Theory of Berry phases for Bloch states: Polarization and more

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Outline

• Intro to Berry phases and curvatures
• Electric polarization and Wannier functions
• Anomalous Hall effect
• Orbital magnetization
• Linear magnetoelectric coupling
• Topological insulators: Next lecture
• Summary
Berry phases

\[
\begin{align*}
|u_4\rangle & \quad |u_3\rangle \\
|u_2\rangle & \\
|u_n\rangle = |u_1\rangle & \\
|u_{n-1}\rangle & \quad |u_1\rangle \\
|u_y\rangle & \\
|u_x\rangle & \\
|u_z\rangle & \\
\end{align*}
\]

Example:

\[
\phi = -\text{Im} \ln \left[ \langle u_1 | u_2 \rangle \langle u_2 | u_3 \rangle \ldots \langle u_{n-1} | u_n \rangle \right]
\]

Check: \( |\tilde{u}_2\rangle = e^{i\beta} |u_2\rangle \) has no effect.
Example

Let \(|u_z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\)

Let \(|u_x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}\)

Let \(|u_y\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}\)

Then \(\phi = \text{Arg} \langle u_z | u_x \rangle \langle u_x | u_y \rangle \langle u_y | u_z \rangle\)

\[= \text{Arg} (1) (1 + i) (1)\]

\[= \pi / 4\]
Berry phases

Now take limit that density of points $\to \infty$

$$\phi = -\text{Im} \ln \left[ \langle u_1 | u_2 \rangle \langle u_2 | u_3 \rangle \ldots \langle u_{n-1} | u_n \rangle \right]$$
Berry phases

\[ \phi = -\text{Im} \int d\lambda \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle \]

\[ \phi = -\text{Im} \int d\lambda \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle \]

\[ \phi \text{ is well-defined modulo } 2\pi \]

\[ \Rightarrow \phi \text{ is a phase} \]
Berry phases

$$\phi = -\text{Im} \int d\lambda \left| u_\lambda \right\rangle \frac{d}{d\lambda} \left| u_\lambda \right\rangle$$

Let

$$|\tilde{u}_\lambda\rangle = e^{-i\beta(\lambda)} |u_\lambda\rangle \text{ with } \beta(1) - \beta(0) = 2\pi m$$

$$\Rightarrow \tilde{\phi} = \phi + 2\pi m$$

$\phi$ is well-defined modulo $2\pi$

$\Rightarrow \phi$ is a phase
Berry phases

Berry potential

\[ A(\lambda) = i \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle \]

Berry phase

\[ \phi = \int A(\lambda) \, d\lambda \]

Gauge transformation:

\[ |\tilde{u}_\lambda\rangle = e^{-i\beta(\lambda)} |u_\lambda\rangle \]

A is gauge-dependent but \( \phi \) is well-defined modulo 2\( \pi \)
Berry phase and curvature

Famous example: Spinor in magnetic field

\[ \phi = -\text{Im} \int d\lambda \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle \]

\[ \phi = \text{(solid angle)}/2 \]
Berry curvature

\[ F = \frac{\Delta \phi}{\Delta A_\lambda} \]

\[ \phi = \int \mathcal{F}(\lambda) \, dS_\lambda \]

\[ \mathcal{F} = -2 \text{Im} \left\langle \frac{du}{d\lambda_x} \left| \frac{du}{d\lambda_y} \right\rangle \right\rangle \]

Berry phase per unit area
The integral of the Berry curvature over any closed 2D manifold must be $2\pi C$ where $C$ is an integer known as the Chern number.
Chern theorem

Stokes applied to A:

\[ \phi = \int_{A} \mathcal{F}(\lambda) \, dS_\lambda \mod 2\pi \]

Stokes applied to B:

\[ \phi = -\int_{B} \mathcal{F}(\lambda) \, dS_\lambda \mod 2\pi \]

Subtract:

\[ 0 = \int \mathcal{F}(\lambda) \, dS_\lambda \mod 2\pi \]

Chern theorem:

\[ \int \mathcal{F}(\lambda) \, dS_\lambda = 2\pi C \]
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\[ P = \frac{d_{cell}}{V_{cell}} \]

\[ d_{cell} = \int_{cell} r \rho(r) d^3r \]

\[ d_{cell} \approx 0 \]
$P = d_{\text{cell}} \div V_{\text{cell}}$ ?

$d_{\text{cell}} = \int_{\text{cell}} r \rho(r) \, d^3r$

$d_{\text{cell}} = \uparrow$
$P = \frac{d_{\text{cell}}}{V_{\text{cell}}}$?

\[ d_{\text{cell}} = \int_{\text{cell}} r \, \rho(r) \, d^3r \]

\[ d_{\text{cell}} = \downarrow \]
Modern Theory of Polarization

Problem:

Knowledge of bulk charge density $\rho(r)$ is not enough, even in principle, to determine $\mathbf{P}$!

Solution:

Go beyond $|\psi_{nk}(r)|^2$ to access Berry phase information hidden in $\psi_{nk}(r)$

Resta, Ferroelectrics 136, 51 (1992)

King-Smith and Vanderbilt, PRB 47, 1651 (1993)
Berry phases in crystalline insulators

$(\lambda_x, \lambda_y) \Rightarrow (k, \lambda)$

General Parametric Hamiltonian

1D insulator with adiabatic parameter
Change of notation

Berry curvature: \( \mathcal{F} \rightarrow \Omega \)

\[
\phi = \int \Omega(\lambda) \, dS_\lambda
\]

\[
\Omega = -2 \text{Im} \left\langle \frac{du}{d\lambda_x} \left| \frac{du}{d\lambda_y} \right. \right\rangle
\]
1D: BZ is really a loop

- Reciprocal space is really periodic
- Brillouin zone can be regarded as a loop
Parametric 1D Ham. (Open path)

Berry curvature $\Omega^{(k\lambda)}$

$$\Delta P = -\frac{e}{2\pi} \int dk \int_{\lambda_1}^{\lambda_2} d\lambda \Omega^{(k\lambda)}$$

$$= \frac{e}{2\pi} \phi(\lambda_2) - \frac{e}{2\pi} \phi(\lambda_1)$$

$$P(\lambda) = \frac{e}{2\pi} \phi(\lambda) \pmod{e}$$

(Resta, 1993)
1D: Polarization

\[ \phi = -\text{Im} \int dk_x \langle u_k | \frac{d}{dk_x} | u_k \rangle \]

\[ P = \frac{-e}{2\pi} \sum_{n}^{\text{occ}} \phi_n \]

King-Smith & V., 1993
Under an adiabatic cycle,

\[ \Delta P = \frac{e}{2\pi} \oint d\lambda \oint dk \Omega(k, \lambda) \]

By Chern theorem,

\[ \Delta P = n e \]

( \( n = \) TKNN invariant = integer )
Polarization in a 2D insulator

\[ \phi(k_x) = -\text{Im} \ln \left[ \langle u_1 | u_2 \rangle \langle u_2 | u_3 \rangle \ldots \langle u_{n-1} | u_n \rangle \right] \]

\[ P_y(k_x) \propto \phi(k_x) \]
Discretized formula in 3D

\[ P_n = \frac{-1}{2\pi} \frac{e}{\Omega} \sum_j \phi_{n,j} R_j \quad \text{where} \quad \phi_{n,j} = \frac{1}{N_{k\perp}} \sum_{k\perp} \phi_n(k\perp) \]

\[ P = P^{\text{elec}} + P^{\text{ion}} \quad \text{where} \quad P^{\text{ion}} = \frac{e}{V_{\text{cell}}} \sum_{\tau} Z^{\text{ion}}_{\tau} r_{\tau} \]
Sample Application: Born $Z^*$

$$Z^*_{j\alpha\beta} = \frac{dP_\alpha}{dR_{j\beta}} \sim \frac{\Delta P_\alpha}{\Delta R_{j\beta}}$$

$Z^*(Ba) = +2 \text{ e}$?

$Z^*(Ti) = +4 \text{ e}$?

$Z^*(O_{I}) = -2 \text{ e}$?

$Z^*(O_{II}) = -2 \text{ e}$?
Summary: Theory of Polarization

- $P$ cannot be expressed in terms of the bulk charge density
- $P$ can be expressed in terms of the Berry phases of the Bloch bands
- Provides practical approach to calculation of $P$
- Alternate and equivalent view: Wannier functions
Choose Wannier functions as

\[ w_n(r - R) = \int_{BZ} \psi_{nk}(r) e^{-i\mathbf{k} \cdot \mathbf{R}} d\mathbf{k} \]

Form wave-packet = “Wannier function”
Tutorial on Wannier functions

Crystal in real space:

Brillouin zone in reciprocal space:
Tutorial on Wannier functions

Crystal in real space:

Brillouin zone in reciprocal space:
Tutorial on Wannier functions

Crystal in real space:

Brillouin zone in reciprocal space:

\[ w_R(r) = \sum_k \psi_k(r) e^{-i k \cdot R} \, dk \]

\[ w_0(r) = \sum_k \psi_k(r) \, dk \]
Tutorial on Wannier functions

Centers of Wannier functions:

\[ \langle w_0 \mid r \mid w_0 \rangle = ? \]
Tutorial on Wannier functions

Centers of Wannier functions:

\[ |w_0\rangle = \frac{V}{(2\pi)^3} \int_{BZ} dk \ |\psi_k\rangle \]

\[ = \frac{V}{(2\pi)^3} \int_{BZ} dk \ e^{ik \cdot r} \ |u_k\rangle \]

\[ r \ |w_0\rangle = \frac{V}{(2\pi)^3} \int_{BZ} dk \ ( - i \nabla_k e^{ik \cdot r} ) \ |u_k\rangle \]

\[ = i \frac{V}{(2\pi)^3} \int_{BZ} dk \ e^{ik \cdot r} \ ( \nabla_k \ |u_k\rangle ) \]

\[ \langle w_0 | r | w_0 \rangle = i \frac{V}{(2\pi)^3} \int_{BZ} dk \ \langle u_k | \nabla_k | u_k \rangle \]
Polarization $\leftrightarrow$ Wannier centers

Centers of Wannier functions:

\[
\langle w_0 | x | w_0 \rangle = i \frac{a}{2\pi} \int_{BZ} dk \langle u_k | \frac{d}{dk} | u_k \rangle = a \frac{\phi}{2\pi}
\]
Polarization ↔ Wannier centers
Total polarization

\[ P = \frac{e}{V_{\text{cell}}} \sum_{\tau} Z^{\text{ion}}_{\tau} \mathbf{r}_{\tau} + \frac{-e}{V_{\text{cell}}} \sum_{n} \mathbf{r}_{n} \]

- Ionic polarization
- Electronic polarization

Each term only well defined modulo \( eR/V_{\text{cell}} \)
Quantum of polarization

\[ \Delta \phi \rightarrow \phi + 2\pi \quad \Rightarrow \quad \mathbf{P} \rightarrow \mathbf{P} + \Delta \mathbf{P} \]

- Spin-polarized systems (spinor bands)
  - 1D: \( \Delta P = ea/a = e \ (C) \)
  - 2D: \( \Delta \mathbf{P} = e\mathbf{R}/A_{\text{cell}} \ (C/m) \) (\( \mathbf{R} = \) lattice vector)
  - 3D: \( \Delta \mathbf{P} = e\mathbf{R}/V_{\text{cell}} \ (C/m^2) \)

- Spin-paired systems (non-magnetic)
  - 1D: \( \Delta P = 2ea/a = 2e \ (C) \)
  - 2D: \( \Delta \mathbf{P} = 2e\mathbf{R}/A_{\text{cell}} \ (C/m) \)
  - 3D: \( \Delta \mathbf{P} = 2e\mathbf{R}/V_{\text{cell}} \ (C/m^2) \)
Quantum of polarization

\[ \Delta P = e \frac{R}{V_{cell}} \]
Quantum of $\mathbf{P}$ under adiabatic cycle

\[
\Delta \mathbf{P} = 0
\]

\[
\Delta \mathbf{P} = e \frac{R}{V_{\text{cell}}}
\]
Quantum of $P$ and surface charge

\[ \Delta P = e \frac{R}{V_{\text{cell}}} \quad \leftrightarrow \quad \Delta \sigma = \Delta P \cdot \hat{n} = e / A_{\text{surf}} \]
Polarization as a lattice-valued quantity

\[ \Delta \mathbf{P} = e \mathbf{R} / V_{\text{cell}} \]

Cubic crystal

\[ \mathbf{P}_0 = 0 \]
\[ \mathbf{P}_0 = (a, 0) \]
\[ \text{etc.} \]

\( \mathbf{P}_0 \) = “Formal polarization”

Cubic crystal

\[ \mathbf{P}_0 = (-a/2, a/2) \]
\[ \mathbf{P}_0 = (a/2, a/2) \]
\[ \text{etc.} \]

\[ \mathbf{P}_0 + \Delta \mathbf{P} \]

Distorted Cubic crystal

\[ \Delta \mathbf{P} = “\text{Effective pol.”} \]
\[ = “\text{Spontaneous pol.”} \]
Examples

Unit cell of “2D Ar crystal”

$P = 0$ etc.

Unit cell of “2D KCl crystal”

$P = (a/2, a/2)$ etc.
Review articles on theory of polarization

• Three useful reviews:

  MACROSCOPIC POLARIZATION IN CRYSTALLINE DIELECTRICS - THE GEOMETRIC PHASE APPROACH
  By: RESTA, R
  REVIEWS OF MODERN PHYSICS Volume: 66 Issue: 3 Pages: 899-915 Published: JUL 1994


• Currently posted at
  http://www.physics.rutgers.edu/~dhv/tmp
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Berry phase and curvature in the BZ

Berry potential:
\[ A(k) = -\text{Im} \langle u_k | \nabla_k | u_k \rangle \]

Berry phase:
\[ \phi = \oint A(k) \cdot dk \]

Berry curvature:
\[ \Omega(k) = \nabla \times A \]
\[ \Omega_z(k) = -2\text{Im} \left\langle \frac{du}{dk_x}, \frac{du}{dk_y} \right\rangle \]

Stoke’s theorem:
\[ \phi = \int \Omega_z(k) \, d^2k \]
Bandstructure of a metal

Fermi Energy $E_F$
Non-magnetic metal: no net Berry curvature

\[ \Omega(\mathbf{k}) = -\Omega(-\mathbf{k}) \]

Time-reversal symmetry

If centrosymmetric too, then \( \Omega = 0 \)

\[ u(k_x, k_y) = u^*(-k_x, -k_y) \]

\[ \Omega(k) = -\Omega(-k) \]

\[ \phi = 0 \]
Magnetic metal: things get interesting

\[ \Omega_z(k) = -2\text{Im} \left\langle \frac{du}{dk_x} \right| \frac{du}{dk_y} \right\rangle \]

\[ \phi = \int_{FS} \Omega_z(k) \, d^2k \]

\[ \sigma_{xy}^{\text{AHE}} = \frac{-e^2}{(2\pi)^3 \hbar} \sum_n \int d^3k \, f_{nk} \Omega_{n,z}(k) \]

(3D)
Ordinary Hall conductivity

\[ R_H = \frac{E_y}{j_x B} = \frac{dV_H}{IB} = -\frac{1}{ne} \]
Anomalous Hall conductivity (AHC)

\[ R_{AH} = \frac{E_y}{j_x} \]
Anomalous Hall conductivity (AHC)

- Karplus-Luttinger theory (1954)
  - Scattering-free, intrinsic
- Skew-scattering mechanism (1955)
  - Impurity scattering
- Side-jump mechanism (1970)
  - Impurity or phonon scattering
- Berry-phase theory (1999)
  - Restatement of Karplus-Luttinger

Sundaram and Niu, PRB 59, 14925 (1999).

\[ \sigma_{xy}^{AHE} = \frac{-e^2}{(2\pi)^3 \hbar} \sum_n \int d^3k \ f_{nk} \Omega_{n,z}(k) \]
A pure bandstructure effect!
Summary of Results

**AHC (Ωcm)$^{-1}$**

<table>
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<th>Bcc Fe</th>
<th>Fcc Ni</th>
<th>Hcp Co</th>
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<tr>
<td><strong>Experimental Value</strong></td>
<td>1032</td>
<td>-752</td>
<td>500</td>
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<tr>
<td><strong>Our theory</strong></td>
<td>771</td>
<td>-2362</td>
<td>478</td>
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</table>

bcc Fe: Calculated Berry curvature over \( k_y = 0 \) plane

DFT (LSDA):
Non-collinear
With spin-orbit

Plane-wave basis
(PWSCF)

Wannier interpolation

\( \Omega(k) \) (atomic units)
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Interstitial regions are not empty!

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

Real crystals look like not

Previous work is mostly based on integrating currents inside muffin-tin spheres

But a knowledge of \( J(\mathbf{r}) \) is insufficient, in principle, to determine \( M \)!
Modern theory of orbital magnetization

• Semiclassical derivation

• Wannier representation derivation

• Long-wave derivation

• Calculations for Fe, Ni, Cu

• Relation to magnetic circular dichroism
Orbital magnetization of 2D insulator

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

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

Is this all?
What is missing?

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

- **Local Circulation (LC)**
- **Itinerant Circulation (IC)**
$M_{\text{orb}}$ in Wannier representation

Local circulation

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

Itinerant circulation

$$M_{\text{IC}} = \frac{-q}{2 A_0 \hbar c} \Im \sum_{\mathbf{R}} \left( R_x \langle 0 | y | \mathbf{R} \rangle - R_y \langle 0 | x | \mathbf{R} \rangle \right) \langle \mathbf{R} | H | 0 \rangle$$
Convert two terms to k-space

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

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

\[ \Omega_z(k) = -2\text{Im} \left\langle \frac{du}{dk_x} \left| \frac{du}{dk_y} \right\rangle \right. \]

(Berry curvature)

\[ M = -\frac{q}{\hbar c} \text{Im} \int_{\text{BZ}} \frac{d^2k}{(2\pi)^2} \left\langle \frac{\partial u_k}{\partial k_x} \right| H_k + E_k \left| \frac{\partial u_k}{\partial k_y} \right\rangle \]
Results for $M_{\text{orb}}$ of Fe, Co and Ni

<table>
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<tr>
<th>Axis</th>
<th>Expt.</th>
<th>This Work</th>
<th>Ref. 14</th>
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</tbody>
</table>

*Experimental easy axis.

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Linear magnetoelectric coupling (MEC)

\[ \alpha_{ij} = -\frac{d^2 E}{d\varepsilon_i d B_j} = \frac{dP_i}{dB_j} = \frac{dM_j}{d\varepsilon_i} \]

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

Spin  Orb.

Spin  Orb.
Frozen-ion orbital MEC

\[ M^{\text{orb}}(\mathcal{E}) \propto \int d\mathbf{k} \langle \nabla_\mathbf{k} u^\mathcal{E}_\mathbf{k} | \times (H_\mathbf{k} + E_\mathbf{k}) | \nabla_\mathbf{k} u^\mathcal{E}_\mathbf{k} \rangle \\
+ e\mathcal{E} \int d\mathbf{k} \epsilon_{ijl} \text{tr} \left[ A_i \nabla_{kj} A_l - \frac{2i}{3} A_i A_j A_l \right] \]

Note

where \( A(k) = \langle u^\mathcal{E}_k | i\nabla_k | u^\mathcal{E}_k \rangle \)

Chern-Simons

Malashevich, Souza, Coh, and Vanderbilt
NJP 12 053032 (2010)
Frozen-ion orbital MEC

\[ \alpha_{da} = \alpha_{da}^{LC} + \alpha_{da}^{IC} + \alpha_{da}^{\text{geom}} \]

\[ \alpha_{da}^{LC} = -\frac{e}{\hbar c} \epsilon_{abc} \int \frac{d^3 k}{(2\pi)^3} \sum_n \text{Im} \langle \tilde{\partial}_b u_{nk} | (\partial_c H_k) | \tilde{\partial}_d u_{nk} \rangle \]

\[ \alpha_{da}^{IC} = -\frac{e}{\hbar c} \epsilon_{abc} \int \frac{d^3 k}{(2\pi)^3} \sum_{mn} \text{Im} \left\{ \langle \tilde{\partial}_b u_{nk} | \tilde{\partial}_d u_{mk} \rangle \langle u_{mk} | (\partial_c H_k) | u_{nk} \rangle \right\} \]

\[ \alpha_{da}^{\text{geom}} = \frac{\theta}{2\pi} \frac{e^2}{\hbar c} \delta_{da} \]

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

NG = non-geometric

CS = Chern-Simons

RUTGERS

MASTANI School, Pune, India, July 10 2014
Gauge properties of CS piece

It turns out that:

• $\theta_{\text{geom}}$ is only well-defined modulo $2\pi$
• Just as $\phi_{\text{Berry}}$ is only well-defined modulo $2\pi$
• In fact, there are close mathematical relations between the two...

Consequences for topological insulators...

$$\alpha_{da}^{\text{geom}} = \frac{\theta}{2\pi} \frac{e^2}{hc} \delta_{da}$$

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

$$A(k) = -\text{Im} \langle u_k | \nabla_k | u_k \rangle$$

CS = Chern-Simons
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