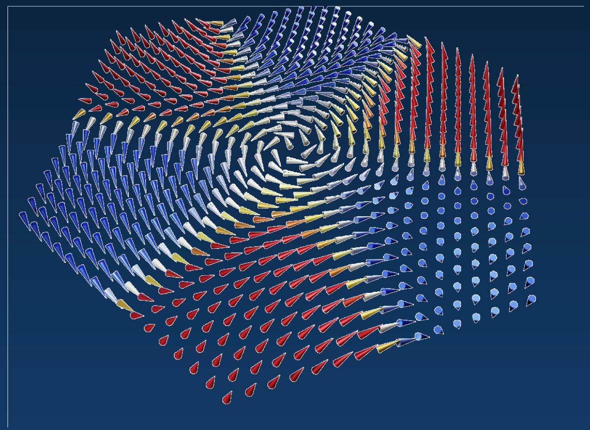
1) Adiabatic approximation in quantum mechanics.
2) Geometric phase, Berry connection and Berry curvature
3) Example 1: spin ½ in a rotating magnetic field.
4) Anomalous transport.
5) Berry curvature of a two-level system.
6) Example 2: Berry curvature of a Rashba two-dimensional electron system.
7) Example 3: Berry curvature of a trigonal Rashba two-dimensional electron system.
8) Application: quantum geometry at oxide interfaces.



Lecture notes available at caviglia.unige.ch/teaching

Learning objectives

1) Discuss geometric properties of wavefunctions.
2) Compute geometric quantities of model two-level systems.
3) Identify condensed matter systems with quantum geometric properties.
4) Apply these ideas to your research?



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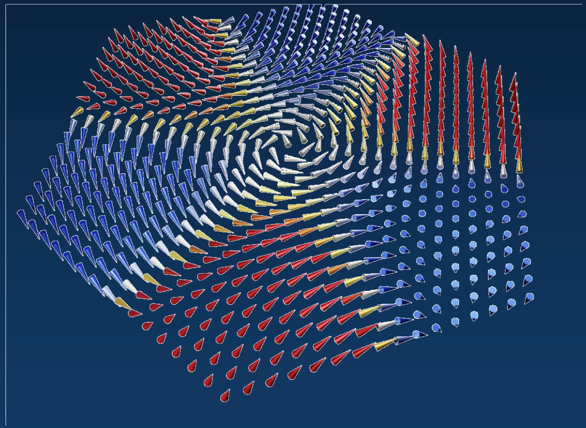

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Adiabatic approximation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

Time-dependent Schrödinger equation

Adiabatic approximation

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H\left|\Psi(t)\right\rangle$$

$$\left|\Psi(t)\right\rangle = \sum_n \Psi_n(t) = \sum_n c_n(t)\left|\psi_n(t)\right\rangle$$

Time-dependent Schrödinger equation

Ansatz

Adiabatic approximation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

Time-dependent Schrödinger equation

$$|\Psi(t)\rangle = \sum_n \Psi_n(t) = \sum_n c_n(t)\,|\psi_n(t)\rangle$$

Ansatz

$$H(t)\psi_n(t) = E_n(t)\psi_n(t)$$

Instantaneous Schrödinger-like eq

Adiabatic approximation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

Time-dependent Schrödinger equation

$$|\Psi(t)\rangle = \sum_n \Psi_n(t) = \sum_n c_n(t)\,|\psi_n(t)\rangle$$

Ansatz

$$H(t)\psi_n(t) = E_n(t)\psi_n(t)$$

Instantaneous Schrödinger-like eq

$$i\hbar\dot{c}_k(t) \approx \Big(E_k(t) - i\hbar\,\langle\psi_k(t)|\dot{\psi}_k(t)\rangle\Big)\,c_k(t).$$

$$c_k(t) = \exp\left\{\frac{1}{i\hbar}\int_0^t \Big(E_k(t') - i\hbar\,\langle\psi_k(t')|\dot{\psi}_k(t')\rangle\Big)\,\mathrm{d}t'\right\}$$

Approx solutions neglecting transitions, during the evolution the system remains in its instantaneous eigenstates

Valid for $T_{ext} >> T_{int}$

Adiabatic approximation

$$c_k(t) = \exp\left\{\frac{1}{i\hbar}\int_0^t \left(E_k(t') - i\hbar \langle \psi_k(t')|\dot{\psi}_k(t')\rangle\right) \mathrm{d}t'\right\}$$

$$\Psi_n(t) \approx e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t)$$

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\mathrm{d}t'$$

Dynamical phase

$$\gamma_n(t) = \int_0^t i \langle \psi_n(t')|\dot{\psi}_n(t')\rangle \,\mathrm{d}t'$$

Geometric phase or Berry phase

Why geometric?

Geometric phase

$$H(\mathbf{k})\,|\psi_n(\mathbf{k})\rangle = E_n(\mathbf{k})\,|\psi_n(\mathbf{k})\rangle$$

k is a vector field containing a set of parameters describing the Hamiltonian

Geometric phase

$$H(\mathbf{k})\left|\psi_n(\mathbf{k})\right\rangle = E_n(\mathbf{k})\left|\psi_n(\mathbf{k})\right\rangle$$

$$\mathbf{k}(t) = (k_1(t), \dots, k_N(t))$$

k is a vector field containing a set of parameters describing the Hamiltonian

Path in the configuration space

Geometric phase

$$H(\mathbf{k})\,|\psi_n(\mathbf{k})\rangle = E_n(\mathbf{k})\,|\psi_n(\mathbf{k})\rangle$$

$$\mathbf{k}(t) = (k_1(t), \dots, k_N(t))$$

$$\gamma_n(t) = \int_0^t i\,\langle\psi_n\left(\mathbf{k}(t')\right)|\frac{\mathrm{d}}{\mathrm{d}t'}\psi_n\left(\mathbf{k}(t')\right)\rangle\,\mathrm{d}t' =$$

k is a vector field containing a set of parameters describing the Hamiltonian

Path in the configuration space

Geometric phase

$$H(\mathbf{k})\,|\psi_n(\mathbf{k})\rangle = E_n(\mathbf{k})\,|\psi_n(\mathbf{k})\rangle$$

k is a vector field containing a set of parameters describing the Hamiltonian

$$\mathbf{k}(t) = (k_1(t), \ldots, k_N(t))$$

Path in the configuration space

$$\gamma_n(t) = \int_0^t i\,\langle\psi_n\left(\mathbf{k}(t')\right)|\frac{\mathrm{d}}{\mathrm{d}t'}\psi_n\left(\mathbf{k}(t')\right)\rangle\,\mathrm{d}t' =$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_n\left(\mathbf{k}(t)\right) = \frac{\mathrm{d}}{\mathrm{d}t}\psi_n\left(k_1(t), \ldots, k_N(t)\right) =$$

$$= \frac{\partial\psi_n}{\partial k_1}\frac{\mathrm{d}k_1}{\mathrm{d}t} + \ldots + \frac{\partial\psi_n}{\partial k_N}\frac{\mathrm{d}k_N}{\mathrm{d}t} = \nabla_{\mathbf{k}}\psi_n \cdot \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}$$

Geometric phase acquired along the path

Geometric phase

$$\gamma_n(t) = \int_0^t i \langle \psi_n(\mathbf{k}(t')) | \nabla_{\mathbf{k}} | \psi_n(\mathbf{k}(t')) \rangle \cdot \frac{\mathrm{d}\mathrm{k}}{\mathrm{d}t'} \mathrm{d}t'$$

$$\gamma_n = \oint_C i \langle \psi_n(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi_n(\mathbf{k}) \rangle \cdot \mathrm{d}\mathbf{k}$$

The geometric phase can be calculated as a purely geometric quantity

Geometric phase

$$\gamma_n(t) = \int_0^t i \left\langle \psi_n\left(\mathbf{k}(t')\right) \middle| \nabla_{\mathbf{k}} \middle| \psi_n\left(\mathbf{k}(t')\right) \right\rangle \cdot \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t'} \mathrm{d}t'$$

$$\gamma_n = \oint_C i \left\langle \psi_n(\mathbf{k}) \middle| \nabla_{\mathbf{k}} \middle| \psi_n(\mathbf{k}) \right\rangle \cdot \mathrm{d}\mathbf{k}$$

$$\mathcal{A}_n(\mathbf{k}) = i \left\langle \psi_n(\mathbf{k}) \middle| \nabla_{\mathbf{k}} \middle| \psi_n(\mathbf{k}) \right\rangle$$

The geometric phase can be calculated as a purely geometric quantity

Berry connection

Geometric phase

$$\mathcal{A}_n(\mathbf{k}) = i \langle \psi_n(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi_n(\mathbf{k}) \rangle$$

Berry connection

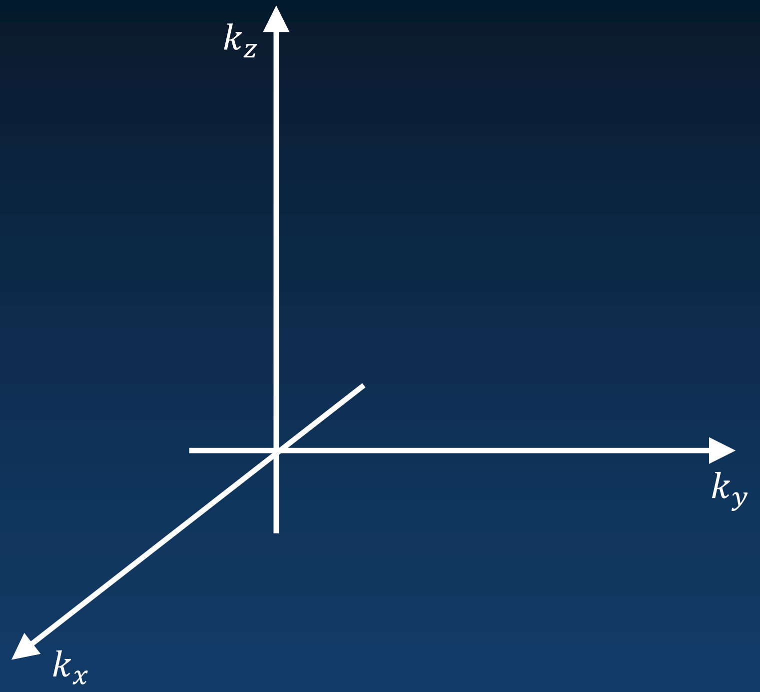
$$\gamma_n = \oint_{\mathcal{C}} \mathcal{A}_n(\mathbf{k}) \cdot \mathrm{d}\mathbf{k} = \iint_{\mathcal{S}} \nabla_{\mathbf{k}} \times \mathcal{A}_n(\mathbf{k}) \cdot \mathrm{d}^2\mathbf{k} \,.$$

In 3D configuration space
we can use Stoke's theorem

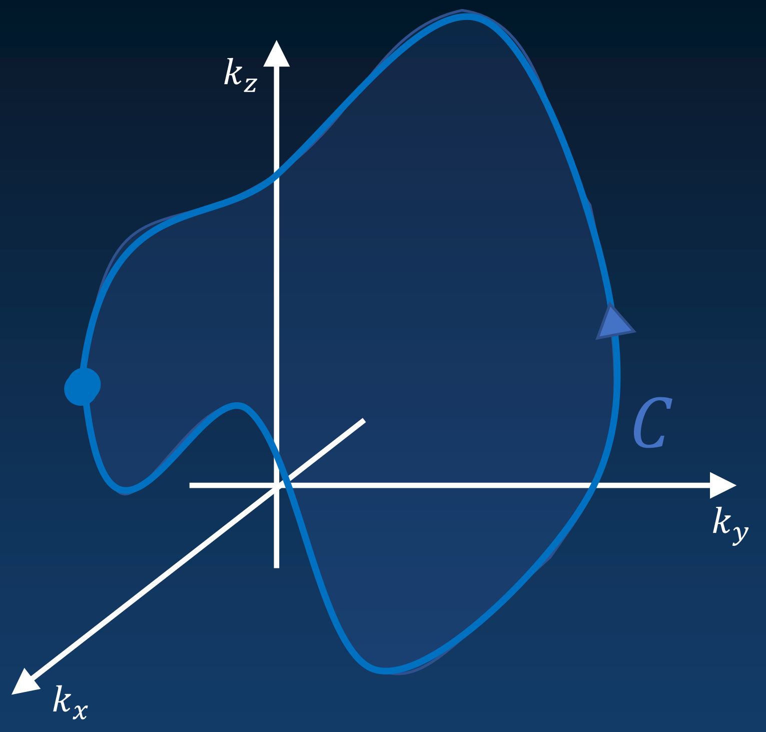
$$\mathcal{B}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}_n(\mathbf{k})$$

Berry curvature

Geometric phase



Geometric phase

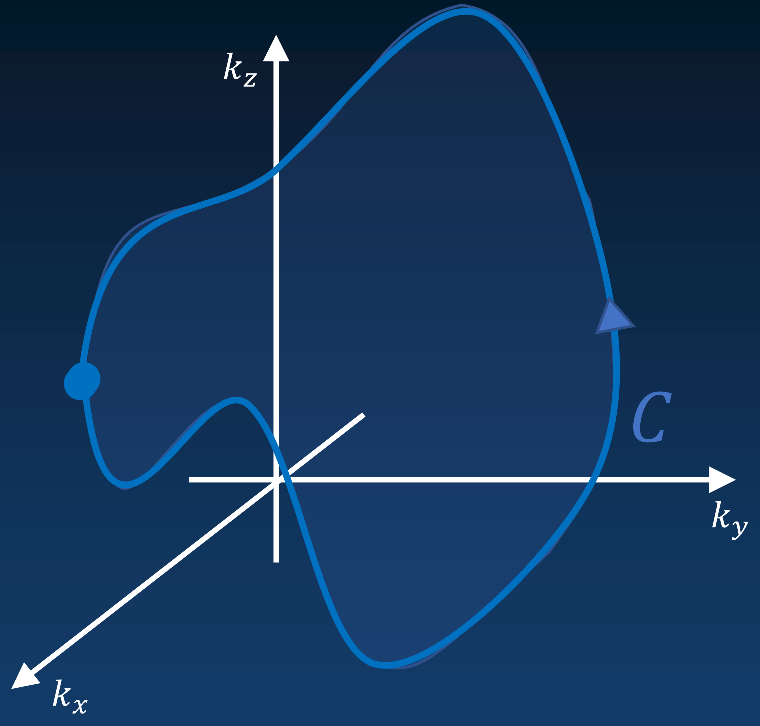


Geometric phase

$$\gamma_n = \int_C \boldsymbol{A}_n(\boldsymbol{k}) \cdot d\boldsymbol{k}$$

$$\boldsymbol{A}_n(\boldsymbol{k}) = i\langle u_n(\boldsymbol{k})|\nabla_{\boldsymbol{k}}|\, u_n(\boldsymbol{k})\rangle$$

Berry
Connection



Geometric phase

$$\gamma_n = \int_C \boldsymbol{A}_n(\boldsymbol{k}) \cdot d\boldsymbol{k}$$

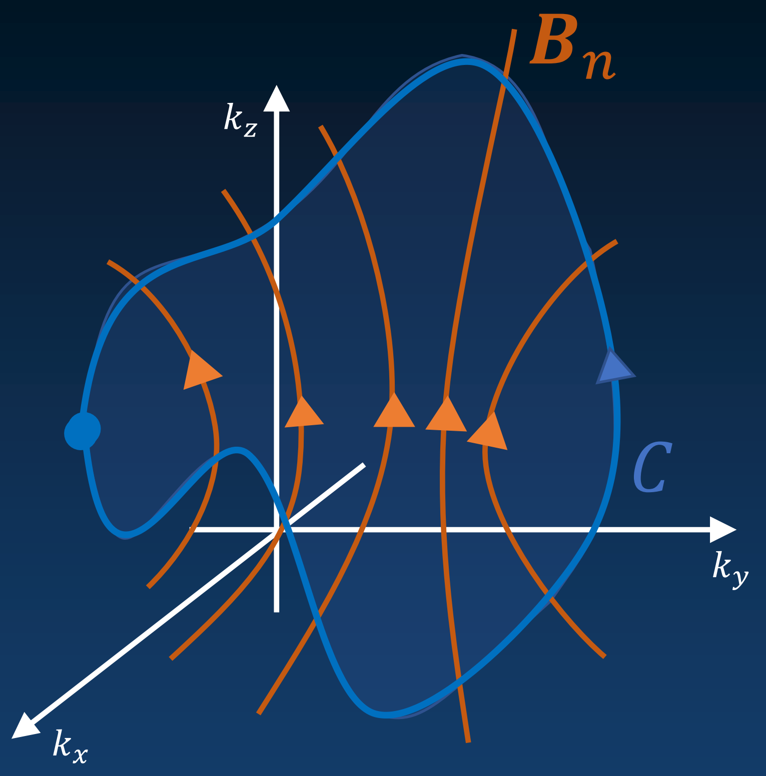
$$\gamma_n = \oiint_\Omega \boldsymbol{B}_n(\boldsymbol{k}) \cdot d\boldsymbol{\Omega}$$

$$\boldsymbol{A}_n(\boldsymbol{k}) = i\langle u_n(\boldsymbol{k})|\nabla_{\boldsymbol{k}}|\, u_n(\boldsymbol{k})\rangle$$

Berry Connection

$$\boldsymbol{B}_n(\boldsymbol{k}) = \nabla_{\mathbf{k}} \times \boldsymbol{A}_n(\boldsymbol{k})$$

Berry Curvature



Example 1. Spin in a rotating B field

$$\mathcal{H}(t) = -\frac{\mu}{2}\,\vec{\sigma}\cdot\vec{\mathbf{B}}(t)$$

$$\vec{\mathbf{B}}(t) = B_0[\sin\theta\cos\omega t\ \hat{\mathbf{x}} + \sin\theta\sin\omega t\ \hat{\mathbf{y}} + \cos\theta\ \hat{\mathbf{z}}]$$

Spin ½ immersed in a homogeneous magnetic field rotating on a two-dimensional plane

Example 1. Spin in a rotating B field

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$$\vec{\mathbf{B}}(t) = B_0[\sin\theta\cos\omega t\ \hat{\mathbf{x}} + \sin\theta\sin\omega t\ \hat{\mathbf{y}} + \cos\theta\ \hat{\mathbf{z}}]$$

$$\gamma_n = i\int_{\mathcal{C}} \langle n,\vec{\mathbf{B}}|\,\boldsymbol{\nabla}_B\,|n,\vec{\mathbf{B}}\rangle\cdot \mathrm{d}\vec{\mathbf{B}}$$

Geometric phase

Example 1. Spin in a rotating B field

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$$\vec{\mathbf{B}}(t) = B_0[\sin\theta\cos\omega t\ \hat{\mathbf{x}} + \sin\theta\sin\omega t\ \hat{\mathbf{y}} + \cos\theta\ \hat{\mathbf{z}}]$$

$$\det\{E\mathbb{1} - \mathcal{H}(t)\} = 0$$

$$E_\pm = \pm\frac{\mu B}{2}$$

Spin ½ immersed in a homogeneous magnetic field rotating on a two-dimensional plane

Eigenvalues

Example 1. Spin in a rotating B field

$$\mathcal{H}(t) = -\frac{\mu}{2}\vec{\sigma}\cdot\vec{\mathbf{B}}(t)$$

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$$E_\pm = \pm\frac{\mu B}{2}$$

Eigenvalues

$$\vec{\mathbf{v}}_+ = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2)e^{i\omega t} \end{pmatrix} \qquad \vec{\mathbf{v}}_- = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\omega t} \end{pmatrix}$$

Eigenvectors

Example 1. Spin in a rotating B field

$$\mathcal{H}(t) = -\frac{\mu}{2}\vec{\sigma} \cdot \vec{\mathbf{B}}(t)$$

$$\vec{\mathbf{B}}(t) = B_0[\sin\theta \cos\omega t \ \hat{\mathbf{x}} + \sin\theta \sin\omega t \ \hat{\mathbf{y}} + \cos\theta \ \hat{\mathbf{z}}]$$

$$\gamma_n = i \int_{\mathcal{C}} \langle n, \vec{\mathbf{B}}| \boldsymbol{\nabla}_B |n, \vec{\mathbf{B}}\rangle \cdot \mathrm{d}\vec{\mathbf{B}}$$

$$\boldsymbol{\nabla}_B \, \vec{\mathbf{v}}_{\pm} = \left(\frac{\partial}{\partial B_0} \quad \frac{1}{B_0}\frac{\partial}{\partial \theta} \quad \frac{1}{B_0 \sin\theta}\frac{\partial}{\partial \omega t} \right) \vec{\mathbf{v}}_{\pm}$$

Spin ½ immersed in a homogeneous magnetic field rotating on a two-dimensional plane

Gradient operator in configuration space in spherical coordinates

Example 1. Spin in a rotating B field

$$\mathcal{H}(t) = -\frac{\mu}{2}\vec{\sigma}\cdot\vec{\mathbf{B}}(t)$$

$$\vec{\mathbf{B}}(t) = B_0[\sin\theta\cos\omega t\ \hat{\mathbf{x}} + \sin\theta\sin\omega t\ \hat{\mathbf{y}} + \cos\theta\ \hat{\mathbf{z}}]$$

$$\gamma_n = i\int_{\mathcal{C}} \langle n, \vec{\mathbf{B}}|\,\boldsymbol{\nabla}_B\,|n,\vec{\mathbf{B}}\rangle \cdot \mathrm{d}\vec{\mathbf{B}}$$

$$\boldsymbol{\nabla}_B\,\vec{\mathbf{v}}_+ = \frac{1}{2B_0}\begin{pmatrix} -\cos\frac{\theta}{2}\hat{\boldsymbol{\theta}} \\ -\sin\frac{\theta}{2}e^{i\omega t}\hat{\boldsymbol{\theta}} + \frac{i}{\sin\frac{\theta}{2}}e^{i\omega t}\hat{\boldsymbol{\phi}} \end{pmatrix}$$

$$\boldsymbol{\nabla}_B\,\vec{\mathbf{v}}_- = \frac{1}{2B_0}\begin{pmatrix} -\sin\frac{\theta}{2}\hat{\boldsymbol{\theta}} \\ \cos\frac{\theta}{2}e^{i\omega t}\hat{\boldsymbol{\theta}} + \frac{i}{\cos\frac{\theta}{2}}e^{i\omega t}\hat{\boldsymbol{\phi}} \end{pmatrix}$$

Spin ½ immersed in a homogeneous magnetic field rotating on a two-dimensional plane

Geometric phase, expectation value of the gradient

Example 1. Spin in a rotating B field

$$\mathcal{H}(t) = -\frac{\mu}{2}\vec{\sigma}\cdot\vec{\mathbf{B}}(t)$$

$$\vec{\mathbf{B}}(t) = B_0[\sin\theta\cos\omega t\ \hat{\mathbf{x}} + \sin\theta\sin\omega t\ \hat{\mathbf{y}} + \cos\theta\ \hat{\mathbf{z}}]$$

$$\gamma_{v_+} = -\pi(1+\cos\theta)$$

$$\gamma_{v_-} = -\pi(1-\cos\theta)$$

Spin ½ immersed in a homogeneous magnetic field rotating on a two-dimensional plane

Geometric phase acquired after a full rotation

Example 1. Spin in a rotating B field

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$$\langle\psi^{\pm}\left(t=\frac{2\pi}{\omega}\right)|\,|\psi^{\pm}(t=0)\rangle = \underbrace{e^{\pm i\frac{2\pi}{\omega}\mu B_0}}_{\text{dynamical phase}} \quad \underbrace{e^{-i\pi(1\pm\cos\theta)}}_{\text{geometric phase}}$$

Spin ½ immersed in a homogeneous magnetic field rotating on a two-dimensional plane

Geometric phase acquired after a full rotation

Anomalous transport

$$\nabla_{\mathbf{k}} \to \nabla_{\mathbf{k}} - i\mathcal{A}_{\mathbf{k}}.$$

Geometric riformulation of QM
J. Anandan and Y. Aharonov
Geometry of quantum evolution
Phys. Rev. Lett. 65, 1697 (1990)

Quantum Geometric Tensor (QGT)

Re (QGT) : geodesic distance on the Bloch's sphere that is endowed with a Fubini–Study metric

Im (QGT): Berry curvature, associated with geometric phase of the wavefunction

Anomalous transport

$$\nabla_{\mathbf{k}} \to \nabla_{\mathbf{k}} - i\mathcal{A}_{\mathbf{k}}.$$

Gradient needs to be redefined

$$\hat{x} = \nabla_{k_x} - i\mathcal{A}_{k_x}$$
$$\hat{y} = \nabla_{k_y} - i\mathcal{A}_{k_y}.$$

Position operators

Anomalous transport

$$\nabla_{\mathbf{k}} \to \nabla_{\mathbf{k}} - i\mathcal{A}_{\mathbf{k}}.$$

Gradient needs to be redefined

$$\hat{x} = \nabla_{k_x} - i\mathcal{A}_{k_x}$$
$$\hat{y} = \nabla_{k_y} - i\mathcal{A}_{k_y}.$$

Position operators

$$\hat{H}' = -e\mathcal{E}_x\hat{x}$$

Static homogeneous electric field

Anomalous transport

$$\hat{H}' = -e\mathcal{E}_x\hat{x}$$

Static homogeneous electric field

$$\begin{aligned}\left\langle \frac{\mathrm{d}\hat{y}}{\mathrm{d}t} \right\rangle &= \frac{i}{\hbar}\left[\hat{H}', \hat{y}\right] \\ &= -\frac{ie\mathcal{E}_x}{\hbar}[\hat{x}, \hat{y}] \\ &= \frac{e\mathcal{E}_x}{\hbar}\left(\frac{\partial \mathcal{A}_{k_y}}{\partial k_x} - \frac{\partial \mathcal{A}_{k_x}}{\partial k_y}\right) \\ &= \frac{e}{\hbar}\mathcal{E}_x\mathcal{B}^z_{\mathrm{k}} = v^{\mathrm{AH}}_y\end{aligned}$$

In the absence of Berry curvature we do not expect any dynamics

The z-component of the curl of A

Anomalous velocity

Anomalous transport

Static homogeneous electric field

$$\hat{H}' = -e\mathcal{E}_x\hat{x}$$

Anomalous conductance

$$\sigma_{xy}^{\mathrm{AH}} = -v_y^{\mathrm{AH}} e/\mathcal{E}_x .$$

Anomalous conductance in a Fermi liquid

$$\sigma_{xy}^{\mathrm{AH}} = -\frac{e^2}{2\pi h}\sum_n \iint_{\mathrm{BZ}} f(\epsilon_{\mathbf{k}}^n)\mathcal{B}_n^z \, \mathrm{d}^2\mathbf{k} \, .$$

Anomalous conductance in a Chern insulator

$$\sigma_{xy,n}^{\mathrm{AH}} = -\frac{e^2}{2\pi h}\iint_{\mathrm{BZ}} \mathcal{B}_n^z \, \mathrm{d}^2\mathbf{k} = -\frac{e^2}{h}C_n .$$

Geometric phase

$$\gamma_n = \int_C \boldsymbol{A}_n(\boldsymbol{k}) \cdot d\boldsymbol{k}$$

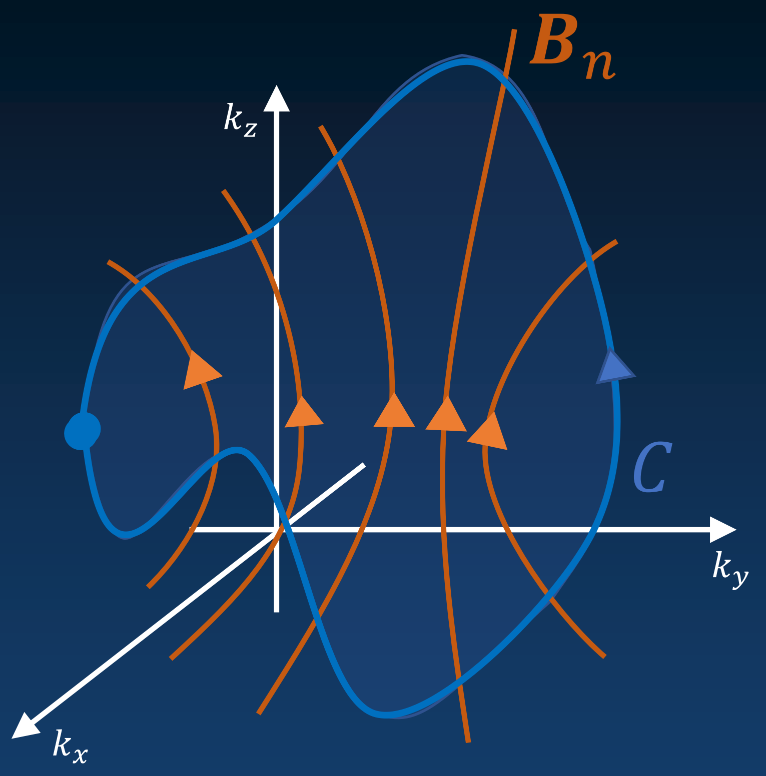
$$\gamma_n = \oiint_\Omega \boldsymbol{B}_n(\boldsymbol{k}) \cdot d\boldsymbol{\Omega}$$

$$\boldsymbol{A}_n(\boldsymbol{k}) = i\langle u_n(\boldsymbol{k})|\nabla_{\boldsymbol{k}}|\, u_n(\boldsymbol{k})\rangle$$

Berry Connection

$$\boldsymbol{B}_n(\boldsymbol{k}) = \nabla_{\mathbf{k}} \times \boldsymbol{A}_n(\boldsymbol{k})$$

Berry Curvature



Anomalous velocity and Berry phase

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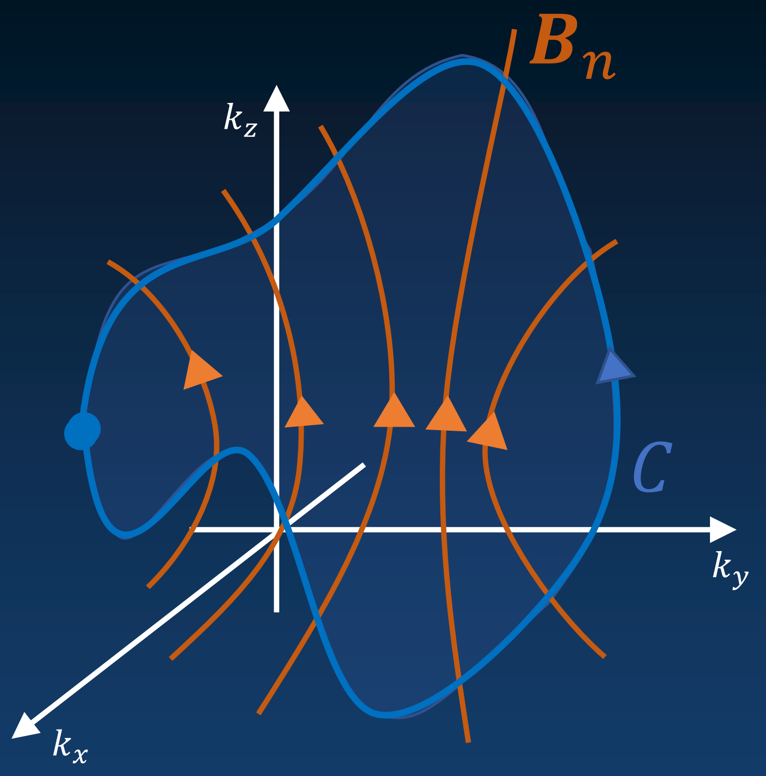


$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\epsilon_n(\boldsymbol{k}) - \frac{e}{\hbar}\boldsymbol{E} \times \boldsymbol{B}_n(\boldsymbol{k})$$

Anomalous velocity and Berry phase

$$\gamma_n = \int_C \boldsymbol{A}_n(\boldsymbol{k}) \cdot d\boldsymbol{k}$$

$$\gamma_n = \oiint_\Omega \boldsymbol{B}_n(\boldsymbol{k}) \cdot d\boldsymbol{\Omega}$$

$$\boldsymbol{A}_n(\boldsymbol{k}) = i\langle u_n(\boldsymbol{k})|\nabla_{\boldsymbol{k}}|\, u_n(\boldsymbol{k})\rangle$$

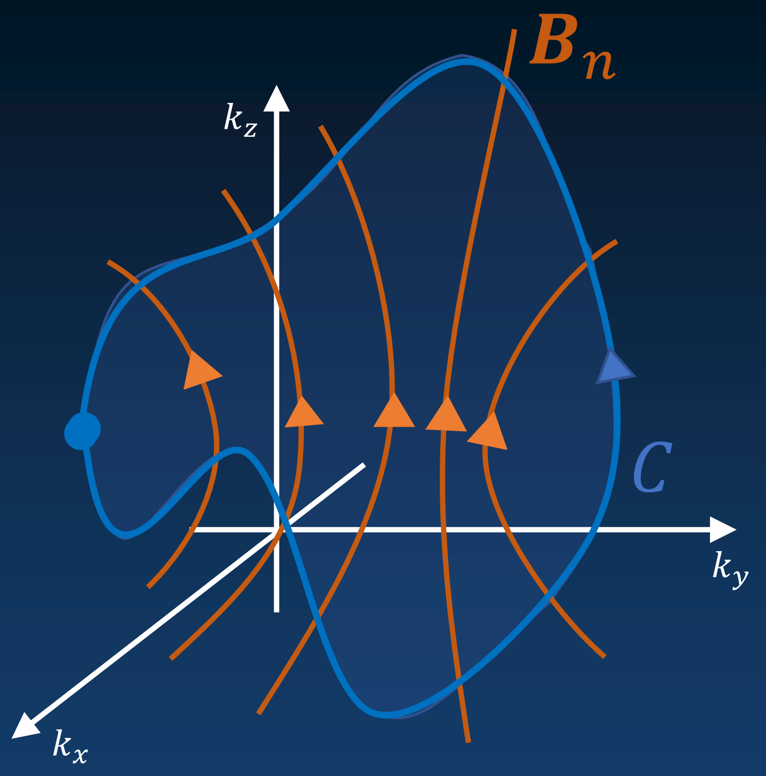
Berry Connection

Effective Vector Potential

$$\boldsymbol{B}_n(\boldsymbol{k}) = \nabla_{\mathbf{k}} \times \boldsymbol{A}_n(\boldsymbol{k})$$

Berry Curvature

Effective Magnetic Field



$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\epsilon_n(\boldsymbol{k}) - \frac{e}{\hbar}\,\boldsymbol{E} \times \boldsymbol{B}_n(\boldsymbol{k})$$

Karplus, Luttinger Phys. Rev. 95, 1154 (1954)
Berry Proc. R. Soc. London A 392, 45 (1984)
Chang, Niu PRL 75, 1348 (1995)

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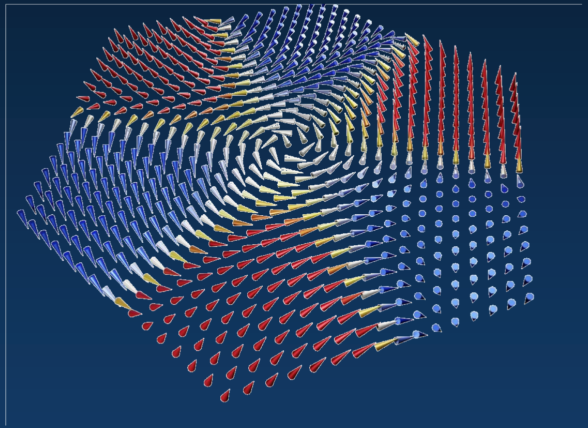

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Berry curvature of a two-level system

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = d_1\sigma_x + d_2\sigma_y + d_3\sigma_z$$

$$d = |\mathbf{d}| = \sqrt{d_1^2 + d_2^2 + d_3^2}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Hamiltonian of a two-level system

Relevant for systems such as gapped graphene

$$\mathcal{H}(\mathbf{k}) = v_F[\sigma_x k_x + \sigma_y k_y] + m\sigma_z$$

Weyl semimetal

$$\mathcal{H}(\mathbf{k}) = v_F^x \sigma_x k_x + v_F^y \sigma_y k_y + v_F^z \sigma_z k_z$$

Berry curvature of a two-level system

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = d_1\sigma_x + d_2\sigma_y + d_3\sigma_z$$

Hamiltonian of a two-level system

$$\mathcal{A}^{\pm}(\mathbf{k}) = i \langle \psi^{\pm}(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi^{\pm}(\mathbf{k}) \rangle$$

We want to compute BC

$$\psi^- = \frac{1}{\sqrt{2d(d-d_3)}} \begin{bmatrix} d_3 - d \\ d_1 + id_2 \end{bmatrix}$$

$$\psi^+ = \frac{1}{\sqrt{2d(d+d_3)}} \begin{bmatrix} d_3 + d \\ d_1 + id_2 \end{bmatrix}$$

$$E_{\pm} = \pm|\mathbf{d}|.$$

Eigenvectors and eigenvalues

Berry curvature of a two-level system

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = d_1\sigma_x + d_2\sigma_y + d_3\sigma_z$$

Hamiltonian of a two-level system

$$\mathcal{A}^{\pm}(\mathbf{k}) = i\,\langle \psi^{\pm}(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi^{\pm}(\mathbf{k}) \rangle$$

We want to compute BC

$$\nabla_{\mathbf{k}}|\psi^{\pm}\rangle = \nabla_{\mathbf{k}} \frac{1}{\sqrt{2d(d \pm d_3)}} \begin{bmatrix} d_3 \pm d \\ d_1 + id_2 \end{bmatrix} =$$

$$= \frac{1}{\sqrt{2d(d \pm d_3)}} \begin{bmatrix} \nabla_{\mathbf{k}}(d_3 \pm d) \\ \nabla_{\mathbf{k}}(d_1 + id_2) \end{bmatrix} - \frac{\nabla_{\mathbf{k}} d(d \pm d_3)}{[2d(d \pm d_3)]^{3/2}} \begin{bmatrix} d_3 \pm d \\ d_1 + id_2 \end{bmatrix}$$

Gradient

Berry curvature of a two-level system

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = d_1\sigma_x + d_2\sigma_y + d_3\sigma_z$$

Hamiltonian of a two-level system

$$\mathcal{A}^{\pm}(\mathbf{k}) = i \langle \psi^{\pm}(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi^{\pm}(\mathbf{k}) \rangle$$

We want to compute BC

$$\nabla_{\mathbf{k}} |\psi^{\pm}\rangle = \nabla_{\mathbf{k}} \frac{1}{\sqrt{2d(d \pm d_3)}} \begin{bmatrix} d_3 \pm d \\ d_1 + i d_2 \end{bmatrix} =$$

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Hamiltonian of a two-level system

$$\mathcal{A}^{\pm}(\mathbf{k}) = i \langle \psi^{\pm}(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi^{\pm}(\mathbf{k}) \rangle$$

We want to compute BC

$$\begin{aligned}\langle \psi^{\pm}(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi^{\pm}(\mathbf{k}) \rangle = &\frac{1}{2d(d \pm d_3)}[(d \pm d_3)\nabla_{\mathbf{k}}(d \pm d_3) + (d_1 - id_2)\nabla_{\mathbf{k}}(d_1 + id_2)] \\ &- \frac{1}{[2d(d \pm d_3)]^2}\nabla_{\mathbf{k}} d(d \pm d_3)[(d \pm d_3)^2 + d_1^2 + d_2^2]\end{aligned}$$

Expectation of gradient

Berry curvature of a two-level system

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = d_1\sigma_x + d_2\sigma_y + d_3\sigma_z$$

Hamiltonian of a two-level system

$$\mathcal{A}^{\pm}(\mathbf{k}) = i \langle \psi^{\pm}(\mathbf{k}) | \nabla_{\mathbf{k}} | \psi^{\pm}(\mathbf{k}) \rangle$$

We want to compute BC

$$\mathcal{A}^{\pm}(\mathbf{k}) = \frac{d_2 \nabla_{\mathbf{k}} d_1 - d_1 \nabla_{\mathbf{k}} d_2}{2d(d \pm d_3)}$$

Berry connection

Berry curvature of a two-level system

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} = d_1\sigma_x + d_2\sigma_y + d_3\sigma_z$$

Hamiltonian of a two-level system

$$\mathcal{B}_z^{\pm} = \nabla_{k_x}\mathcal{A}_{k_y}^{\pm} - \nabla_{k_y}\mathcal{A}_{k_x}^{\pm}$$

Berry curvature in two-dimensions

$$\boxed{\mathcal{B}_z^{\pm} = \mp\frac{1}{2}\hat{\mathbf{d}} \cdot (\nabla_{k_x}\hat{\mathbf{d}} \times \nabla_{k_y}\hat{\mathbf{d}})}$$

Berry curvature of a two-level system

Example 2. BC of a Rashba 2DEG

$$\mathcal{H}_{\mathrm{R}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\sigma_0 - \alpha_{\mathrm{R}}\,\boldsymbol{\sigma}\cdot\mathbf{k}\times\hat{\mathbf{z}}\,,$$

$$H = \frac{\mathbf{k}^2}{2m}\sigma_0 + \alpha_{\mathrm{R}}(k_y\sigma_x - k_x\sigma_y)$$

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k})\cdot\boldsymbol{\sigma} = d_1\sigma_x + d_2\sigma_y + d_3\sigma_z$$

Hamiltonian of a Rashba 2DEG

Example 2. BC of a Rashba 2DEG

$$\mathcal{H}_{\mathrm{R}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\sigma_0 - \alpha_{\mathrm{R}}\,\boldsymbol{\sigma}\cdot\mathbf{k}\times\hat{\mathbf{z}}\,,$$

Hamiltonian of a Rashba 2DEG

$$H = \frac{\mathbf{k}^2}{2m}\sigma_0 + \alpha_{\mathrm{R}}(k_y\sigma_x - k_x\sigma_y)$$

We want to find its spin texture

$$\mathbf{k} = k(\cos\phi, \sin\phi, 0),$$

In-plane crystal momentum

Example 2. BC of a Rashba 2DEG

$$\mathcal{H}_{\mathrm{R}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\sigma_0 - \alpha_{\mathrm{R}}\,\boldsymbol{\sigma}\cdot\mathbf{k}\times\hat{\mathbf{z}}\,,$$

Hamiltonian of a Rashba 2DEG

$$H = \frac{\mathbf{k}^2}{2m}\sigma_0 + \alpha_{\mathrm{R}}(k_y\sigma_x - k_x\sigma_y)$$

We want to find its spin texture

$$\mathbf{k} = k(\cos\phi, \sin\phi, 0),$$

In-plane crystal momentum

$$H = \frac{\hbar^2 k^2}{2m}\begin{pmatrix} 1 & i\eta e^{-i\phi} \\ -i\eta e^{i\phi} & 1 \end{pmatrix} \quad \eta = 2m\alpha/(\hbar^2 k).$$

Matrix form

$$\det\begin{pmatrix} 1-\lambda & i\eta e^{-i\phi} \\ -i\eta e^{i\phi} & 1-\lambda \end{pmatrix} = (1-\lambda)^2 - \eta^2 = 0$$

Example 2. BC of a Rashba 2DEG

$$\mathcal{H}_{\mathrm{R}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\sigma_0 - \alpha_{\mathrm{R}}\,\boldsymbol{\sigma}\cdot\mathbf{k}\times\hat{\mathbf{z}}\,,$$

Hamiltonian of a Rashba 2DEG

$$E^{\pm} = \frac{\hbar^2 k^2}{2m} \pm \alpha k$$

Eigenvalues

$$|\psi^{+}\rangle = \frac{1}{\sqrt{2}}(ie^{-i\phi}, 1)$$

$$|\psi^{-}\rangle = \frac{1}{\sqrt{2}}(-ie^{-i\phi}, 1)$$

Eigenvectors

Example 2. BC of a Rashba 2DEG

$$\mathcal{H}_{\mathrm{R}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\sigma_0 - \alpha_{\mathrm{R}}\,\boldsymbol{\sigma}\cdot\mathbf{k}\times\hat{\mathbf{z}}\,,$$

Hamiltonian of a Rashba 2DEG

$$E^{\pm} = \frac{\hbar^2 k^2}{2m} \pm \alpha k$$

Eigenvalues

$$|\psi^{+}\rangle = \frac{1}{\sqrt{2}}(ie^{-i\phi}, 1)$$

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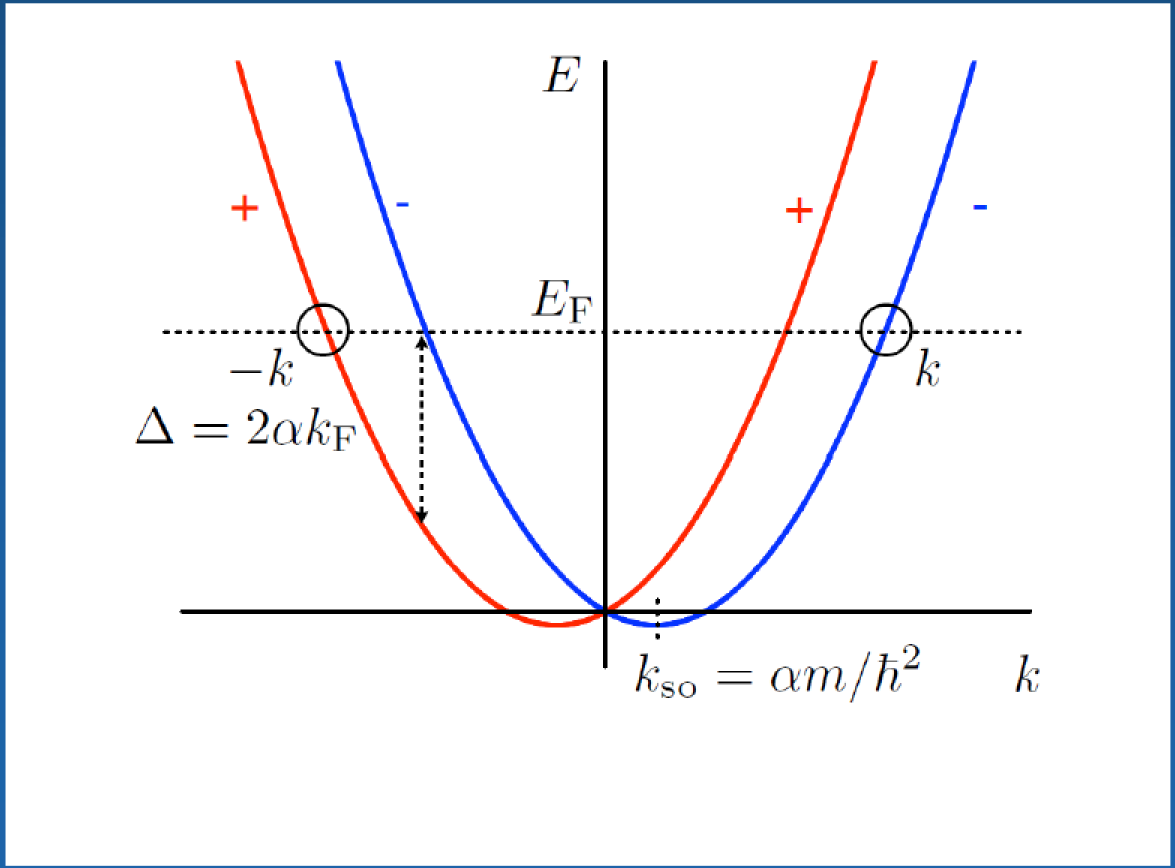
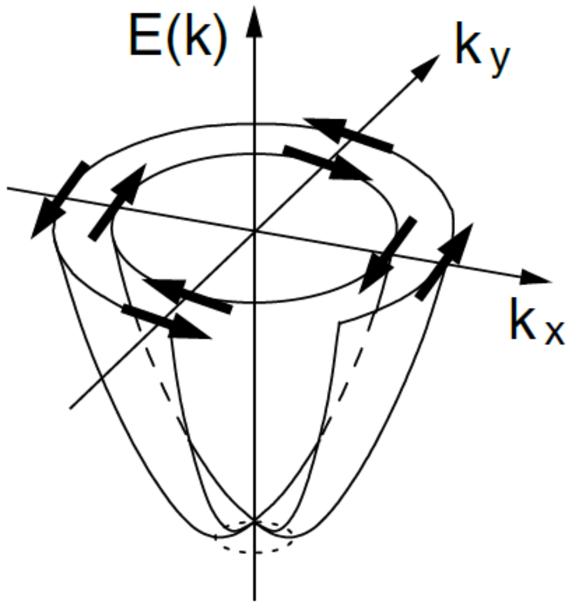
Eigenvectors

Example 2. BC of a Rashba 2DEG



Spin splitting of the Fermi surface

Example 2. BC of a Rashba 2DEG

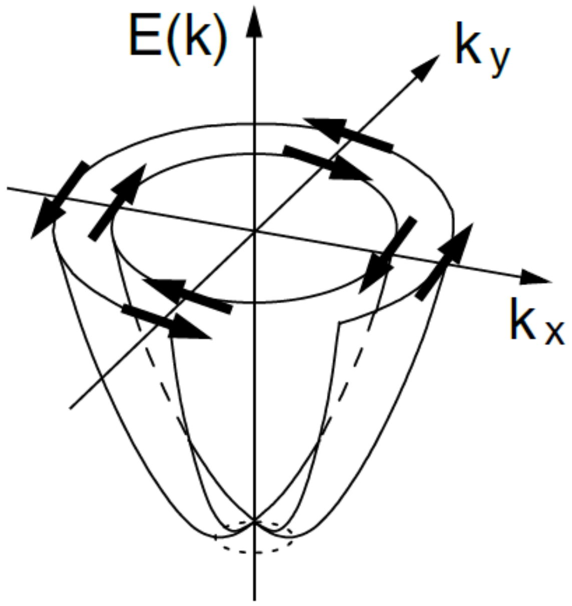


$$\widehat{S}^{\pm} = \pm\widehat{\mathbf{k}} \times \widehat{z}$$

Spin splitting of the Fermi surface

Spin-momentum locking

Example 2. BC of a Rashba 2DEG



$$\mathcal{B}_z^{\pm} = \mp\frac{1}{2}\hat{\mathbf{d}}\cdot(\nabla_{k_x}\hat{\mathbf{d}}\times\nabla_{k_y}\hat{\mathbf{d}})$$

Spin splitting of the Fermi surface

Spin-momentum locking

Example 3. BC of a trigonal Rashba 2DEG

$$\mathcal{H}_{\mathrm{R}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\sigma_0 - \alpha_{\mathrm{R}}\,\boldsymbol{\sigma}\cdot\mathbf{k}\times\hat{\mathbf{z}}\,,$$

$$\mathcal{H}_w(\mathbf{k}) = \frac{\lambda}{2}(k_+^3 + k_-^3)\sigma_z\,. \qquad k_\pm = k_x \pm ik_y$$

$$\mathbf{d} = \left\{-k_y, k_x, \lambda\left(k_+^3 + k_-^3\right)/2\right\}.$$

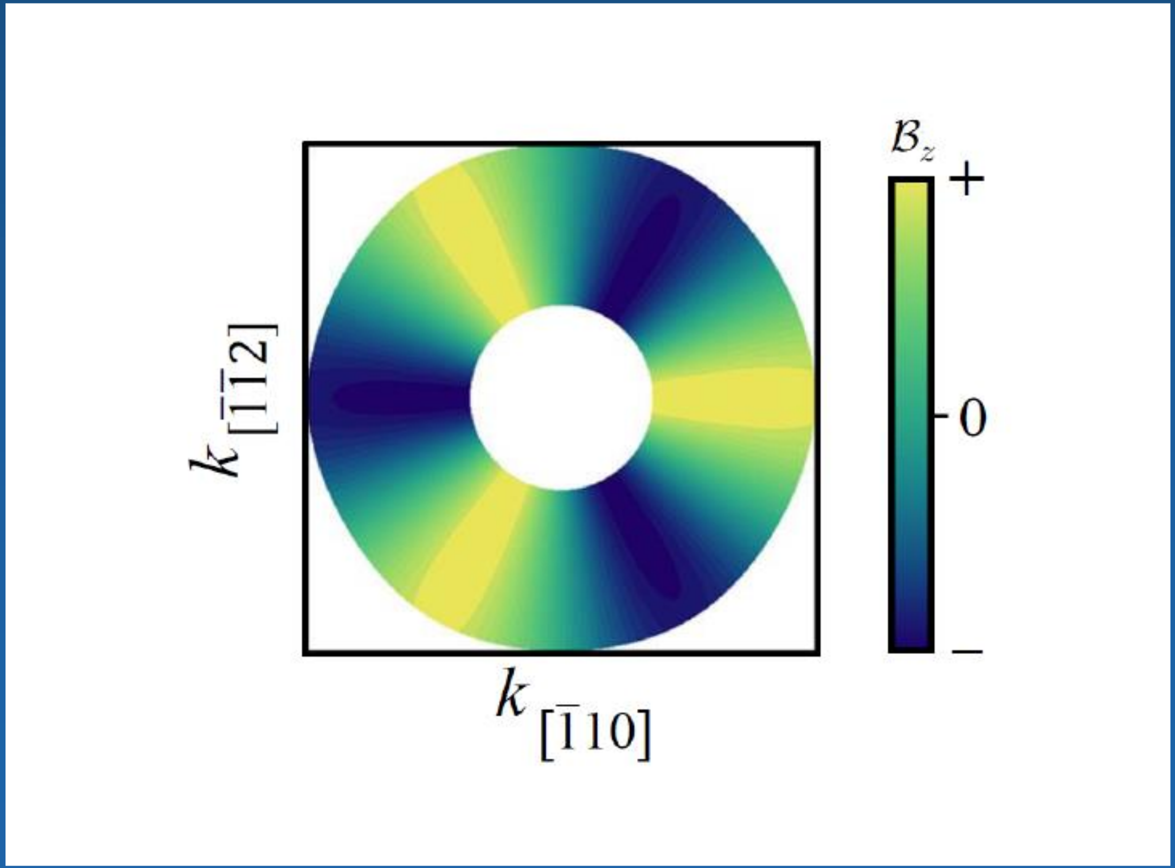
$$\mathcal{B}_z^\pm = \mp\frac{1}{2}\hat{\mathbf{d}}\cdot(\nabla_{k_x}\hat{\mathbf{d}}\times\nabla_{k_y}\hat{\mathbf{d}})$$

Example 3. BC of a trigonal Rashba 2DEG

$$\mathcal{B}_z^{\pm} = \mp\frac{1}{2}\hat{\mathbf{d}} \cdot (\nabla_{k_x}\hat{\mathbf{d}} \times \nabla_{k_y}\hat{\mathbf{d}})$$

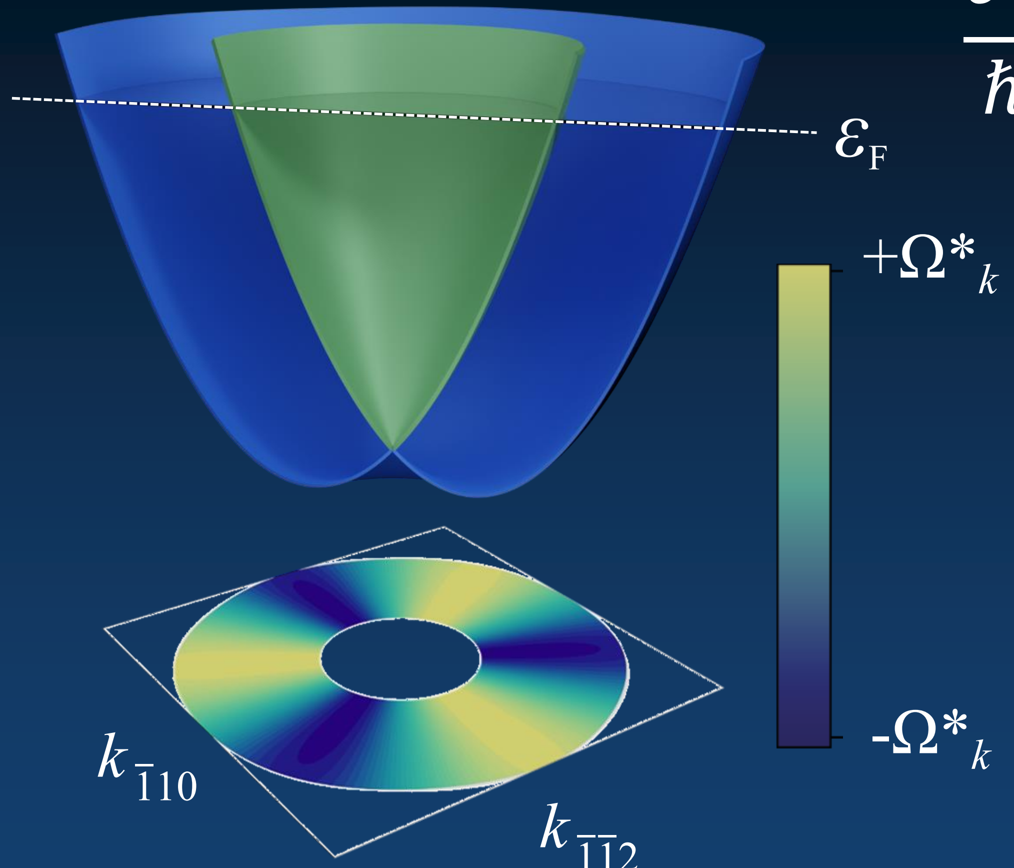
$$\mathcal{B}_z^{\pm}(k,\theta) = \pm\frac{2\sqrt{2}\lambda\alpha_{\mathrm{R}}^2 k^3\cos(3\theta)}{\left[2\alpha_{\mathrm{R}}^2 k^2 + \lambda^2 k^6\cos(6\theta) + \lambda^2 k^6\right]^{3/2}},$$

Example 3. BC of a trigonal Rashba 2DEG



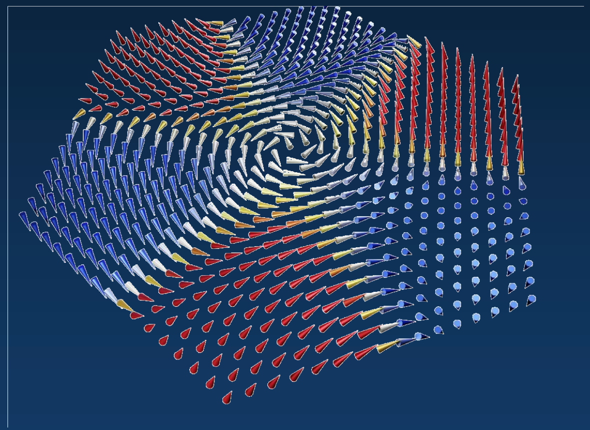
Example 3. BC of a trigonal Rashba 2DEG

$$\frac{e^2}{\hbar}\int \frac{d^2k}{(2\pi)^2}\boldsymbol{B}(\mathbf{k})f^0_{\mathbf{k}} = 0$$



Learning objectives

1) Discuss geometric properties of wavefunctions.
2) Compute geometric quantities of model two-level systems.
3) **Identify condensed matter systems with quantum geometric properties.**
4) Apply these ideas to your research?



Lecture notes available at caviglia.unige.ch/teaching

Sources of Berry curvature

1) Zero for real wavefunctions

$$\Psi_n(t) \approx e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t)$$

$$\gamma_n(t) = \int_0^t i \langle \psi_n(t') | \dot{\psi}_n(t') \rangle \, \mathrm{d}t'$$

Sources of Berry curvature

1) Zero for real wavefunctions

2) Zero for planar spin textures

$$\boldsymbol{B}_{\boldsymbol{z}}^{\pm}(\boldsymbol{k}) = \pm\widehat{\boldsymbol{d}} \cdot (\boldsymbol{\partial}_{\boldsymbol{k}_{\boldsymbol{x}}}\widehat{\boldsymbol{d}} \times \boldsymbol{\partial}_{\boldsymbol{k}_{\boldsymbol{y}}}\widehat{\boldsymbol{d}})/\boldsymbol{2}$$

Sources of Berry curvature

1) Zero for real wavefunctions

2) Zero for planar spin textures

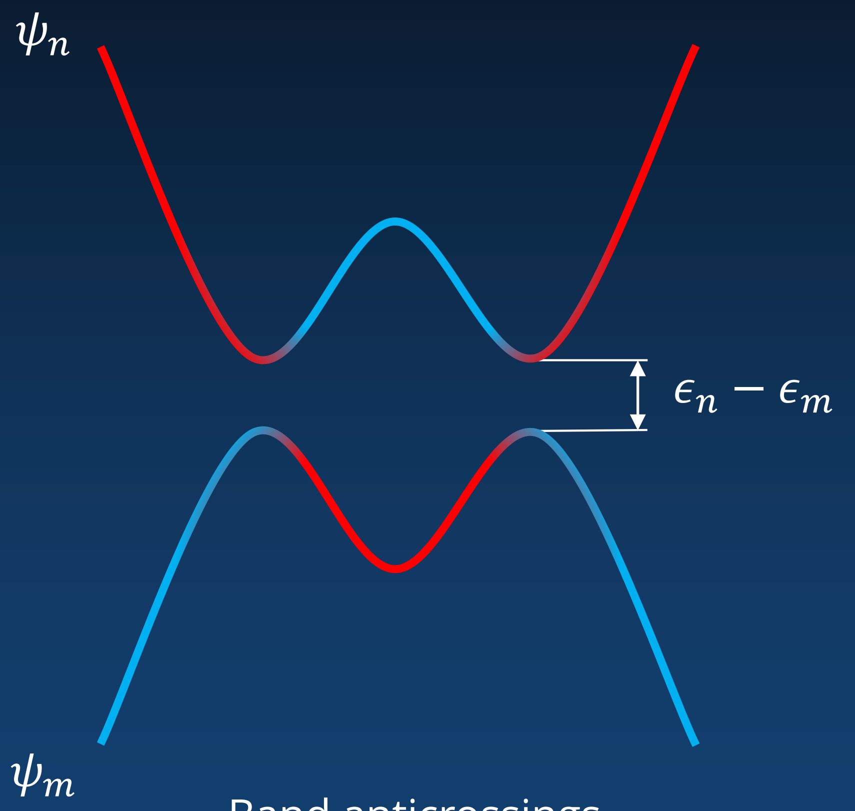
$$\boldsymbol{B}_z^{\pm}(\boldsymbol{k}) = \pm\hat{\boldsymbol{d}} \cdot (\boldsymbol{\partial}_{k_x}\hat{\boldsymbol{d}} \times \boldsymbol{\partial}_{k_y}\hat{\boldsymbol{d}})/2$$

3) Large near avoided band crossings

$$\boldsymbol{B}_z(\boldsymbol{k}) = [\langle\psi_m|\nabla\psi_n\rangle \times \langle\nabla\psi_n|\psi_m\rangle]_z$$

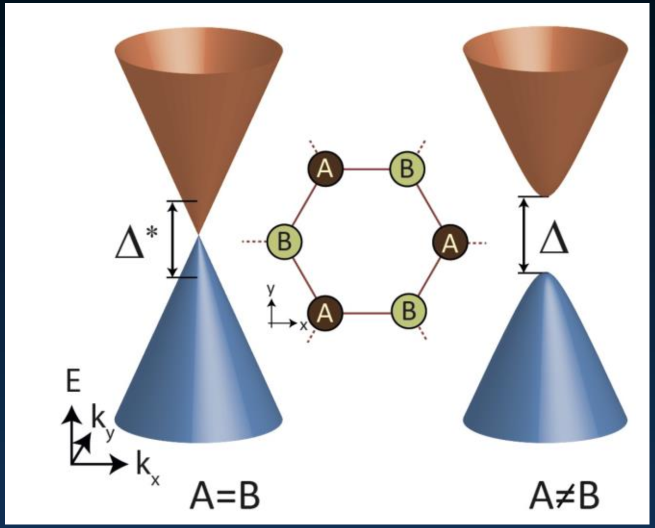
$$= \frac{[\langle\psi_m|\nabla H|\psi_n\rangle \times \langle\psi_n|\nabla H|\psi_m\rangle]_z}{(\epsilon_m - \epsilon_n)^{\,2}}$$

Quantum superposition at finite crystal momentum



Band anticrossings

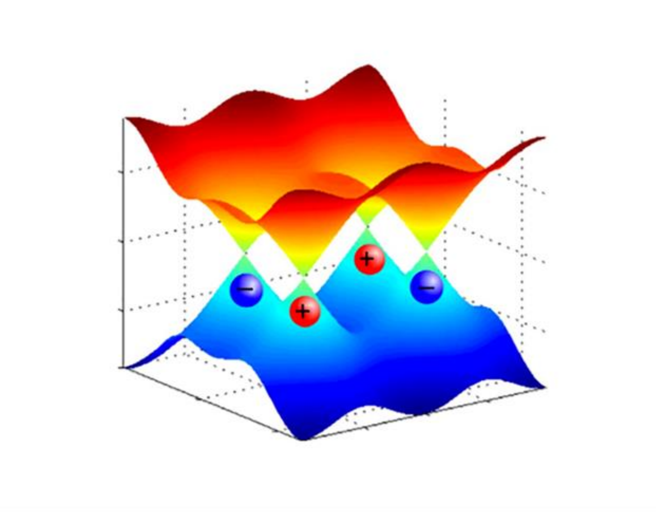
Conventional systems



Gapped graphene

$$\mathcal{H}(\mathbf{k}) = v_F\left[\sigma_x k_x + \sigma_y k_y\right] + m\sigma_z$$

σ sublattice space



Weyl semimetals

$$\mathcal{H}(\mathbf{k}) = v_F^x \sigma_x k_x + v_F^y \sigma_y k_y + v_F^z \sigma_z k_z$$

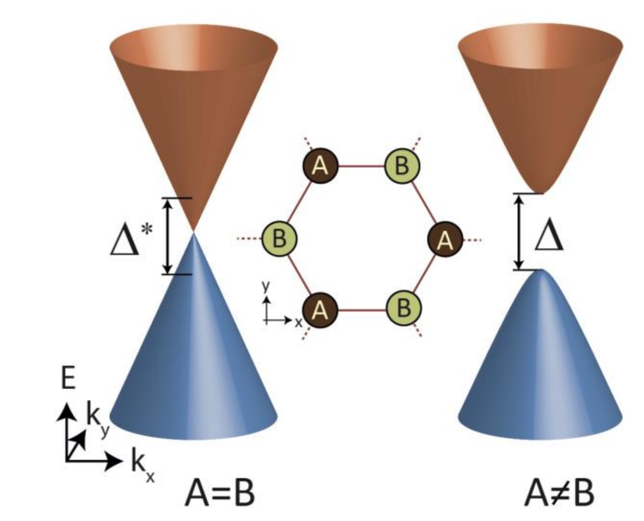
σ spin space

Conventional systems

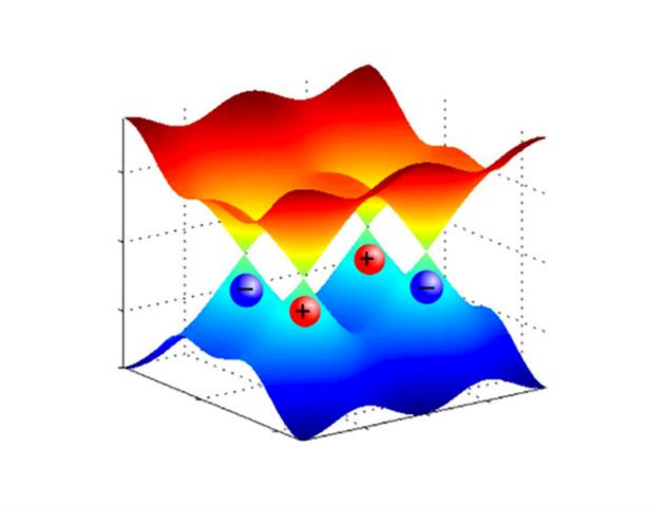
Gapped graphene

$$\mathcal{H}(\mathbf{k}) = v_F[\sigma_x k_x + \sigma_y k_y] + m\sigma_z$$

σ sublattice space



Quantum superposition at finite crystal momentum
of a single quantum number



Weyl semimetals

$$\mathcal{H}(\mathbf{k}) = v_F^x \sigma_x k_x + v_F^y \sigma_y k_y + v_F^z \sigma_z k_z$$

σ spin space

Key questions

Can we design Berry curvature sources
from the quantum superpositions at finite crystal momentum of
multiple quantum numbers?

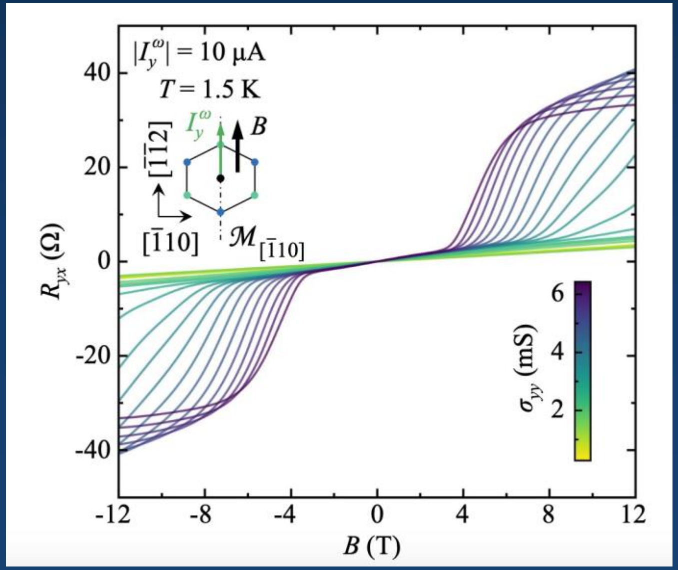
Interplay of correlated and topological physics

(111)LAO/STO: the first material system with coexisting sources of Berry curvature

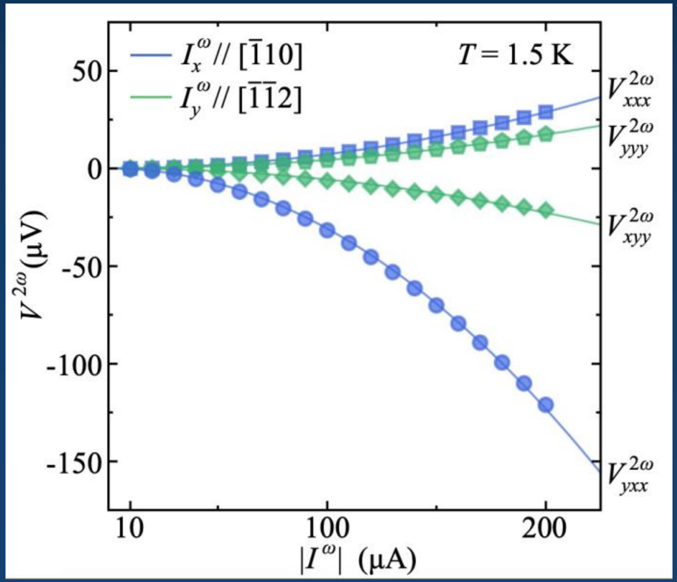
Spin sources

Orbital sources

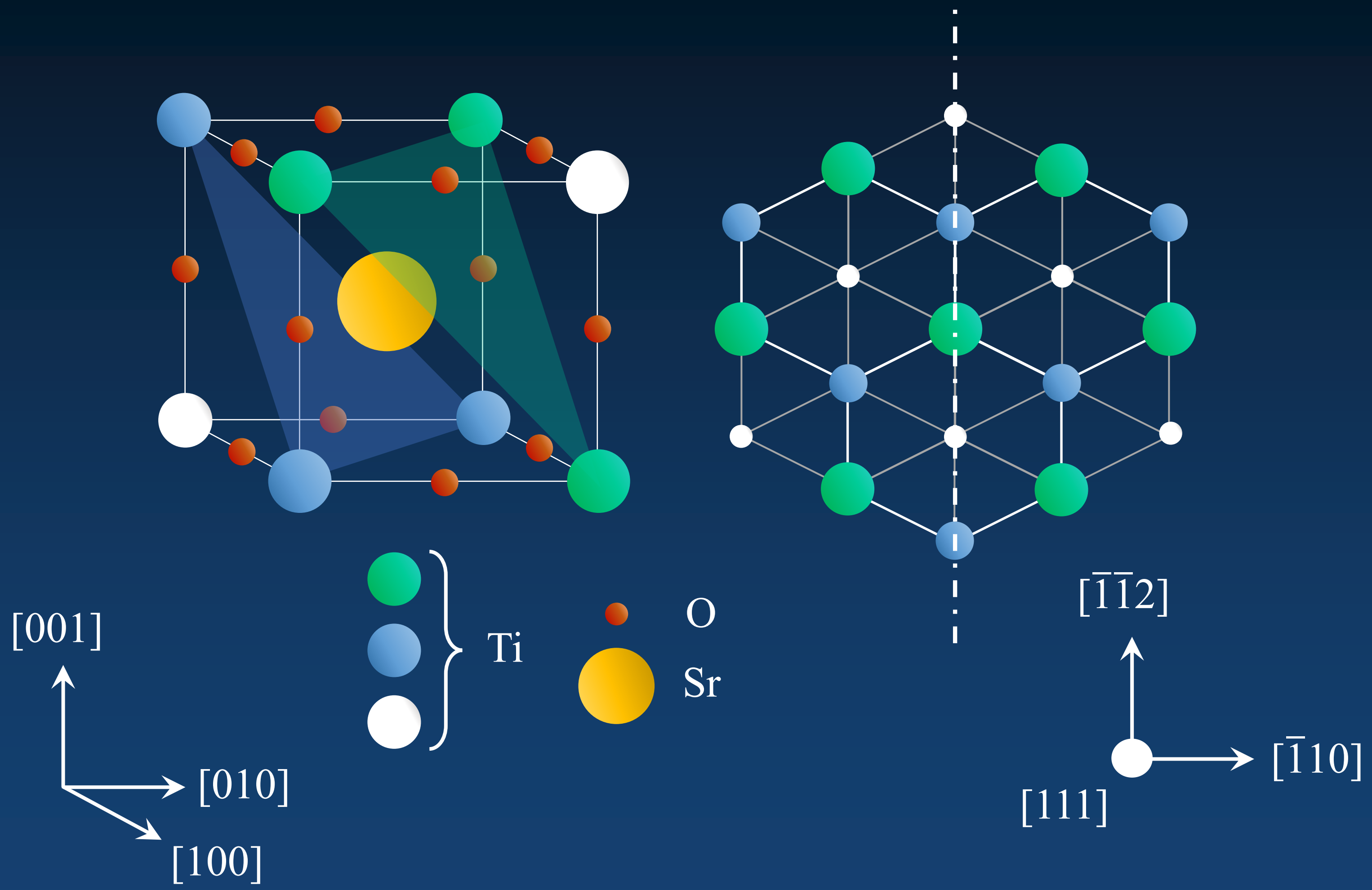
Probed by linear and nonlinear anomalous transport.



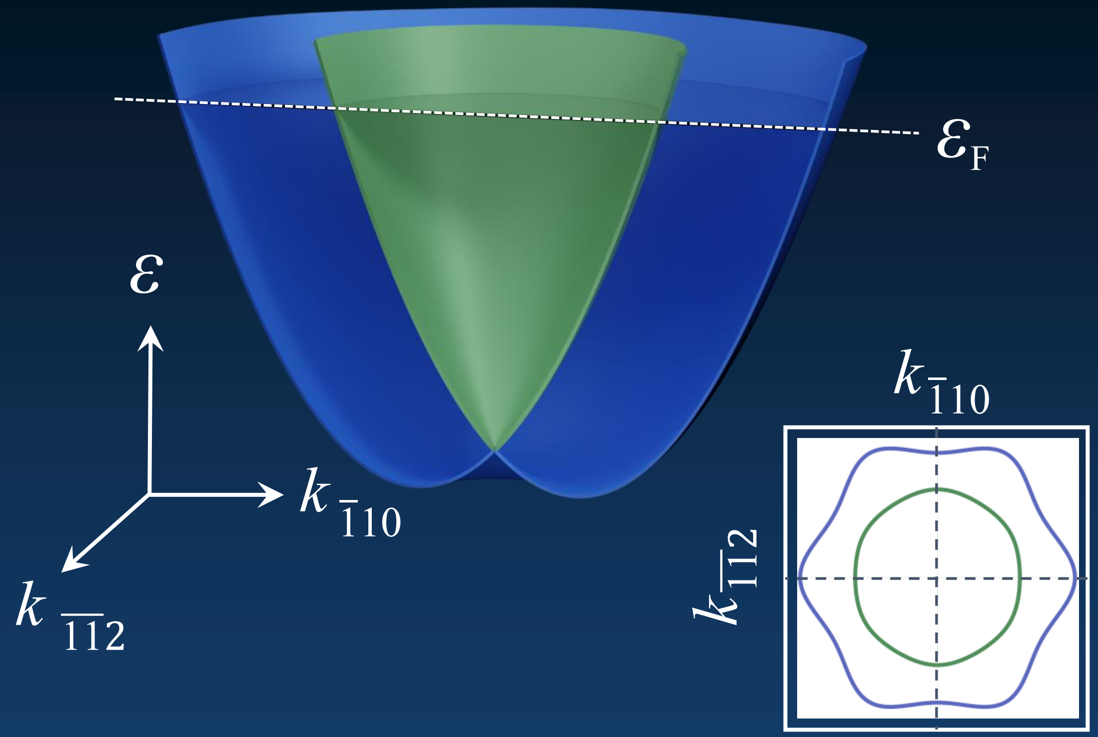
Lesne et al.
Nature Materials 22, 576 (2023)



Exploring hexagonal symmetry



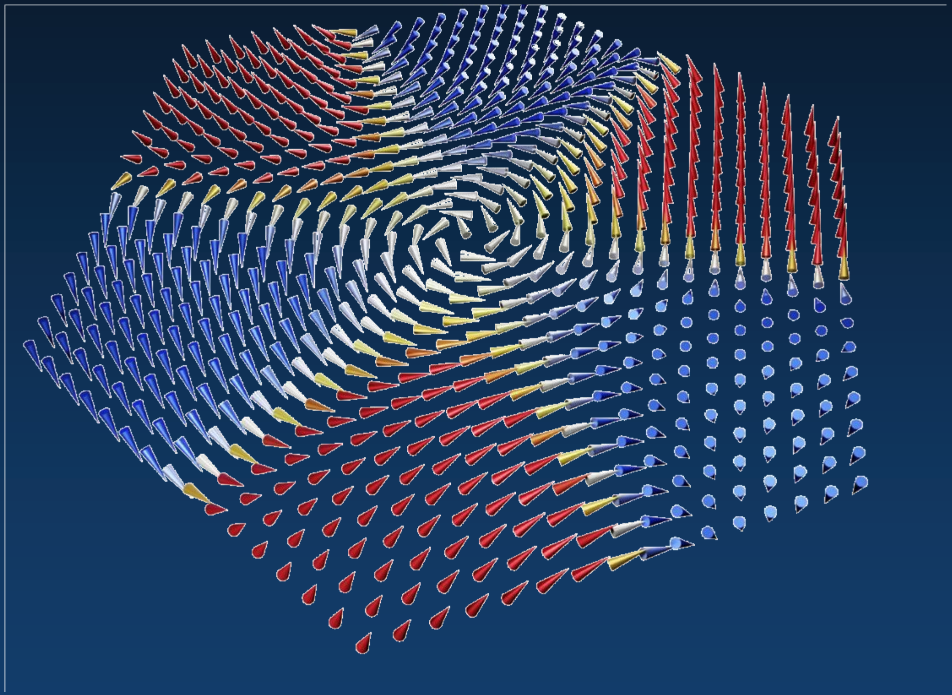
Trigonal warping and spin-orbit coupling

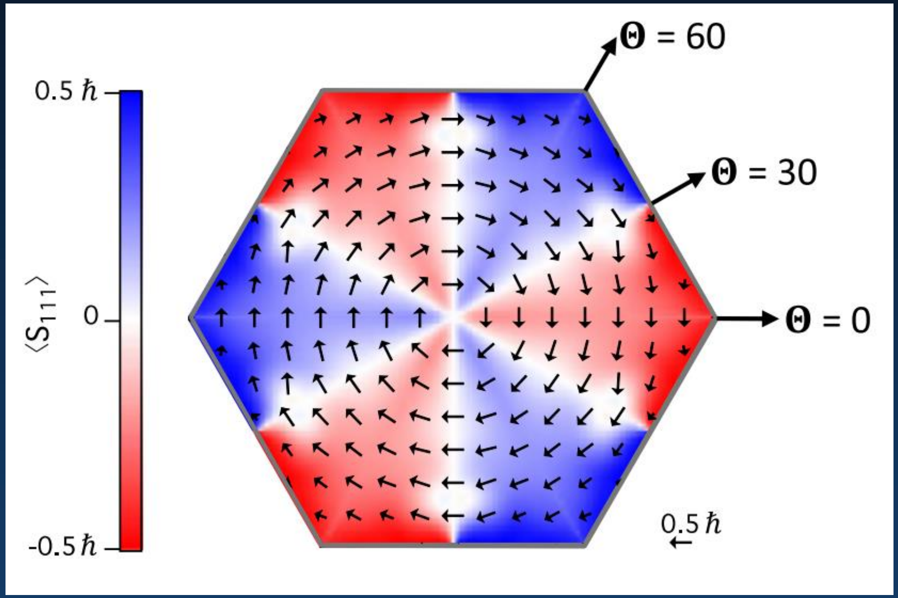


$$\mathcal{H}(\mathbf{k}) = \frac{k^2}{2m}\sigma_0 + (\alpha_R k_x + \mathcal{B}\sin\theta)\sigma_y + (-\alpha_R k_y + \mathcal{B}\cos\theta)\sigma_x + \frac{\lambda}{2}(k_+^3 + k_-^3)\sigma_z$$

$$k_\pm = k_x \pm i k_y$$

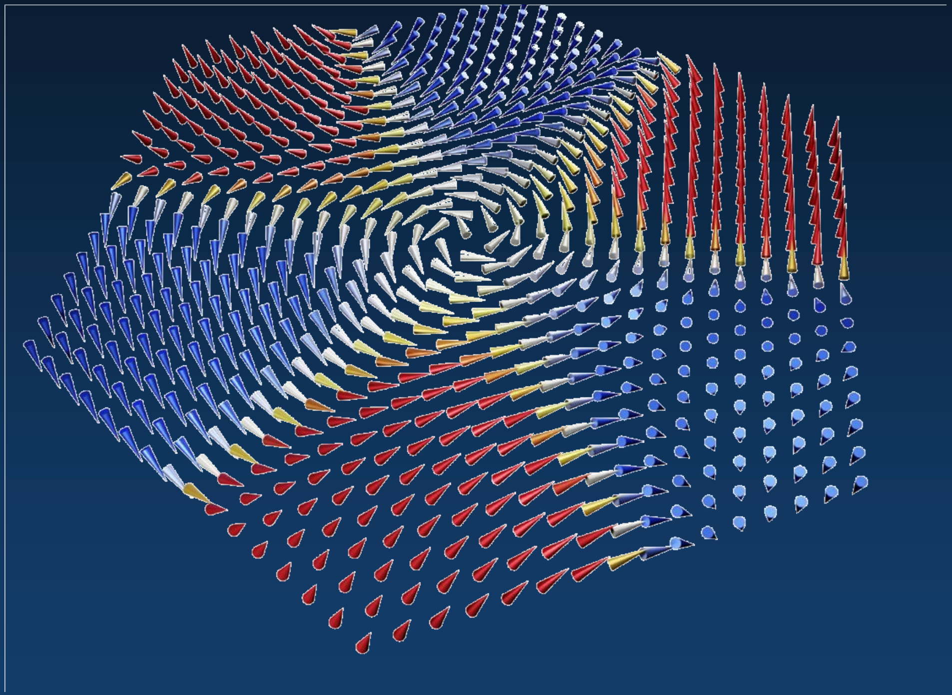
Out-of-plane spin texture

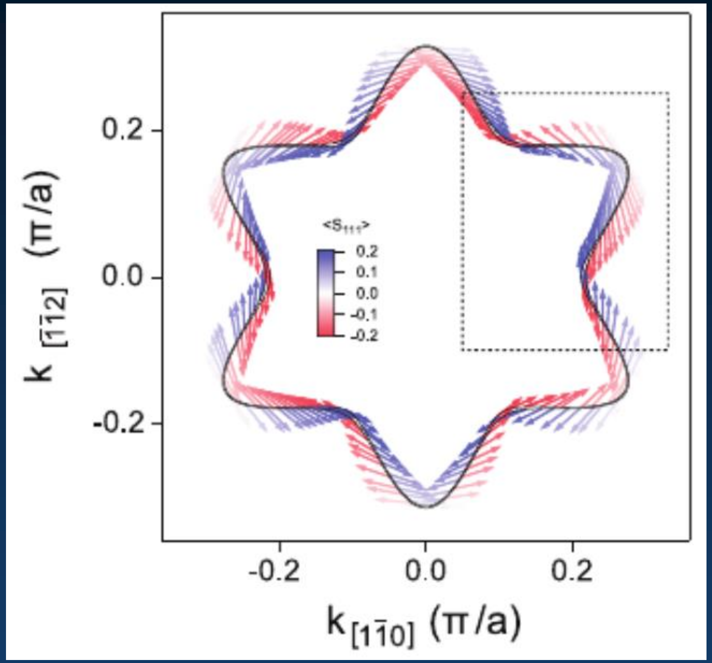




Surface of (111)SrTiO3
He et al. Physical Review Letters 120, 266802 (2018)

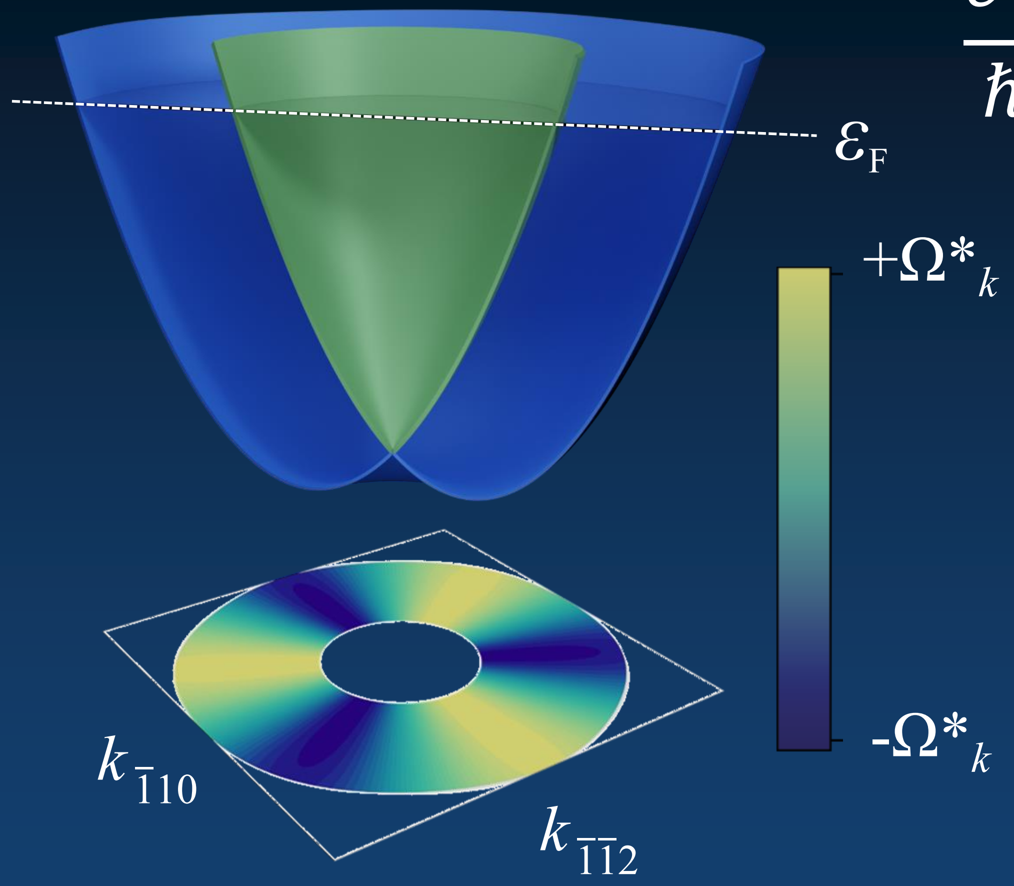
Out-of-plane spin texture





Surface of (111)KTaO3
Bruno et al. Advanced Electronic Materials, 1800860 (2019)

Spin sources of Berry curvature

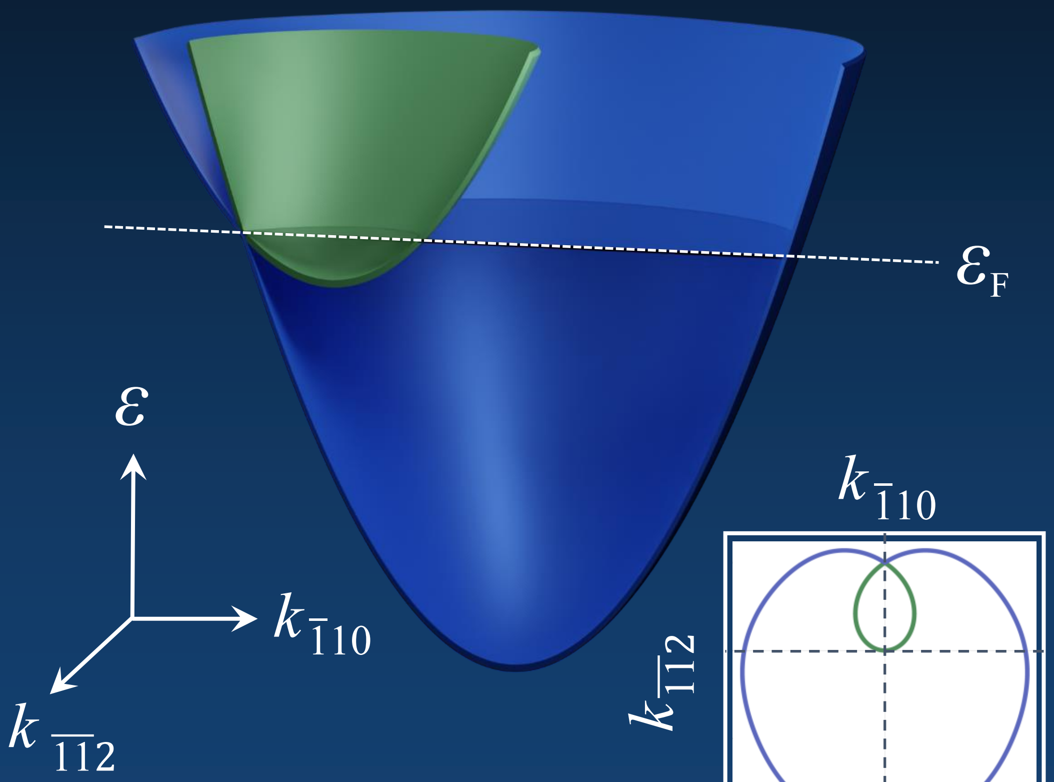


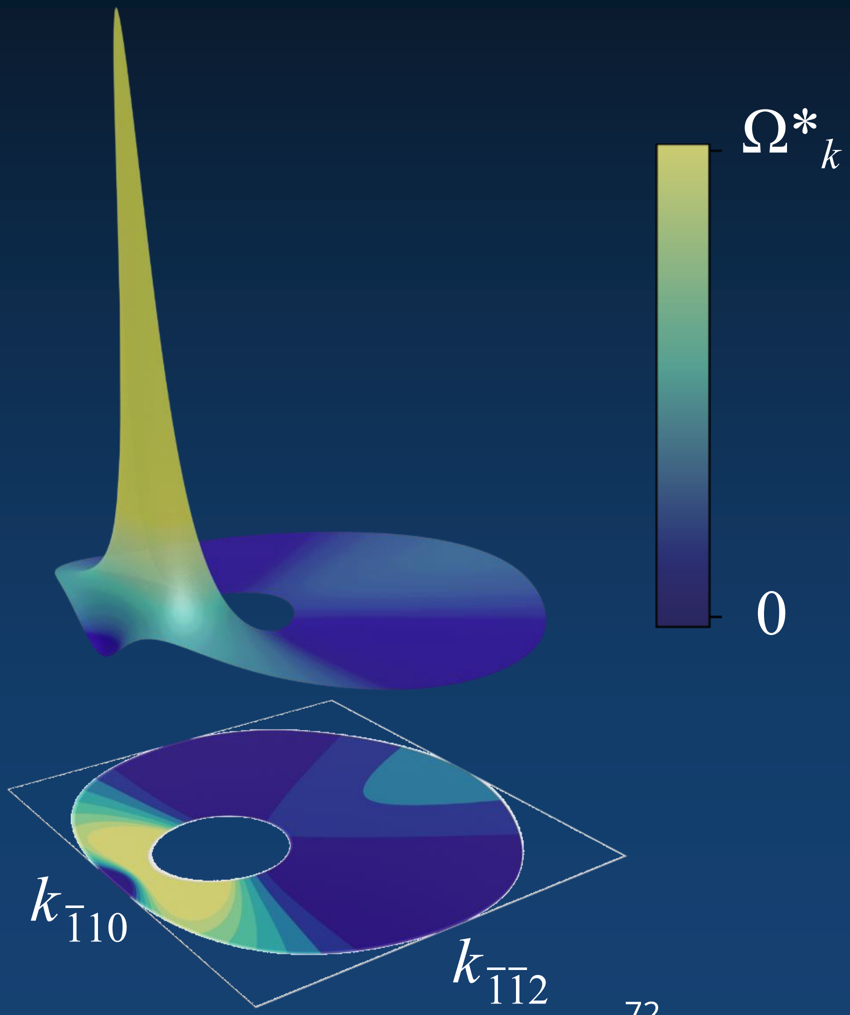
$$\frac{e^2}{\hbar}\int \frac{d^2k}{(2\pi)^2}\boldsymbol{B}(\mathbf{k})f_{\mathbf{k}}^0 = 0$$

No dipolar distribution

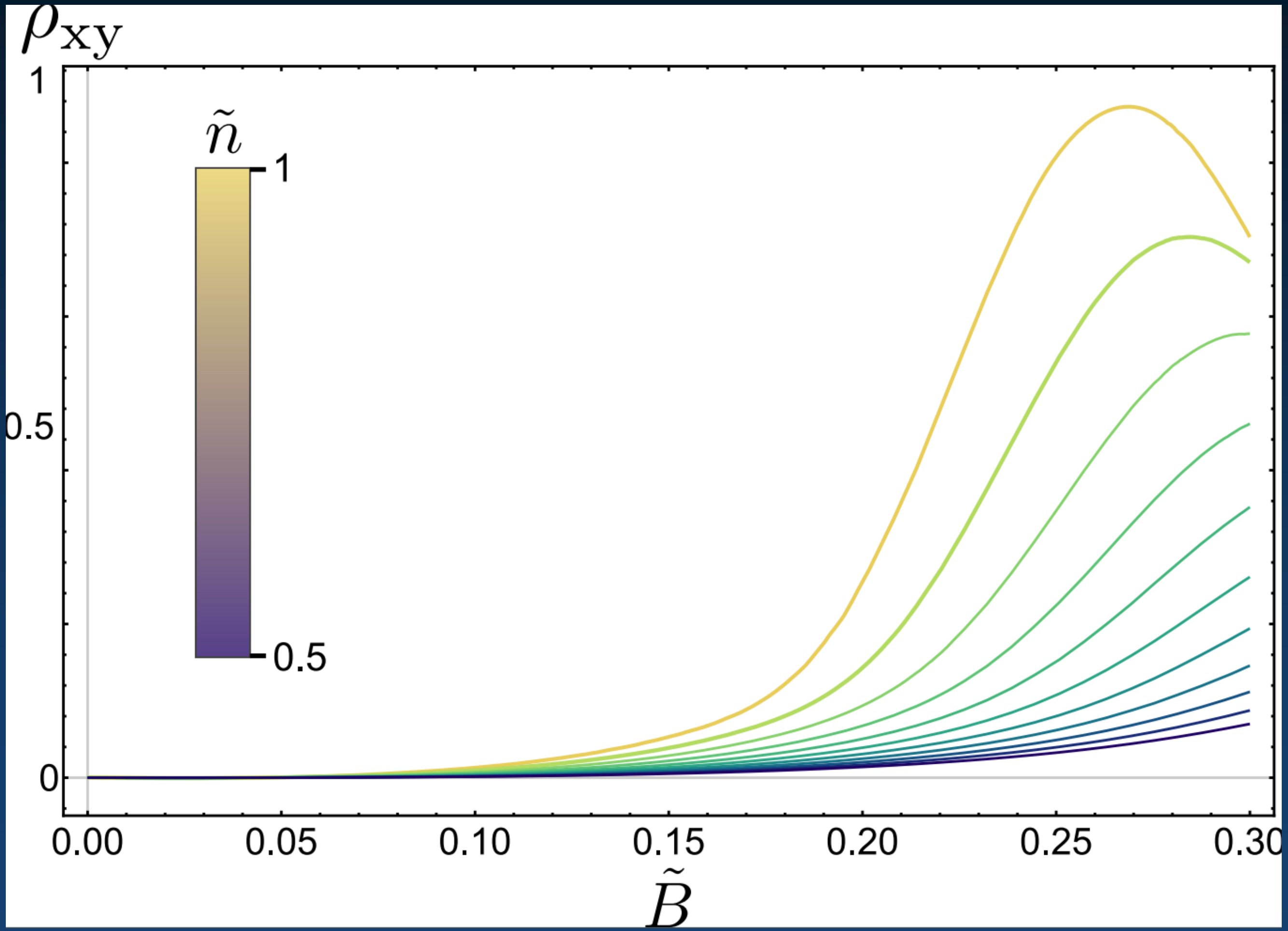
In-plane magnetic field

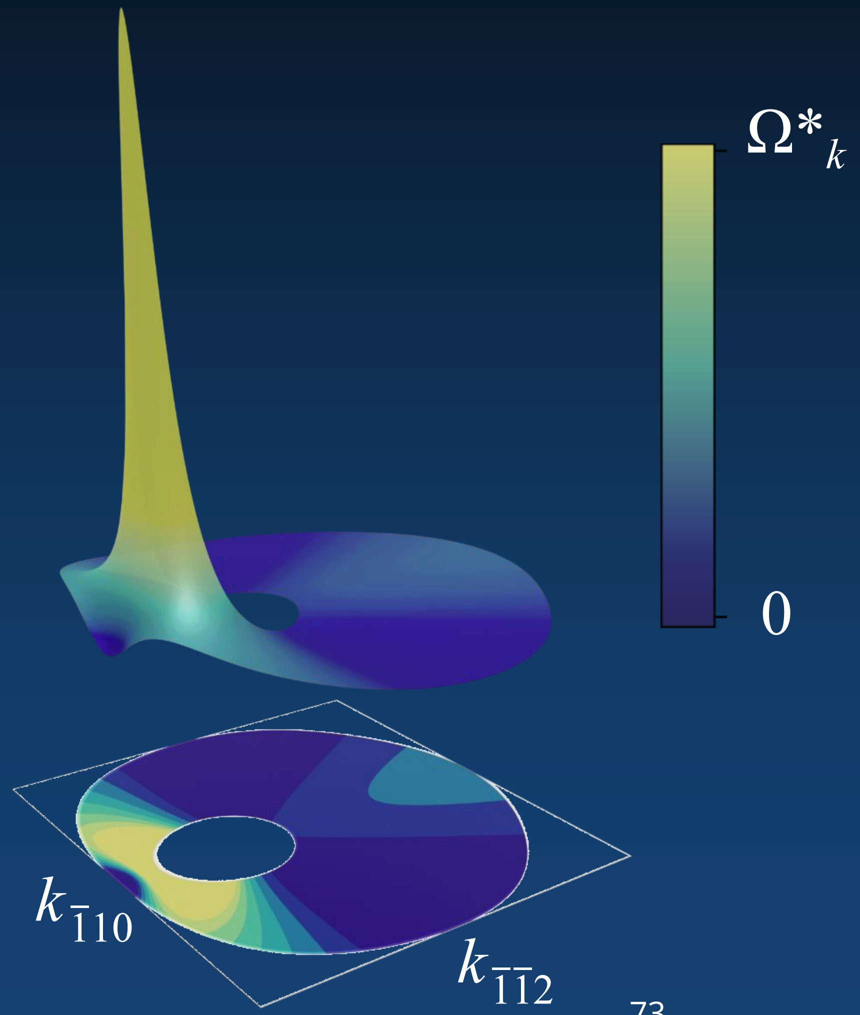
$$\frac{e^2}{\hbar}\int \frac{d^2k}{(2\pi)^2}\boldsymbol{B}(\mathbf{k})f_{\mathbf{k}}^0 \neq 0$$



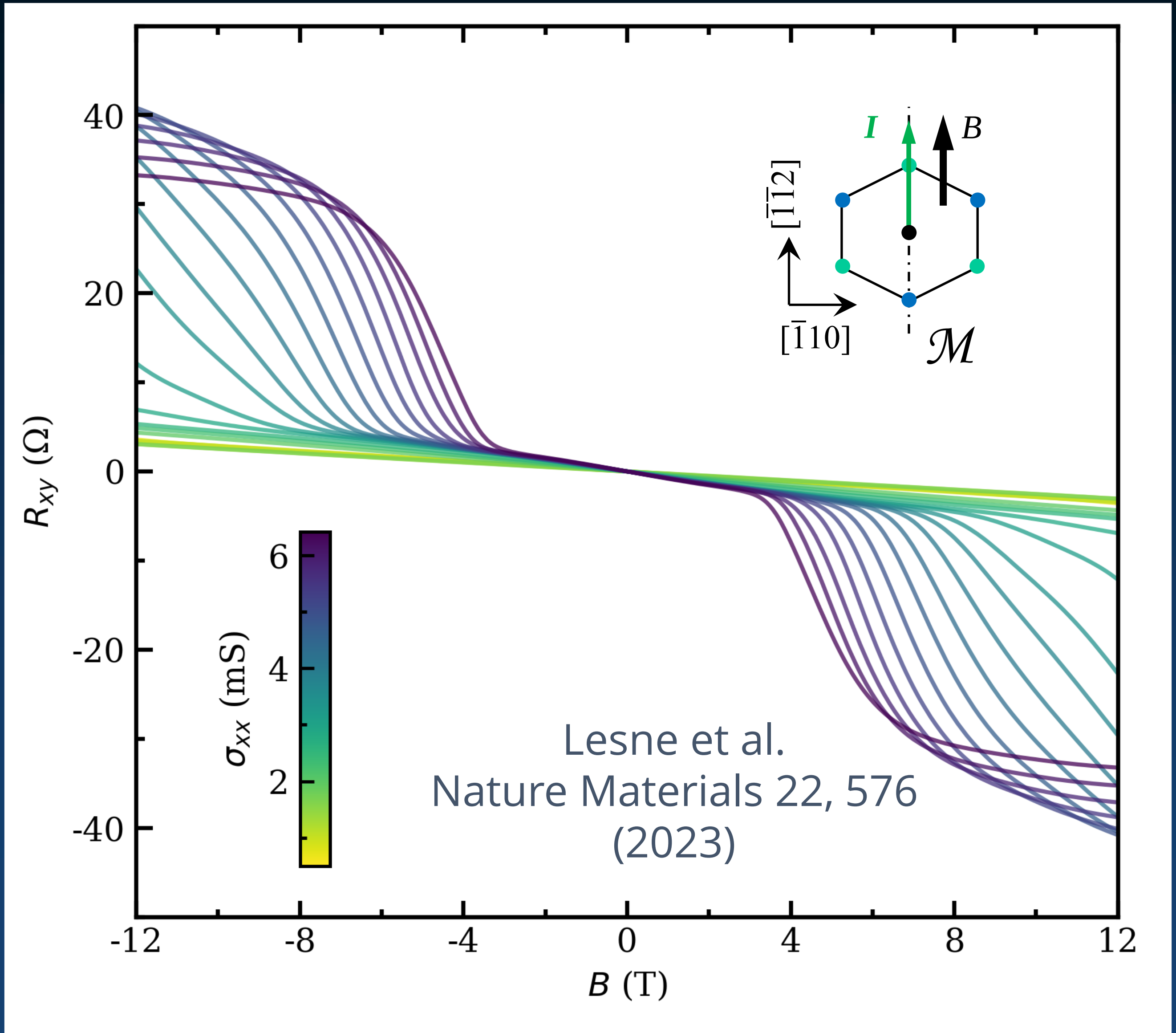


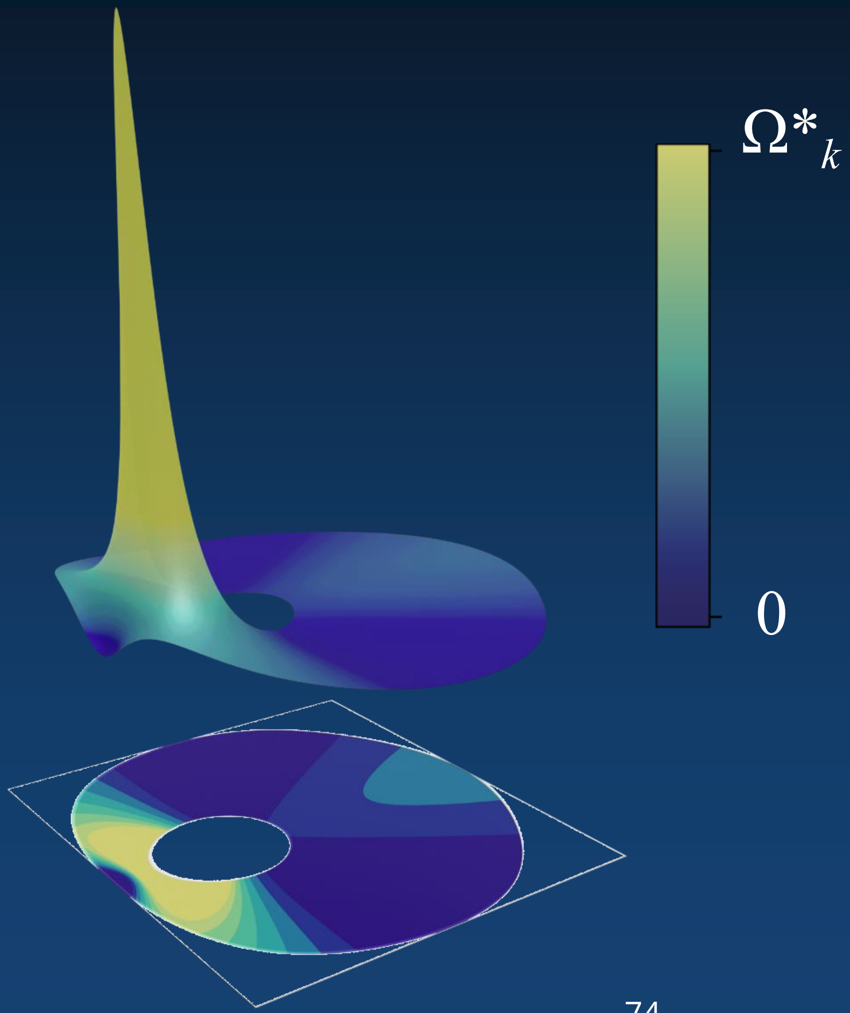
Anomalous planar Hall effect



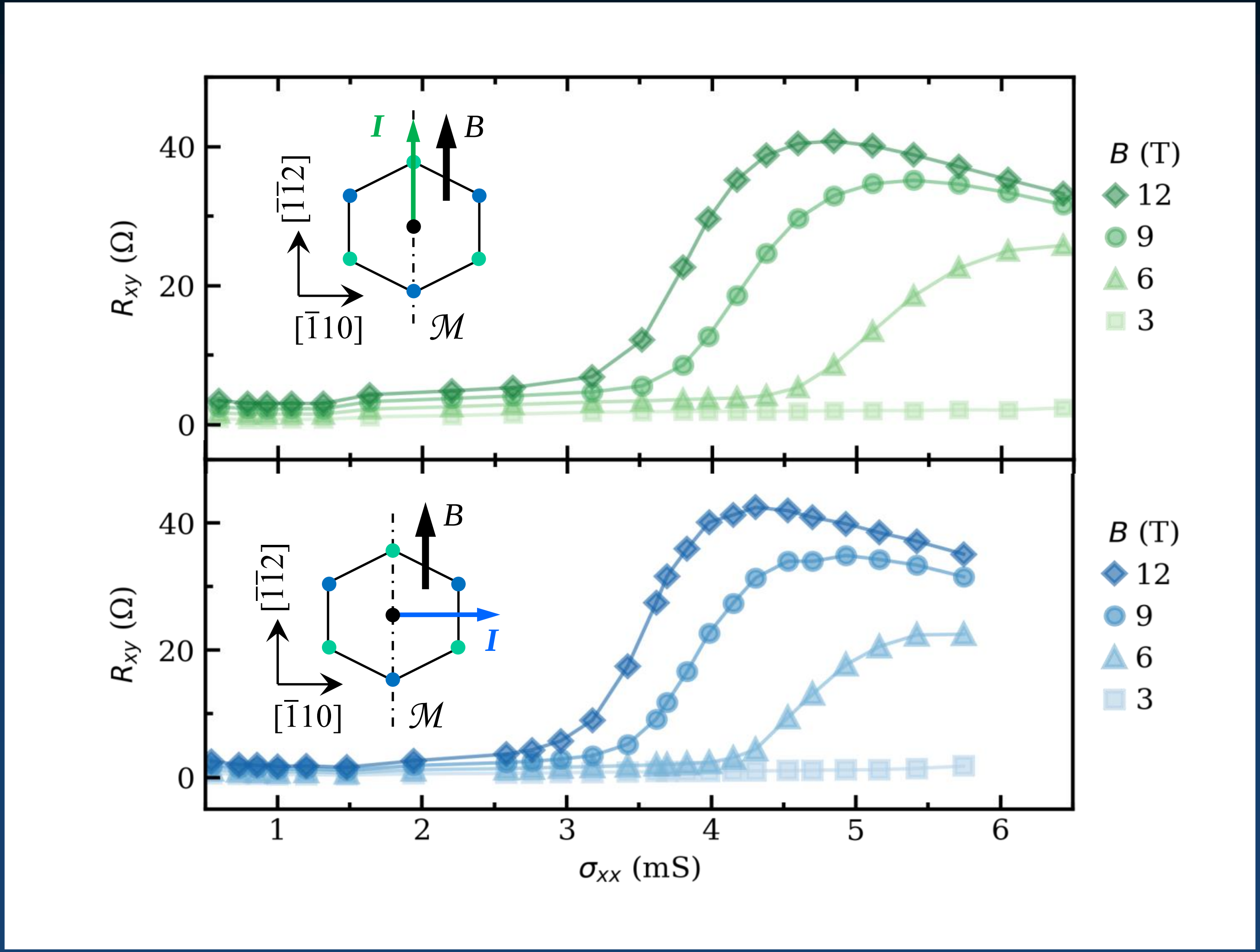


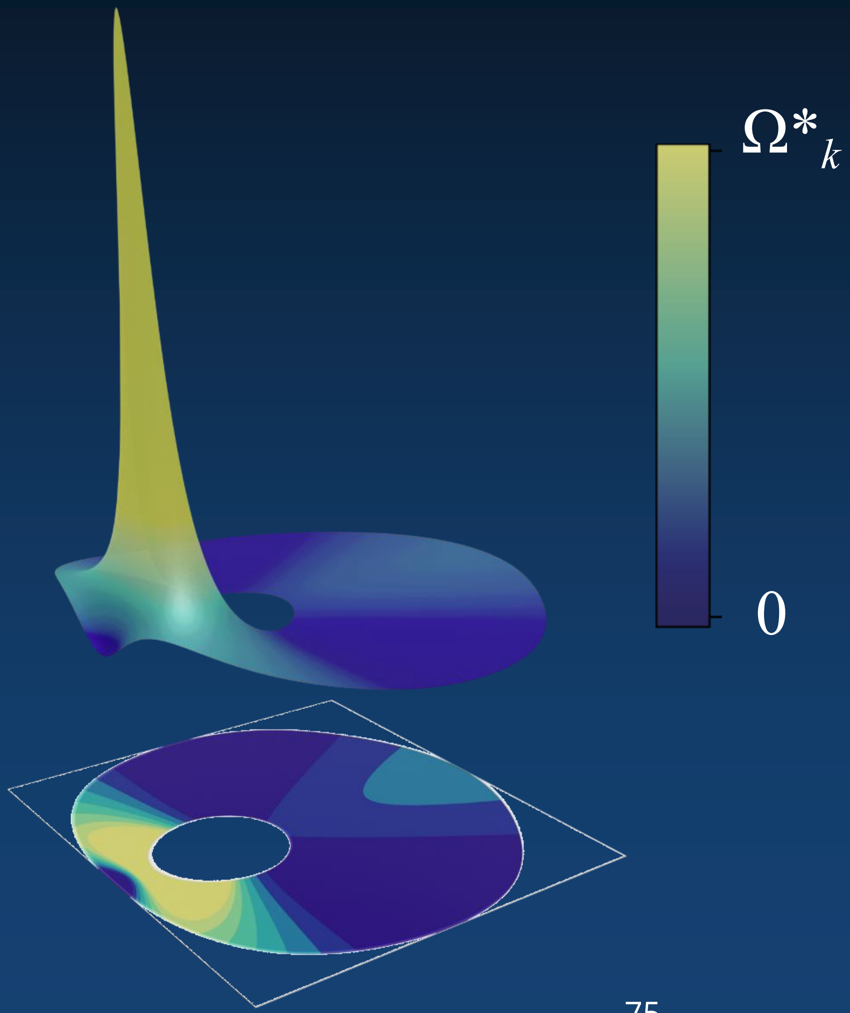
Spin sources of Berry curvature





Spin sources of Berry curvature





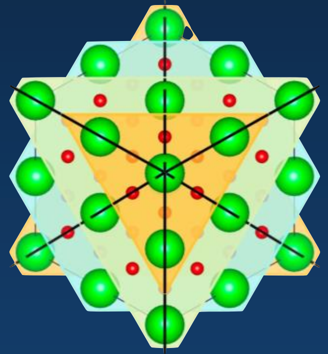
Key questions

Can we design Berry curvature sources
from the quantum superpositions at finite crystal momentum of
multiple quantum numbers?
Can we find transport effects active at B=0?

Structural phase transitions in $SrTiO_3$

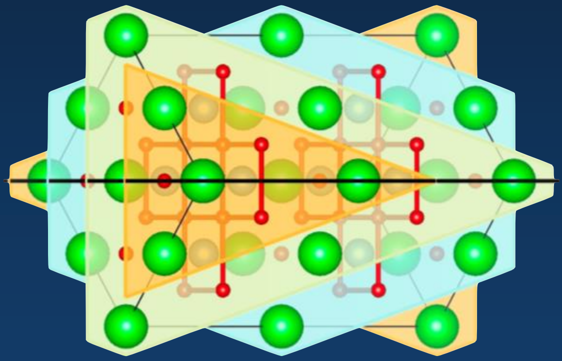
110 K — 40 K — T

$D_{3d}\mathcal{C}_{3v}$



Δ trigonal crystal field

$\mathcal{C}_{2h}\mathcal{C}_s$



Δ_m tetragonal distortion acting at gamma
α_m tetragonal distortion acting at finite k

$\mathcal{C}_s$

Polar order

α_{OR} interfacial breaking of inversion symmetry with polar axis

(Images courtesy A. Lau)

Orbital sources of Berry curvature

t_{2g} orbitals with mixing terms (neglecting spin-orbit coupling)

Δ trigonal crystal field

T < 105 K
Δ_m and α_m tetragonal distortion

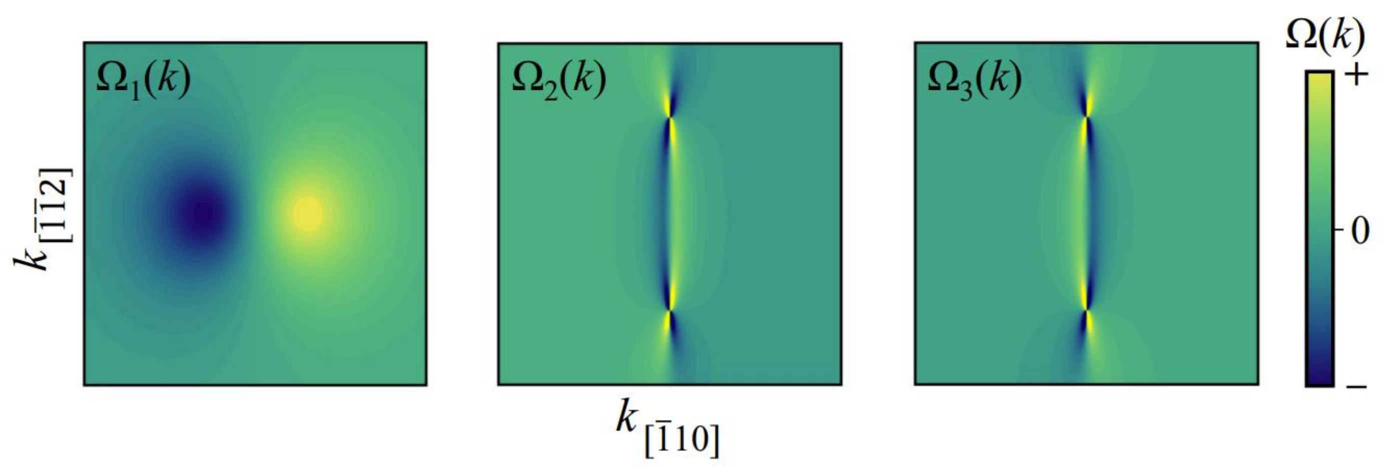
T < 30 K
α_{OR} interfacial breaking of inversion symmetry with polar axis

Mercaldo et al. npj Quantum Materials (2023)
arXiv:2301.04548

$$\mathscr{H}_{OR}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\Lambda_0 + \Delta\left(\Lambda_3 + \frac{1}{\sqrt{3}}\Lambda_8\right) + \Delta_m\left(\frac{1}{2}\Lambda_3 - \frac{\sqrt{3}}{2}\Lambda_8\right) - \alpha_{OR}\left[k_x\Lambda_5 + k_y\Lambda_2\right] - \alpha_m k_x \Lambda_7$$

Orbital sources of Berry curvature

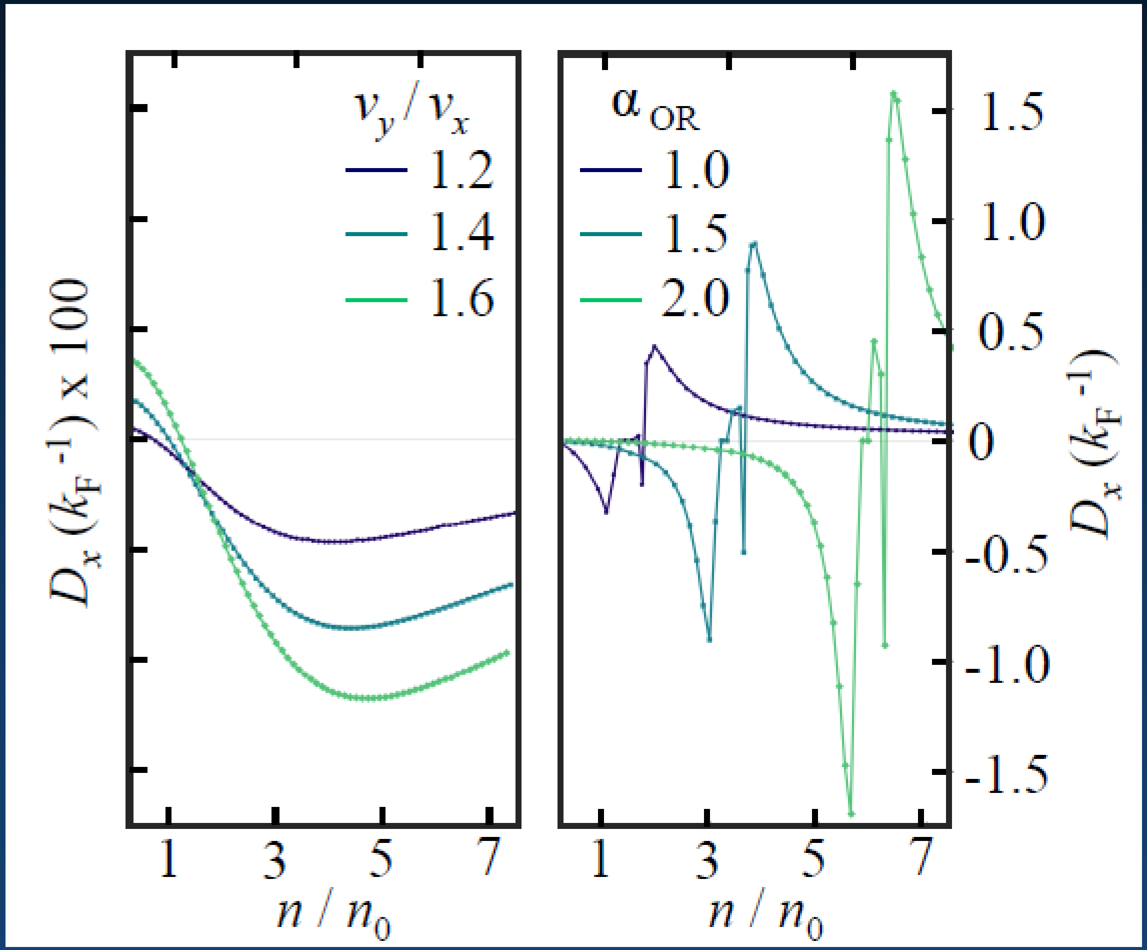
Dipolar distributions: nonlinear transport responses



Hot spots Singular pinch points

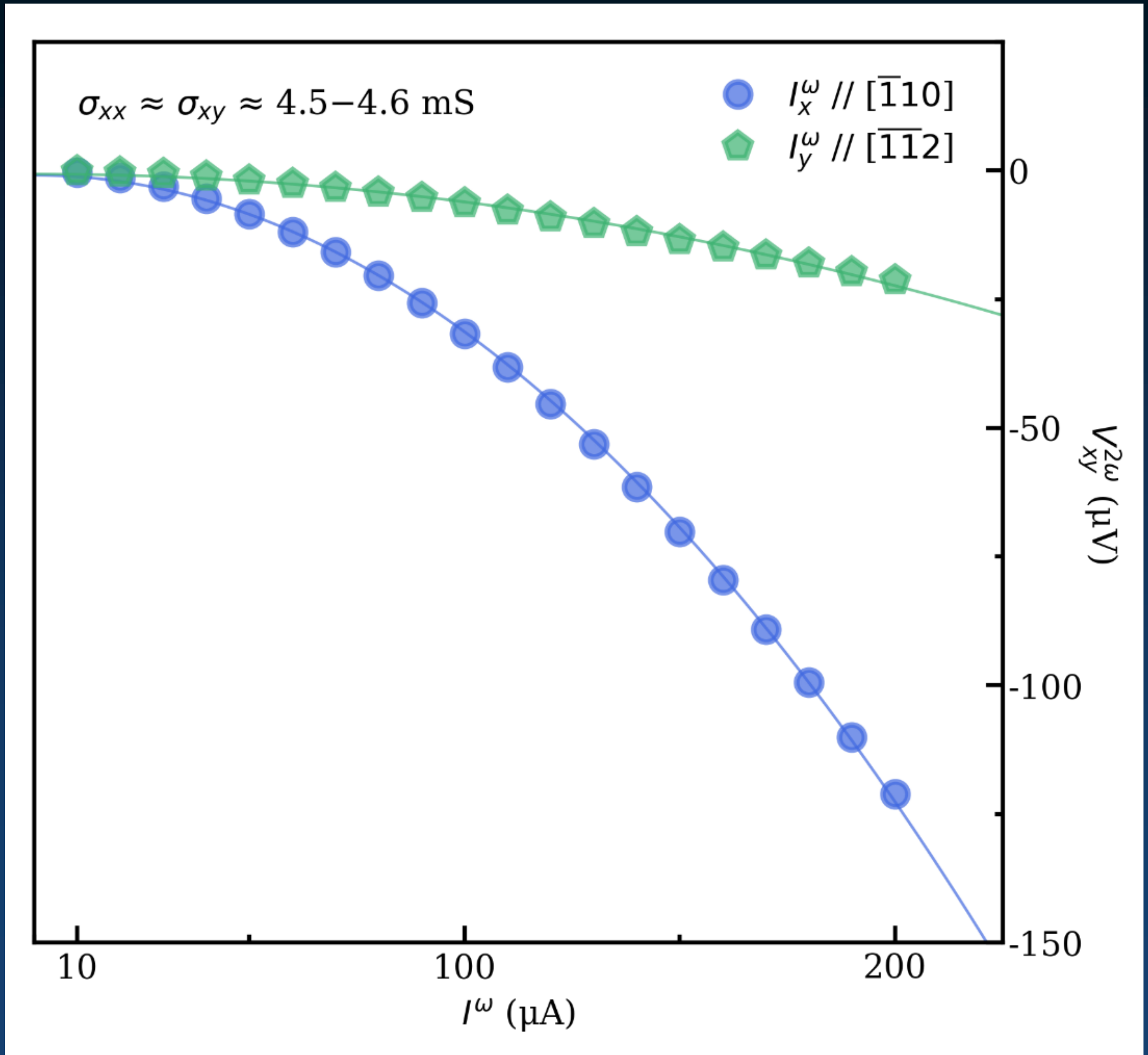
$$\mathscr{H}_{\mathrm{OR}}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m}\Lambda_0 + \Delta\left(\Lambda_3 + \frac{1}{\sqrt{3}}\Lambda_8\right) + \Delta_m\left(\frac{1}{2}\Lambda_3 - \frac{\sqrt{3}}{2}\Lambda_8\right) - \alpha_{\mathrm{OR}}\left[k_x\Lambda_5 + k_y\Lambda_2\right] - \alpha_m k_x \Lambda_7$$

Orbital sources of Berry curvature



Prediction:
BCD in the 10s nm range!

Non linear Hall effect at B=0

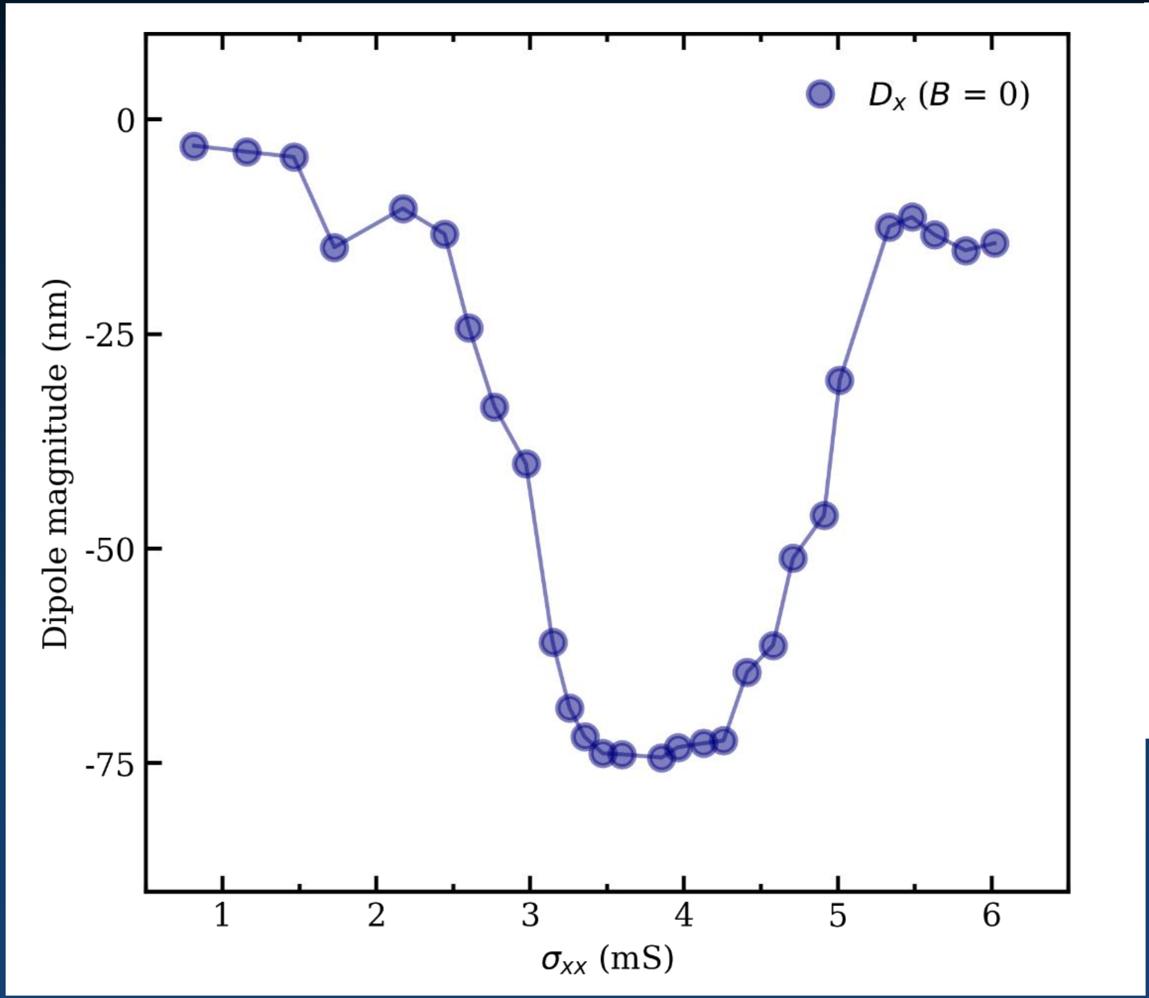


Ulderico Filippozzi

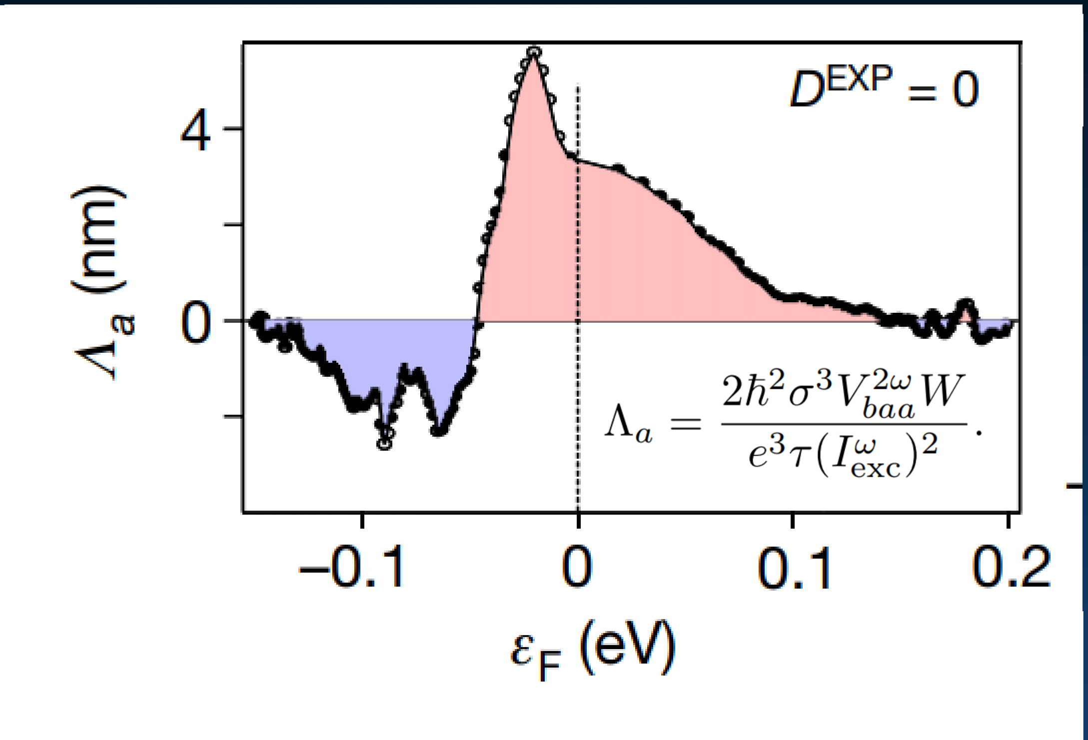
Edouard Lesne

Lesne et al.
Nature Materials 22, 576
(2023)

Dipole magnitude

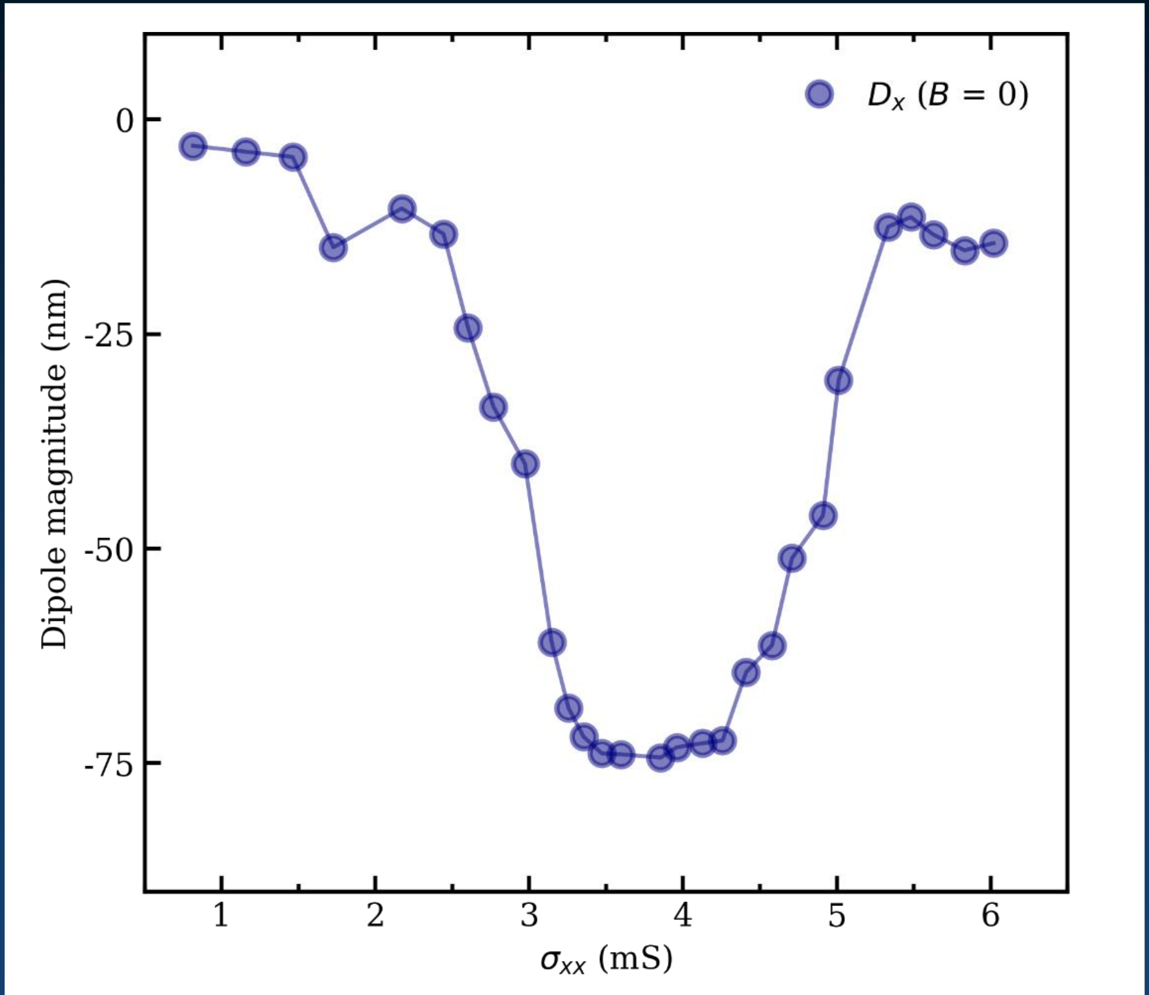


(111)$LaAlO_3$/$SrTiO_3$



WTe_2
Ma et al. Nature 565, 337 (2019)
Sodemann, I. & Fu, L.. Phys. Rev. Lett. 115, 216806 (2015)

Dipole magnitude

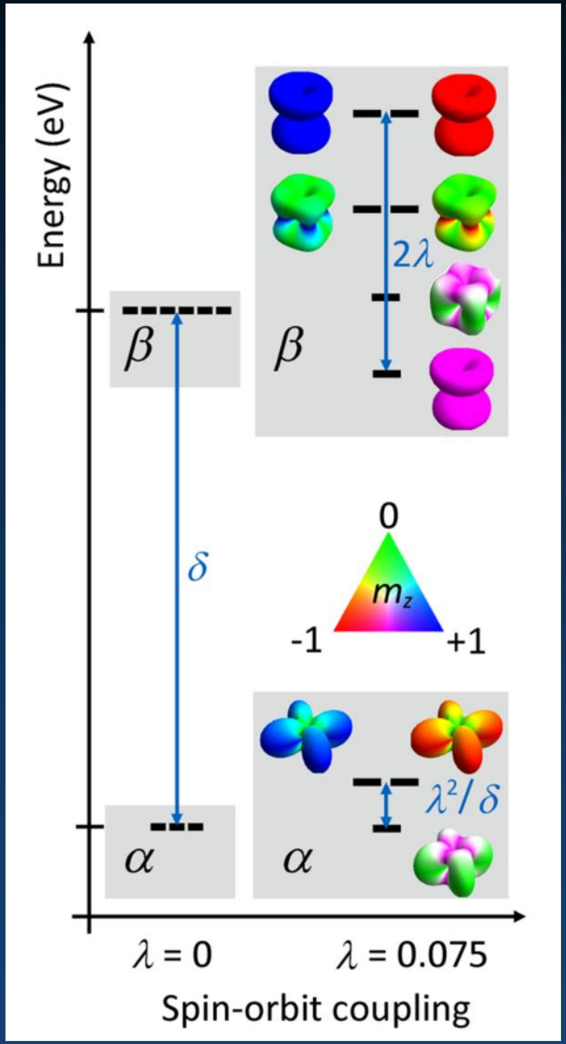


(111)$LaAlO_3/SrTiO_3$

Materials	Dimension	Experimental estimate of Berry curvature dipole (nm)
Bilayer WTe_2	2	5
Few layer WTe_2	2	0.07
Monolayer WTe_2	2	0.06
Corrugated bilayer graphene	2	20
Twisted WSe_2	2	0.5
Strained twisted bilayer graphene	2	20
LAO-STO interface	2	75

Lesne et al.
Nature Materials 22, 576 (2023)

Want to know more? Ruthenates



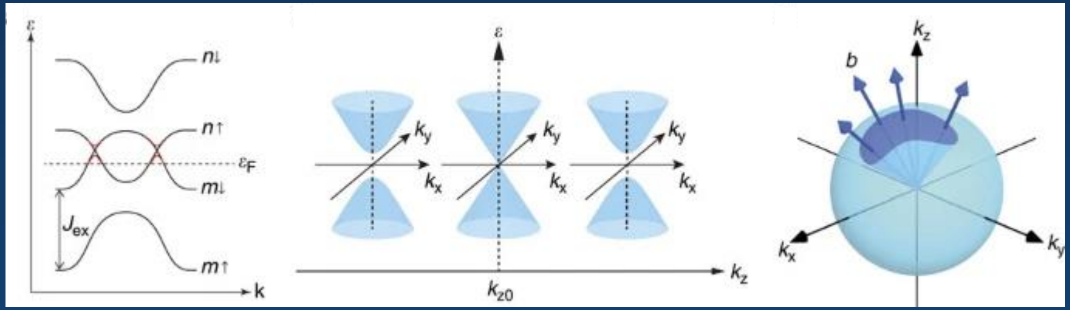
Das et al., Phys. Rev. X 8, 011048 (2018)

Ru^{4+} [Kr] $4d^4$

Tetragonal crystal field splitting of t2g orbitals: δ.

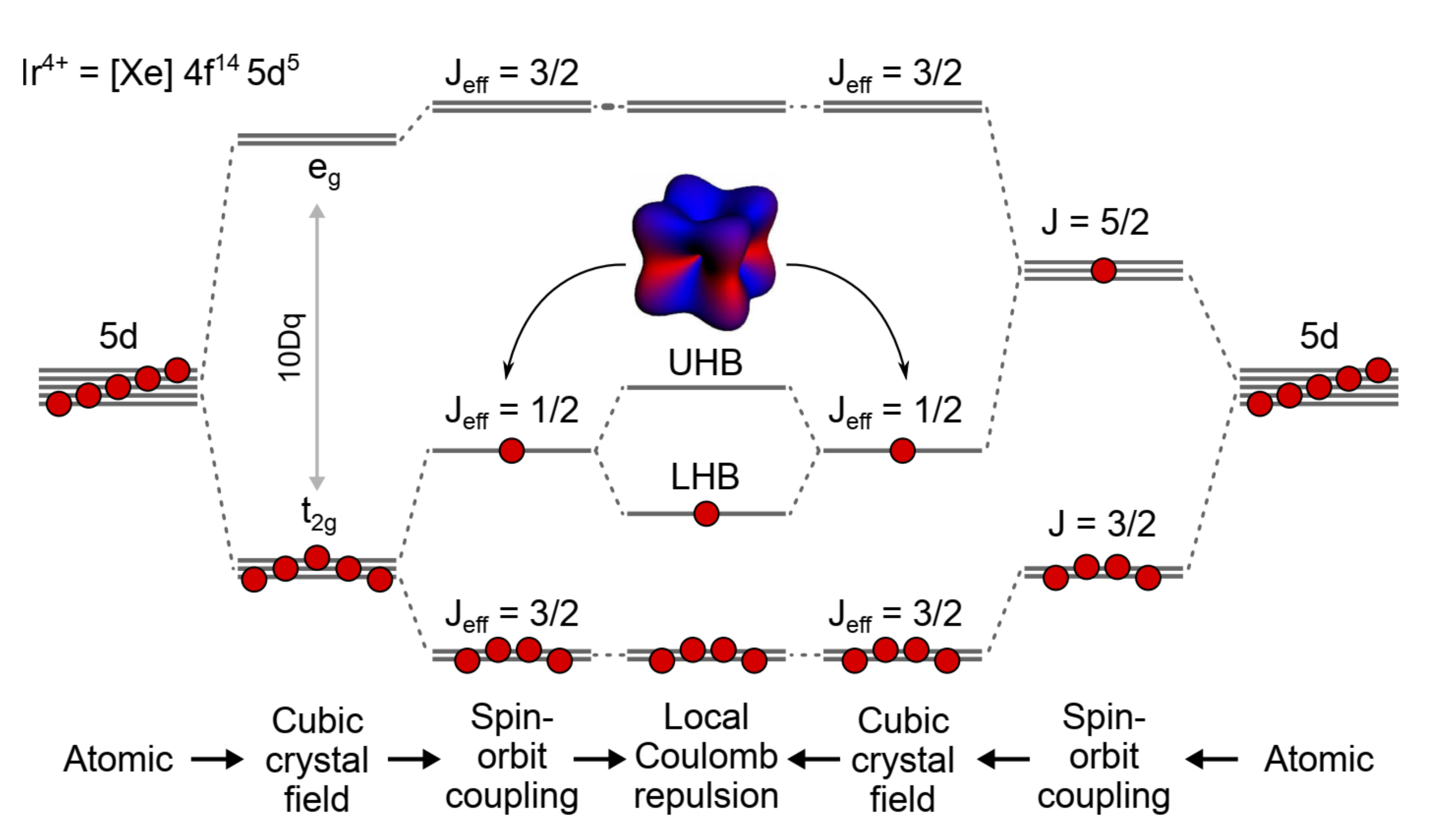
Spin-orbit driven mixing with inherent quantum phase.

Weyl points acting as sources of emergent magnetic fields, anomalous Hall conductivity, and unconventional spin dynamics.



Itoh et al., Nature Comm 7: 11788 (2016)

Want to know more? Iridates



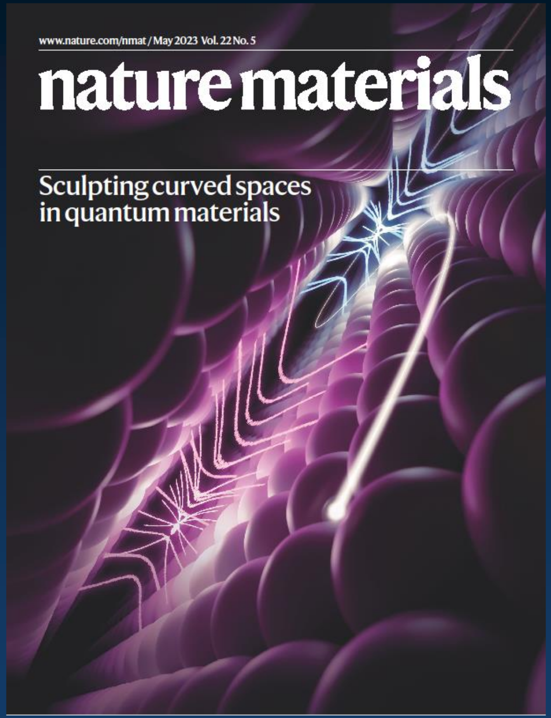
Spin-orbit driven mixing with inherent quantum phase.

$$|J_e = 1/2, +\rangle = \frac{1}{\sqrt{3}}(|xy,\downarrow\rangle - |yz,\uparrow\rangle + i|zx,\uparrow\rangle)$$

$$|J_e = 1/2, -\rangle = \frac{1}{\sqrt{3}}(|xy,\uparrow\rangle + |yz,\downarrow\rangle + i|zx,\downarrow\rangle)$$

P. Schütz et al. Physical Review Letters 119, 256404 (2017)

Collaborators and references



Lesne et al. Nature Materials 22, 576 (2023)
Mercaldo et al. npj Quantum Materials (2023)
van Thiel et al. Physical Review Letters 127 12, 127202 (2021)
van Thiel et al. ACS Materials Letters 2 4, 389-394 (2020)
Physical Review Research 2 2, 023404 (2020)

Image:
Xavier Ravinet
UNIGE

Collaborators and funding

Dmytro Afanasiev, Jorrit Hortensius, Mattias Matthiesen
Thierry van Thiel, Yildiz Saglam, Edouard Lesne,
Ulderico Filippozzi, Patrick Blah, Graham Kimbell,
Mafalda Monteiro, Ian Aupiais, Tancredi Thai Angeloni,
Giacomo Sala

Carmine Autieri,
Wojciech Brzezicki
Polish Academy of Science

Mario Cuoco
CNR Spin

Raffaele Battilomo,
Maria Teresa Mercaldo,
Canio Noce,
Carmine Ortix
Uni Salerno

Nicolas Gauquelin, J. Verbeeck
University of Antwerp

Marc Gabay
Uni Paris-Saclay

B.A. Ivanov, Ukranian Academy of Sciences, Kyiv

Eric Bousquet, Alireza Sazani
Uni Liege

Roberta Citro
CNR Spin
Uni Salerno

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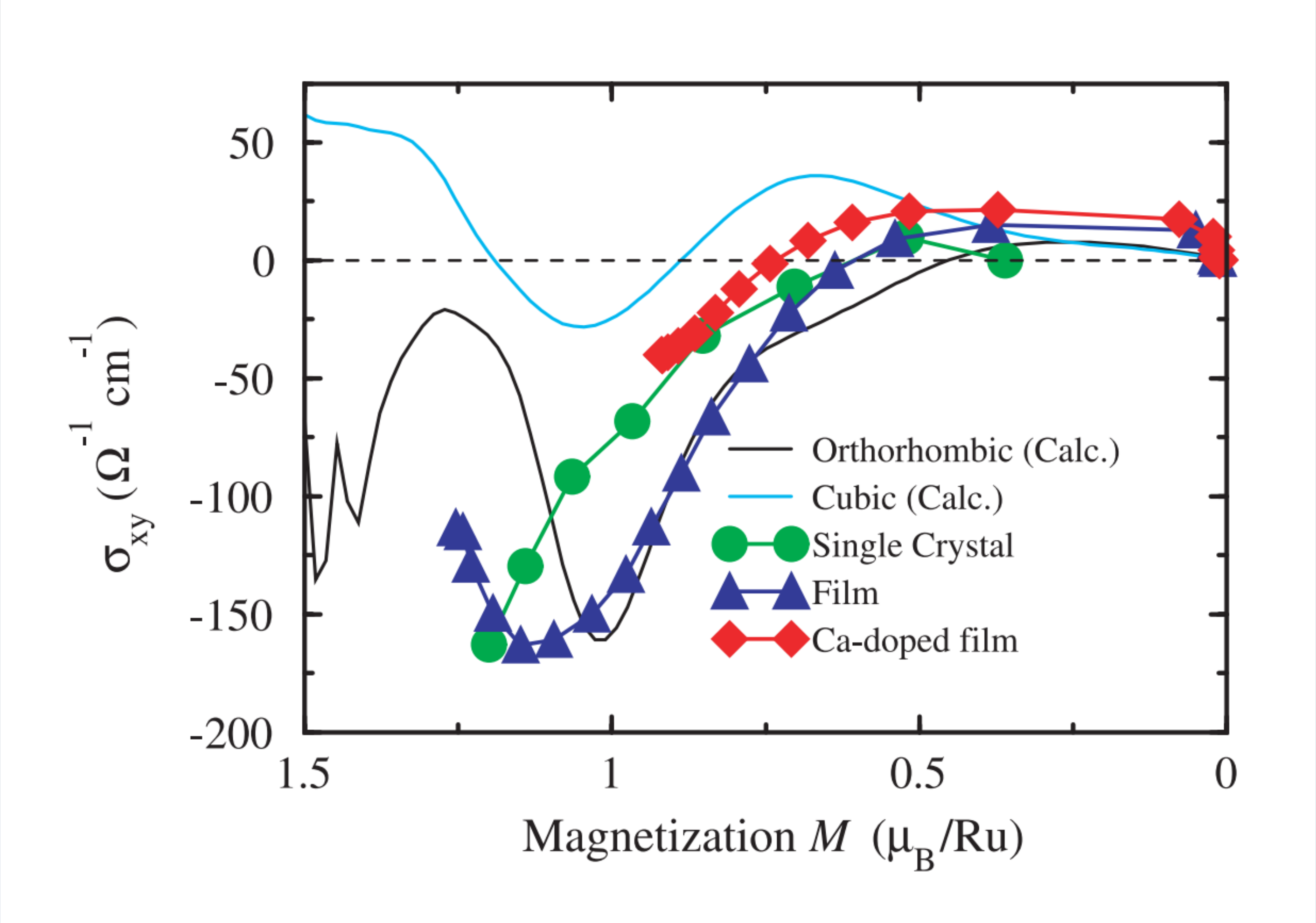
Ruthenates

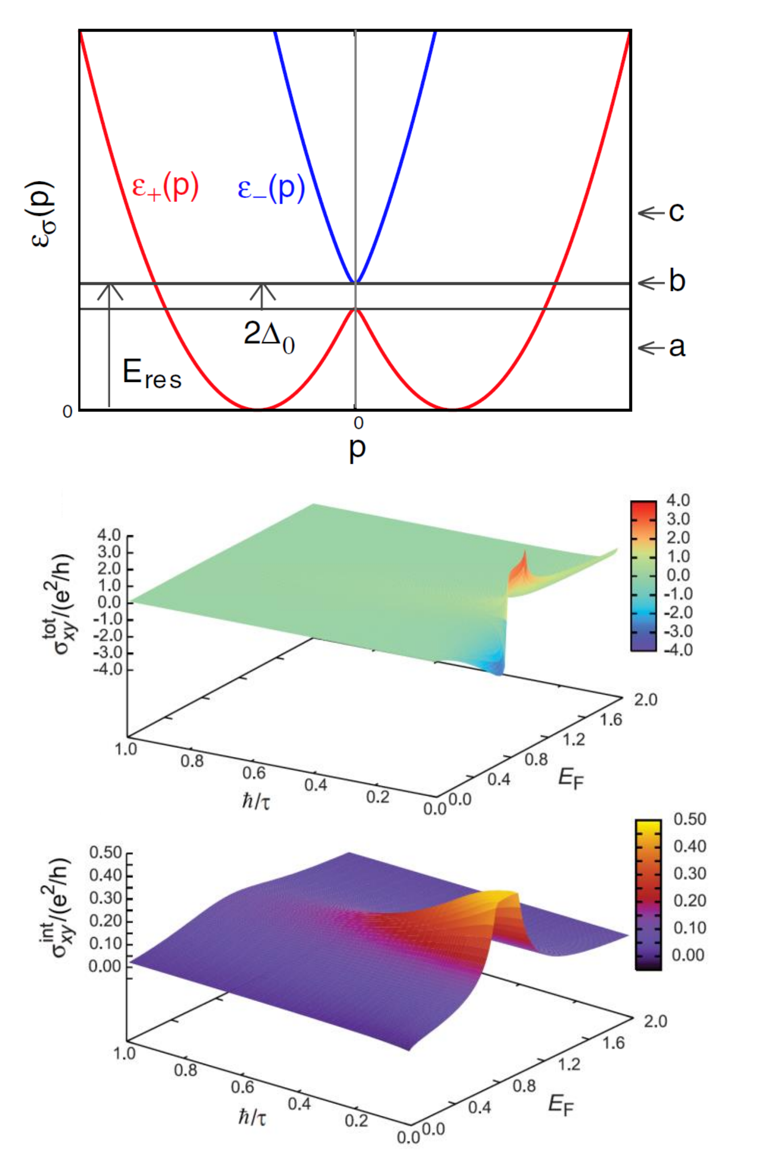


Fang et al. Science 302, 92 (2003)

Anomalous Hall effect from Berry phase

Berry curvature becomes sizable at the anticrossing of spin-orbit split bands with a Zeeman term.

Sign changes well described by theory that includes Berry phase and impurity scattering

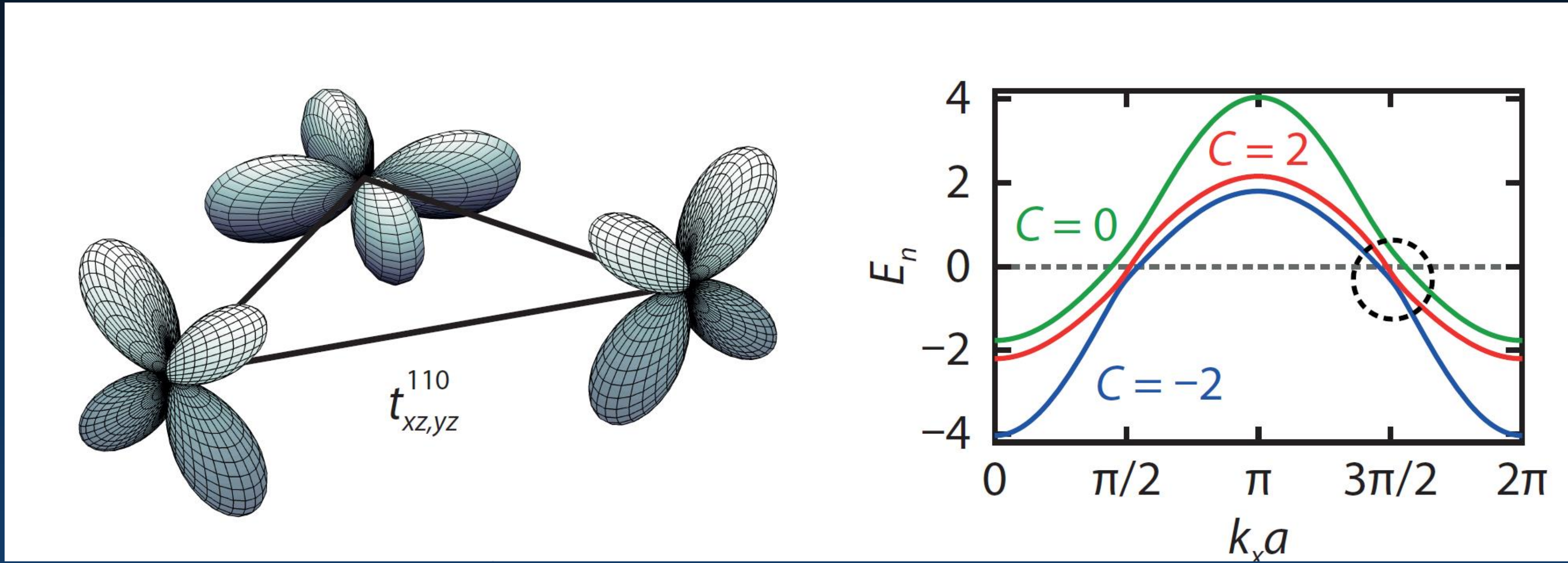


Onoda et al. PRL 97, 126602 (2006)

What is the electronic band topology of the 3D Weyl system $SrRuO_3$ in the two-dimensional limit?

Model system calculations

How do the Weyl points evolve in the two-dimensional limit?



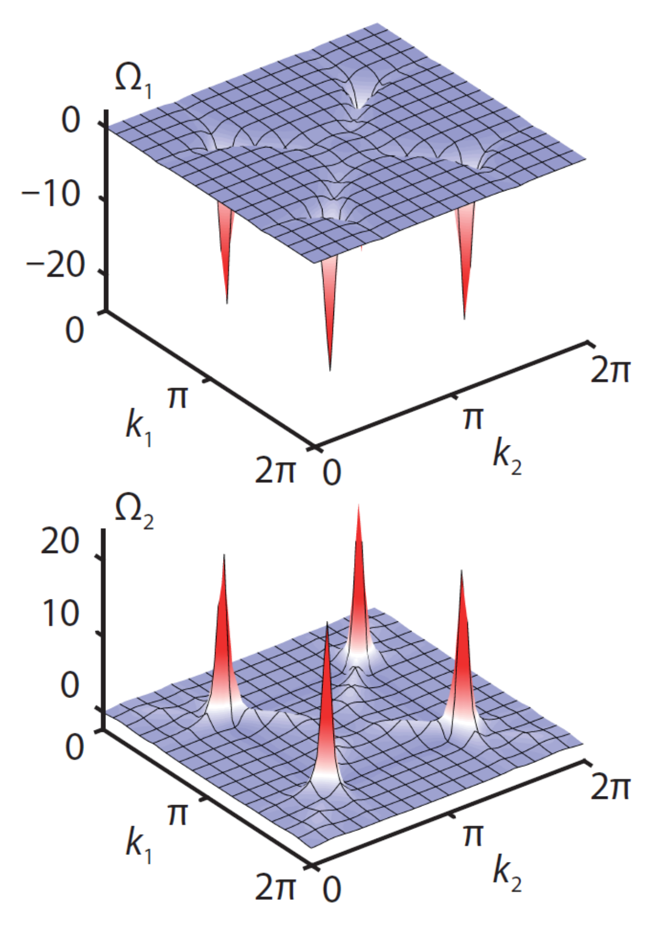
Effective Hamiltonian with spin-orbit coupling and next-nearest neighbours interorbital hopping

Mario Cuoco (CNR Spin)

Physical Review Research 2, 023404 (2020)

2 groups of 3 bands with different spin-orbital parity.
Within each sector, 2 topologically non-trivial bands with Chern numbers +2 and -2 and a single trivial band.
Avoided level crossing at finite k

Model system calculations



Physical Review Research 2, 023404 (2020)

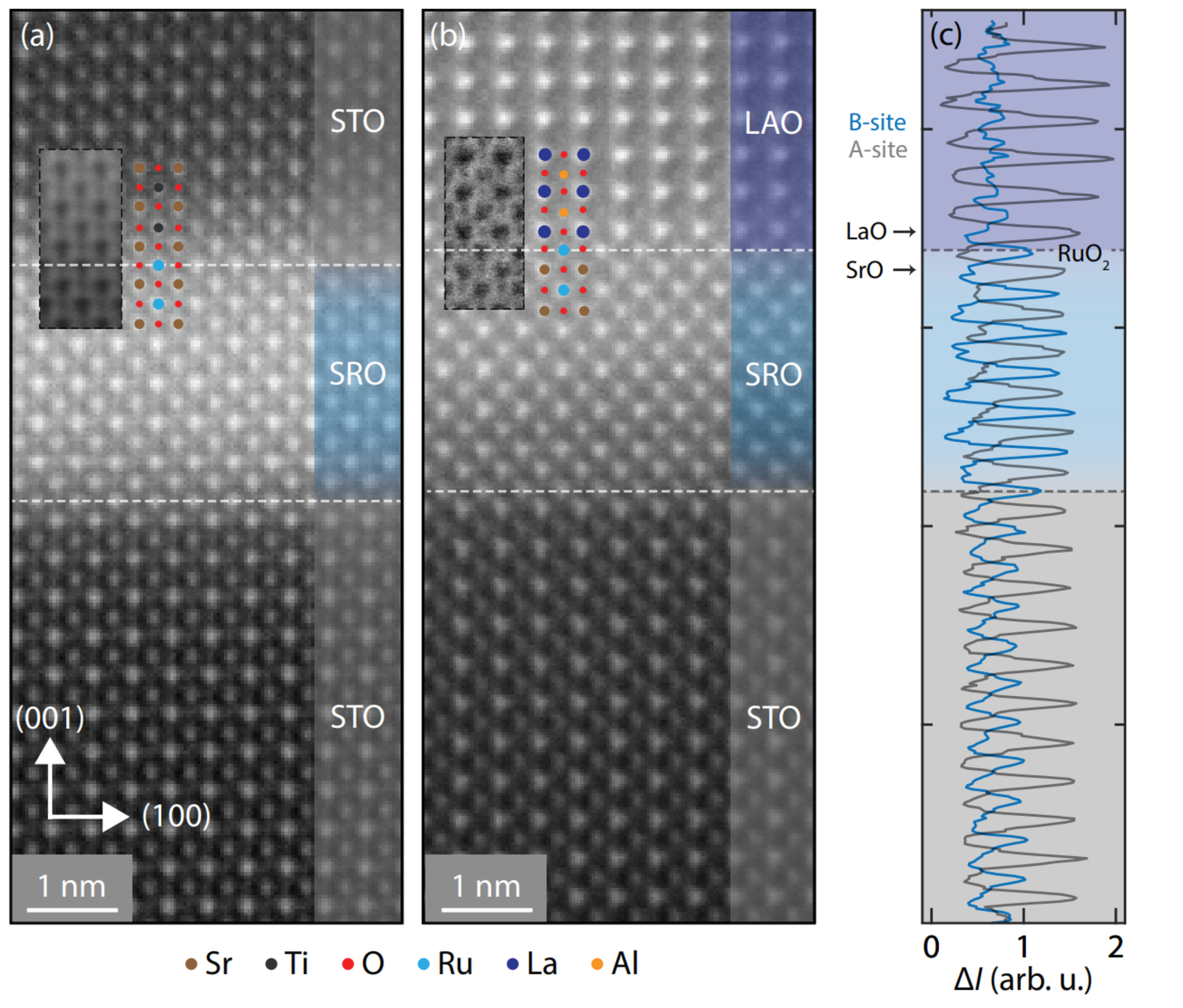
Berry curvature of the topologically non-trivial bands.

Sharp peaks with opposite sign located at the avoided level crossings.

Since the bands have non-trivial Chern number their contribution to the Berry curvature cannot vanish and is robust against variations in electron occupation.

The splitting and relative occupation of the two non-trivial bands determine a competition between positive and negative Berry curvature.

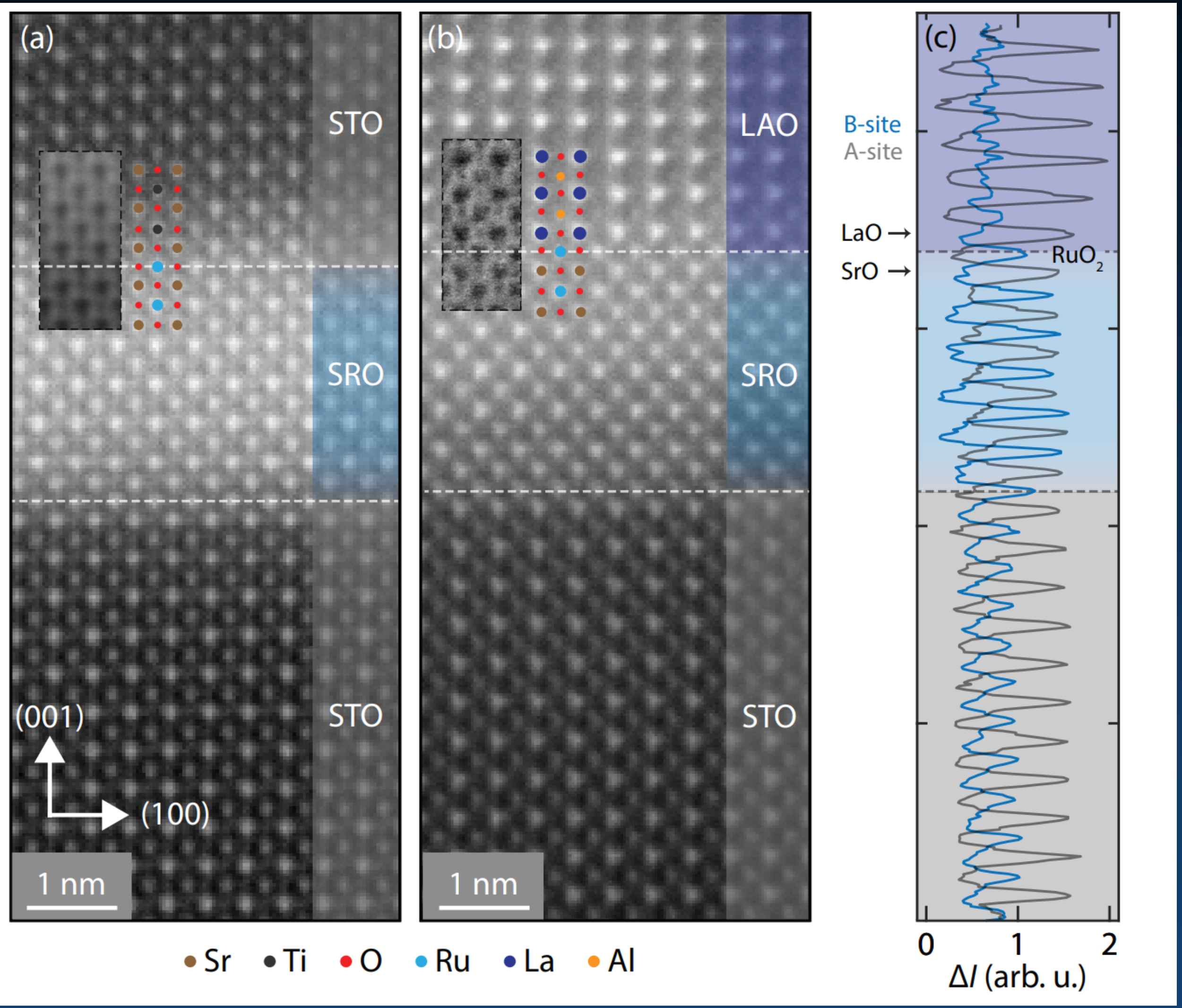
RuO_2/LaO interface

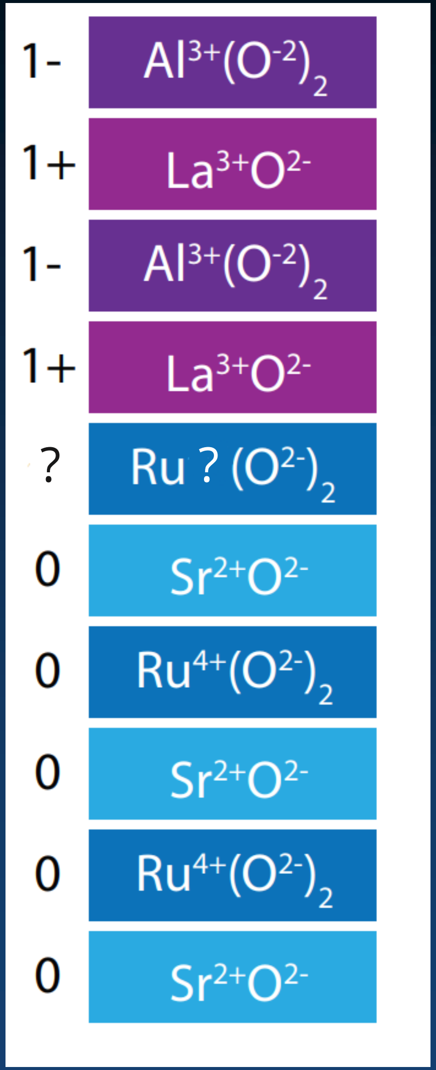


Thierry van Thiel

Physical Review Letters (2021) arXiv:2107.03359

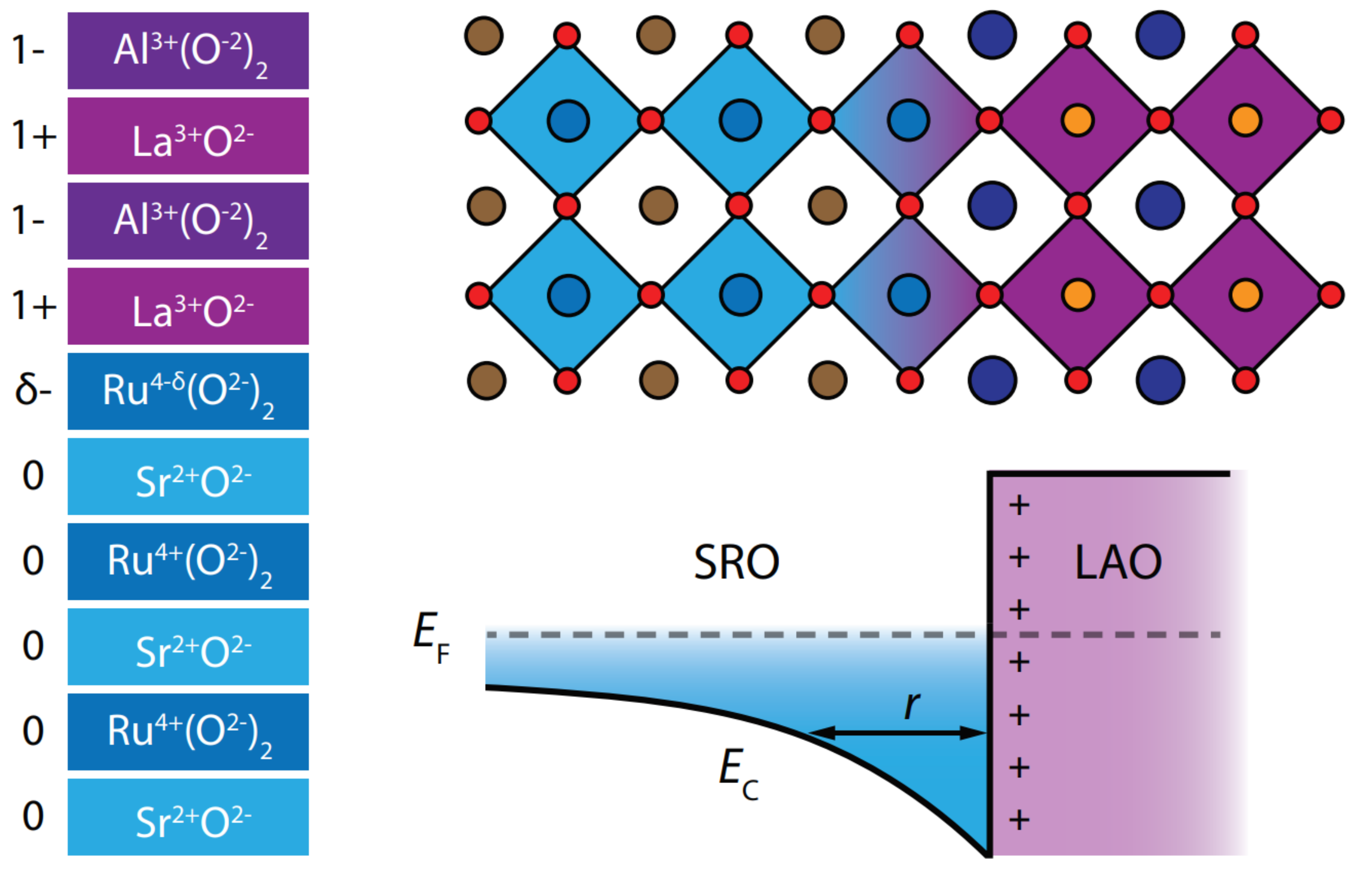
Charge reconstruction



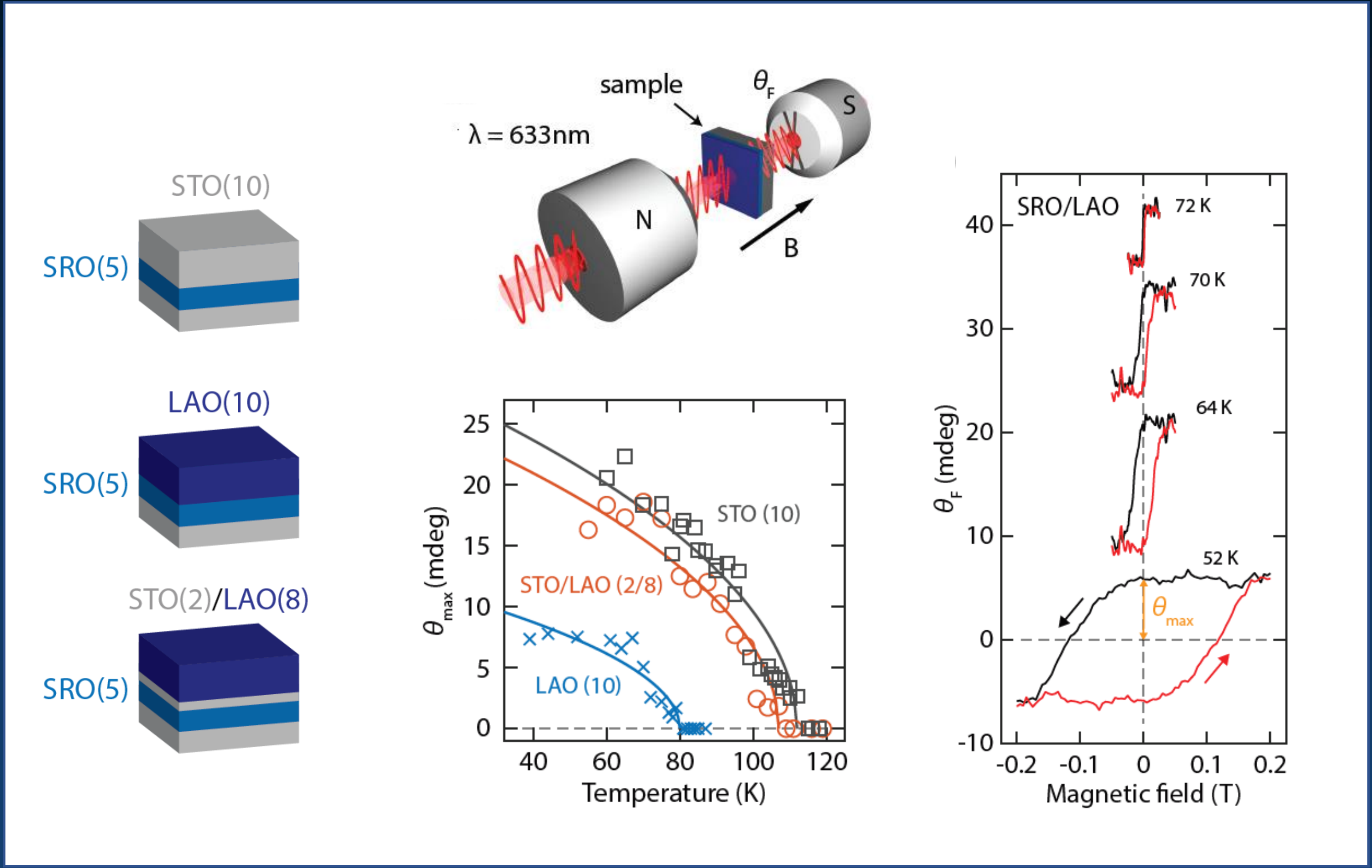


Physical Review Letters 127, 127202 (2021)

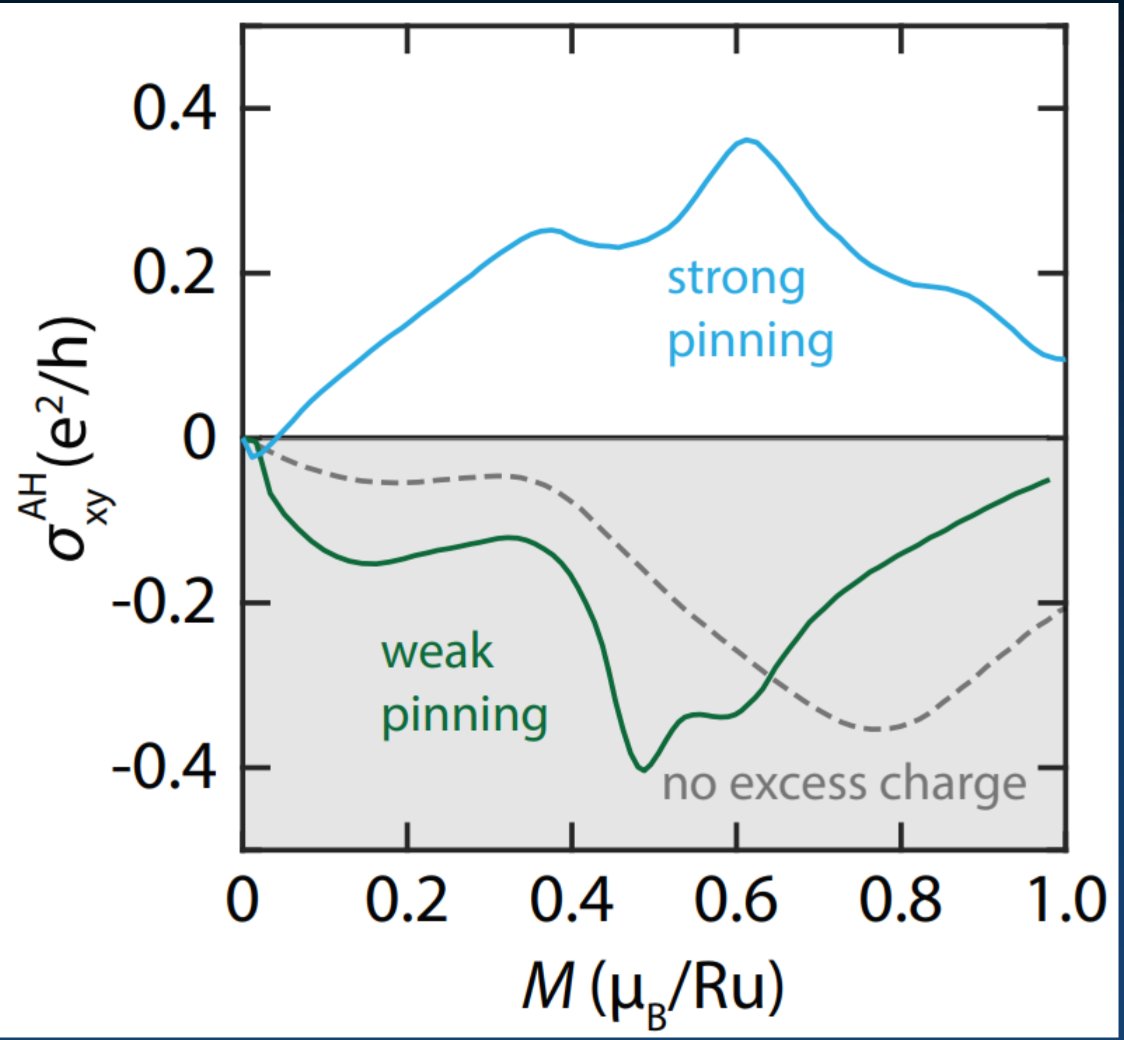
Charge reconstruction

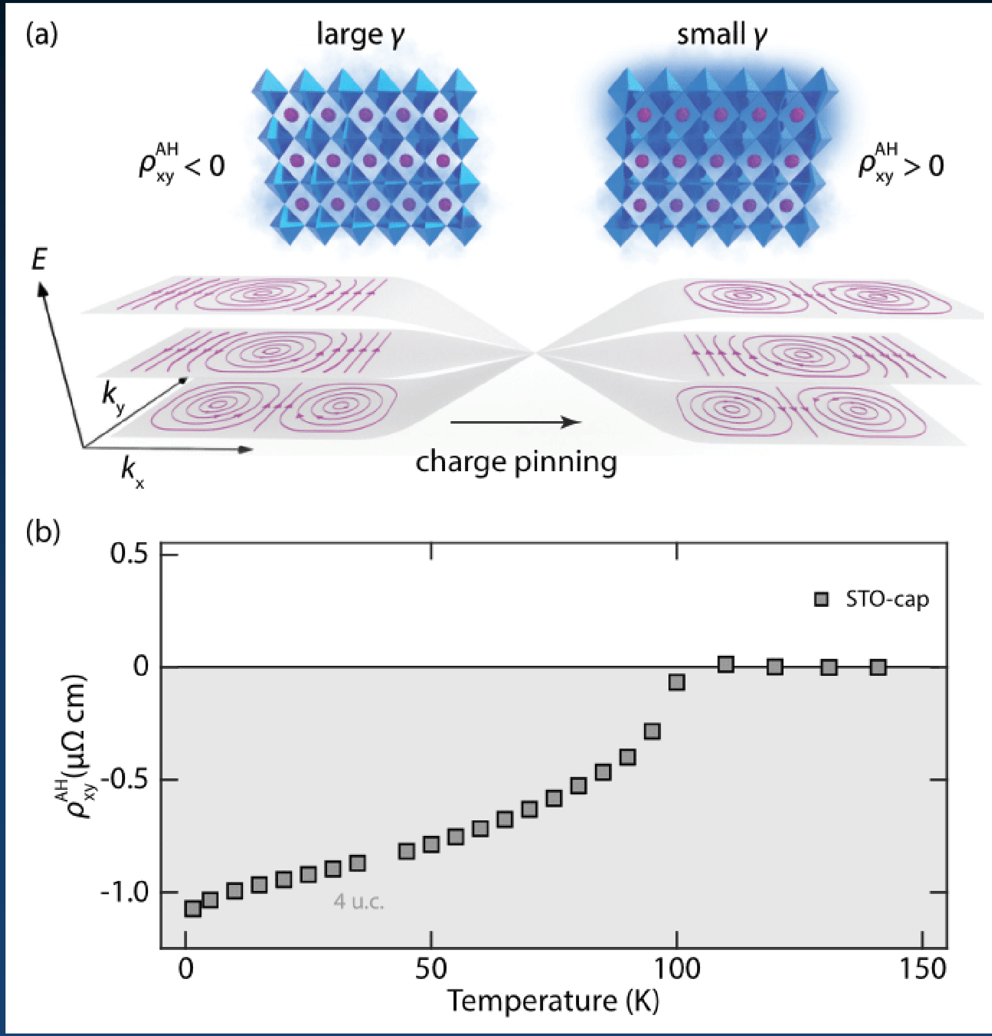


Magnetic reconstruction

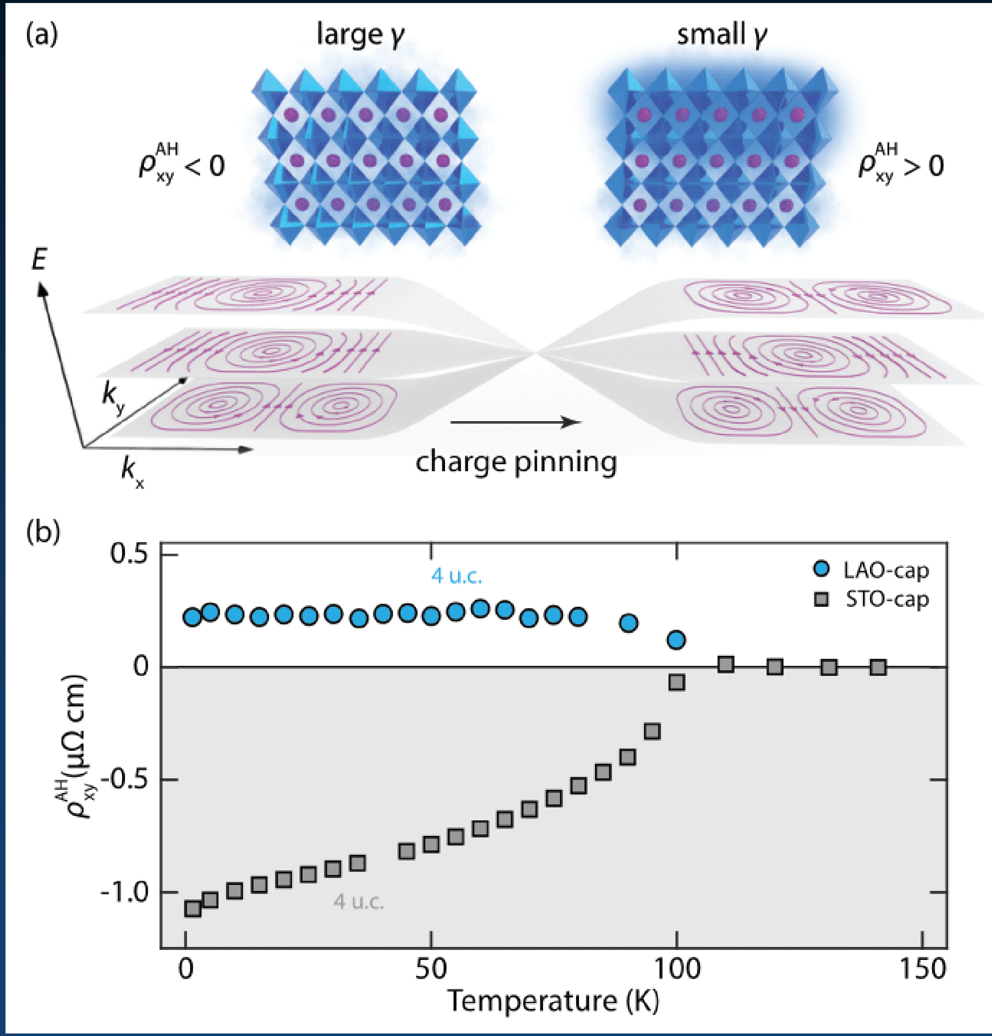


Berry curvature reconstruction in bilayer SRO

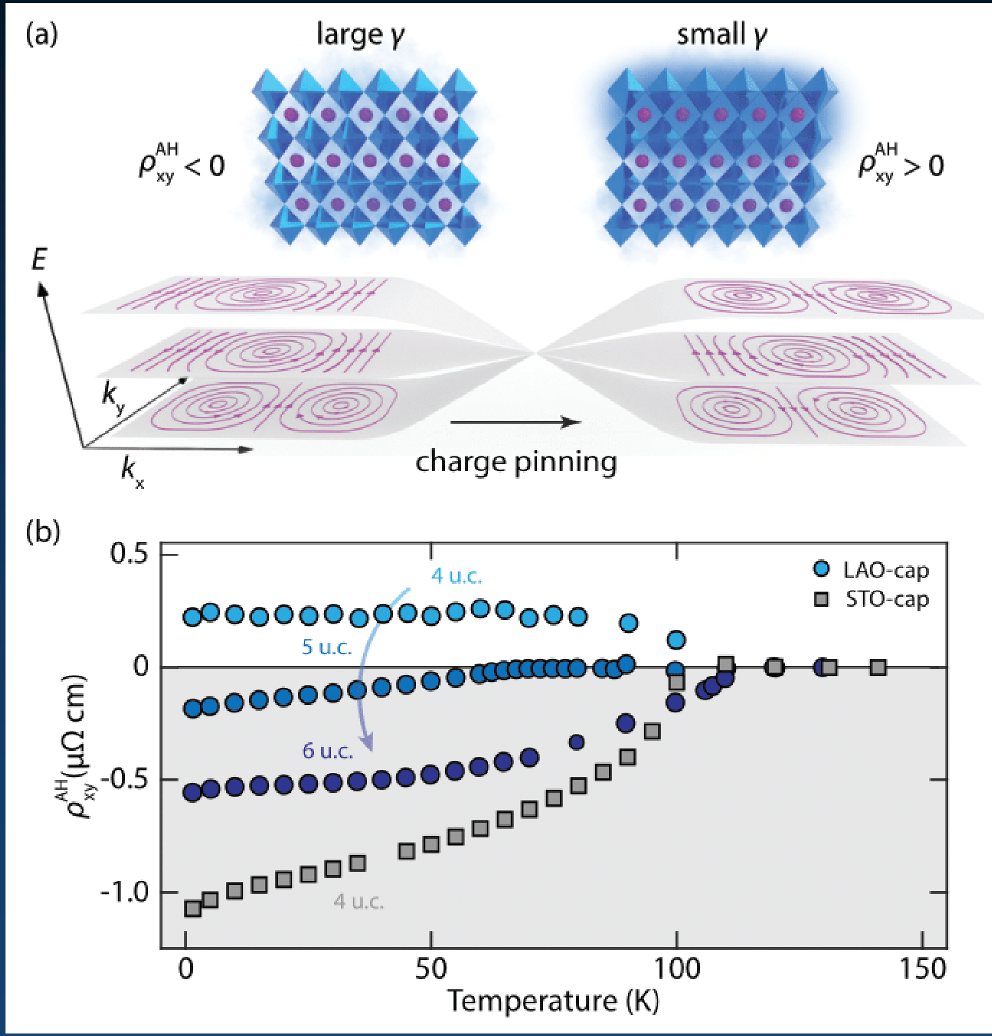




Physical Review Letters 127, 127202 (2021)



Physical Review Letters 127, 127202 (2021)



Physical Review Letters 127, 127202 (2021)