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Total Energy and Force Methods**

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Orbital magnetization in periodic solids and its connection to NMR

Timo THONHAUSER
Massachusetts Institute of Technology
Department of Materials Science & Engineering
77 Massachusetts Ave.
Cambridge, MA 02139-4307
U.S.A.

Orbital magnetization in periodic solids and its connection to NMR

Timo Thonhauser

Department of Physics & Astronomy
Rutgers, The State University of New Jersey

THE STATE UNIVERSITY OF NEW JERSEY
RUTGERS

Department of Materials Science and Engineering
Massachusetts Institute of Technology

How can we calculate the orbital magnetization in periodic solids

Why is this important?

$$\vec{H} = \vec{B} - 4\pi\vec{M}$$

$$\vec{M} = \vec{M}_{\text{spin}} + \vec{M}_{\text{orbital}}$$

No theory for periodic solids!

- Interesting in and of itself
- Spintronics
- Magnetic semiconductors
- Anom. Hall effect

Vocabulary (one band in 2D)

Berry connection

$$A_\alpha(\vec{k}) = i\langle u_{\vec{k}}|\partial/\partial k_\alpha|u_{\vec{k}}\rangle$$

Berry curvature

$$\Omega(\vec{k}) = \nabla \times \vec{A}$$

Electric polarization

$$P_\alpha = \frac{q}{(2\pi)^2}\int_{BZ} A_\alpha(\vec{k})\, d^2k$$

Anomalous Hall conductivity

$$\sigma_{xy} = \frac{q^2}{(2\pi)^2\hbar}\int \Omega(\vec{k}) f(E_{\vec{k}} - \mu)\, d^2k$$

Chern number

$$C = \frac{1}{2\pi}\int_{BZ} \Omega(\vec{k})\, d^2k = \frac{1}{2\pi}\oint_{BZ} \vec{A}(\vec{k}) \cdot d\vec{k}$$

Terms & conditions

- one-particle H, broken TR
- B=0, or commensurate

1-particle states labeled by k

- ferromagnetic insulator
- zero Chern numbers

Wannier representable

- spinless electrons
- two dimensional
- isolated occupied band

for simplicity of presentation

- tight-binding model

for tests

Theory

Polarization

Magnetization

fi

eigenstates

$$\vec{d} = -e \sum_i \langle \psi_i | \vec{r} | \psi_i \rangle$$

$$= -e \sum_i \langle w_i | \vec{r} | w_i \rangle$$

loc. mol. orb.

thermod

Theory

Polarization

Magnetization

finite samples

$$\vec{d} = -e\sum_i \langle \psi_i|\vec{r}|\psi_i\rangle$$
$$= -e\sum_i \langle w_i|\vec{r}|w_i\rangle$$

therm

bulk Wannier functions |R>

$$\vec{P} = \frac{\vec{d}}{A} = -\frac{e}{A_0}\langle\vec{0}|\vec{r}|\vec{0}\rangle$$

Theory

Polarization

[…]netization

finite samp[…]

circulation operator

$$\vec{d} = -e\sum_i \langle \psi_i | \vec{r} | \psi_i \rangle = -e\sum_i \langle w_i | \vec{r} | w_i \rangle$$

$$\vec{m} = -\frac{e}{2c}\sum_i \langle \psi_i | \vec{r} \times \vec{v} | \psi_i \rangle = -\frac{e}{2c}\sum_i \langle w_i | \vec{r} \times \vec{v} | w_i \rangle$$

thermodynamic limit

$$\vec{P} = \frac{\vec{d}}{A} = -\frac{e}{A_0}\langle \vec{0} | \vec{r} | \vec{0} \rangle$$

Theory

Polarization | **Magnetization**

finite samples

$$\vec{d} = -e\sum_i \langle \psi_i | \vec{r} | \psi_i \rangle = -e\sum_i \langle w_i | \vec{r} | w_i \rangle$$

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thermodynamic limit

$$\vec{P} = \frac{\vec{d}}{A} = -\frac{e}{A_0}\langle \vec{0} | \vec{r} | \vec{0} \rangle$$

$$\vec{M}_{\mathrm{LC}} = \frac{\vec{m}}{A} = -\frac{e}{2cA_0}\langle \vec{0} | \vec{r} \times \vec{v} | \vec{0} \rangle$$

Theory

Polarization

Magnetization

$$\vec{m} = -\frac{e}{2c}\sum_i \langle \psi_i | \vec{r} \times \vec{v} | \psi_i \rangle$$
$$= -\frac{e}{2c}\sum_i \langle w_i | \vec{r} \times \vec{v} | w_i \rangle$$

compare in a simple tight-binding model

$$\vec{M}_{\rm LC} = \frac{\vec{m}}{A} = -\frac{e}{2cA_0}\langle \vec{0} | \vec{r} \times \vec{v} | \vec{0} \rangle$$

A simple tight-binding model

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

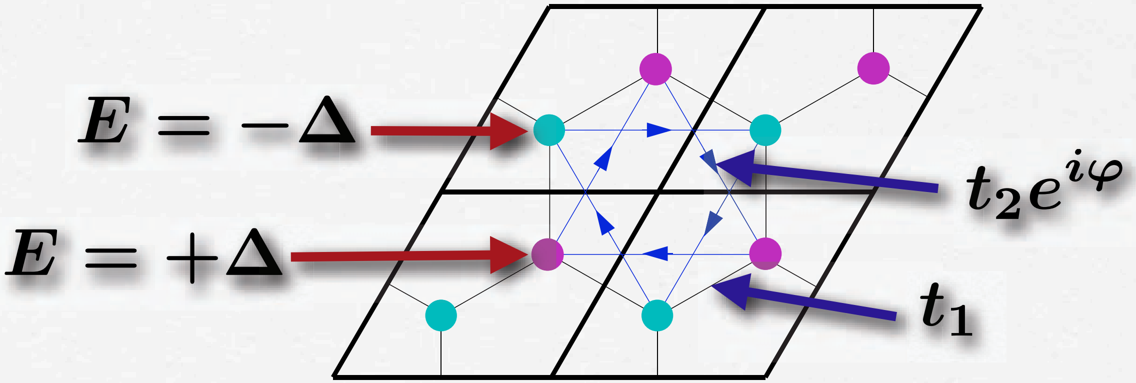
Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

F. D. M. Haldane

Department of Physics, University of California, San Diego, La Jolla, California 92093

(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance σ^{xy} in the *absence* of an external magnetic field. Massless fermions *without spectral doubling* occur at critical values of the model parameters, and exhibit the so-called "parity anomaly" of (2+1)-dimensional field theories.



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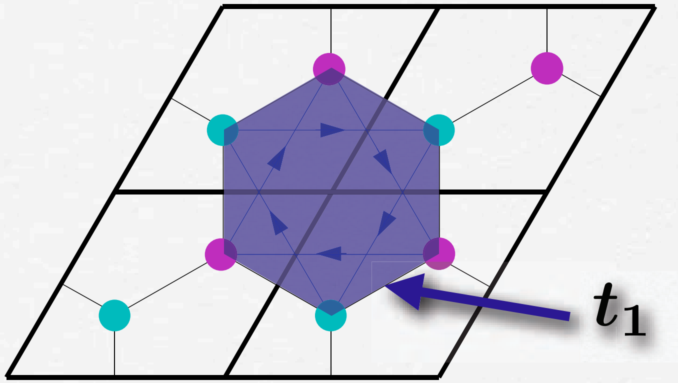
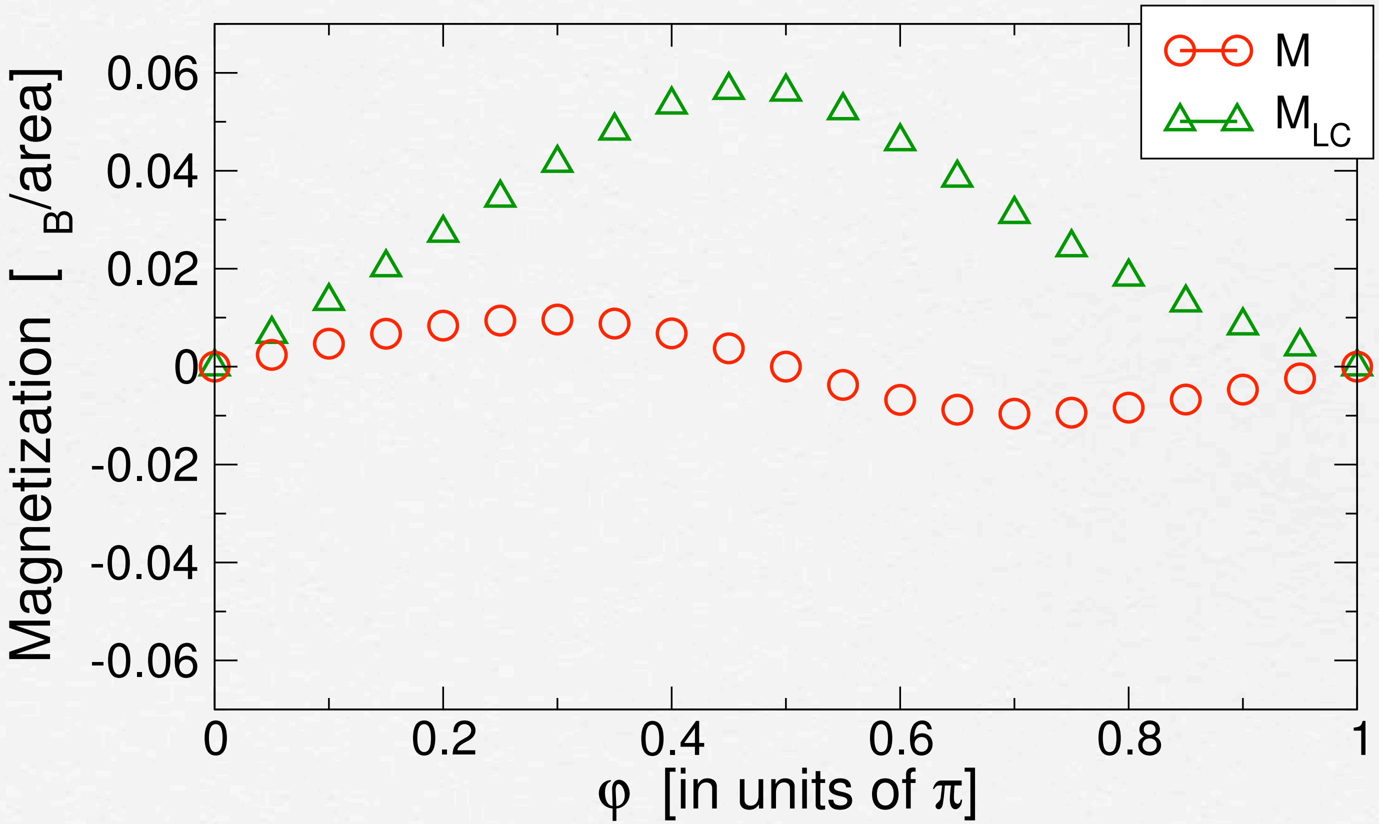


Compare - Numerical results



Something has gone wrong!

compare in a simple tight-binding model

$$\vec{m} = -\frac{e}{2c}\sum_i \langle \psi_i | \vec{r} \times \vec{v} | \psi_i \rangle$$
$$= -\frac{e}{2c}\sum_i \langle w_i | \vec{r} \times \vec{v} | w_i \rangle$$

$$\vec{M}_{\mathrm{LC}} = \frac{\vec{m}}{A} = -\frac{e}{2cA_0}\langle \vec{0} | \vec{r} \times \vec{v} | \vec{0} \rangle$$

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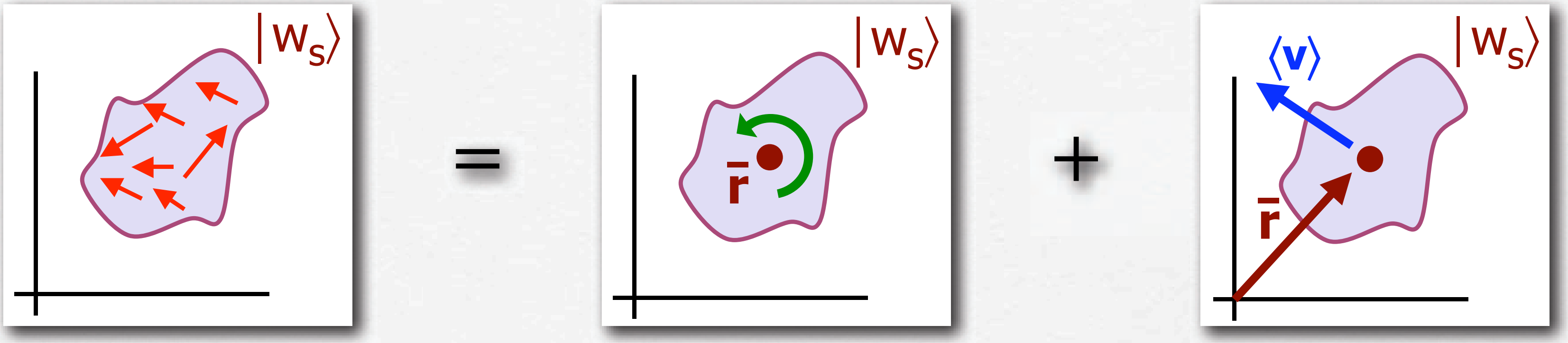
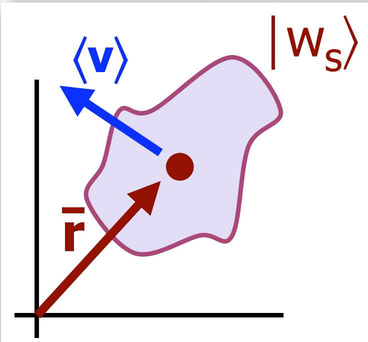


$$\langle w_s|\vec{r}\times\vec{v}|w_s\rangle = \langle w_s|(\vec{r}-\bar{r})\times\vec{v}|w_s\rangle + \bar{r}\times\langle w_s|\vec{v}|w_s\rangle$$

(LC) local circulation

(IC) itinerant circulation

Itinerant circulation



$$\bar{r} \times \langle w_s | \vec{v} | w_s \rangle$$

(IC) itinerant circulation

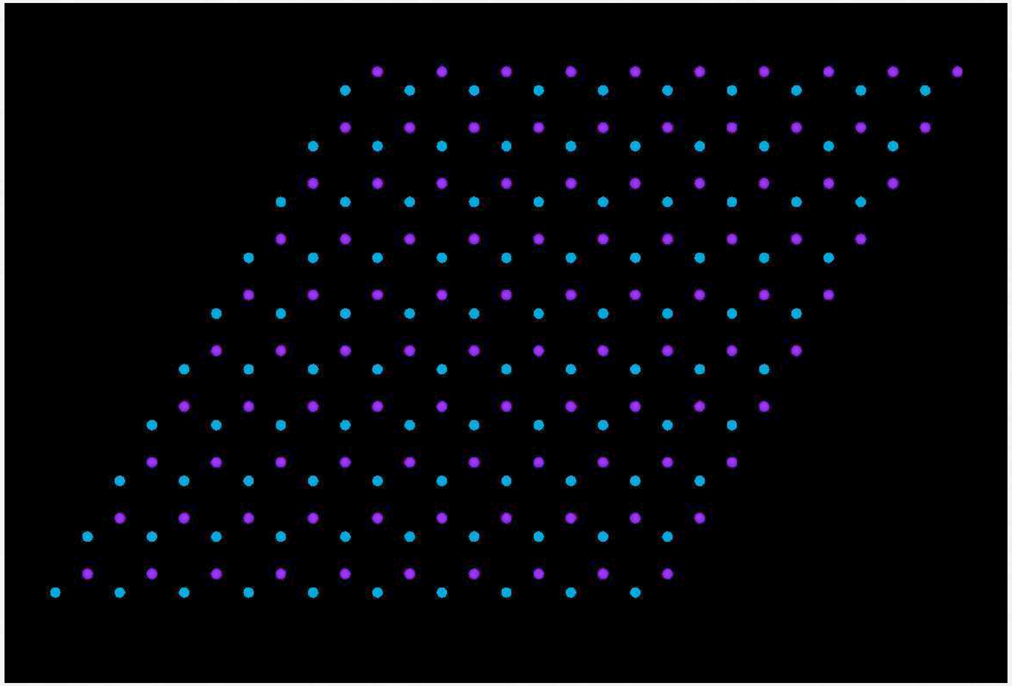
- bulk WF: bulk band carries no net current

  so <v>=0
  so r x <v>=0

- but what about surface WF?

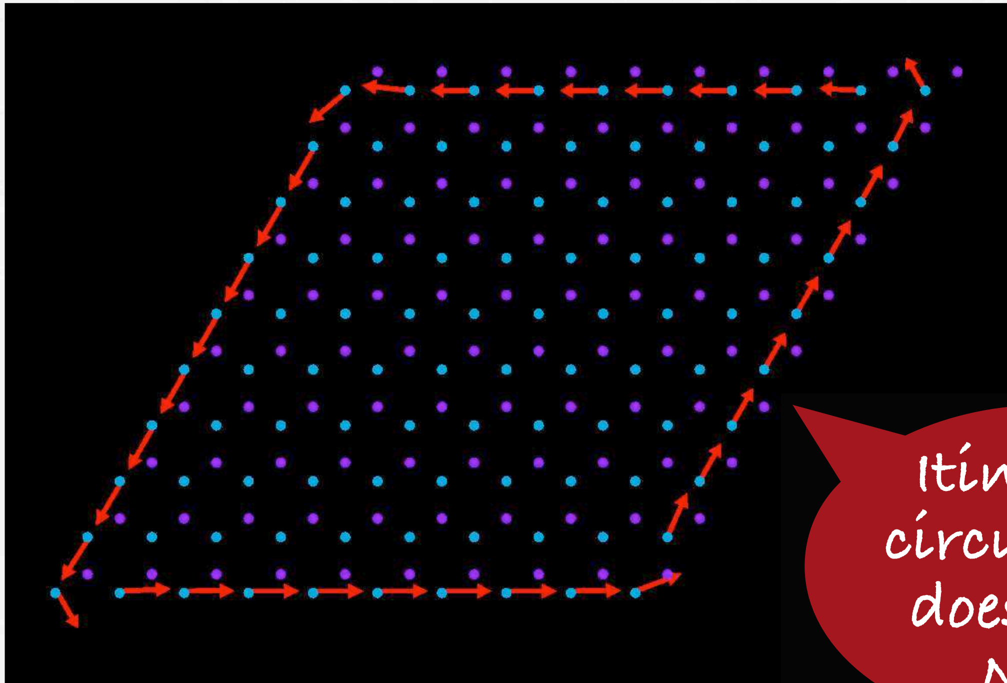
Itinerant circulation

WF currents $-e\langle w_i|\vec{v}|w_i\rangle$



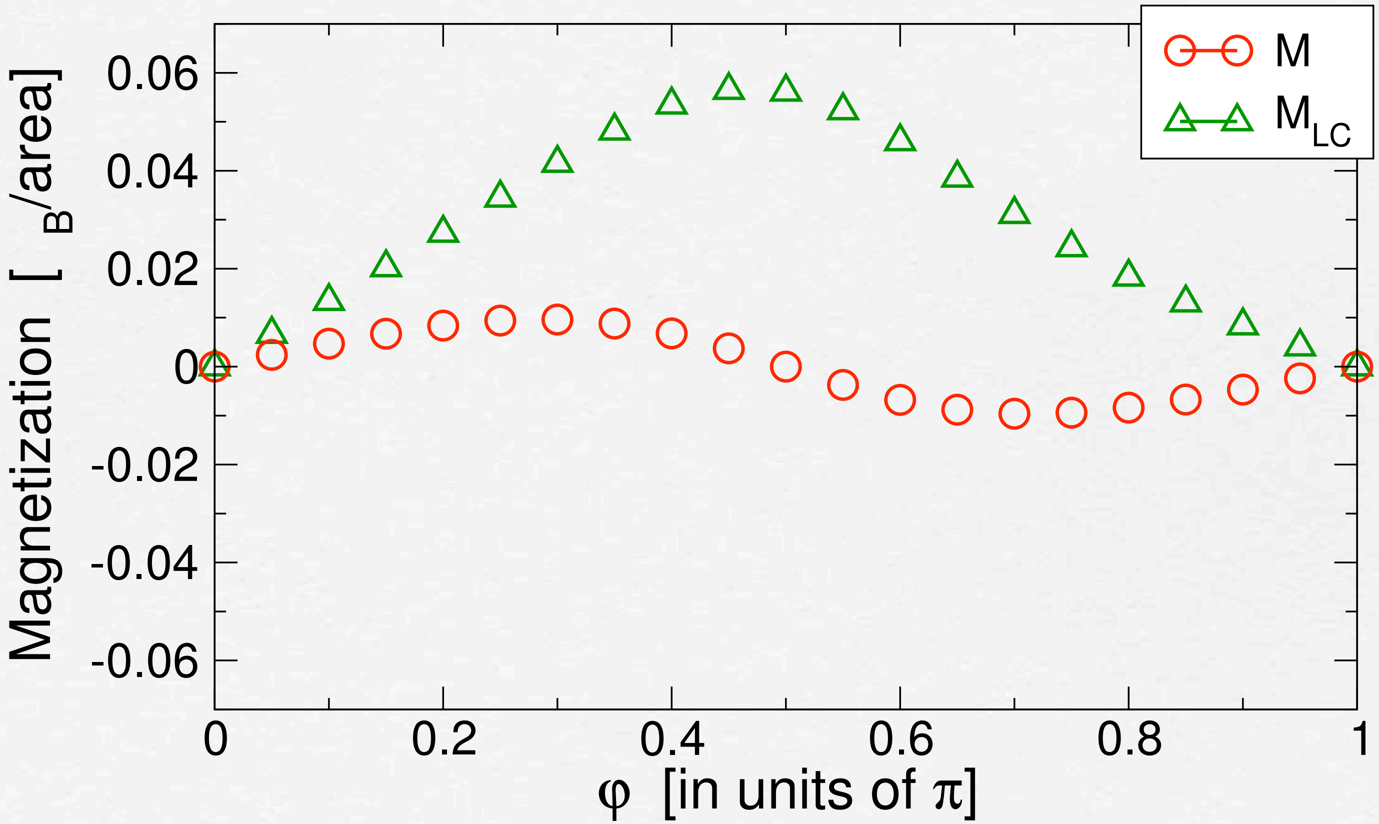
Itinerant circulation

WF currents $-e\langle w_i|\vec{v}|w_i\rangle$

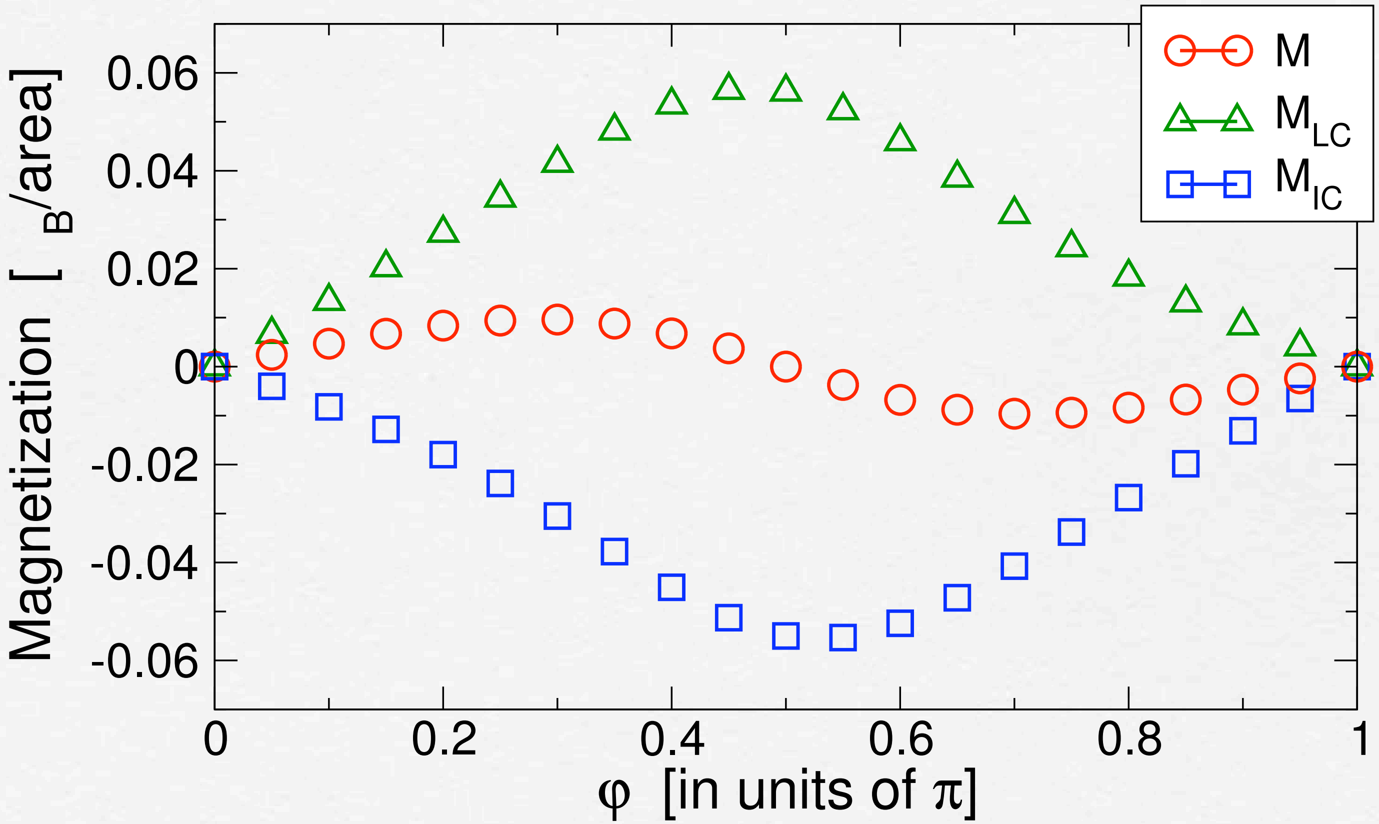


Itinerant circulation does exist M_{IC} !

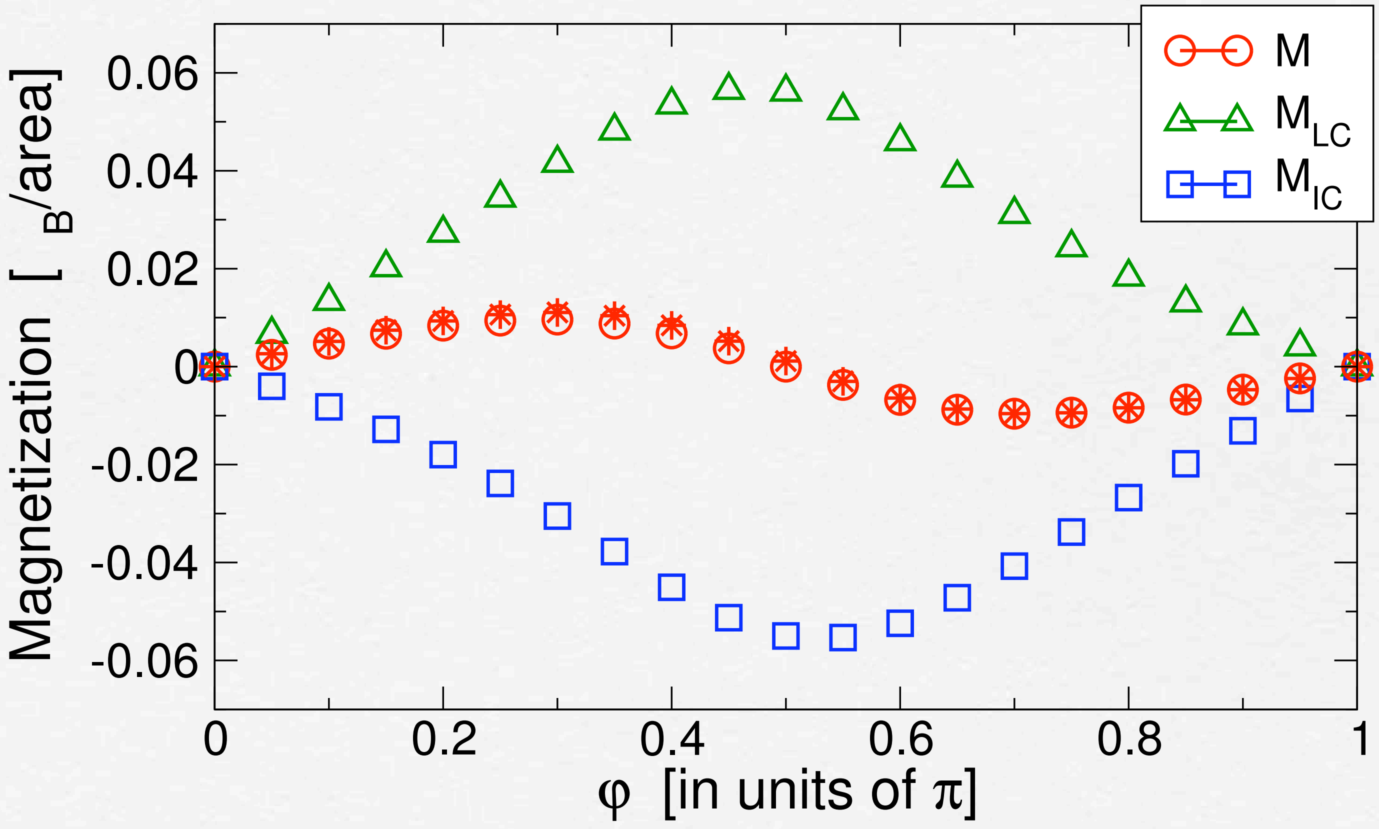
Compare again!



Compare again!

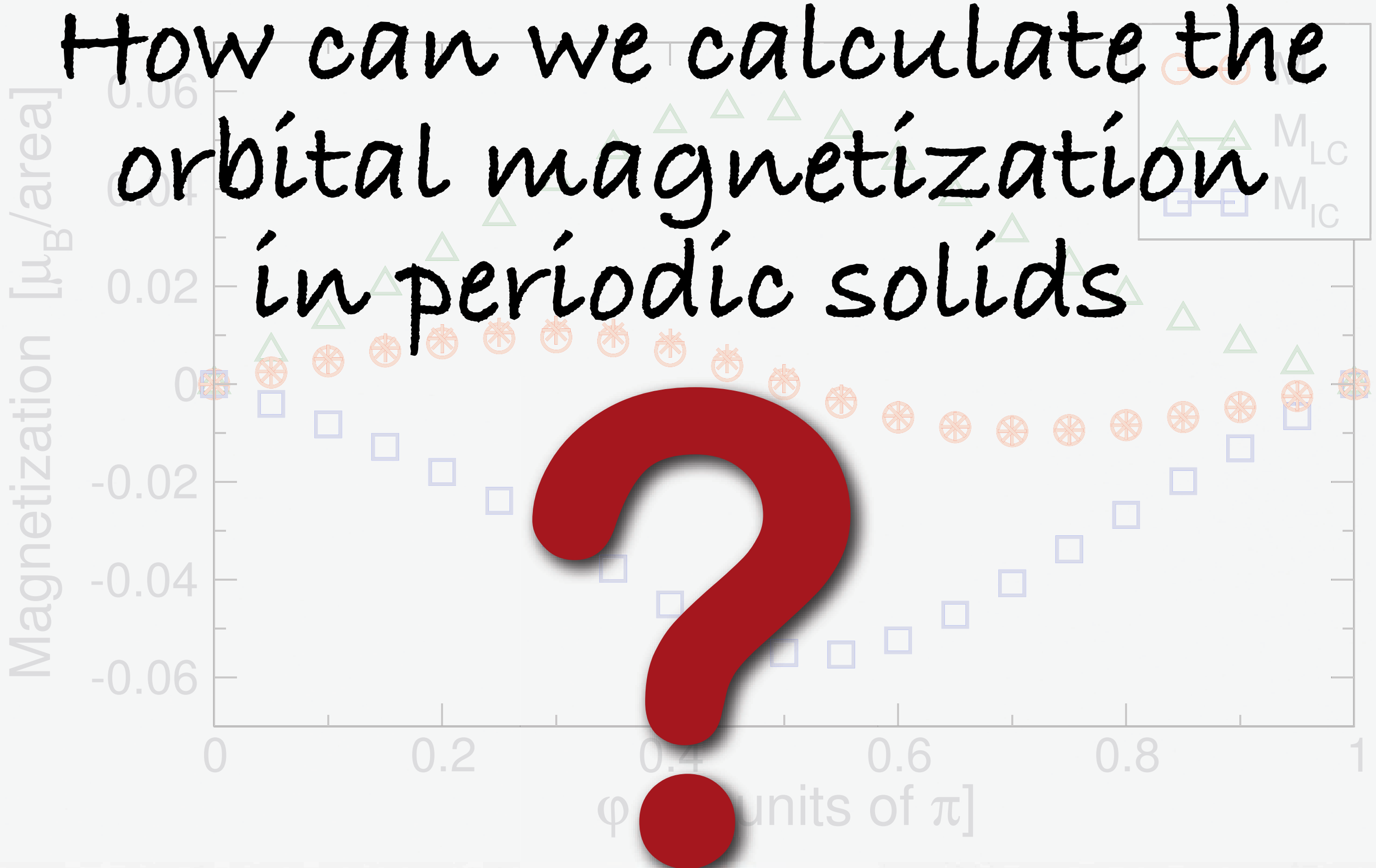


Compare again!



Compare again!

How can we calculate the orbital magnetization in periodic solids



Final result

$$\vec{M}_{\mathrm{LC}} = -\frac{e}{2A_0 c}\langle\vec{0}|\vec{r}\times\vec{v}|\vec{0}\rangle$$

$$\vec{M}_{\mathrm{IC}} = -\frac{e}{2A_0 c\hbar}\sum_{\vec{R}} \mathrm{Im}\left[R_x y_{\vec{R},\vec{0}} H_{\vec{0},\vec{R}} - R_y x_{\vec{R},\vec{0}} H_{\vec{0},\vec{R}}\right]$$

Final result

$$\vec{M}_{\rm LC} = \frac{e}{2\hbar c}\,{\rm Im}\int \frac{d^2k}{(2\pi)^2}\langle \partial_{\vec{k}} u_{\vec{k}}| \times H_{\vec{k}}\,|\partial_{\vec{k}} u_{\vec{k}}\rangle$$

$$\vec{M}_{\rm IC} = -\frac{e}{2\hbar c}\int \frac{d^2k}{(2\pi)^2}\,E_{\vec{k}}\,\Omega_{\vec{k}}$$

Final result

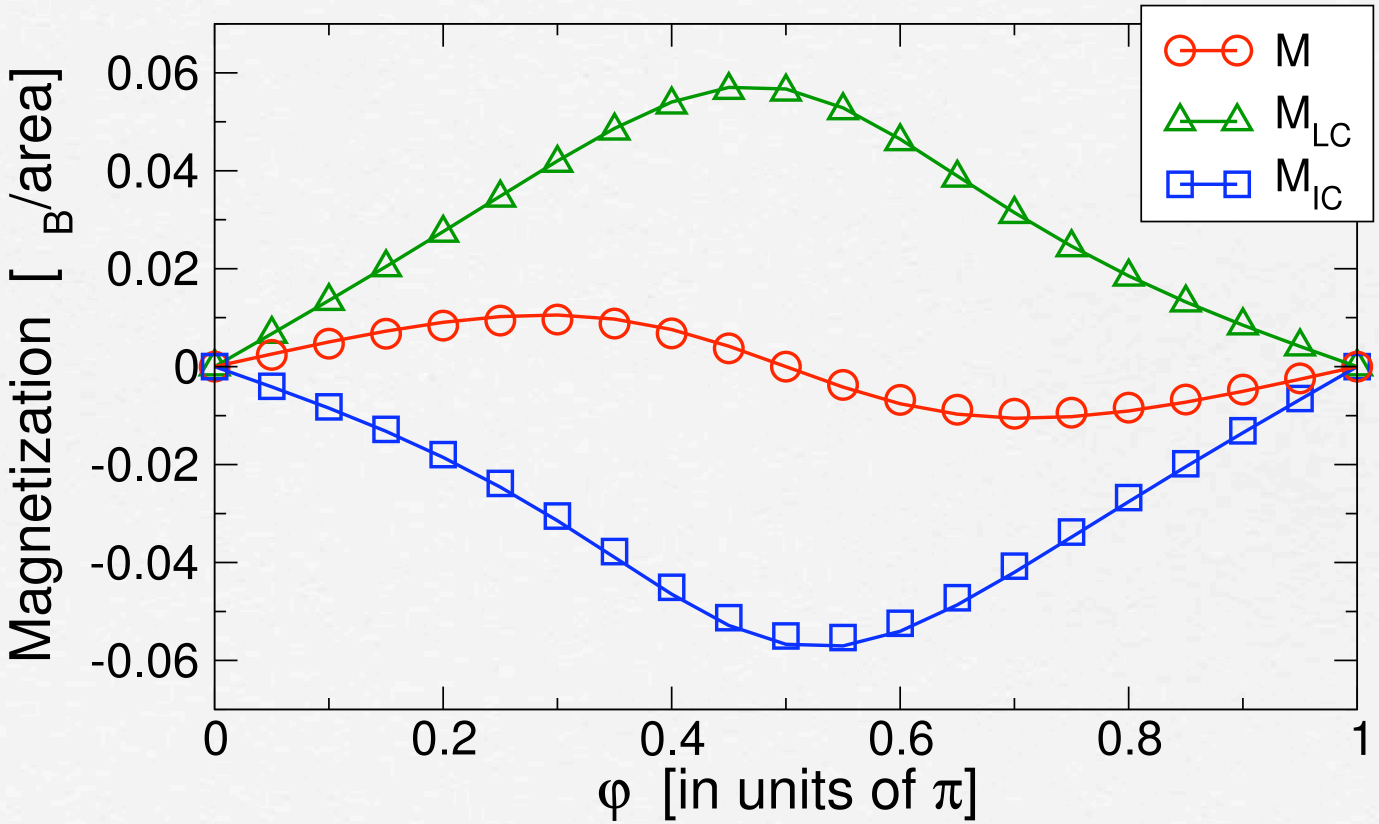
$$\vec{M} = \frac{e}{2\hbar c} \operatorname{Im} \int \frac{d^2k}{(2\pi)^2} \langle \partial_{\vec{k}} u_{\vec{k}} | \times (H_{\vec{k}} + E_{\vec{k}}) | \partial_{\vec{k}} u_{\vec{k}} \rangle$$

Final result

$$\vec{M} = \frac{e}{2\hbar c} \operatorname{Im} \int \frac{d^2k}{(2\pi)^2} \langle \partial_{\vec{k}} u_{\vec{k}} | \times (H_{\vec{k}} + E_{\vec{k}}) | \partial_{\vec{k}} u_{\vec{k}} \rangle$$

- Invariant under H ! H+ΔE
- Gauge invariant $|u_{\vec{k}}\rangle \rightarrow e^{i\phi(\vec{k})}|u_{\vec{k}}\rangle$
- Easy to discretize and implement
- Consistent with Xiao et al.
  PRL 95, 137204 (2005)

Perfect agreement!



Extensions

$$\vec{M} = \frac{e}{2\hbar c} \mathrm{Im} \sum_n \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} \; f(E_{n,\vec{k}} - \mu)$$

$$\langle \partial_{\vec{k}} u_{n,\vec{k}} | \times (H_{\vec{k}} + E_{n,\vec{k}} - 2\mu) | \partial_{\vec{k}} u_{n,\vec{k}} \rangle$$

Extensions

$$\vec{M} = \frac{e}{2\hbar c} \mathrm{Im} \sum_n \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} f(E_{n,\vec{k}} - \mu)$$

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- three dimensions

Extensions

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- ☐ three dimensions
- ☐ multi-band

Extensions

$$\vec{M} = \frac{e}{2\hbar c} \mathrm{Im} \sum_n \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} f(E_{n,\vec{k}} - \mu)$$

$$\langle \partial_{\vec{k}} u_{n,\vec{k}} | \times (H_{\vec{k}} + E_{n,\vec{k}} - 2\mu) | \partial_{\vec{k}} u_{n,\vec{k}} \rangle$$

- ☐ three dimensions
- ☐ multi-band
- ☐ metals ?
- ☐ Non-zero Chern No. ?

Papers & posters

PRL 95, 137205 (2005) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2005

Orbital Magnetization in Periodic Insulators

T. Thonhauser,[1] Davide Ceresoli,[2] David Vanderbilt,[1] and R. Resta[3]

[1]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
[2]*International School for Advanced Studies (SISSA/ISAS) and INFM-DEMOCRITOS, via Beirut 4, 34014, Trieste, Italy*
[3]*Dipartimento di Fisica Teorica Università di Trieste and INFM-DEMOCRITOS, strada Costiera 11, 34014, Trieste, Italy*

(Received 20 May 2005; published 22 September 2005)

Working in the Wannier representation, we derive an expression for the orbital magnetization of a periodic insulator. The magnetization is shown to be comprised of two contributions, an obvious one associated with the internal circulation of bulklike Wannier functions in the interior, and an unexpected one arising from net currents carried by Wannier functions near the surface. Each contribution can be expressed as a bulk property in terms of Bloch functions in a gauge-invariant way. Our expression is verified by comparing numerical tight-binding calculations for finite and periodic samples.

PRL 95, 137205 (2005)

Orbital magnetization in crystalline solids: Multi-band insulators, Chern insulators, and metals

Davide Ceresoli,[1] T. Thonhauser,[2] David Vanderbilt,[2] and R. Resta[3]

[1] International School for Advanced Studies (SISSA/ISAS) and DEMOCRITOS, via Beirut 2-4, 34014 Trieste, Italy
[2] Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA
[3] Dipartimento di Fisica Teorica Università di Trieste and DEMOCRITOS, strada Costiera 11, 34014 Trieste, Italy

We derive a multi-band formulation of the orbital magnetization in a normal periodic insulator (i.e., one in which the Chern invariant, or in 2d the Chern number, vanishes). Following the approach used recently to develop the single-band formalism [T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta, Phys. Rev. Lett. 95, 137205 (2005)], we work in the Wannier representation and find that the magnetization is comprised of two contributions, an obvious one associated with the internal circulation of bulk-like Wannier functions in the interior and an unexpected one arising from net currents carried by Wannier functions near the surface. Unlike the single-band case, where each of these contributions is separately gauge-invariant, in the multi-band formulation only the sum of

PRB 74, 024408 (2006)

Papers & posters

Magnetic circular dichroism and the orbital magnetization of ferromagnets

Ivo Souza[1] and David Vanderbilt[2]

Department of Physics, University of California, Berkeley (USA)

Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey (USA)

Orbital magnetization in a supercell framework: Single k-point formula

D. Ceresoli[1] and R. Resta[2]

1. Scuola Internazionale Superiore di Studi Avanzati (SISSA) and DEMOCRITOS, Trieste, Italy.
2. University of Trieste and DEMOCRITOS, Trieste, Italy.

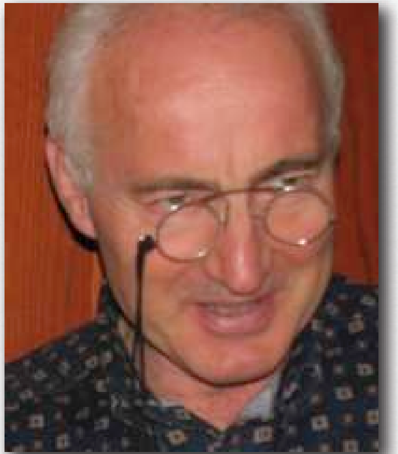
Summary

- Solved long-standing problem and developed a theory of orbital magnetization
- Orbital magnetization is a bulk property
- Sum of two distinct contributions
- Suitable for calculations using standard band-structure codes
- Closely related to NMR

Acknowledgments

Davide Ceresoli

David Vanderbilt



Raffaele Resta

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