Linear magnetoelectric coupling (MEC)

Non-centrosymmetric magnetic insulator:

$$\alpha_{ij} = -\frac{d^2 E}{d\mathcal{E}_i dB_j} = \frac{dP_i}{dB_j} = \frac{dM_j}{d\mathcal{E}_i}$$

$$\alpha = \alpha_{\text{lattice}} + \alpha_{\text{frozen-ion}}$$

$$\alpha^{\text{Zeeman}}_{\text{frozen-ion}} + \boxed{\alpha^{\text{orbital}}_{\text{frozen-ion}}}$$

Focus on orbital contribution to frozen-ion MEC.

Theory of orbital MEC

$$\alpha_{da} = \boxed{\alpha^{\rm LC}_{da} + \alpha^{\rm IC}_{da}} + \boxed{\alpha^{\rm geom}_{da}}$$

$$\alpha^{\rm LC}_{da} = -\frac{e}{\hbar c}\,\epsilon_{abc}\int\frac{d^3k}{(2\pi)^3}\sum_n^N {\rm Im}\langle\widetilde{\partial}_b u_{n\mathbf{k}}|(\partial_c H_{\mathbf{k}})|\widetilde{\partial}_{\mathcal{E}_d} u_{n\mathbf{k}}\rangle$$

"Kubo terms"

$$\alpha^{\rm IC}_{da} = -\frac{e}{\hbar c}\,\epsilon_{abc}\int\frac{d^3k}{(2\pi)^3}\sum_{mn}^N {\rm Im}\Big\{\langle\widetilde{\partial}_b u_{n\mathbf{k}}|\widetilde{\partial}_{\mathcal{E}_d} u_{m\mathbf{k}}\rangle\langle u_{m\mathbf{k}}|(\partial_c H_{\mathbf{k}})|u_{n\mathbf{k}}\rangle\Big\}$$

Chern-Simons piece

$$\alpha^{\rm geom}_{da} = \frac{\theta}{2\pi}\frac{e^2}{hc}\,\delta_{da}$$

$$\theta_{\rm geom} = -\frac{1}{4\pi}\int d^3k\,\epsilon_{abc}{\rm tr}\left[A_a\partial_b A_c - \frac{2i}{3}A_a A_b A_c\right]$$

A.M. Essin, A.M. Turner, J.E. Moore, and DV, Phys. Rev. B 81, 205104 (2010).
A. Malashevich, I. Souza, S. Coh, and DV, New J. Phys. 12, 053032 (2010).

Insulator in finite electric field

Ak is the Berry connection, acting for the charges

$$H_{\mathbf{k}} = H_{\mathbf{k}}^0 + \boxed{e\boldsymbol{\mathcal{E}} \cdot \mathbf{A}_{\mathbf{k}}}$$

$$F_{mn\underline{k},\mu\nu} = \langle \partial_\mu u_{m\underline{k}} | Q | \partial_\nu u_{n\underline{k}} \rangle$$

$$\Gamma_{mn\underline{k},\mu\nu} = \langle \partial_\mu u_{m\underline{k}} | Q H_k Q | \partial_\nu u_{n\underline{k}} \rangle$$

$$\mathbf{M} = \widetilde{\mathbf{M}}^{\mathrm{LC}} + \widetilde{\mathbf{M}}^{\mathrm{IC},0} + \widetilde{\mathbf{M}}^{\mathrm{IC},\mathcal{E}}$$

$$\widetilde{M}_\alpha^{\mathrm{LC}} = \frac{e}{2\hbar c} \frac{1}{(2\pi)^3} \int_{\mathrm{BZ}} \varepsilon_{\alpha\mu\nu} \, \mathrm{Im}\, \mathrm{Tr}\, [\Gamma_{\mu\nu}]\, d^3k \,, \tag{6.40}$$

$$\widetilde{M}_\alpha^{\mathrm{IC},0} = \frac{e}{2\hbar c} \frac{1}{(2\pi)^3} \int_{\mathrm{BZ}} \varepsilon_{\alpha\mu\nu} \, \mathrm{Im}\, \mathrm{Tr}\, [H^0 F_{\mu\nu}]\, d^3k \,, \tag{6.41}$$

$$\widetilde{M}_\alpha^{\mathrm{IC},\mathcal{E}} = \frac{-e^2}{2\hbar c} \mathcal{E}_\alpha \frac{1}{(2\pi)^3} \int_{\mathrm{BZ}} \varepsilon_{\mu\nu\sigma} \, \mathrm{Tr} \left[A_\mu^0 \partial_\nu A_\sigma^0 - \frac{2i}{3} A_\mu^0 A_\nu^0 A_\sigma^0 \right] d^3k \,. \tag{6.42}$$

$$\alpha_{\mathrm{iso}} = \frac{e^2}{hc} \frac{\theta}{2\pi}$$

Chern-Simons 3-form

$$\theta_{\mathrm{CS}} = -\frac{1}{4\pi} \int_{\mathrm{BZ}} \varepsilon_{\mu\nu\sigma} \, \mathrm{Tr} \left[A_\mu \partial_\nu A_\sigma - \frac{2i}{3} A_\mu A_\nu A_\sigma \right] d^3k$$

$$A_{mn,\mu} = i \langle u_{m\underline{k}} | \partial_\mu u_{n\underline{k}} \rangle$$

$$\sum_{mn} A_{mn,\mu} \partial_\nu A_{nm,\sigma} - \frac{2i}{3} \sum_{mnp} A_{mn,\mu} A_{np,\nu} A_{pm,\sigma}$$

m, n : band index

Gauge dependence of theta

See
Appendix C

$$\theta_{\mathrm{CS}} = -\frac{1}{4\pi}\int_{\mathrm{BZ}} \varepsilon_{\mu\nu\sigma}\,\mathrm{Tr}\left[A_\mu \partial_\nu A_\sigma - \frac{2i}{3} A_\mu A_\nu A_\sigma\right] d^3k$$

$$|\tilde{u}_{n\mathbf{k}}\rangle = \sum_m U_{mn}(\mathbf{k})\,|u_{m\mathbf{k}}\rangle$$

Radical Gauge transformation in the book

$$\widetilde{A}_\mu = U^\dagger A_\mu U + U^\dagger i\partial_\mu U$$

$$\Delta\theta_{\mathrm{CS}} = \frac{1}{12\pi}\int_{\mathrm{BZ}} \varepsilon_{\mu\nu\sigma}\,\mathrm{Tr}\left[U^\dagger(\partial_\mu U)U^\dagger(\partial_\nu U)U^\dagger(\partial_\sigma U)\right] d^3k$$

Assume
- Not a Chern insulator, C_j=0
- det (U) does not wind in any reciprocal direction

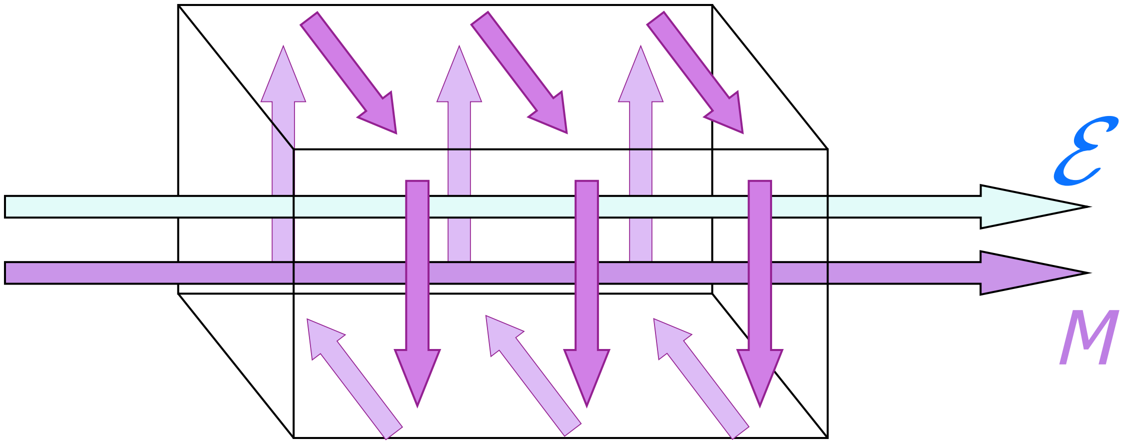
There is a new kind of gauge transformation that changes θ by 2π:

$$U(\mathbf{k}) = \begin{cases} -e^{-i\,\mathbf{q}\cdot\boldsymbol{\sigma}}\,, & q \le \pi \\ I\,, & q \ge \pi \end{cases} \qquad \mathbf{q} = \pi\mathbf{k}/k_0$$

"Z homotopy invariant for mapping from T^3 onto SU(2)"

Result: θ is well defined modulo 2π (like Berry phase)

Magnetoelectric coupling (MEC)



$$\mathbf{M} = \alpha\,\mathcal{E}$$

α = "magnetoelectric coefficient"

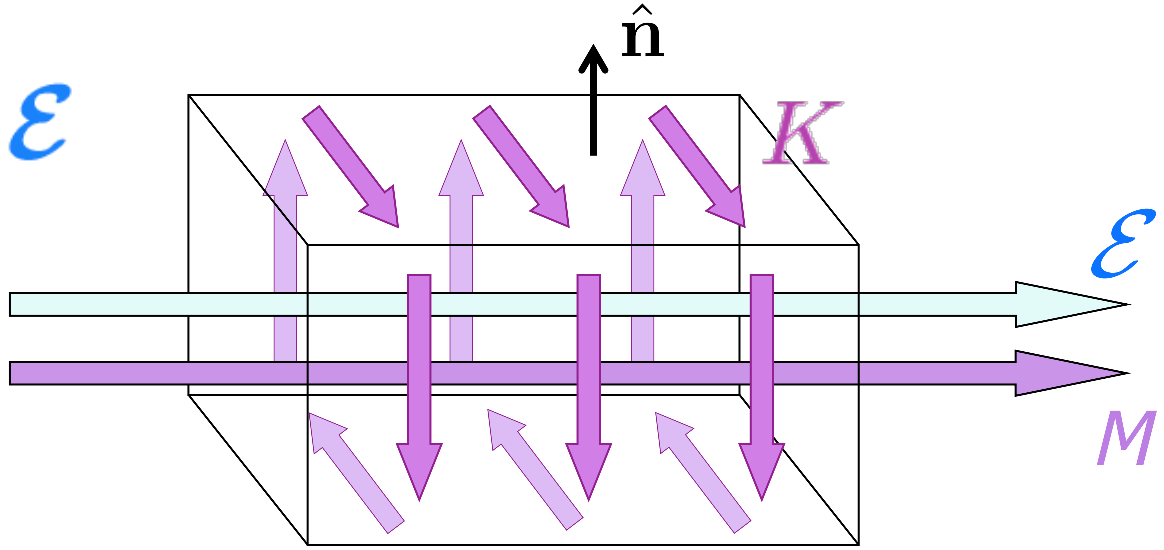
Comments:

- Consider electronic (not lattice-mediated) part
- Consider orbital (not spin) part
- Assume α is isotropic (in general, it is a 3x3 tensor)

"axion"

Surface σ_{AHC} = MEC

$$\mathbf{M} = \alpha\, \mathcal{E}$$

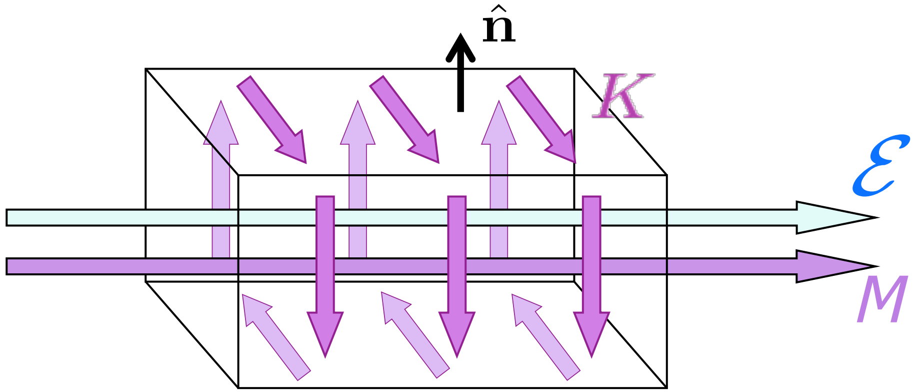


$$\mathbf{K} = \mathbf{M} \times \hat{\mathbf{n}}$$

$$\mathbf{K} = \sigma_{\mathrm{AHC}}^{\mathrm{surf}}\, \hat{\mathbf{n}} \times \mathcal{E}$$

$$\boxed{\sigma_{\mathrm{AHC}}^{\mathrm{surf}} = -\alpha}$$

MEC = "axion coupling"



Let

$$\alpha = \frac{\theta}{2\pi}\frac{e^2}{h}$$

- θ has Berry-phase like formula
- θ is only well-defined modulo 2π
- θ = "axion coupling"

Axion (Chern-Simons) θ coupling

*Qi, Hughes and Zhang, PRB **78**, 195424 (2008)*
*Essin, Moore and Vanderbilt, PRL **120**,146805 (2009)*

$$\boxed{\theta = -\frac{1}{4\pi}\int_{\mathrm{BZ}} d^3k\,\epsilon_{abc}\,\mathrm{tr}\left[\mathrm{A_a}\partial_\mathrm{b}\mathrm{A_c} - \frac{2\mathrm{i}}{3}\mathrm{A_a A_b A_c}\right]}$$

$$\text{Berry connection:}\quad A_{a,nm} = i\,\langle u_{n\mathbf{k}}|\,\frac{\partial}{\partial k_a}\,|u_{m\mathbf{k}}\rangle$$

Compare Berry phase:

$$\phi = \int_{\mathrm{BZ}} dk\;\mathrm{tr}[\mathrm{A}]$$

θ and ϕ are gauge-invariant only modulo 2π

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Theory of orbital MEC

($\boldsymbol{E}\cdot\boldsymbol{B}$ term in Lagrangian)

Drop Kubo terms:

"geometrical" = "axion" = "Chern-Simons"

$$\boxed{\alpha_{ij} = \frac{e^2}{h}\frac{\theta}{2\pi}\delta_{ij}}$$

$$\boxed{\theta = -\frac{1}{4\pi}\int d^3k\,\epsilon_{abc}\mathrm{tr}\left[A_a\partial_b A_c - \frac{2i}{3}A_aA_bA_c\right]}$$

Berry connection: $A_{a,nm} = i\,\langle u_{n\mathbf{k}}|\partial_a|u_{m\mathbf{k}}\rangle$

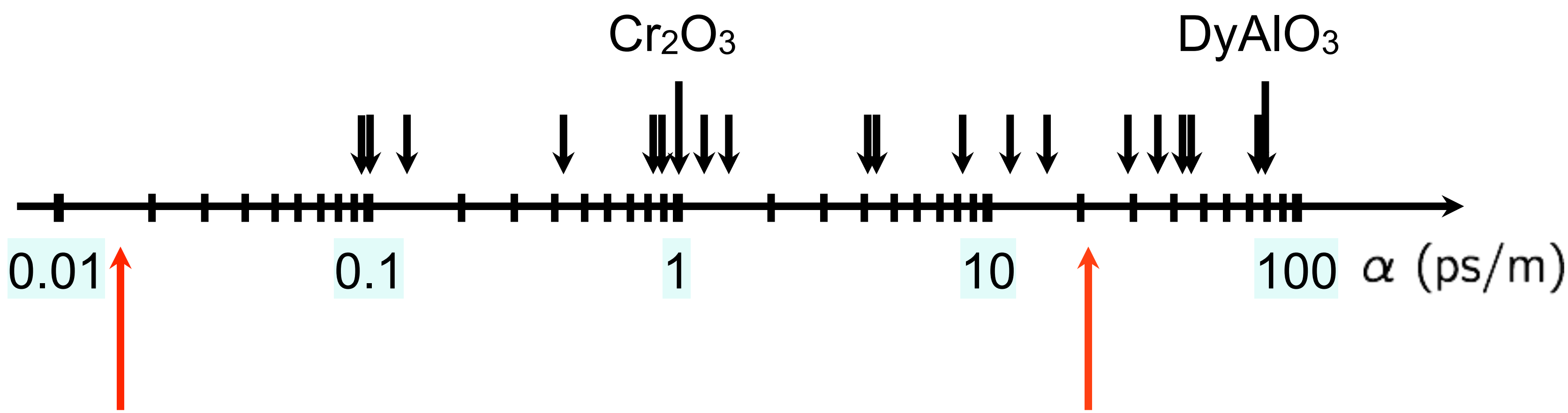
Theory of orbital MEC

$$\theta = -\frac{1}{4\pi}\int d^3k\,\epsilon_{abc}\mathrm{tr}\left[A_a\partial_b A_c - \frac{2i}{3}A_aA_bA_c\right]$$

*Qi, Hughes and Zhang, PRB **78**, 195424 (2008)*
*Essin, Moore and Vanderbilt, PRL **120**, 146805 (2009)*

- Integrand is called Chern-Simons 3-form
- Integrand is *not* gauge-invariant
- But integral over 3D BZ *is* gauge-invariant, modulo 2π
- Typically, $\theta << 2\pi$ and quantum of MEC is unimportant

Order of magnitude values



Orbital electronic

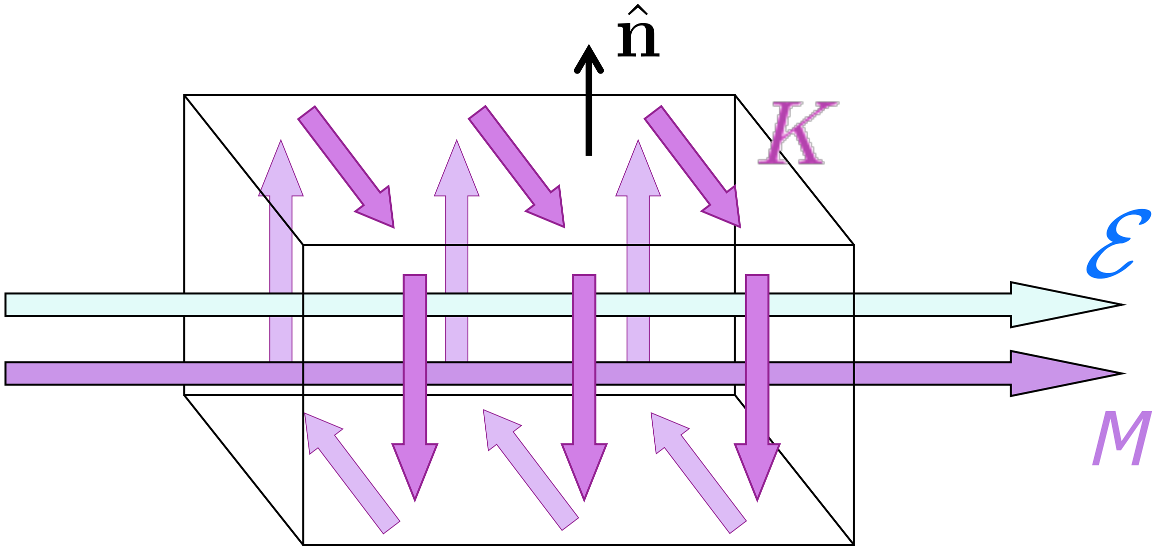
Chern-Simons θ in conventional magnetoelectrics like Cr_2O_3

$$\alpha = \frac{e^2}{h}\frac{\theta}{2\pi}$$

Orbital electronic

$$\theta = \pi$$

Surface $\sigma_{\text{AHC}} \Leftrightarrow$ axion coupling



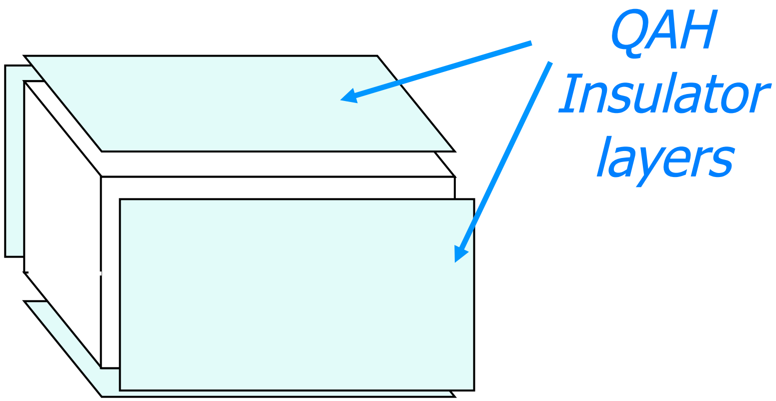
$$\sigma_{\text{AHC}}^{\text{surf}} = -\alpha = -\frac{\theta}{2\pi}\frac{e^2}{h}$$

θ only defined modulo 2π

Start with crystal having α given by θ.

Glue on 2D QAH insulator layer

$$\alpha = \frac{e^2}{h}\frac{\theta}{2\pi}$$



This increments $\sigma_{xy}^{\mathrm{surf}}$ by $\dfrac{e^2}{h}$, i.e., $\theta_{\mathrm{new}} = \theta + 2\pi$

So θ as a bulk property is ill-defined modulo 2π !

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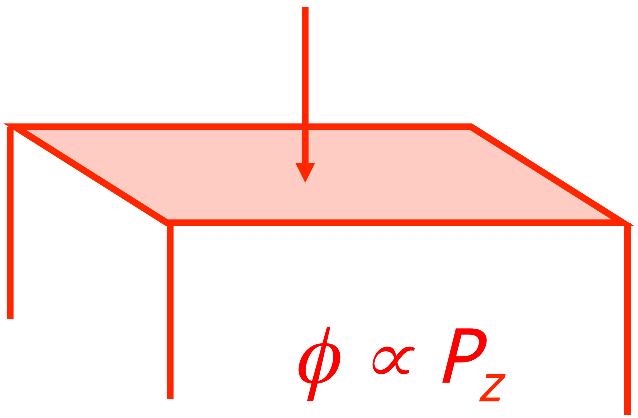
Insulating surface of bulk insulator

Surface charge

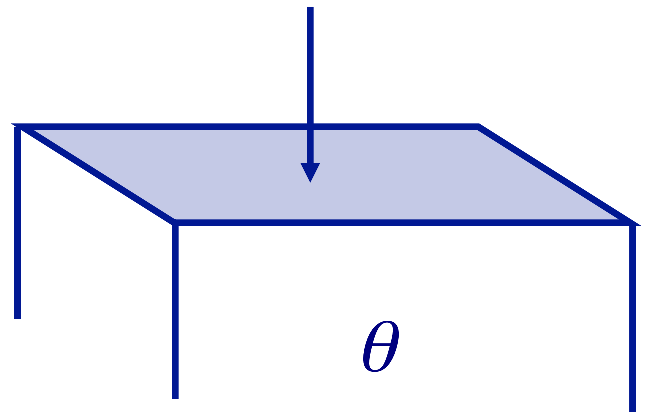
$$\boxed{\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{integer}\right]}$$



ϕ is ill-defined modulo 2π

Surface AHC

$$\boxed{\sigma^{\mathrm{AH}} = \frac{e^2}{h}\left[\frac{\theta}{2\pi} + \text{integer}\right]}$$



θ is ill-defined modulo 2π

When can θ be equal to π ?

- θ is gauge-invariant, modulo 2π
- T or I symmetry operator maps θ into $-\theta$
- Two values of θ are allowed (Z_2 classification):
  - Case of $\theta = 0$ $\Leftrightarrow$ trivial insulator
  - Case of $\theta = \pi$ $\Leftrightarrow$ strong topological insulator (T)
    axion insulator (I)
- $\theta = \pi$ implies half-integer surface quantum AHC !

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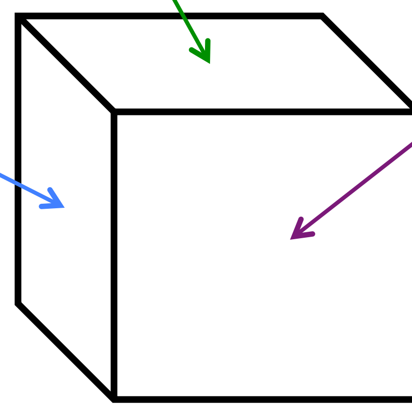
Half-integer surface QAH?

- $\theta = \pi$ implies half-integer surface quantum AHC !

$$\sigma_{\mathrm{AHC}}^{\mathrm{surf}} = +\frac{1}{2}\frac{e^2}{h}$$

$$\sigma_{\mathrm{AHC}}^{\mathrm{surf}} = +\frac{3}{2}\frac{e^2}{h}$$

$$\sigma_{\mathrm{AHC}}^{\mathrm{surf}} = -\frac{1}{2}\frac{e^2}{h}$$



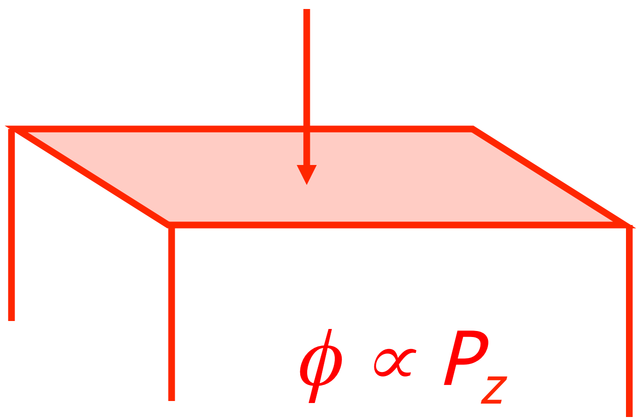
But if T is a symmetry ⇒ surface AHC = 0.

Is this a contradiction?

Insulating surface of bulk insulator

Surface charge

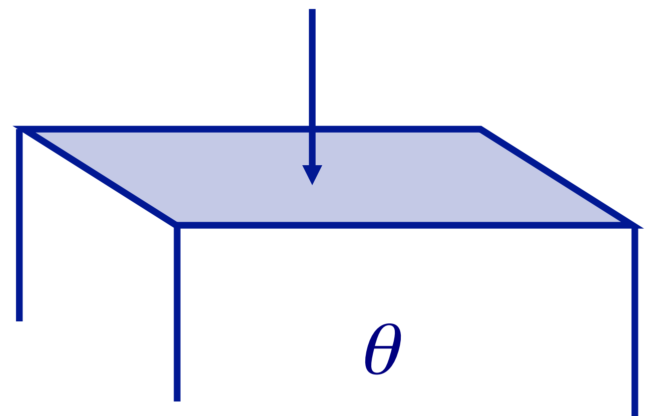
$$\boxed{\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{integer}\right]}$$



ϕ is ill-defined modulo 2π

Surface AHC

$$\boxed{\sigma^{\mathrm{AH}} = \frac{e^2}{h}\left[\frac{\theta}{2\pi} + \text{integer}\right]}$$

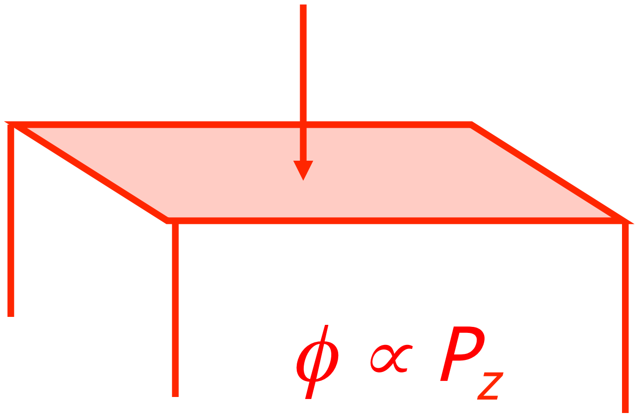


θ is ill-defined modulo 2π

Metallic surface of bulk insulator

Surface charge

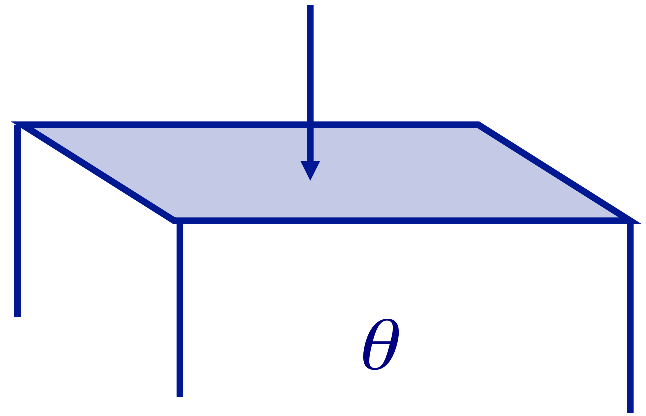
$$\sigma = \frac{-e}{A}\left[\frac{\phi}{2\pi} + \text{int} + \frac{A}{(2\pi)^2}\int d^2k\, f(\mathbf{k})\right]$$



ϕ is ill-defined modulo 2π

Anom. Hall conductivity

$$\sigma^{\mathrm{AH}} = \frac{e^2}{h}\left[\frac{\theta}{2\pi} + \text{int} + \frac{1}{2\pi}\int d^2k\, f(\mathbf{k})\,\Omega(\mathbf{k})\right]$$

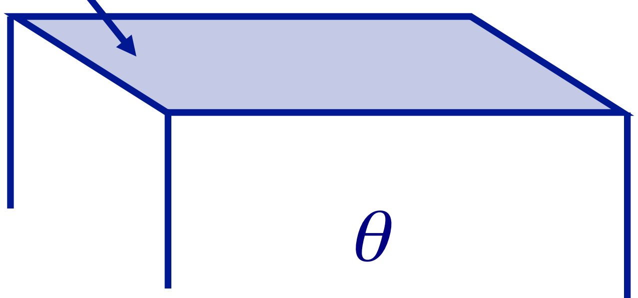


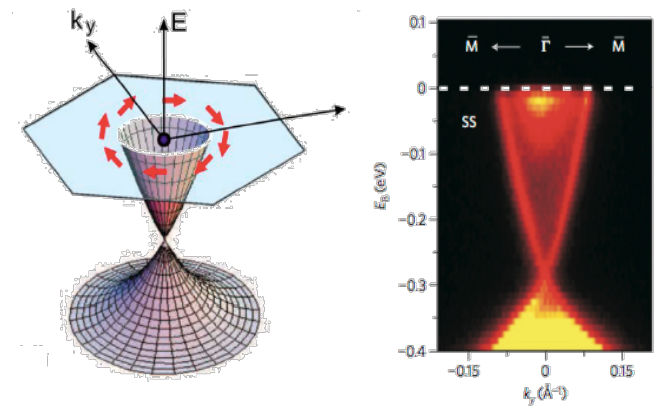
θ is ill-defined modulo 2π

Surface AHC of strong topological insulator

if surface is metallic

$$\sigma^{\rm surf}_{\rm AHC} = -\frac{e^2}{h}\Big[-\frac{\overset{\pi}{\theta}}{2\pi} + \boxed{\frac{1}{2\pi}\overbrace{\int d^2k\, f(\mathbf{k})\,\Omega(\mathbf{k})}^{\pi}}\,\Big]$$





Figures from Hasan and Kane, RMP, 2010 (Adapted from Xia et al., 2008; Hsieh, Xia, Qian, Wray, et al., 2009a; and Xia, Qian, Hsieh, Wray, et al., 2009).

Bulk θ is defined modulo 2π

Total surface AHC = 0 !

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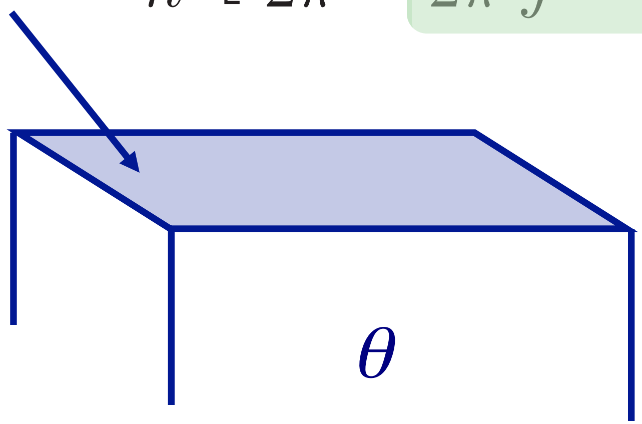
Surface AHC of axion insulator

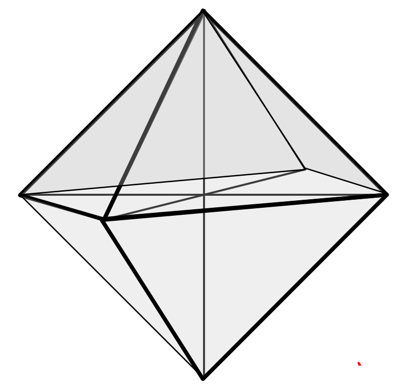
π

0

if surface is metallic

$$\sigma^{\rm surf}_{\rm AHC} = -\frac{e^2}{h}\left[-\frac{\theta}{2\pi} + \frac{1}{2\pi}\int d^2k\, f(\mathbf{k})\,\Omega(\mathbf{k}) \right]$$





Bulk θ is defined modulo 2π

Surface AHC = $\pm\, e^2/2h$!

Polarization	Orbital ME coupling
Berry phase ϕ	Axion angle θ
Surface charge	Surface AHC
Adiabatic charge pump	Adiabatic axion pump
First Chern number	Second Chern number