Orbital magnetization in insulators with broken time-reversal symmetry

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Collaboration

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Preprints

Motivations: Orbital Magnetization

Much current interest in “spintronics”

- Magnetic semiconductors
- Half metallic magnets
- Spin injection
- Anomalous Hall conductivity
- Spin Hall effect
- Etc.

Back to basics:

\[ H = B - 4\pi M \]

\[ K_{surf} = M \cdot n \]

\[ M = M_{\text{spin}} + M_{\text{orbital}} \]
Motivations: Orbital Magnetization

Condensed Matter, abstract
cond-mat/0502340

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Date: Mon, 14 Feb 2005 18:05:30 GMT (10kb)

Berry phase correction to electron density of states in solids

Authors: Di Xiao, Junren Shi, Qian Niu
Comments: submitted to PRL
Subject-class: Mesoscopic Systems and Quantum Hall Effect

Liouville's theorem on the conservation of phase space volume is violated by Berry phase in the semiclassical dynamics of Bloch electrons. This leads to a modification of the phase space density of states, whose significance is discussed in a number of examples: field modification of the Fermi-sea volume, connection to the anomalous Hall effect, and a general formula for orbital magnetization. The effective quantum mechanics of Bloch electrons is also sketched, where the modified density of states plays an essential role.

$$M = \frac{e}{2\hbar} \int^{\mu_0} \frac{dk}{(2\pi)^d} i \left< \frac{\partial u}{\partial k} \right> \times \left[ 2\mu_0 - \varepsilon_0(k) - \hat{H}_0 \right] \left| \frac{\partial u}{\partial k} \right>$$

Semiclassical argument only!
Motivations: Orbital Magnetization

Our approach:

- Fully quantum
- Based on Wannier representation
- Analogous to Berry-phase theory of polarization
Analogy: Electric Polarization

- $\mathbf{P}$ is a bulk property
  - $\mathbf{P} \cdot \mathbf{n}$

- $\mathbf{P}$ is *only apparently* a surface property

**Conditions and caveats:**
- Bulk is periodic insulator
- Surface is
  - Unreconstructed (1x1)
  - Insulating, in gap common to bulk and surface
- $\mathbf{P}$ only determined up to "quantum" $e/A_{\text{surf}}$

**References**
- King-Smith and Vanderbilt, PRB, 1993.
- Vanderbilt and King-Smith, PRB, 1993.
Orbital Magnetization

\[ K = M \times n \]

Is \( M \) a bulk property?

Is \( K \) only apparently a surface property?

**Definition:**

If \( K \) is predetermined at all surfaces in such a way that \( K = M \times n \) for some vector \( M \), then \( M \) is the bulk magnetization.
**Orbital Magnetization**

**Clarification:**

- Microscopic $M(r)$ defined via $\mathbf{n} \times M(r) = J(r)$
- $M(r)$ ill-defined: $M(r) \not= M(r) + M_0 + \mathbb{I}$
- Therefore, cannot define $M$ as cell average of $M(r)$

**Conclusion:** $M$ is not, even in principle, a functional of the bulk current distribution $J(r)$

(Hirst, RMP, 1997)

Just as: $P$ is not, even in principle, a functional of the bulk charge density distribution $\rho(r)$
Strong reasons to expect bulk $M$

- Nearsightedness: Surface current depends only on local environment

- Stationary quantum state: $d\mathcal{J}/dt = 0$

- Conservation of charge: $\Box \cdot \mathbf{J} = 0$

So: $I_y^{(A)} = I_y^{(B)} = M_z$
Central Claims of This Work

- Orbital magnetization is a bulk property
- Expandable in terms of bulk band-structure properties
- Closely related to Berry phases and Berry curvature
- Sum of two distinct contributions
- Suitable for calculation using standard band-structure codes
Theoretical Context

- One-particle Hamiltonian \([H, TR] \neq 0\)
- \(B_{\text{macro}} = 0\) (or commensurate)
- Insulator
- Chern number \(C = 0\)
- Spinless electrons
- 2D
- Isolated occupied band
- Tight-binding models

\(1\)-particle states labeled by \(k\)

Wannier representable

For simplicity of presentation

For tests
Vocabulary (One band in 2D)

Derivatives act in 2D k-space

\[ k_\alpha, \quad \alpha = \{x, y\} \]

Berry connection

\[ A_\alpha(k) = i \langle u_k | \frac{\partial}{\partial k_\alpha} | u_k \rangle \]

Berry curvature

\[ \Omega(k) = \nabla \times A = \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \]

Chern number

\[ C = \frac{1}{2\pi} \int_{\text{BZ}} \Omega(k) \, d^2k = \frac{1}{2\pi} \oint_{\text{BZ}} A(k) \cdot dk \]

Anomalous Hall conductivity

\[ \sigma_{xy} = \frac{q^2}{(2\pi)^2 \hbar} \int_{\text{BZ}} \Omega(k) f(E_k - \mu) \, d^2k \]

Electric polarization

\[ P_\alpha = \frac{q}{(2\pi)^2} \int_{\text{BZ}} A_\alpha(k) \, d^2k \]

Bloch function

\[ \psi_k(r) = e^{i k \cdot r} u_k(r) \]
Derivation of Electric Polarization

Dipole moment of finite sample

\[ d_x = q \sum_j \langle \psi_j | x | \psi_j \rangle \quad |\psi_j\rangle = \text{Eigenstate} \]
\[ = q \sum_m \langle w_m | x | w_m \rangle \quad |w_m\rangle = \text{Loc. molec. orb.} \]

Thermodynamic limit

\[ |w_m\rangle \rightarrow |R\rangle \quad |R\rangle = \text{Bulk Wannier func.} \]

\[ P_x = \frac{d_x}{A_{\text{sample}}} = \frac{q}{A_0} \langle 0 | x | 0 \rangle \]
Derivation of Electric Polarization

Transform to $k$-space

$$|R\rangle = \frac{A_0}{(2\pi)^2} \int_{BZ} d^2k \ e^{ik \cdot (r-R)} |u_k\rangle$$

$$x \ |R\rangle = i \frac{A_0}{(2\pi)^2} \int_{BZ} d^2k \ e^{ik \cdot (r-R)} \left| \frac{\partial u_k}{\partial k_x} \right\rangle$$

$$y \ |R\rangle = i \frac{A_0}{(2\pi)^2} \int_{BZ} d^2k \ e^{ik \cdot (r-R)} \left| \frac{\partial u_k}{\partial k_y} \right\rangle$$

$$P_\alpha = \frac{iq}{(2\pi)^2} \int_{BZ} d^2k \ \langle u_k | \frac{\partial}{\partial k_\alpha} | u_k \rangle$$
Derivation of Orbital Magnetization?

**Magnetization of finite sample**

\[
M = \frac{q}{2Ac} \sum_j \langle \psi_j | xy - yx | \psi_j \rangle
\]

\[
= \frac{-iq}{2\hbar Ac} \sum_m \langle w_m | x[y, H] - y[x, H] | w_m \rangle
\]

\[
= \frac{-q}{\hbar Ac} \text{Im} \sum_m \langle w_m | xHy | w_m \rangle
\]

**Magnetization in thermodynamic limit**

\[
M_{LC} = \frac{-q}{\hbar c A_0} \text{Im} \langle 0 | xHy | 0 \rangle
\]
Derivation of Orbital Magnetization?

\[ M_{LC} = \frac{-q}{\hbar c A_0} \Im \langle 0 | x H y | 0 \rangle \]

Transform to k-space

\[ M_{LC} = \frac{-q}{\hbar c} \Im \int_{BZ} \frac{d^2 k}{(2\pi)^2} \left\langle \frac{\partial u_k}{\partial k_x} \right| H_k \left| \frac{\partial u_k}{\partial k_y} \right\rangle \]
Numerical Tests: Haldane model

Tight-binding model of Haldane, 1988

\[ E = +D \]

\[ E = -D \]
Complex hoppings and flux tubes

$t_{12} = |t_0| \exp (+i\phi)$

$t_{21} = |t_0| \exp (-i\phi)$
Numerical Tests: Haldane model

Tight-binding model of Haldane, 1988

\[ E = + \]  \[ E = - \]

\[ |t_2| \exp(i\square) \]

\[ t_1 \text{ (real)} \]
Numerical Tests: Haldane model

Tight-binding model of Haldane, 1988

Haldane Model
\[ t_1 = 1, \ t_2 = 1/3 \]

- \( \text{chern} = 0 \)
- \( \text{chern} = -1 \)
- \( \text{chern} = +1 \)

\[ \Delta t_2 \]

\[ \text{flux \ [in \ units \ of \ } \pi \text{]} \]
Numerical Tests: Haldane model

Tight-binding model of Haldane, 1988
Numerical Tests: Haldane model
Derivation of Orbital Magnetization?

Magnetization of finite sample

\[
M = \frac{q}{2Ac} \sum_j \langle \psi_j | xv_y - yv_x | \psi_j \rangle
\]

\[
= \frac{-iq}{2\hbar Ac} \sum_m \langle w_m | x[y, H] - y[x, H] | w_m \rangle
\]

\[
= \frac{-q}{\hbar Ac} \text{Im} \sum_m \langle w_m | xHy | w_m \rangle
\]

Magnetization in thermodynamic limit

\[
M_{LC} = \frac{-q}{\hbar c A_0} \text{Im} \langle 0 | xHy | 0 \rangle
\]
Numerical Tests: Haldane model

\[ M_{\text{LC}} = \frac{-q}{\hbar A_0} \text{Im} \langle 0 | x H y | 0 \rangle \]

\[ M = \frac{q}{2 A c} \sum_j \langle \psi_j | xv_y - yv_x | \psi_j \rangle \]
What is missing?

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

- Local Circulation (LC)
- Itinerant Circulation (IC)
Itinerant Circulation

- **Bulk WF:**
  - Bulk band carries no net current
  - So $\mathbf{v} = 0$
  - So $\mathbf{r} \times \mathbf{v} = 0$

- **But what about a surface WF?**

$\mathbf{r} \times \mathbf{v} = 0$

$\mathbf{r} \times \langle w_s | \mathbf{v} | w_s \rangle$
Numerical Tests: Haldane model

Itinerant circulation does exist!
Numerical Tests: Haldane model
Numerical Tests: Haldane model

Is itinerant circulation a bulk quantity?
I_s = q \langle w_s | v | w_s \rangle

= \frac{-i q}{\hbar} \langle w_s | [r, H] | w_s \rangle \sum_{s'} |w_{s'}\rangle\langle w_{s'}|

= \frac{2q}{\hbar} \sum_{s' \neq s} \text{Im} \langle w_s | r | w_{s'} \rangle \langle w_{s'} | H | w_s \rangle

= \frac{2q}{\hbar} \sum_{s' \neq s} \text{Im} \ r_{ss'} H_{s's}

Understanding Itinerant Circulation
Understanding Itinerant Circulation

Region $S$

\[ I_S = \sum_{s \in S} \sum_{s' \notin S} \frac{2q}{\hbar} \text{Im} \, r_{ss'} \, H_{s's} \]

Sum over blue links only
Understanding Itinerant Circulation

Thickness:
<< Sample size
>> Unit cell

\[ I_y = \frac{q}{A_0 \hbar} \sum_{R} R_x \text{Im} y_{R,0} H_{0,R} \]
Understanding Itinerant Circulation

\[ I_y = \frac{q}{A_0 \hbar} \sum_R R_x \text{Im} \ y_{R,0} \ H_{0,R} \]

\[ M_{IC} = \frac{-q}{2 A_0 \hbar c} \sum_R \text{Im} \left( R_x y_{0,R} \ H_{R,0} - R_y x_{0,R} \ H_{R,0} \right) \]

\[ M_{IC} \text{ can be written in terms of WFs!} \]

\[ \square \ M_{IC} \text{ is a bulk quantity!} \]
Understanding Itinerant Circulation

\[ M_{IC} = \frac{-q}{2A_0\hbar c} \sum_R \text{Im} \left( R_x y_{0,R} H_{R,0} - R_y x_{0,R} H_{R,0} \right) \]

\[ \langle 0|x|R \rangle = \frac{A_0}{(2\pi)^2} \int d^2k A_x(k) e^{-ik\cdot R} \]

\[ \langle 0|y|R \rangle = \frac{A_0}{(2\pi)^2} \int d^2k A_y(k) e^{-ik\cdot R} \]

\[ \langle 0|H|R \rangle = \frac{A_0}{(2\pi)^2} \int d^2k E(k) e^{-ik\cdot R} \]

\[ M_{IC} = \frac{q}{2\hbar c} \int \frac{d^2k}{(2\pi)^2} E(k) \nabla \times A(k) \]

\[ M_{IC} = \frac{q}{2\hbar c} \int \frac{d^2k}{(2\pi)^2} E(k) \Omega(k) \]
Two Contributions to the Magnetization

\[ M = M_{\text{LC}} + M_{\text{IC}} \]

\[ M_{\text{LC}} = \frac{-q}{\hbar c} \text{Im} \int_{\text{BZ}} \frac{d^2k}{(2\pi)^2} \langle \frac{\partial u_k}{\partial k_x} | H_k | \frac{\partial u_k}{\partial k_y} \rangle \]

\[ M_{\text{IC}} = \frac{q}{2\hbar c} \int \frac{d^2k}{(2\pi)^2} E(k) \Omega(k) \]

\[ M = \frac{-q}{\hbar c} \text{Im} \int_{\text{BZ}} \frac{d^2k}{(2\pi)^2} \langle \frac{\partial u_k}{\partial k_x} | H_k + E_k | \frac{\partial u_k}{\partial k_y} \rangle \]
Numerical Tests: Haldane model
Two Contributions to the Magnetization

\[ M = M_{LC} + M_{IC} \]

\[ M = \frac{-q}{\hbar c} \text{Im} \int_{\text{BZ}} \frac{d^2 k}{(2\pi)^2} \left\langle \frac{\partial u_k}{\partial k_x} \middle| H_k + E_k \middle| \frac{\partial u_k}{\partial k_y} \right\rangle \]

- Each contribution invariant under \( H \otimes H + \otimes E \)
- Each contribution gauge invariant \( (|u_k\rangle \otimes e^{i\theta(k)}|u_k\rangle) \)
- Consistent with result of Xiao et al.

\[ M = \frac{e}{2\hbar} \int_{\mu_0} \frac{d k}{(2\pi)^d} i \left\langle \frac{\partial u}{\partial k} \right| \times [2\mu_0 - \epsilon_0(k) - \hat{H}_0] \left| \frac{\partial u}{\partial k} \right\rangle \]

Needed for metals or non-zero Chern
Future Challenges

- One-particle Hamiltonian $[H, TR] 
eq 0$
- $B_{\text{macro}} = 0$ (or commensurate)
- Insulator
- Chern number $C = 0$
- Spinless electrons
- 2D
- Isolated occupied band
- Tight-binding models

1-particle states labeled by $k$
Summary

• Orbital magnetization is a bulk property
• Expandable in terms of bulk band-structure properties
• Closely related to Berry phases and Berry curvature
• Sum of two distinct contributions
• Suitable for calculation using standard band-structure codes
• Generalizable for metals, Chern insulators?