Theory of Berry phases for Bloch states: Polarization and more

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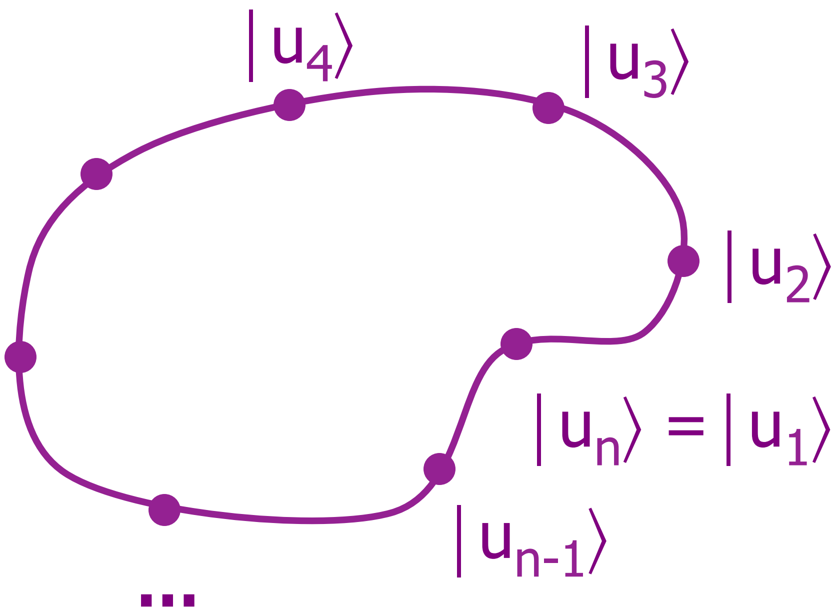
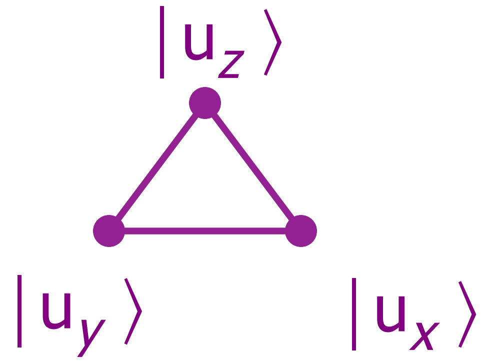
Outline

- 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



Example:



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

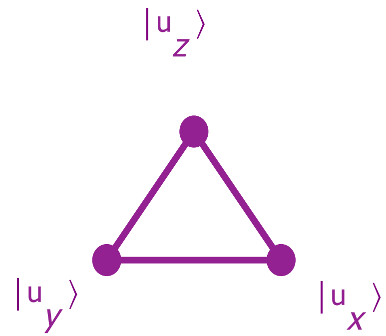
Check: $|\widetilde{u}_2\rangle = e^{i\beta}\,|u_2\rangle$ has no effect.

Example

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

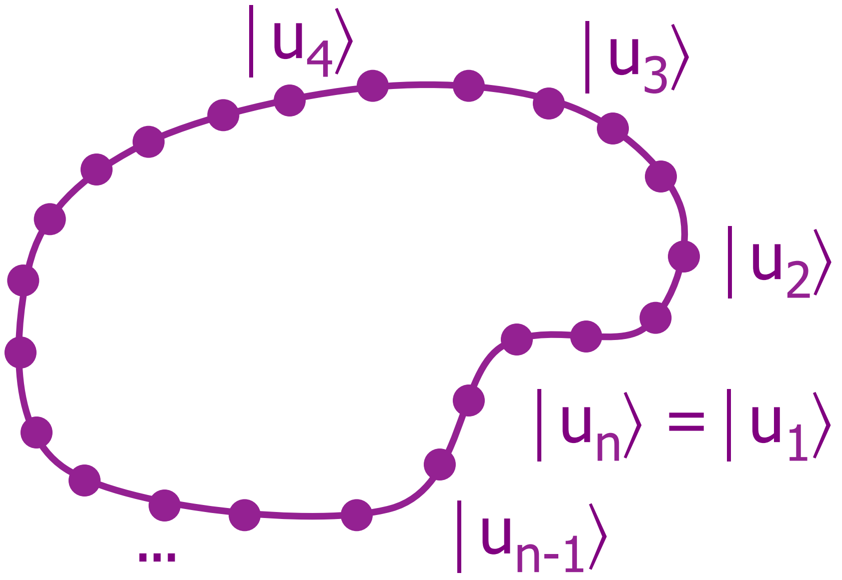
Let $|u_x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

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



Then $$\begin{aligned} \phi &= \mathrm{Arg}\, \langle u_z|u_x\rangle \langle u_x|u_y\rangle \langle u_y|u_z\rangle \\ &= \mathrm{Arg}\, (1)\,(1+i)\,(1) \\ &= \pi/4 \end{aligned}$$

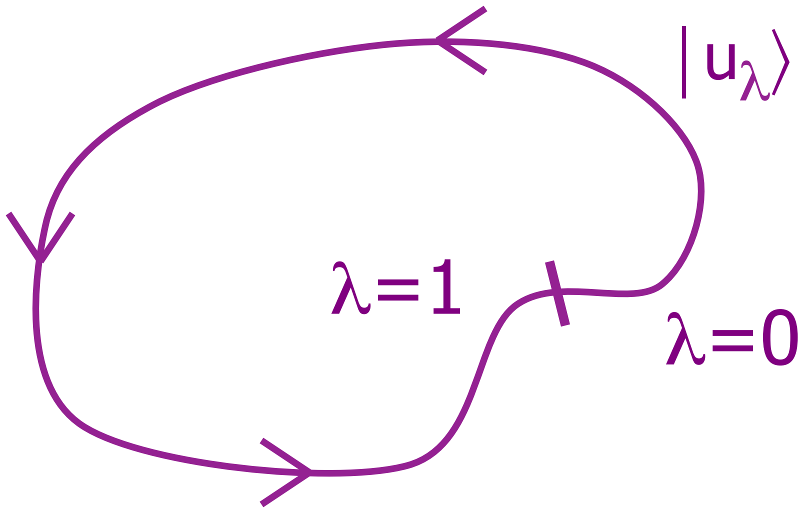
Berry phases



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

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

Berry phases



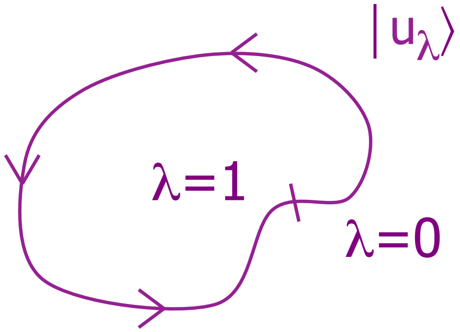
$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{du_\lambda}{d\lambda} \rangle$$

$$\boxed{\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle}$$

ϕ is well-defined modulo 2π

$\Rightarrow$ ϕ is a phase

Berry phases



ϕ is well-defined modulo 2π

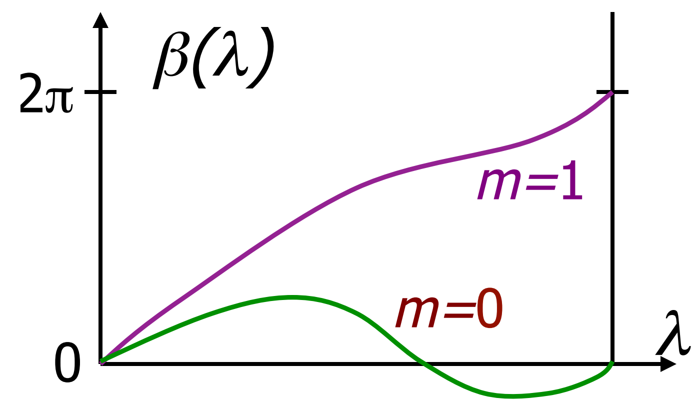
$\Rightarrow$ ϕ is a phase

$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle$$

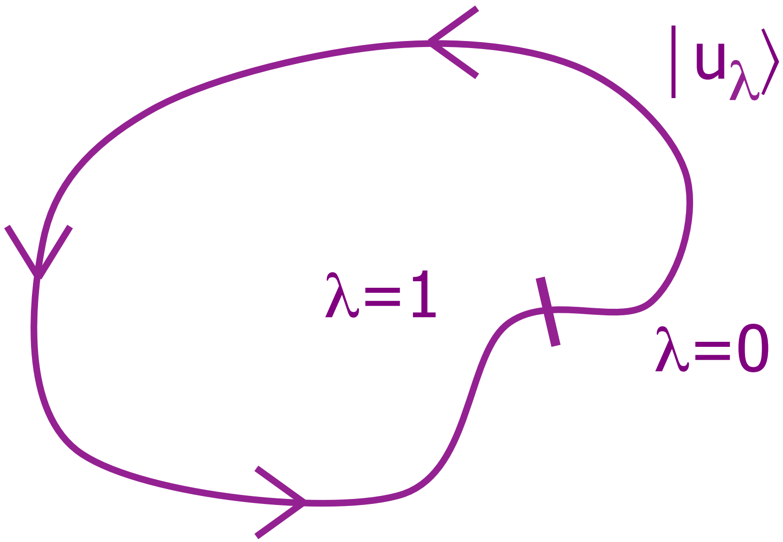
Let

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

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



Berry phases



Berry potential

$$A(\lambda) = i\,\langle u_\lambda|\frac{d}{d\lambda}|u_\lambda\rangle$$

Berry phase

$$\phi = \oint A(\lambda)\,d\lambda$$

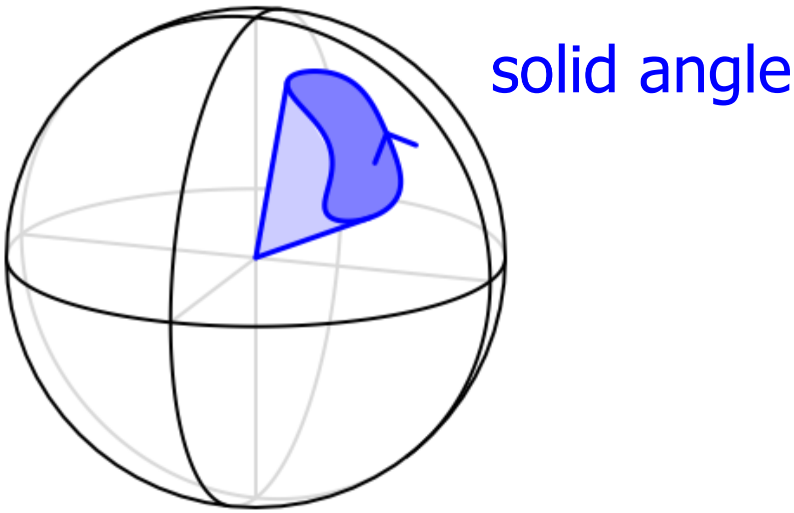
Gauge transformation:

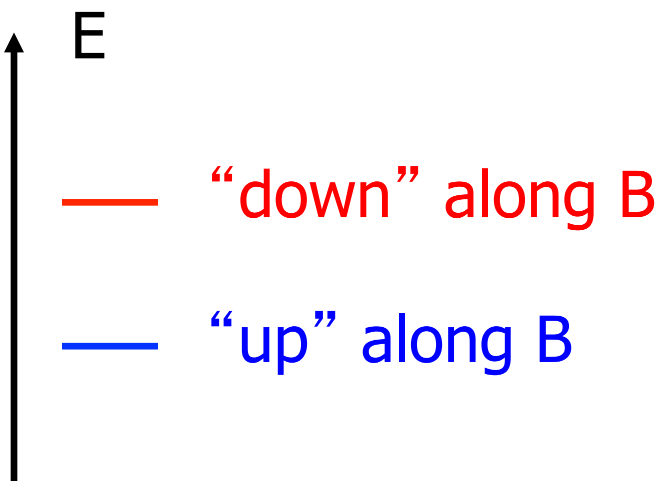
$$|\widetilde{u}_\lambda\rangle = e^{-i\beta(\lambda)}\,|u_\lambda\rangle$$

A is gauge-dependent but
ϕ is well-defined modulo 2π

Berry phase and curvature

Famous example: Spinor in magnetic field

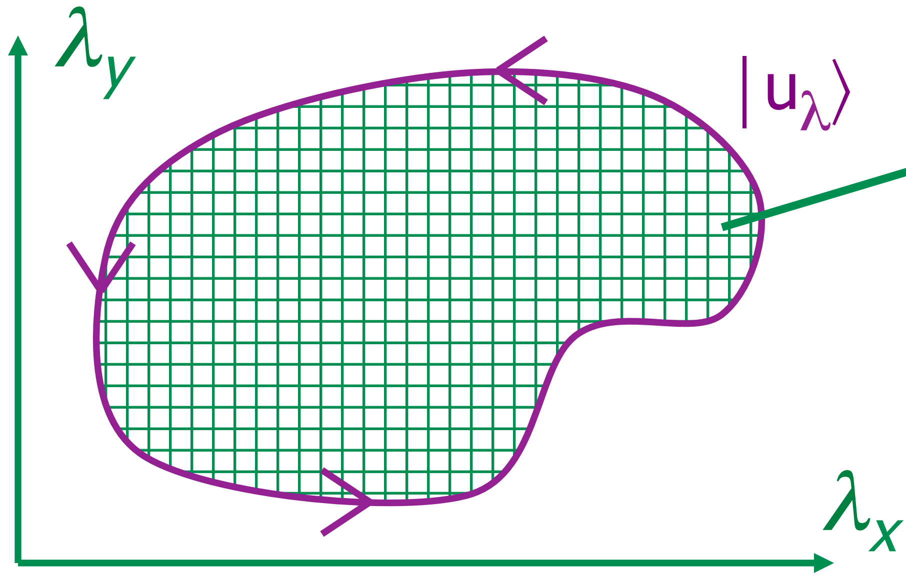




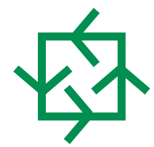
$$\boxed{\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \tfrac{d}{d\lambda} | u_\lambda \rangle}$$

$$\boxed{\phi = (\text{solid angle})/2}$$

Berry curvature



Berry phase per unit area



$\mathcal{F} = \Delta\phi/\Delta A_\lambda$

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

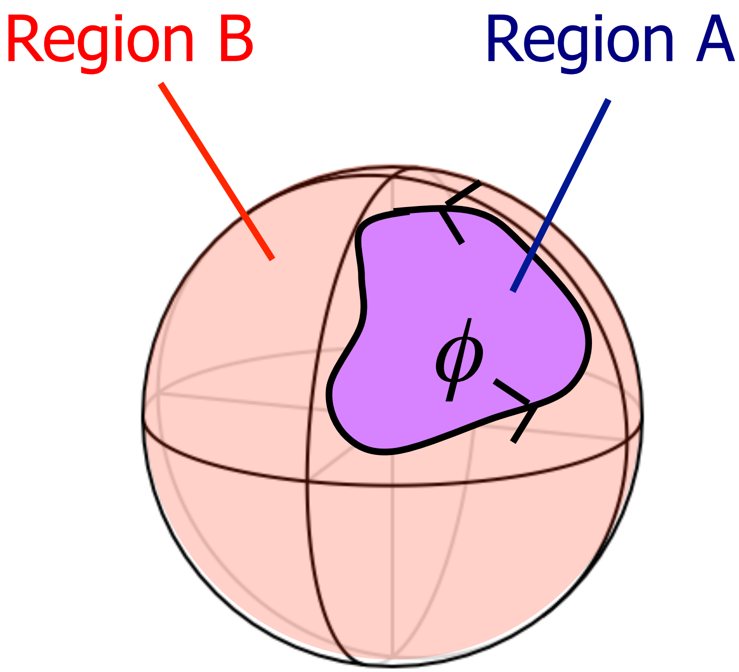
$$\mathcal{F} = -2\,\mathrm{Im}\,\left\langle \frac{du}{d\lambda_x} \middle| \frac{du}{d\lambda_y} \right\rangle$$

$$\phi = -\mathrm{Im} \oint d\lambda\, \langle u_\lambda | \tfrac{d}{d\lambda} | u_\lambda \rangle$$

Chern theorem

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:

$$0 = \oint \mathcal{F}(\lambda)\, dS_\lambda \mod 2\pi$$

Chern theorem: $$\oint \mathcal{F}(\lambda)\, dS_\lambda = 2\pi\, C$$

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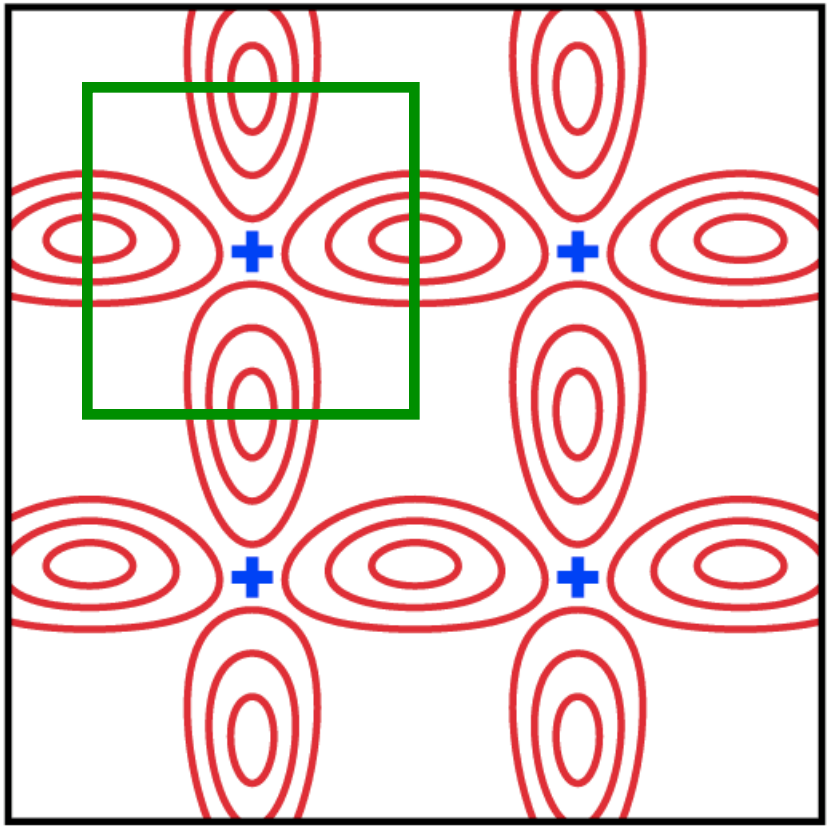
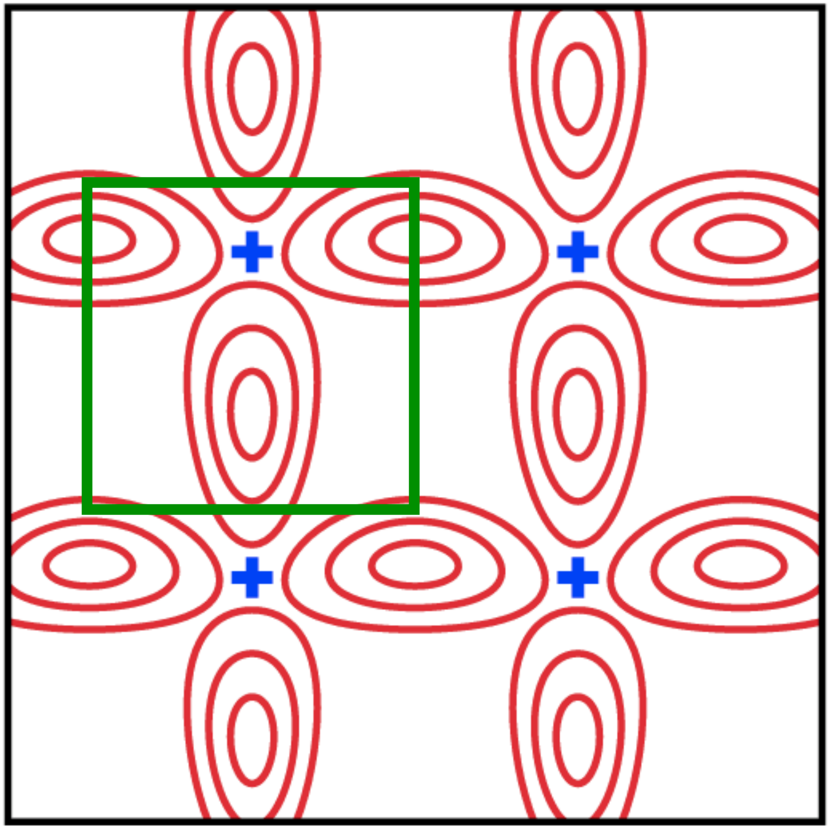
$\boldsymbol{P} = \boldsymbol{d}_{cell} / V_{cell}$?



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

$\boldsymbol{d}_{cell} \approx \mathbf{0}$

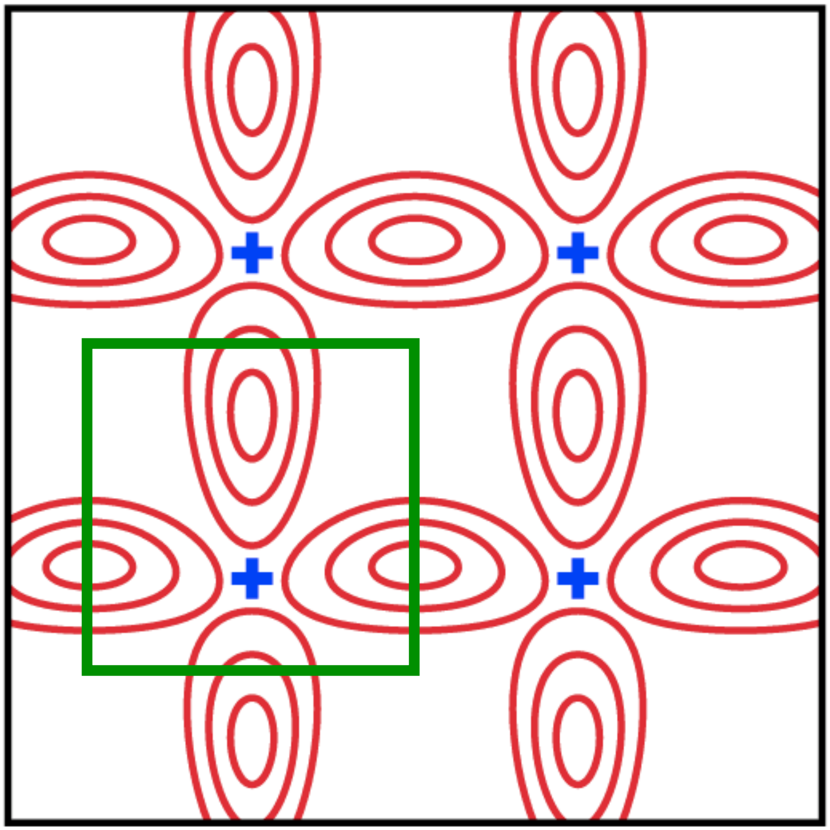
$\boldsymbol{P} = \boldsymbol{d}_{cell} / V_{cell}$?



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

$\boldsymbol{d}_{cell} =$ ⬆

$\boldsymbol{P} = \boldsymbol{d}_{cell} \,/\, V_{cell}$?



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

$\boldsymbol{d}_{cell} =$ ↓

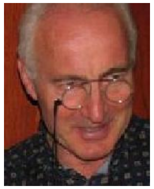
Modern Theory of Polarization

Problem:

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

Solution:

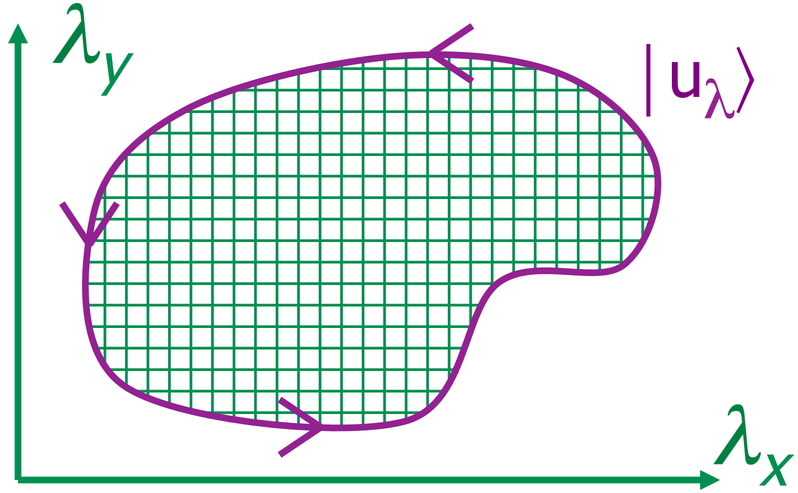
Go beyond $|\psi_{n\mathbf{k}}(\mathbf{r})|^2$ to access Berry phase information hidden in $\psi_{n\mathbf{k}}(\mathbf{r})$



Resta, Ferroelectrics 136, 51 (1992)

King-Smith and Vanderbilt, PRB 47, 1651 (1993)

Berry phases in crystalline insulators



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

General Parametric Hamiltonian

1D insulator with adiabatic parameter

Change of notation

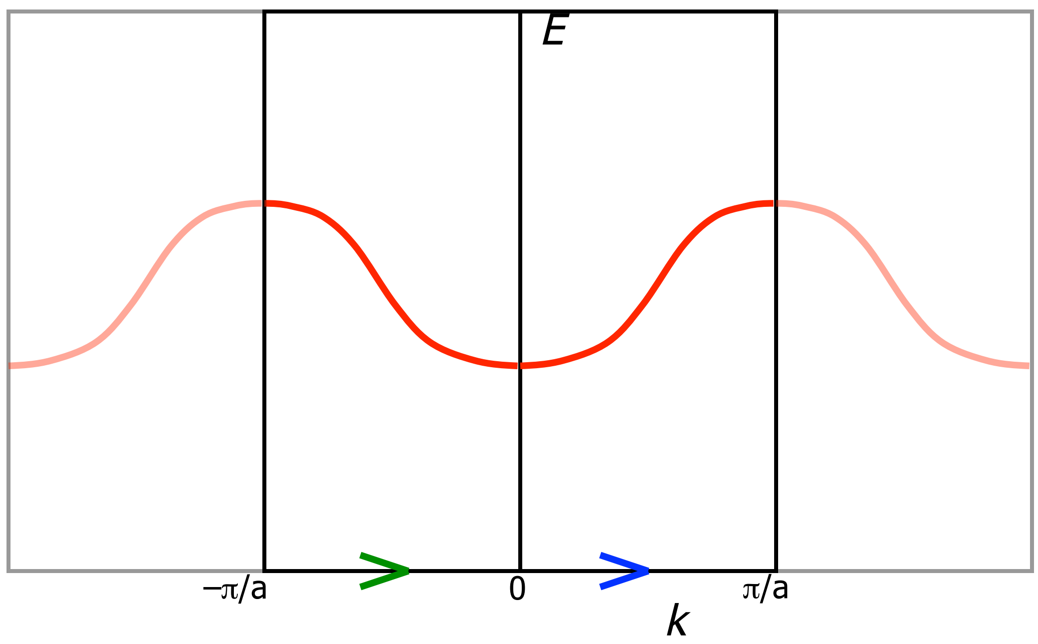
Berry curvature: $\mathcal{F} \rightarrow \Omega$

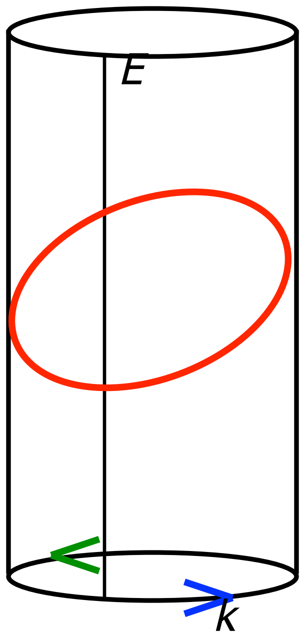
$$\phi = \int \Omega(\lambda)\, dS_\lambda$$

$$\Omega = -2\,\mathrm{Im}\,\left\langle \frac{du}{d\lambda_x} \middle| \frac{du}{d\lambda_y} \right\rangle$$

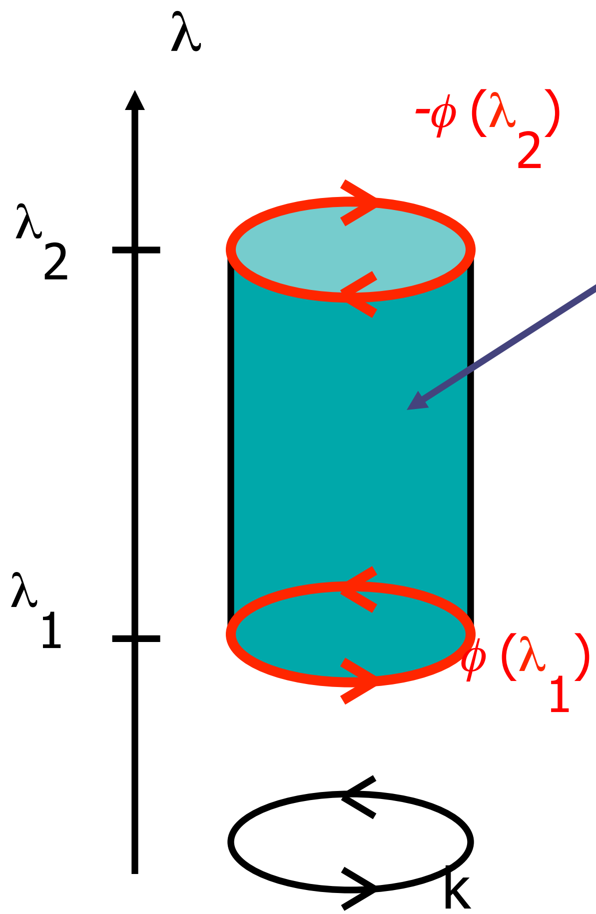
1D: BZ is really a loop

- Reciprocal space is really periodic
- Brillouin zone can be regarded as a loop





Parametric 1D Ham. (Open path)



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

(Resta, 1993)

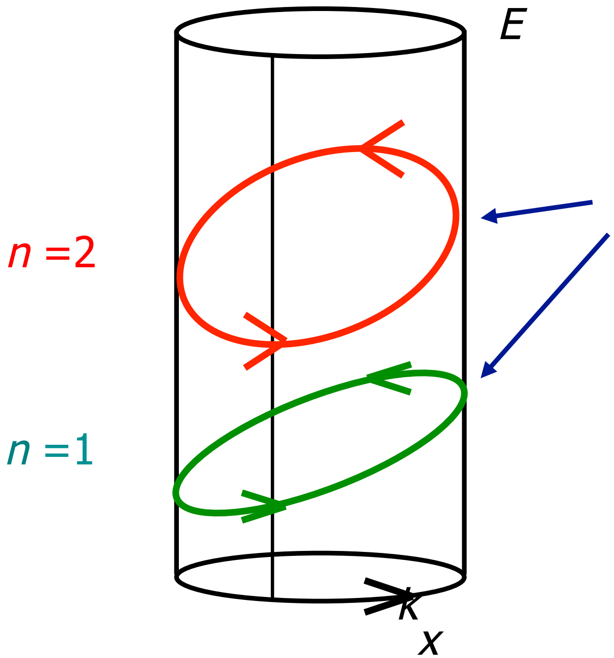
$$\Delta P = -\frac{e}{2\pi}\oint dk \int_{\lambda_1}^{\lambda_2} d\lambda \; \Omega^{(k\lambda)}$$

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

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

(modulo e)

1D: Polarization

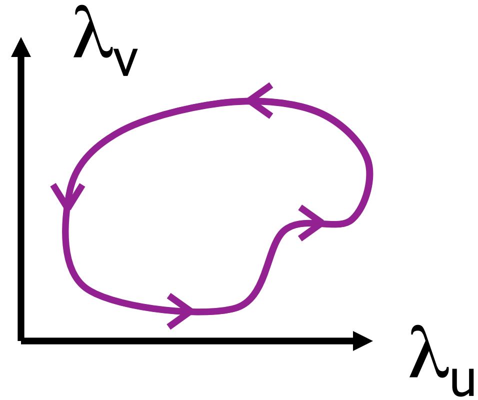


$$\phi = -\mathrm{Im} \int dk_x \langle u_{\mathbf{k}} | \frac{d}{dk_x} | u_{\mathbf{k}} \rangle$$

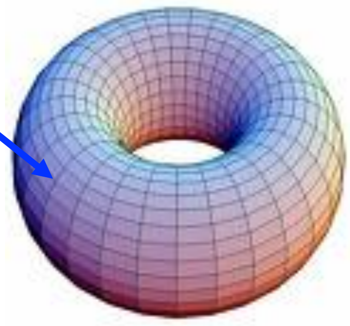
$$\boxed{P = \frac{-e}{2\pi} \sum_{n}^{\mathrm{occ}} \phi_n}$$

King-Smith & V., 1993

Parametric 1D Ham. (Closed path)



Ω (k,λ)



(k, λ) space

Under an adiabatic cycle,

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

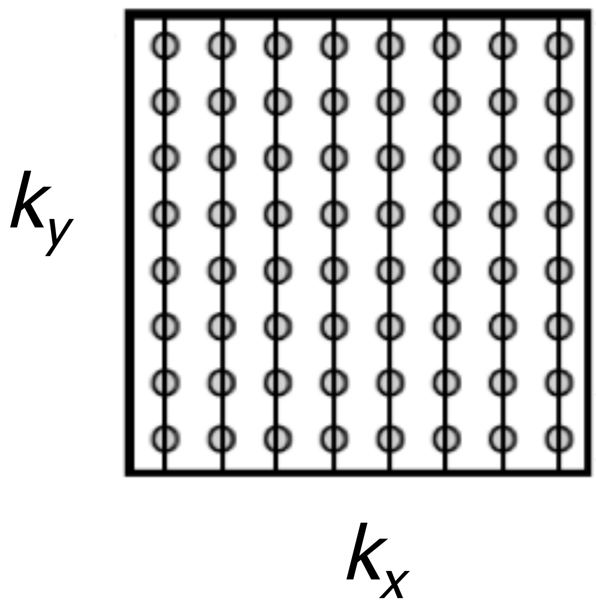
By Chern theorem,

$$\boxed{\Delta P = n\, e}$$

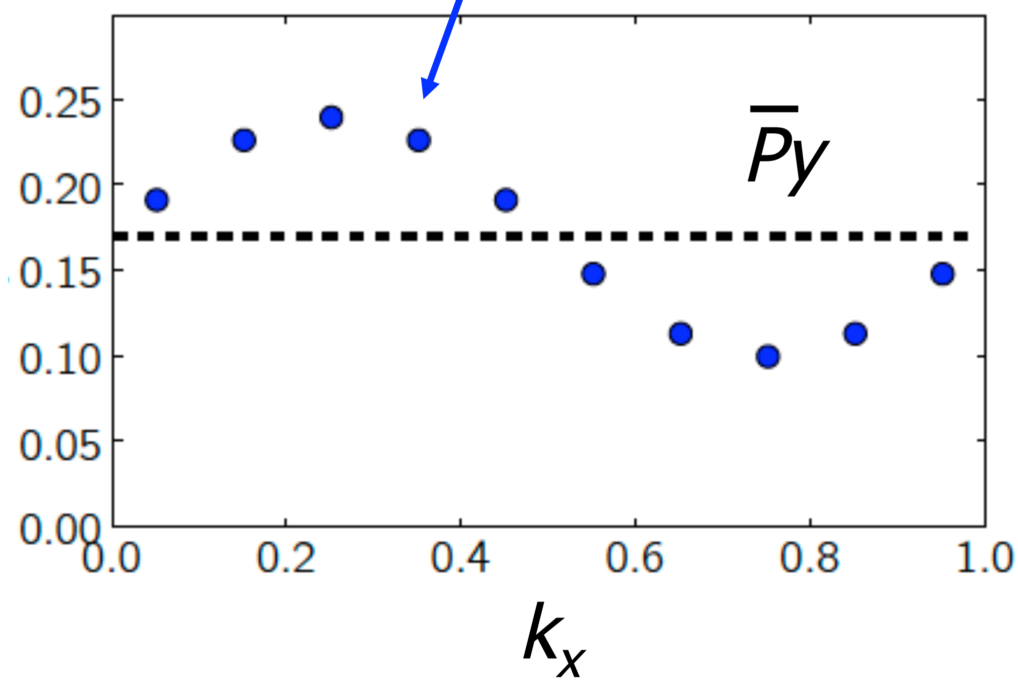
(n = TKNN invariant = integer)

Polarization in a 2D insulator

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

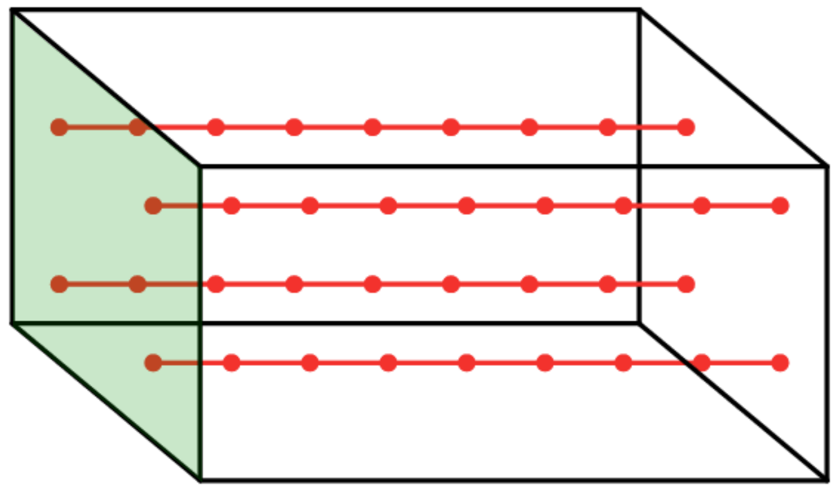


$P_y\,(k_x) \propto \phi\,(k_x)$



Discretized formula in 3D

$\boxed{\phi_n(\mathbf{k}_\perp)}$

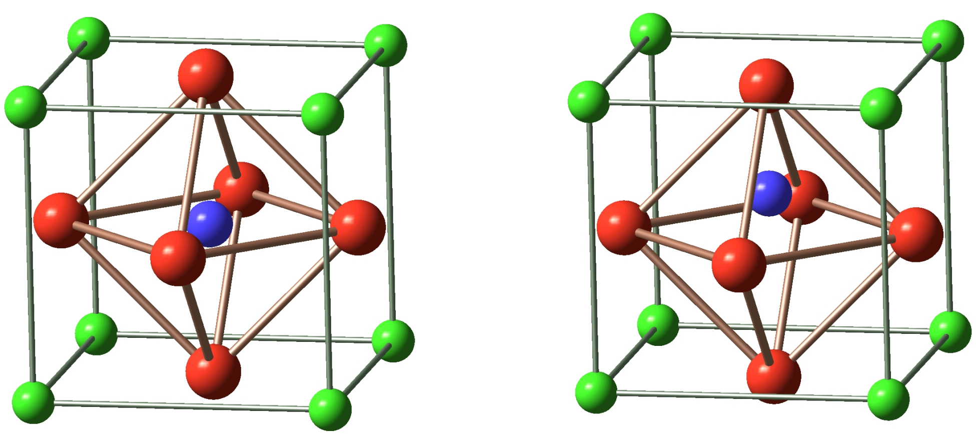


$$\mathbf{P}_n^{\text{elec}} = \frac{-1}{2\pi}\frac{e}{\Omega}\sum_j \phi_{n,j}\,\mathbf{R}_j \quad \text{where} \quad \phi_{n,j} = \frac{1}{N_{\mathbf{k}_\perp}}\sum_{\mathbf{k}_\perp}\phi_n(\mathbf{k}_\perp)$$

$$\mathbf{P} = \mathbf{P}^{\text{elec}} + \mathbf{P}^{\text{ion}} \quad \text{where} \quad \mathbf{P}^{\text{ion}} = \frac{e}{V_{\text{cell}}}\sum_\tau Z_\tau^{\text{ion}}\,\mathbf{r}_\tau$$

Sample Application: Born Z^*

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



Paraelectric *Ferroelectric*

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

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

$Z^*(\mathrm{O_I}) = -2\ e$?

$Z^*(\mathrm{O_{II}}) = -2\ e$?

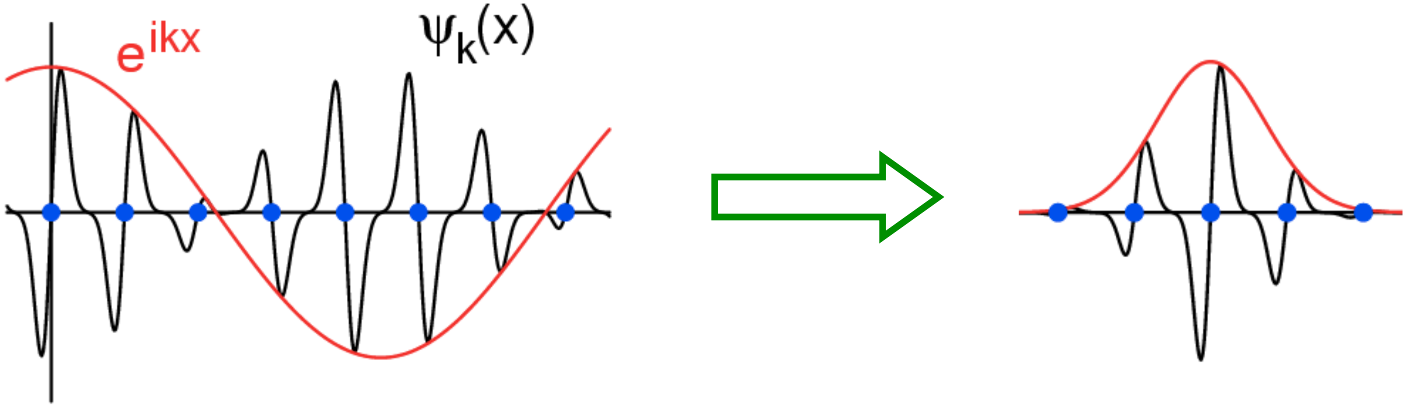
Summary: Theory of Polarization

- ***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

Tutorial on Wannier functions

Choose Wannier functions as

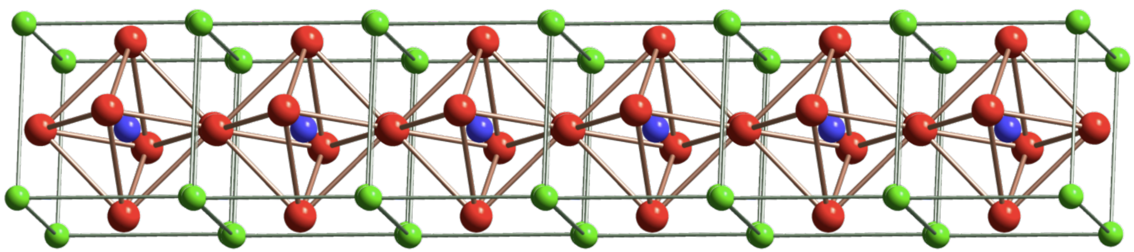
$$w_n(\mathbf{r}-\mathbf{R}) \;=\; \int_{BZ} \psi_{n\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$



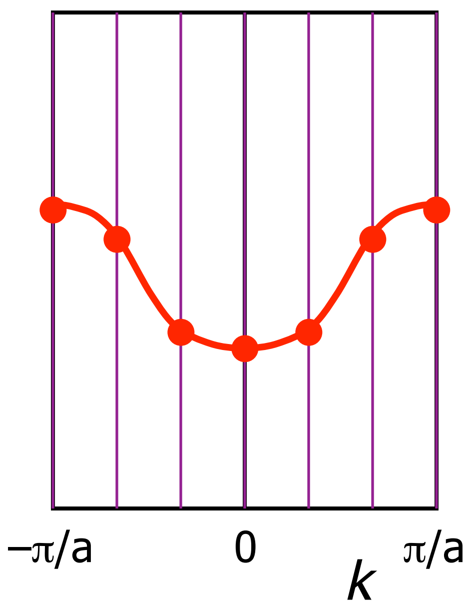
Form wave-packet = "Wannier function"

Tutorial on Wannier functions

Crystal in real space:



Brillouin zone in reciprocal space:



Tutorial on Wannier functions

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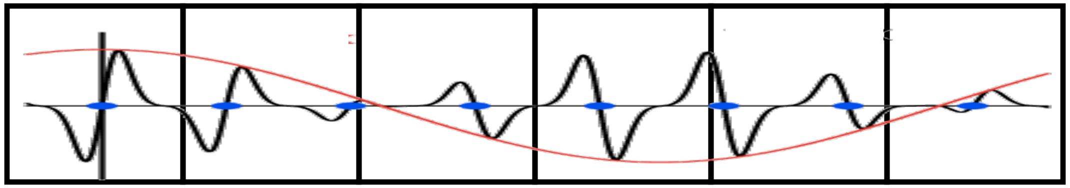

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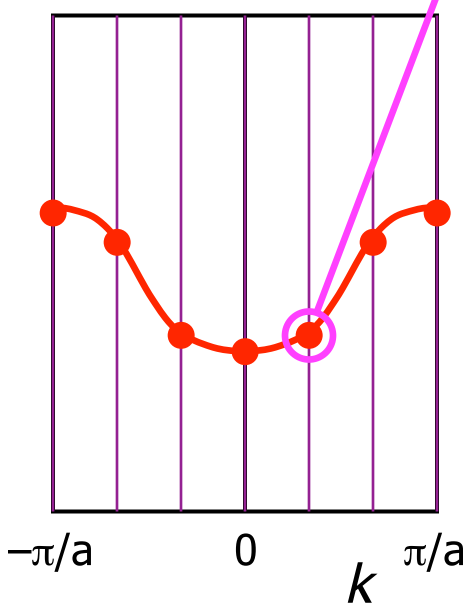
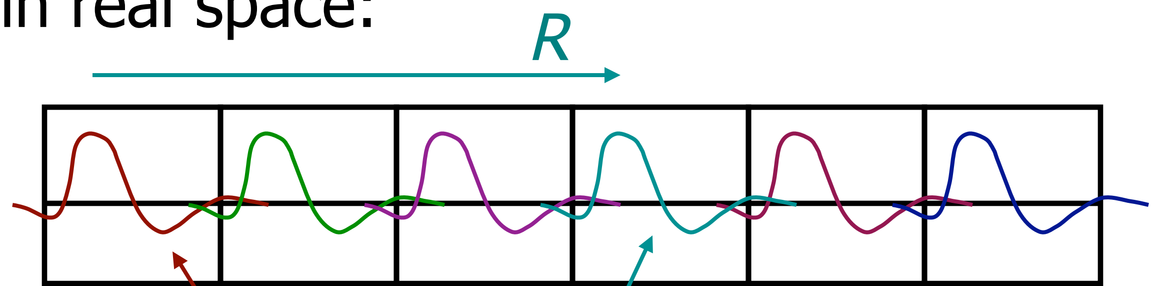
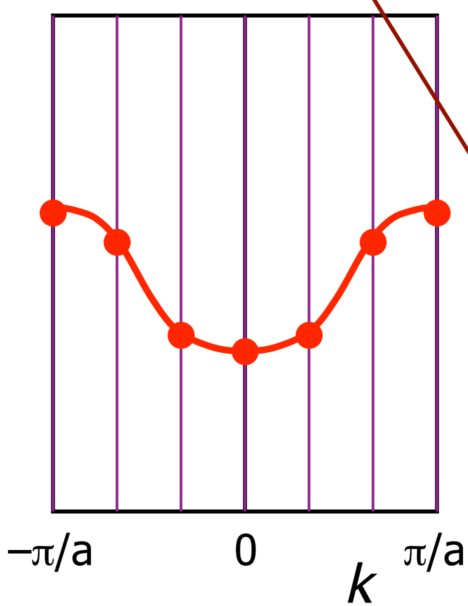


Tutorial on Wannier functions

Crystal in real space:



Brillouin zone in reciprocal space:



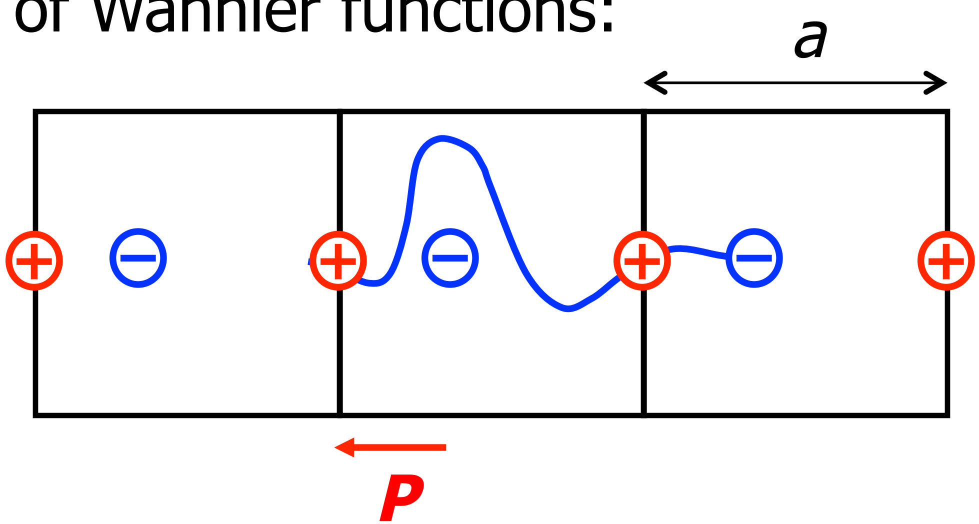
$$w_{\mathbf{R}}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

$$w_{0}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k}$$

Unitary transformation

Tutorial on Wannier functions

Centers of Wannier functions:



$$\langle w_0 | \mathbf{r} | w_0 \rangle = ?$$

Tutorial on Wannier functions

Centers of Wannier functions:

$$|\,w_0\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;|\psi_{\mathbf{k}}\rangle$$

$$= \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\; e^{i\mathbf{k}\cdot\mathbf{r}}\;|u_{\mathbf{k}}\rangle$$

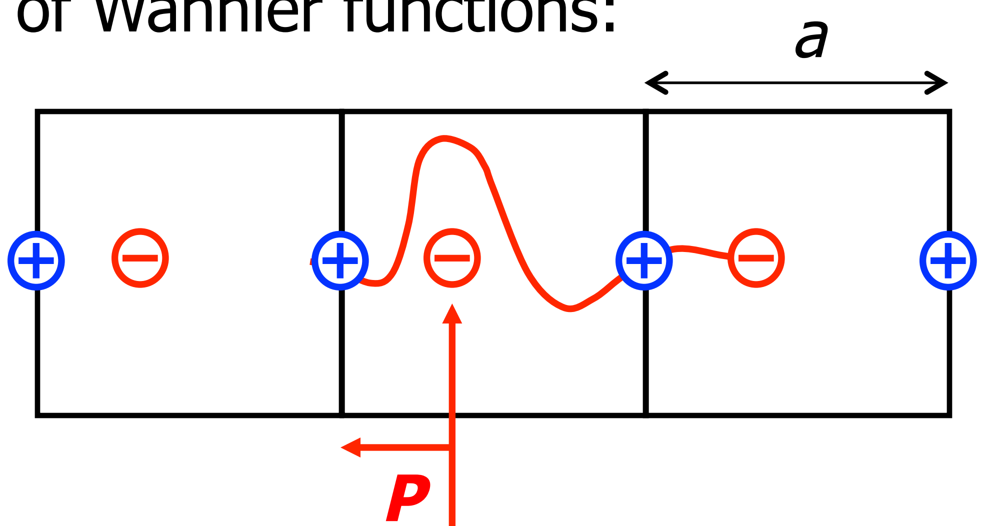
$$\mathbf{r}\,|\,w_0\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;(\,-\,i\nabla_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{r}}\,)\,|u_{\mathbf{k}}\rangle$$

$$= i\,\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\; e^{i\mathbf{k}\cdot\mathbf{r}}\,(\,\nabla_{\mathbf{k}}\,|u_{\mathbf{k}}\rangle\,)$$

$$\boxed{\langle w_0\,|\,\mathbf{r}\,|\,w_0\rangle = i\,\frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k}\;\langle u_{\mathbf{k}}|\,\nabla_{\mathbf{k}}\,|u_{\mathbf{k}}\rangle}$$

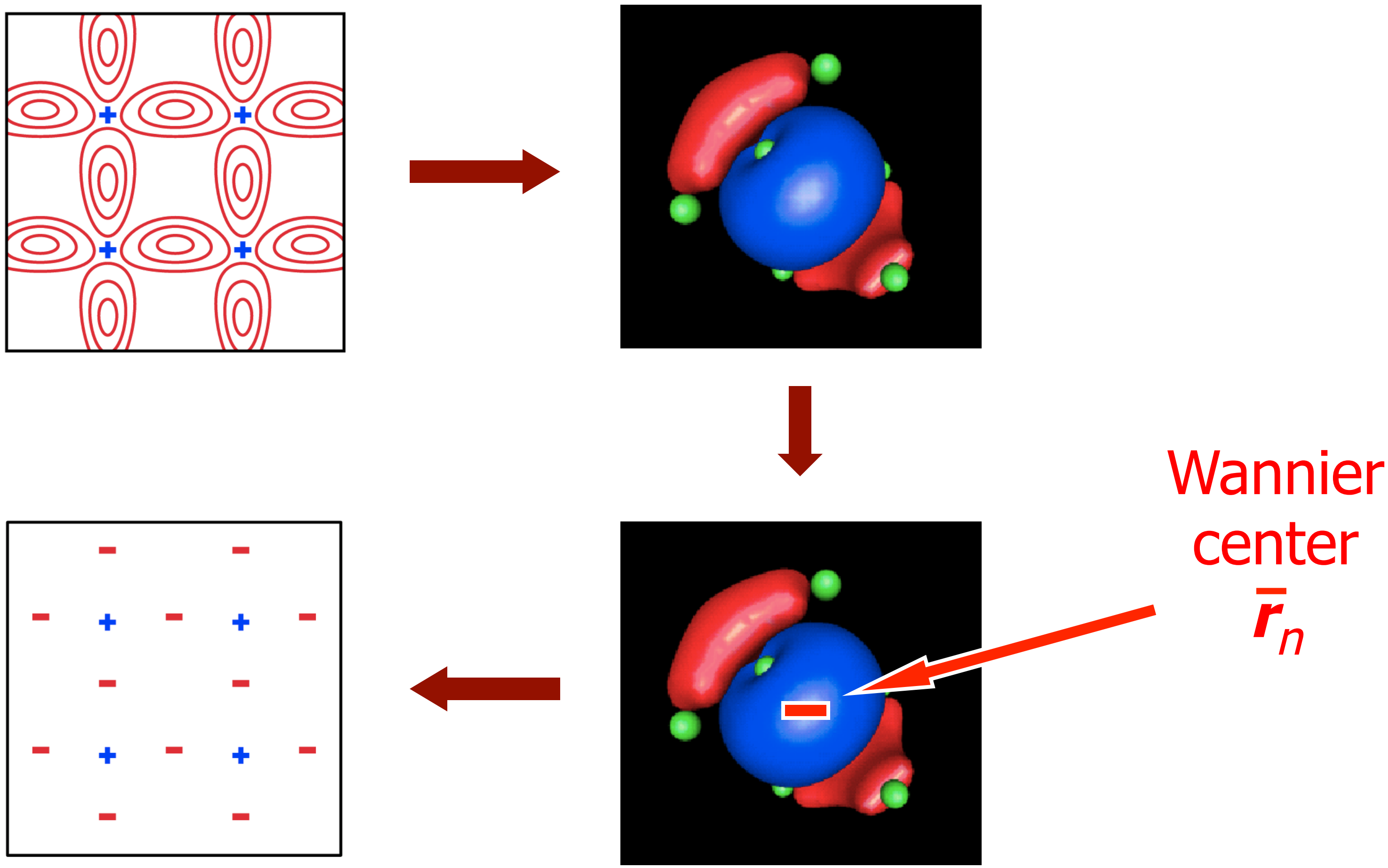
Polarization ↔ Wannier centers

Centers of Wannier functions:



$$\langle w_0|x|w_0\rangle = i\,\frac{a}{2\pi}\int_{\mathrm{BZ}} dk\,\left\langle u_k\middle|\frac{d}{dk}\middle|u_k\right\rangle$$
$$= a\,\frac{\phi}{2\pi}$$

Polarization ↔ Wannier centers



Total polarization

$$\mathbf{P} = \underbrace{\frac{e}{V_{\text{cell}}} \sum_{\tau} Z_{\tau}^{\text{ion}} \, \mathbf{r}_{\tau}}_{\text{Ionic polarization}} + \underbrace{\frac{-e}{V_{\text{cell}}} \sum_{n} \bar{\mathbf{r}}_{n}}_{\text{Electronic polarization}}$$

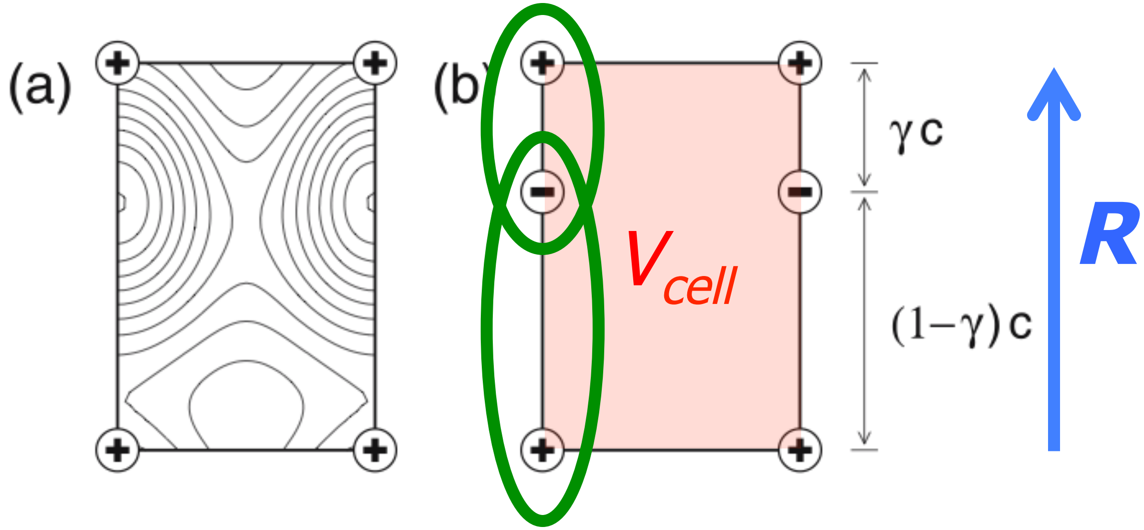
Each term only well defined modulo e**R**/V_{cell}

Quantum of polarization

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

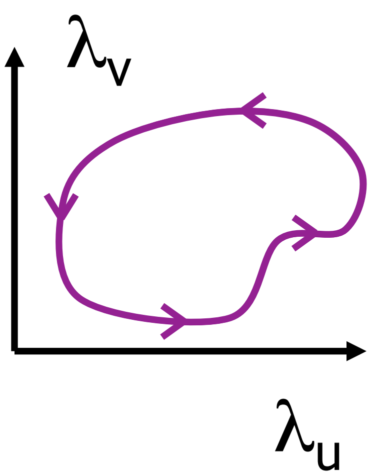
- Spin-polarized systems (spinor bands)
  - 1D: $\Delta P = ea/a = e$ (C)
  - 2D: $\Delta \mathbf{P} = e\mathbf{R}/A_{cell}$ (C/m) ($\mathbf{R}$ = lattice vector)
  - 3D: $\Delta \mathbf{P} = e\mathbf{R}/V_{cell}$ (C/m^2)
- Spin-paired systems (non-magnetic)
  - 1D: $\Delta P = 2ea/a = 2e$ (C)
  - 2D: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

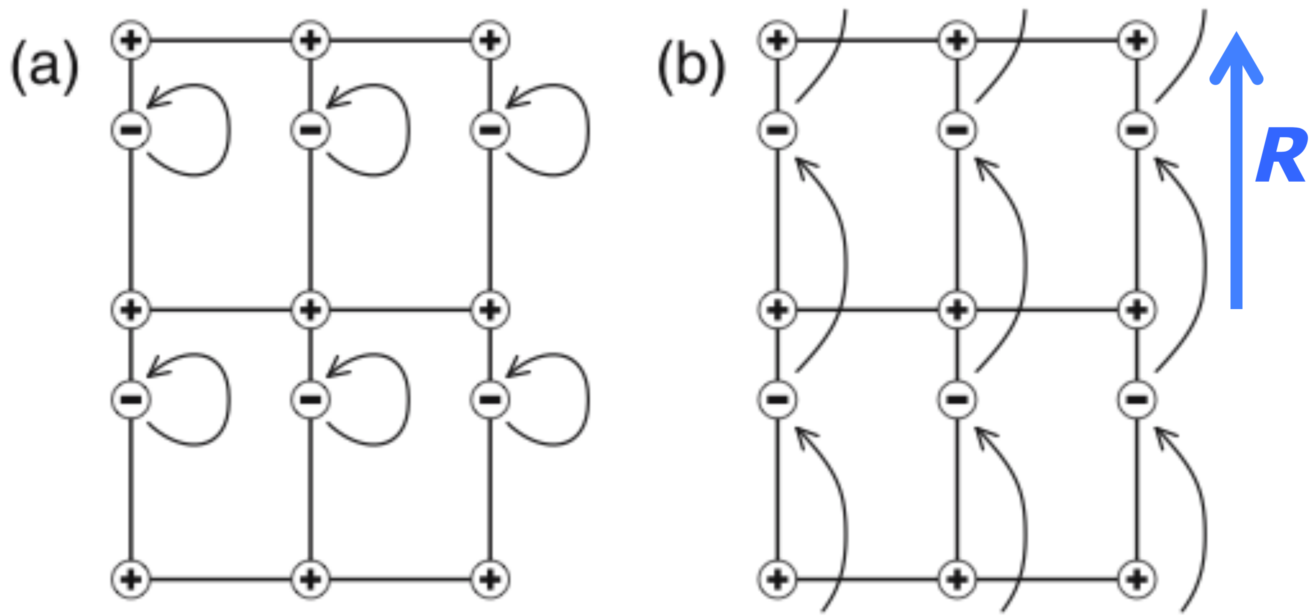
Quantum of polarization



$$\Delta \mathbf{P} = e\,\mathbf{R} \,/\, V_{cell}$$

Quantum of ***P*** under adiabatic cycle

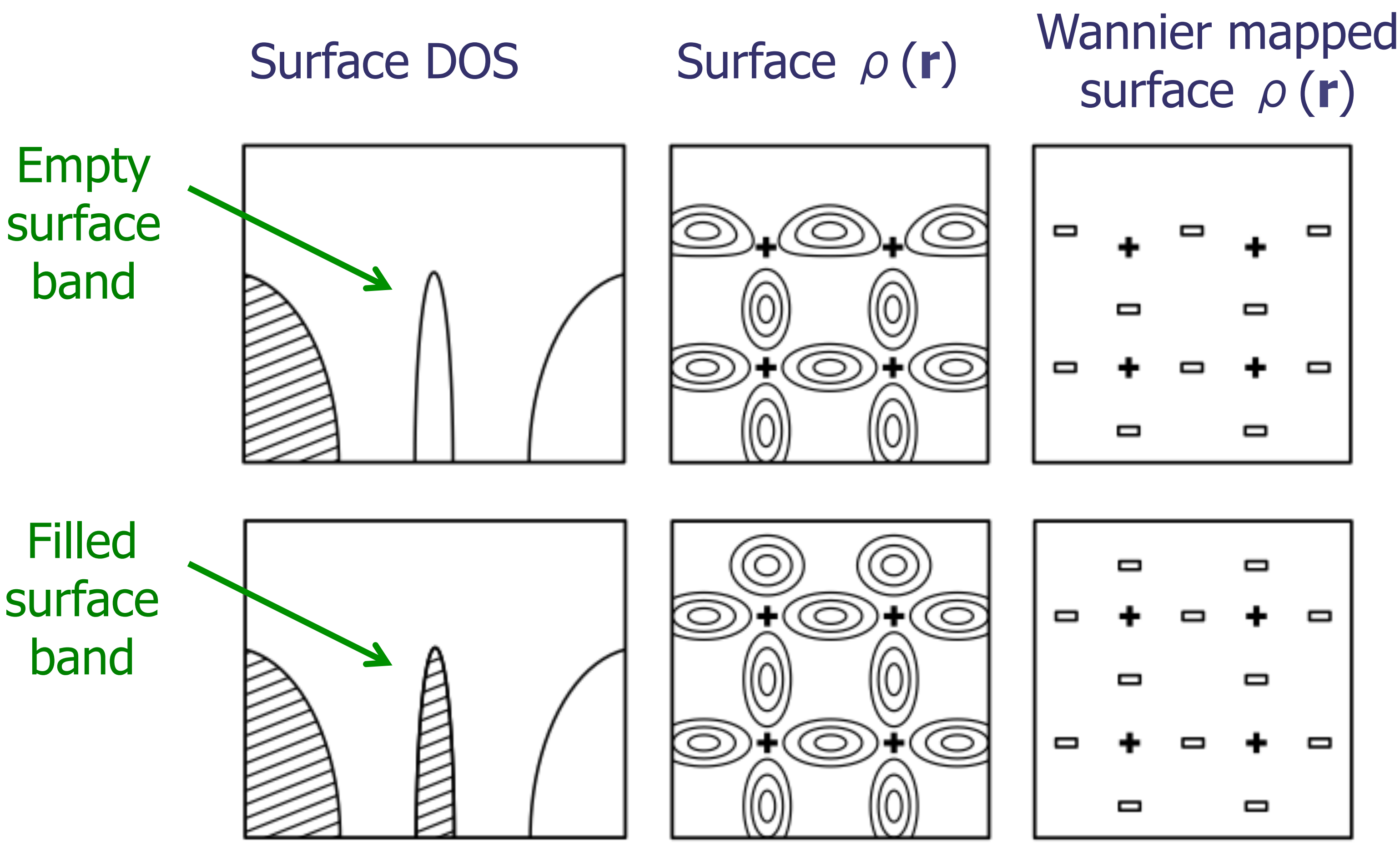




$\Delta \boldsymbol{P} = 0$

$\Delta \boldsymbol{P} = e\,\boldsymbol{R} / V_{cell}$

Quantum of ***P*** and surface charge

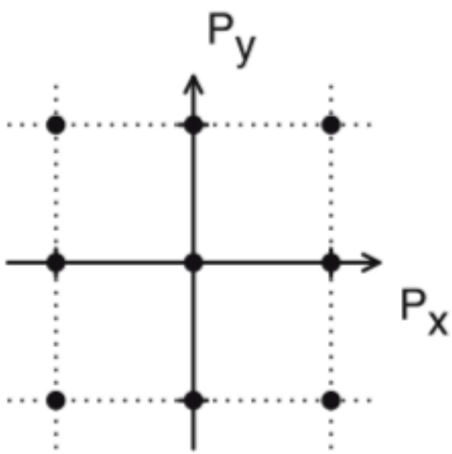


$$\Delta \boldsymbol{P} = e\,\boldsymbol{R} / V_{\mathrm{cell}} \quad \longleftrightarrow \quad \Delta\sigma = \Delta \boldsymbol{P} \cdot \hat{n} = e / A_{\mathrm{surf}}$$

Polarization as a lattice-valued quantity

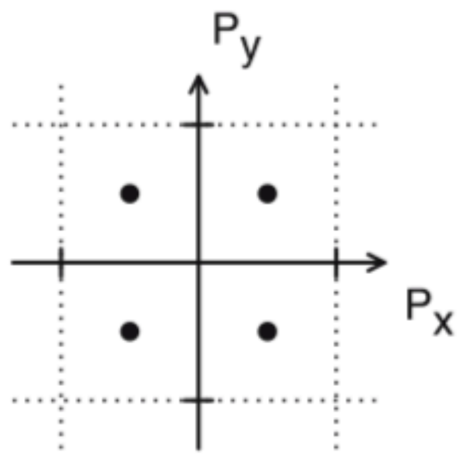
$$\Delta \boldsymbol{P} = e\, \boldsymbol{R} \,/\, V_{\text{cell}}$$

Cubic crystal



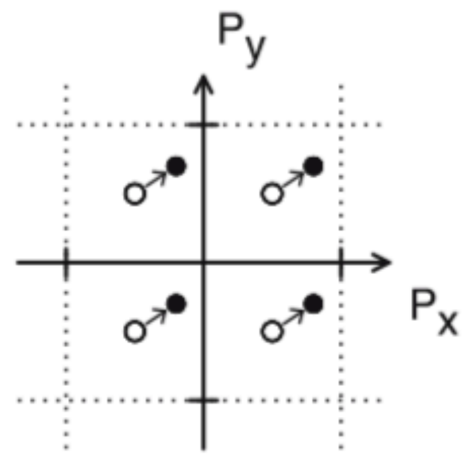
$\boldsymbol{P}_0 = 0$
$\boldsymbol{P}_0 = (a,0)$
etc.

Cubic crystal



$\boldsymbol{P}_0 = (-a/2, a/2)$
$\boldsymbol{P}_0 = (a/2, a/2)$
etc.

Distorted
Cubic crystal

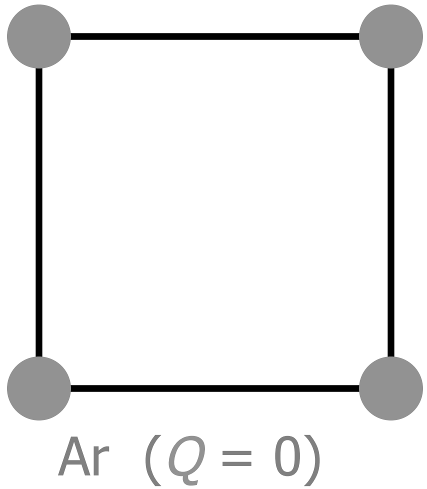


$\boldsymbol{P}_0 + \Delta \boldsymbol{P}$

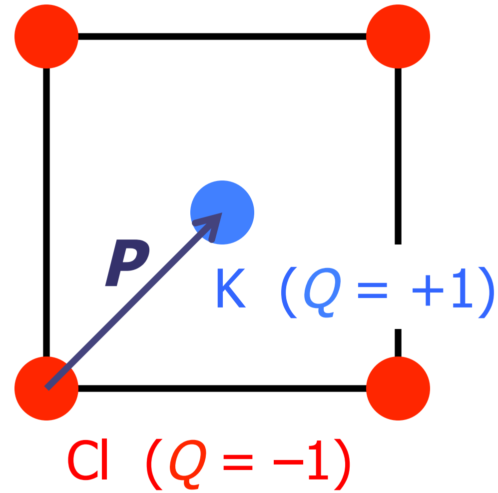
$\boldsymbol{P}_0$ = "Formal polarization"

$\Delta \boldsymbol{P}$ = "Effective pol."
= "Spontaneous pol."

Examples



Unit cell of
“2D Ar crystal”
$\boldsymbol{P} = 0$ etc.



Unit cell of
“2D KCl crystal”
$\boldsymbol{P} = (a/2, a/2)$ 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

D. Vanderbilt and R. Resta, "Quantum electrostatics of insulators: Polarization, Wannier functions, and electric fields," in *Conceptual foundations of materials properties: A standard model for calculation of ground- and excited-state properties*, S.G. Louie and M.L. Cohen, eds. (Elsevier, The Netherlands, 2006), pp. 139-163. *(request article)*

R. Resta and D. Vanderbilt, "Theory of Polarization: A Modern Approach," in {\it Physics of Ferroelectrics: a Modern Perspective}, ed. by K.M. Rabe, C.H. Ahn, and J.-M. Triscone (Springer-Verlag, 2007, Berlin), pp. 31-68. *(local preprint)*

- Currently posted at

  http://www.physics.rutgers.edu/~dhv/tmp

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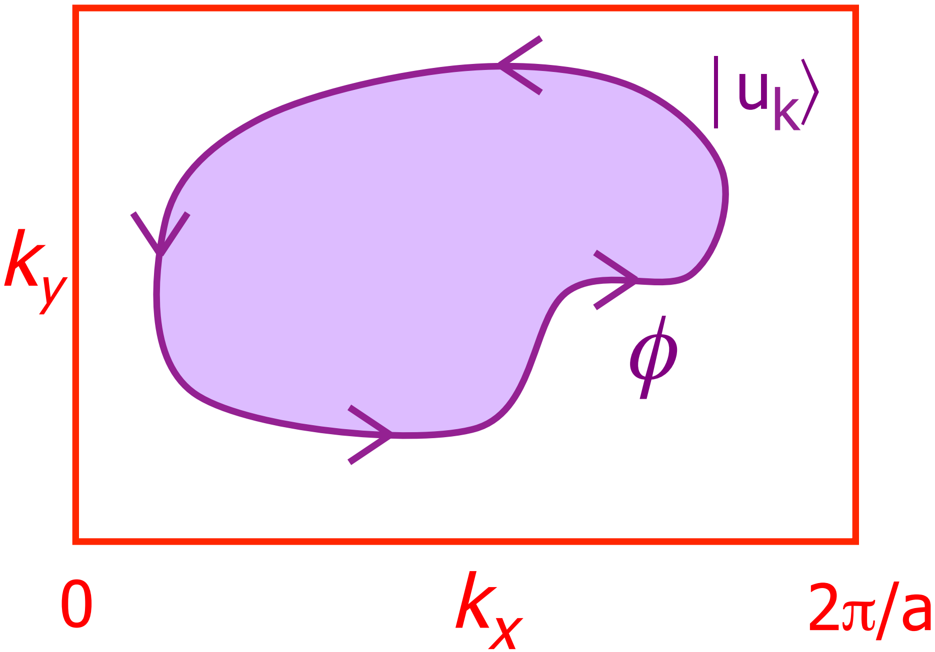
Berry phase and curvature in the BZ



$$u_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}} \underbrace{\psi_{\mathbf{k}}(\mathbf{r})}_{\text{Bloch function}}$$

Berry potential:

$$\mathbf{A}(\mathbf{k}) = -\mathrm{Im}\,\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}}|u_{\mathbf{k}}\rangle$$

Berry phase:

$$\phi = \oint \mathbf{A}(\mathbf{k}) \cdot d\mathbf{k}$$

Berry curvature:

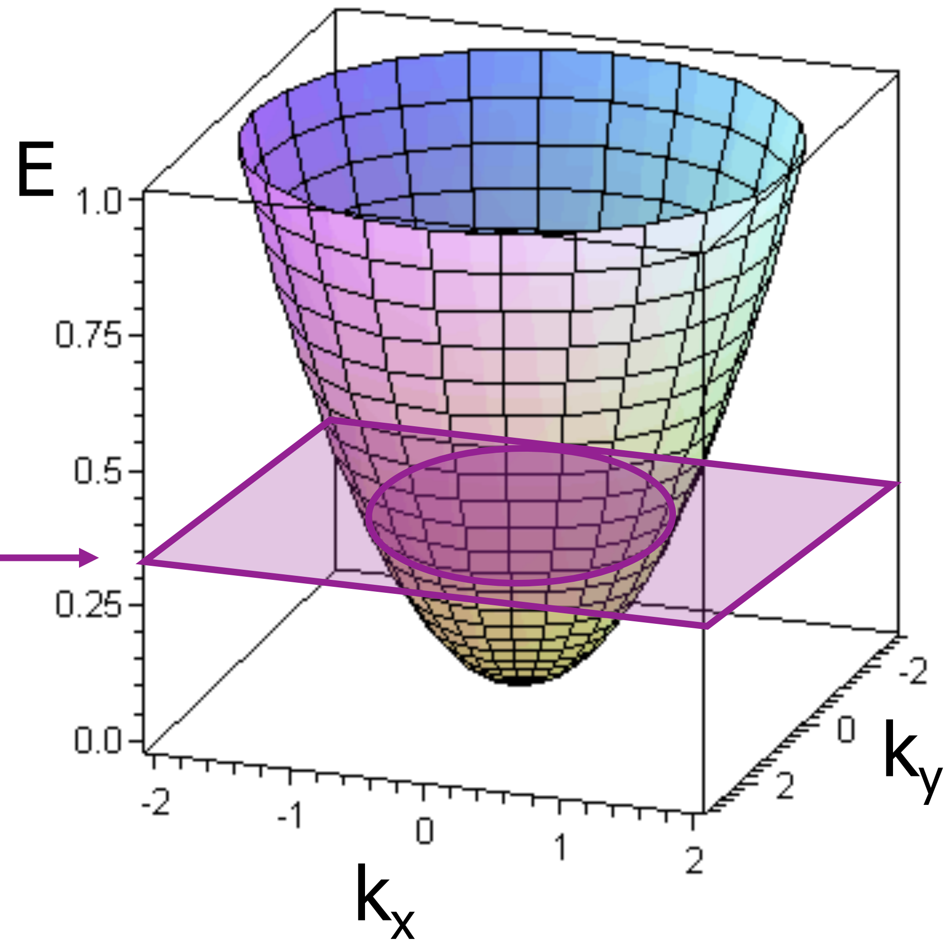
$$\Omega(\mathbf{k}) = \nabla \times \mathbf{A}$$

$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

Stoke's theorem:

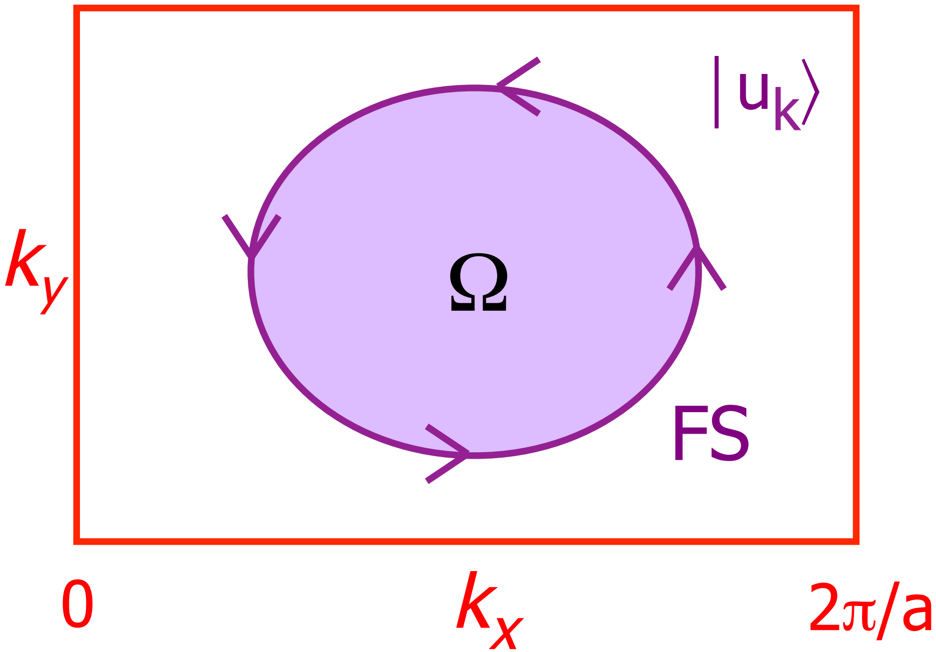
$$\phi = \int \Omega_z(\mathbf{k})\, d^2k$$

Bandstructure of a metal



Fermi Energy E_F

Non-magnetic metal: no net Berry curvature



Time-reversal symmetry

$$\Downarrow$$

$$u(k_x, k_y) = u^*(-k_x, -k_y)$$

$$\Downarrow$$

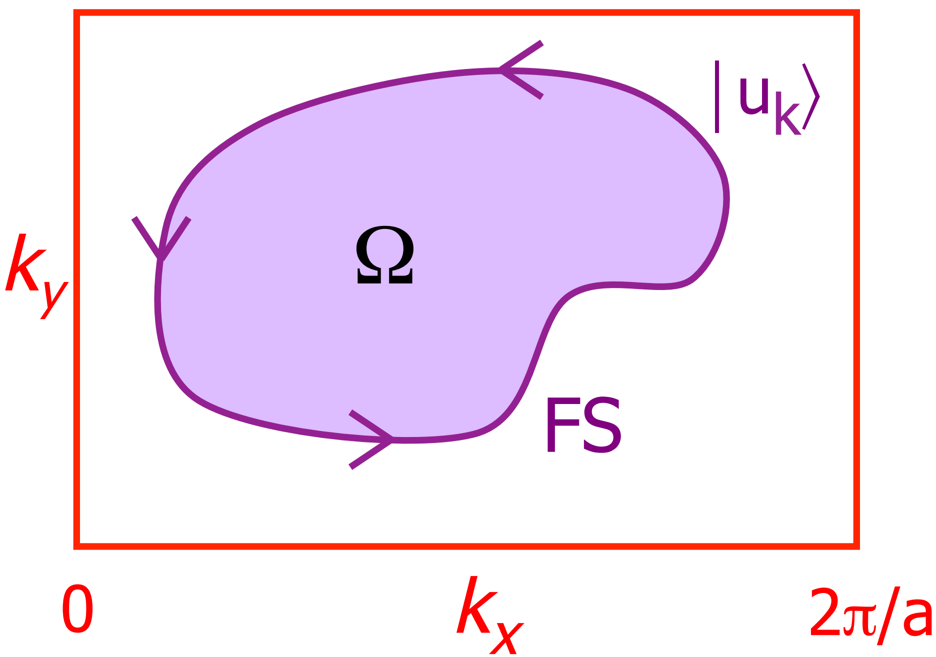
$$\Omega(\mathbf{k}) = -\Omega(-\mathbf{k})$$

$$\Downarrow$$

$$\phi = 0$$

If centrosymmetric too, then Ω=0

Magnetic metal: things get interesting



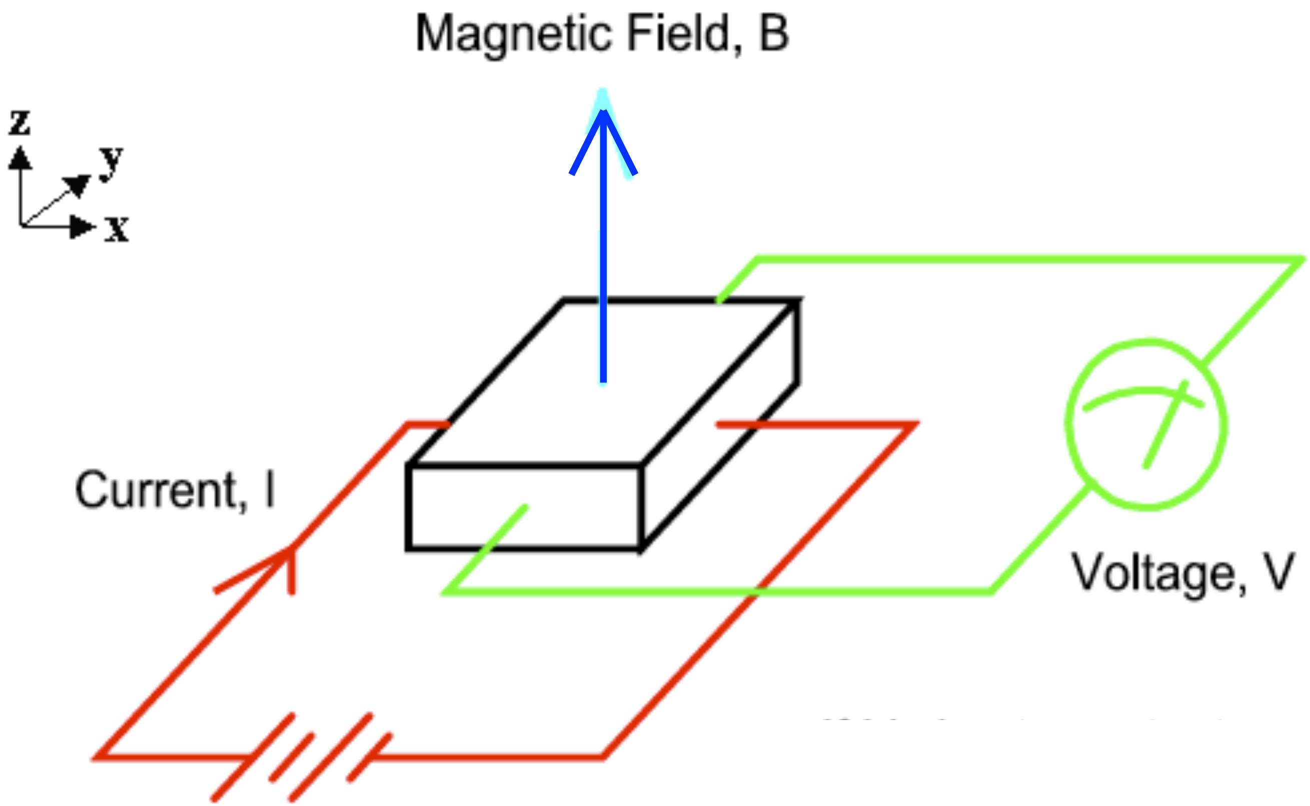
$$\Omega_z(\mathbf{k}) = -2\,\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\phi = \int_{\mathrm{FS}} \Omega_z(\mathbf{k})\, d^2k$$

$$\sigma_{xy}^{\mathrm{AHE}} = \frac{-e^2}{(2\pi)^3\hbar} \sum_n \int d^3k\, f_{n\mathbf{k}}\, \Omega_{n,z}(\mathbf{k})$$

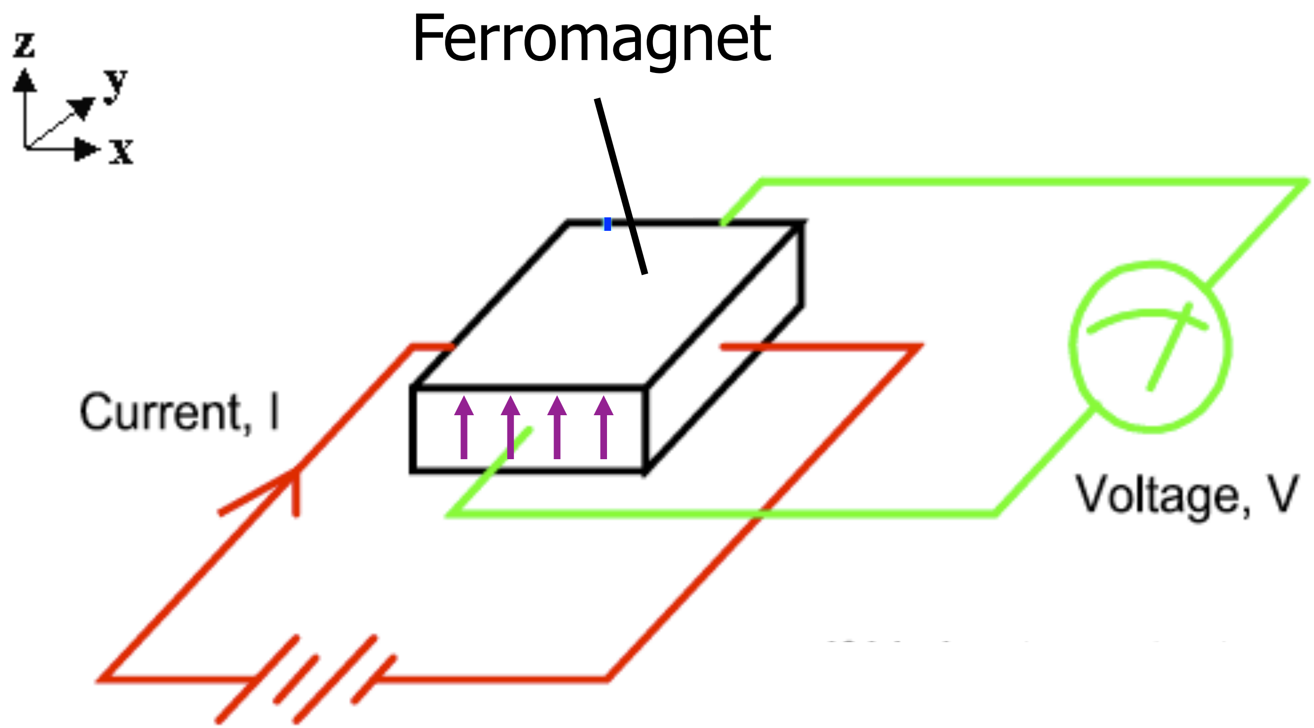
(3D)

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).

$$\sigma_{xy}^{\mathrm{AHE}} = \frac{-e^2}{(2\pi)^3\hbar} \sum_n \int d^3k\, f_{n\mathbf{k}}\, \Omega_{n,z}(\mathbf{k})$$

A pure bandstructure effect!

Summary of Results

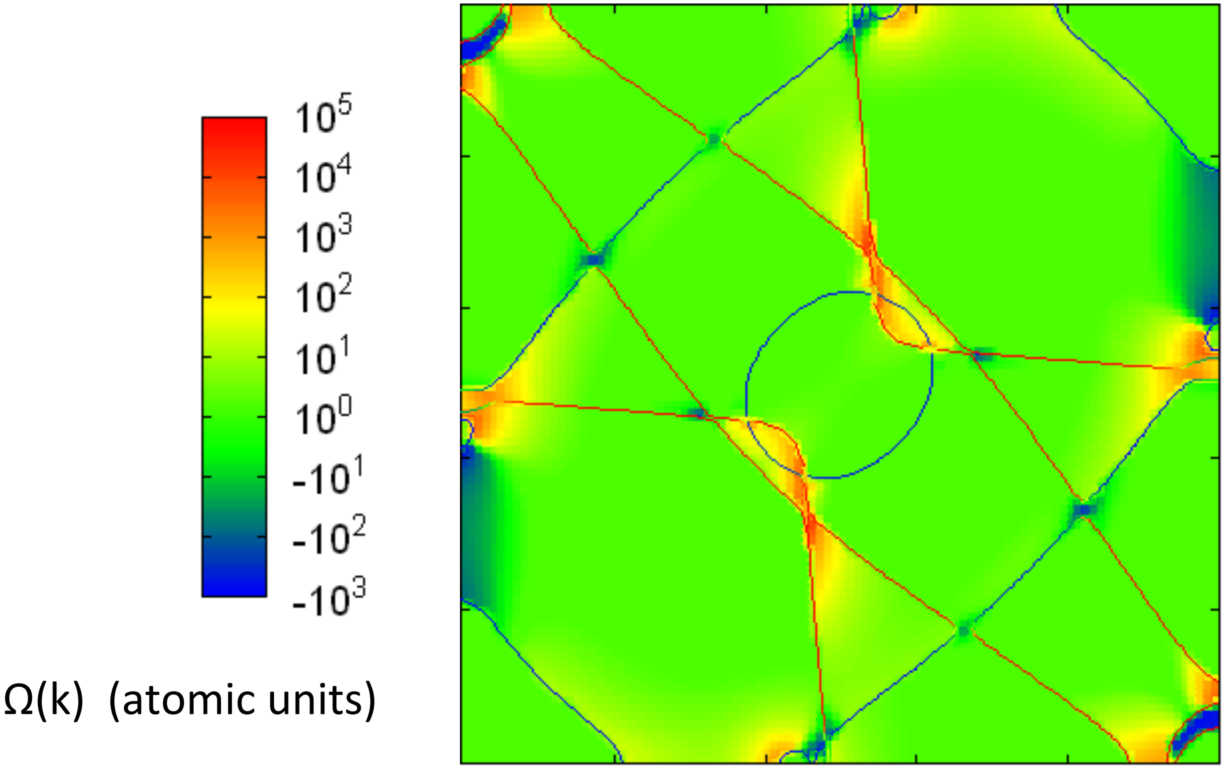
AHC $(\Omega cm)^{-1}$

	Bcc Fe	Fcc Ni	Hcp Co
Experimental Value	1032	-752	500
Our theory	771	-2362	478

- Xinjie Wang, Jonathan R. Yates, Ivo Souza, and David Vanderbilt, *"Ab-initio calculation of the anomalous Hall conductivity by Wannier interpolation,"* Phys. Rev. B 74, 195118 (2006).
- Xinjie Wang, David Vanderbilt, Jonathan R. Yates, and Ivo Souza, *"Fermi-surface calculation of the anomalous Hall conductivity,"* Phys. Rev. B 76, 195109 (2007).




bcc Fe: Calculated Berry curvature over k_y=0 plane



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

Plane-wave basis
(PWSCF)

Wannier
interpolation

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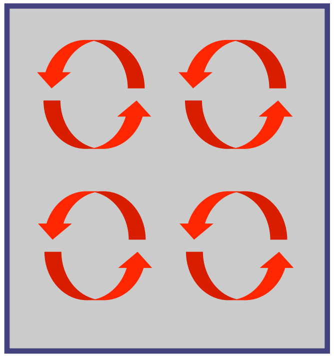
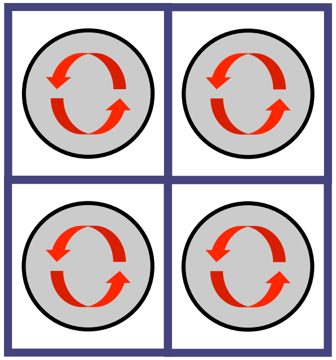
Interstitial regions are not empty!

<u>Magnetizaton:</u> $\mathrm{M} = \mathrm{M}_{\mathrm{spin}} + \boxed{\mathrm{M}_{\mathrm{orbital}}}$

Real crystals look like  not 

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

But a knowledge of **J**(**r**) is insufficient, in principle, to determine ***M*** !

Modern theory of orbital magnetization

- Semiclassical derivation
  - *D. Xiao, J. Shi, and Q. Niu, Phys. Rev. Lett.* ***95****, 137204 (2005).*
- Wannier representation derivation
  - *T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta, Phys. Rev. Lett.* ***95****, 137205 (2005).*
  - *D. Ceresoli, T. Thonhauser, D. Vanderbilt, and R. Resta, Phys. Rev. B* ***74****, 024408 (2006).*
- Long-wave derivation
  - *J. Shi, G. Vignale, D. Xiao, and Q. Niu, Phys. Rev. Lett.* ***99****, 197202 (2007).*
- Calculations for Fe, Ni, Cu
  - *D. Ceresoli, U. Gerstmann, A.P. Seitsonen, and F. Mauri, Phys. Rev. B* ***81****, 060409 (2010).*
- Relation to magnetic circular dichroism
  - *I. Souza and D. Vanderbilt, Phys. Rev. B* ***77****, 054438 (2008).*




Orbital magnetization of 2D insulator

Magnetization of finite sample

$$M = \frac{q}{2Ac} \sum_j \langle \psi_j | x v_y - y v_x | \psi_j \rangle$$

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

$$= \frac{-q}{\hbar Ac} \, \mathrm{Im} \sum_m \langle w_m | \, xHy \, | w_m \rangle$$

"Extended" orbital

Localized molecular orbital

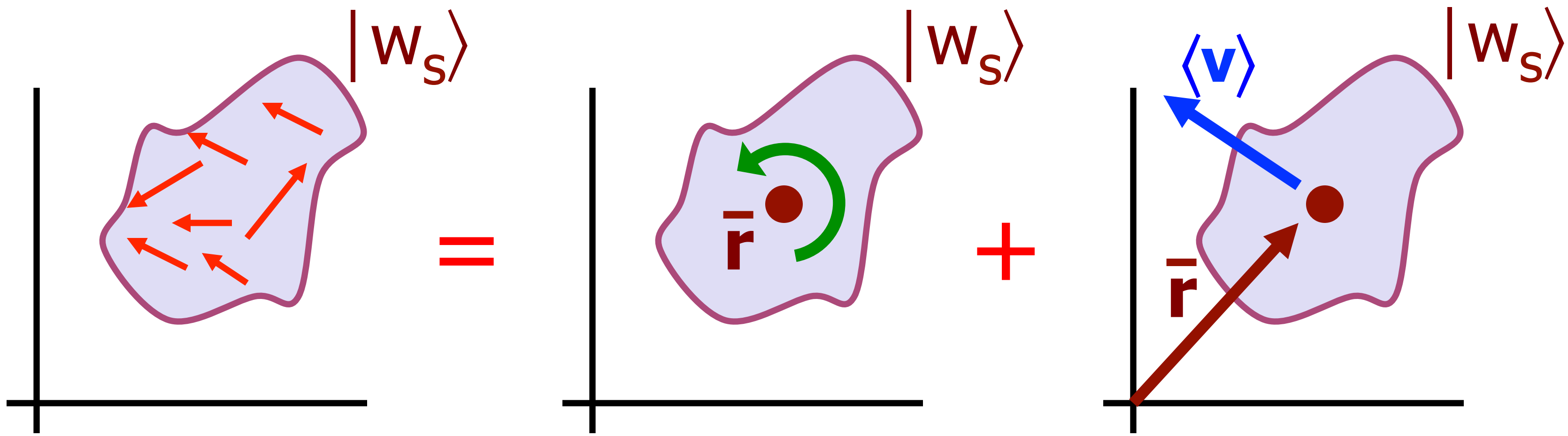
Magnetization in thermodynamic limit

$$M_{\mathrm{LC}} = \frac{-q}{\hbar c A_0} \, \mathrm{Im} \, \langle \mathbf{0} | xHy | \mathbf{0} \rangle$$

Bulk Wannier function

Is this all?

What is missing?



$$\langle w_s | \, \mathbf{r} \times \mathbf{v} \, | w_s \rangle = \underbrace{\langle w_s | \, (\mathbf{r} - \bar{\mathbf{r}}) \times \mathbf{v} \, | w_s \rangle}_{\text{Local Circulation (LC)}} + \underbrace{\bar{\mathbf{r}} \times \langle w_s | \mathbf{v} | w_s \rangle}_{\text{Itinerant Circulation (IC)}}$$

M_{orb} in Wannier representation

Local circulation

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

Itinerant circulation

$$\boxed{M_{\text{IC}} = \frac{-q}{2 A_0 \hbar c} \, \text{Im} \sum_{\mathbf{R}} \Big(R_x \, \langle \mathbf{0} | y | \mathbf{R} \rangle - R_y \, \langle \mathbf{0} | x | \mathbf{R} \rangle \Big) \langle \mathbf{R} | H | \mathbf{0} \rangle}$$

Convert two terms to k-space

$$M_{\mathrm{LC}} = \frac{-q}{\hbar c}\,\mathrm{Im}\int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2} \left\langle \frac{\partial u_{\mathbf{k}}}{\partial k_x} \right| H_{\mathbf{k}} \left| \frac{\partial u_{\mathbf{k}}}{\partial k_y} \right\rangle$$

$$M_{\mathrm{IC}} = \frac{q}{2\hbar c} \int \frac{d^2k}{(2\pi)^2}\; E(\mathbf{k})\,\Omega(\mathbf{k})$$

$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\,\left\langle \frac{du}{dk_x} \right| \left. \frac{du}{dk_y} \right\rangle$$

(Berry curvature)

$$M = \frac{-q}{\hbar c}\,\mathrm{Im}\int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2} \left\langle \frac{\partial u_{\mathbf{k}}}{\partial k_x} \right| H_{\mathbf{k}} + E_{\mathbf{k}} \left| \frac{\partial u_{\mathbf{k}}}{\partial k_y} \right\rangle$$

Results for M_{orb} of Fe, Co and Ni

	Axis	Expt.	Modern Theory: This Work	Modern Theory: Ref. 14	Muffin Tin: Ref. 14
bcc Fe	[001]*	0.081	0.0761	0.0658	0.0433
bcc Fe	[111]		0.0759	0.0660	0.0444
hcp Co	[001]*	0.133	0.0838	0.0957	0.0868
hcp Co	[100]		0.0829	0.0867	0.0799
fcc Ni	[111]*	0.053	0.0467	0.0519	0.0511
fcc Ni	[001]		0.0469	0.0556	0.0409

*Experimental easy axis.

[14] D. Ceresoli, U. Gerstmann, A. P. Seitsonen, and F. Mauri, Phys. Rev. B **81**, 060409(R) (2010).

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Linear magnetoelectric coupling (MEC)

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

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

Spin Orb. Spin Orb.

Frozen-ion orbital MEC

$$\mathbf{M}^{\mathrm{orb}}(\mathcal{E}) \propto \int d\mathbf{k}\, \langle \nabla_{\mathbf{k}} u_{\mathbf{k}}^{\mathcal{E}} | \times (H_{\mathbf{k}} + E_{\mathbf{k}}) | \nabla_{\mathbf{k}} u_{\mathbf{k}}^{\mathcal{E}} \rangle$$

$$+\, e\mathcal{E} \int \underbrace{d\mathbf{k}\, \epsilon_{ijl}\, \mathrm{tr} \left[A_i \nabla_{k_j} A_l - \frac{2i}{3} A_i A_j A_l \right]}_{\text{Chern-Simons}}$$

Note

where $\mathbf{A}(\mathbf{k}) = \langle u_{\mathbf{k}}^{\mathcal{E}} | i\nabla_{\mathbf{k}} | u_{\mathbf{k}}^{\mathcal{E}} \rangle$

Malashevich, Souza, Coh, and Vanderbilt
NJP **12** 053032 (2010)

Frozen-ion orbital MEC

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

NG = non-geometric

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

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

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

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

CS = Chern-Simons

Gauge properties of CS piece

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

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

$$\boxed{\mathbf{A}(\mathbf{k}) = -\text{Im}\,\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}}|u_{\mathbf{k}}\rangle}$$

CS = Chern-Simons

It turns out that:

- θ_{geom} is only well-defined modulo 2π
- Just as ϕ_{Berry} is only well-defined modulo 2π
- In fact, there are close mathematical relations between the two…

Consequences for topological insulators…

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