

Geometric phase formula for the macroscopic polarization

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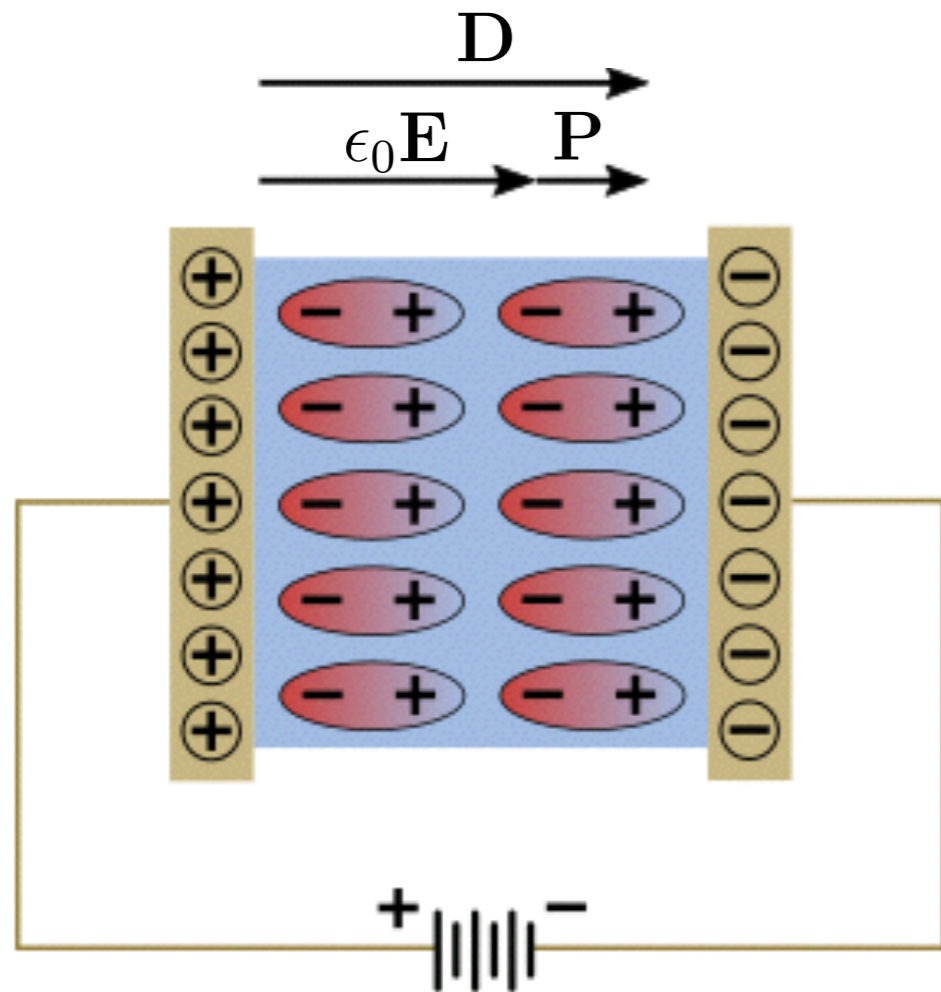
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Outline

- I. Classical theory of macroscopic polarization
 - A. Dielectrics, ferroelectrics, piezoelectrics, etc.
 - B. How to measure macroscopic polarization
 - C. Boundary conditions: finite sample versus infinite crystal
 - D. Clausius-Mossotti theory and its deficiencies
- II. Geometric phase formula for the polarization: mean-field case
 - A. Role of the current
 - B. Derivation of King-Smith-Vanderbilt formula
- III. Geometric phase formula for the polarization: interacting case
 - A. Ortiz-Martin formula
 - B. Twisted boundary conditions
- IV. Reduced geometric phase formula
 - A. Natural orbital geometric phases
 - B. Example: Rice-Mele-Hubbard model

Induced macroscopic polarization



Dielectric materials are polarized by an applied electric field (e.g. in a capacitor)

Induced polarization

$$\mathbf{P} = \epsilon_0 \chi \mathbf{E}$$

$\epsilon_0 =$ vacuum permittivity

$\chi =$ electric susceptibility

$$\nabla \cdot \mathbf{D} = \rho_{\text{free}}$$

$\rho_{\text{free}} =$ free charge

$$\nabla \cdot (\epsilon_0 \mathbf{E} + \mathbf{P}) = \rho_{\text{tot}} - \rho_b$$

$$\Rightarrow \nabla \cdot \mathbf{P} = -\rho_b$$

$\rho_b =$ bound charge

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$$

$$= \epsilon_0 (1 + \chi) \mathbf{E}$$

$$= \epsilon \mathbf{E}$$

$\epsilon =$ permittivity
(dielectric function)

Polarizability under external perturbations

Permittivity

$$\epsilon_{\alpha\beta} = \frac{dP_{\alpha}}{dE_{\beta}}$$

Piezoelectric tensor

$$\gamma_{\alpha\beta\gamma} = \frac{\partial P_{\alpha}}{\partial \epsilon_{\beta\gamma}}$$

Pyroelectric coefficient

$$\Pi_{\alpha} = \frac{dP_{\alpha}}{dT}$$

Born effective charge

$$Z_{s,\alpha\beta}^* = \frac{\Omega}{e} \frac{\partial P_{\alpha}}{\partial u_{s,\beta}}$$

Spontaneous macroscopic polarization

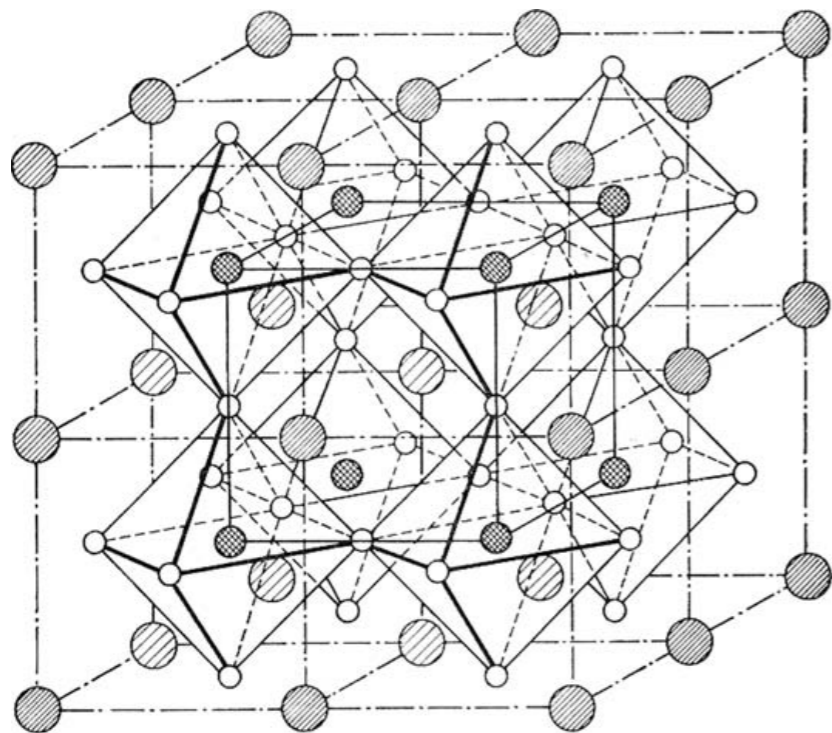
Ferroelectrics are materials with nonzero macroscopic polarization in the absence of externally applied electric fields.

Ferroelectrics have noncentrosymmetric crystal structure.

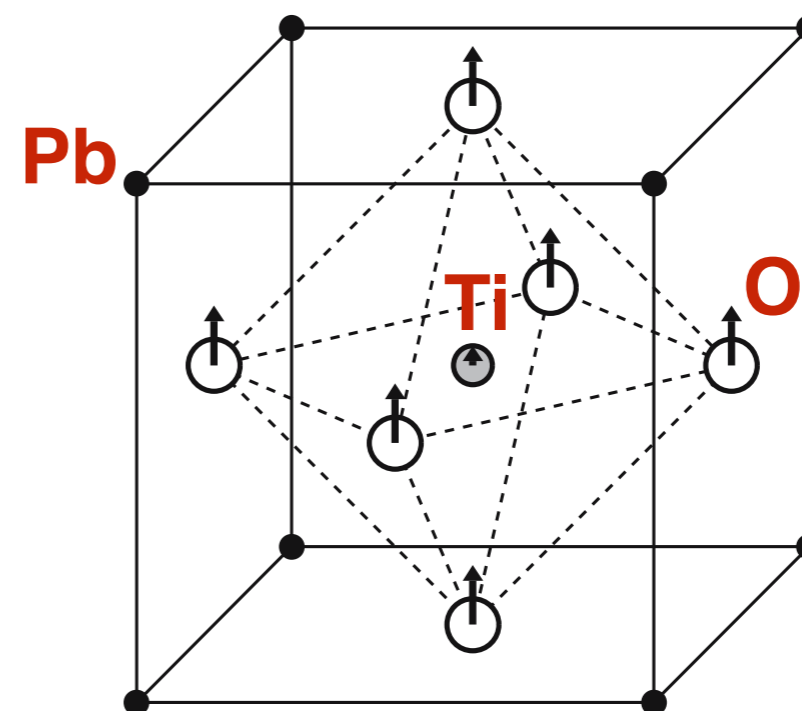
Direction of the polarization can be reversed by applying a field.

Many perovskites are ferroelectrics, e.g. BaTiO_3 , PbTiO_3 and KNbO_3 .

ABO_3 perovskite structure

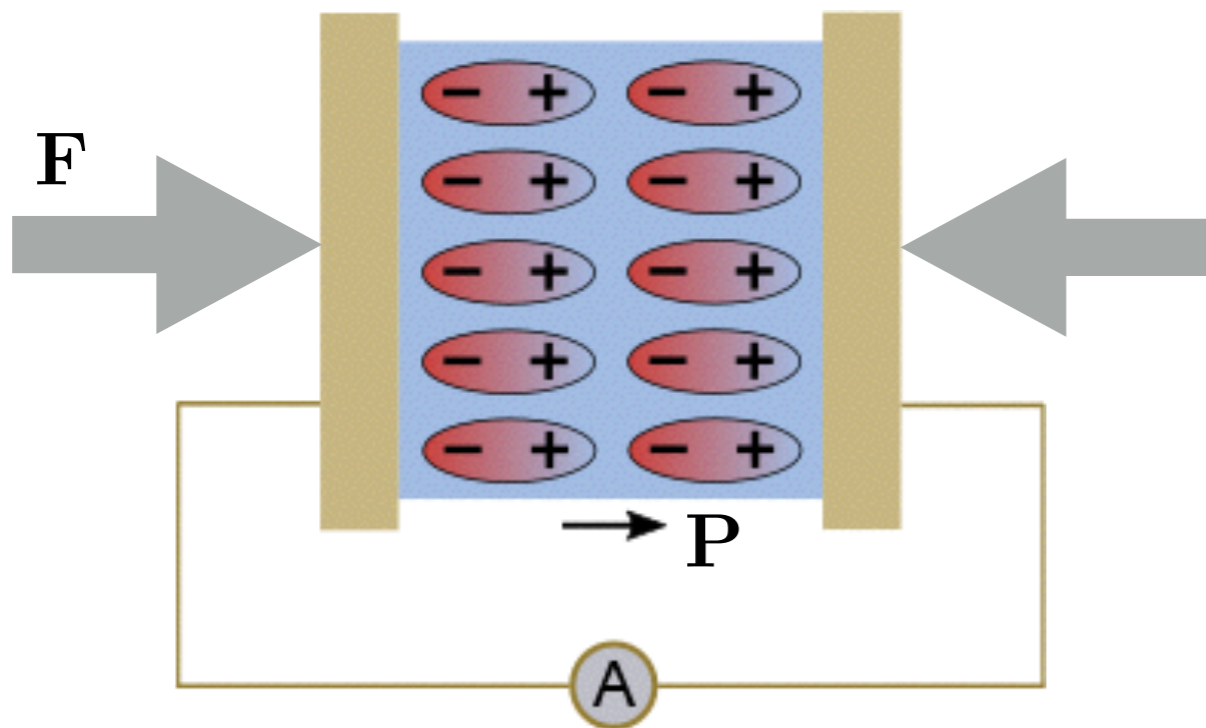


PbTiO_3



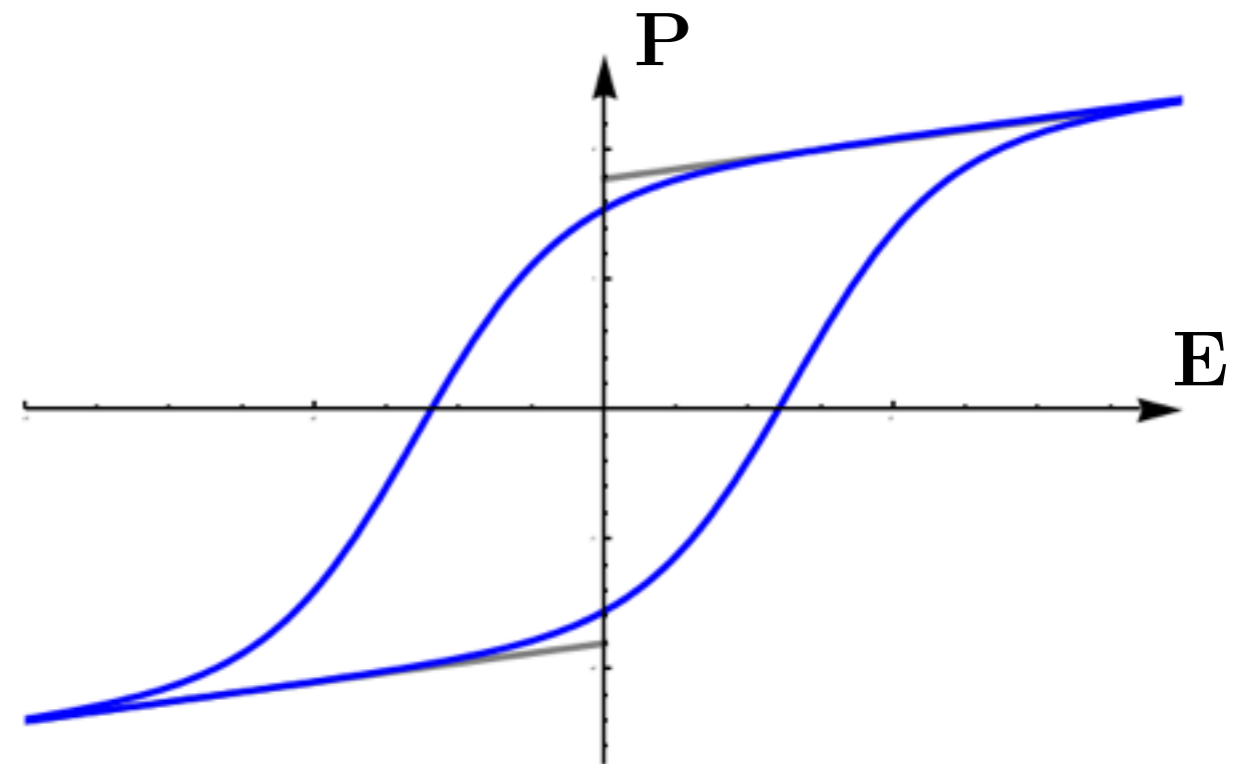
How to measure macroscopic polarization

Piezoelectric polarization



measure integrated current
as sample put under strain

Ferroelectric polarization



hysteresis loop under
cyclic variation of E

Boundary conditions

Finite sample

$$\rho(\mathbf{r}) \rightarrow 0 \text{ as } |\mathbf{r}| \rightarrow \infty$$

Macroscopic polarization is the dipole moment/volume

$$\mathbf{P}_{\text{sample}} = \frac{1}{V_{\text{sample}}} \int \rho(\mathbf{r}) \mathbf{r} d^3r$$

...determined by the charge density as in molecules.

Infinite crystal

$$\rho(\mathbf{r} + \mathbf{L}) = \rho(\mathbf{r}) \quad \text{Born-von Karman boundary conditions}$$

$$\mathbf{L} = n_i M_i \mathbf{a}_i \quad n_i = 0, 1, 2, \dots$$

Macroscopic polarization is a bulk quantity, but...

$$\mathbf{P}_{\text{macro}} \neq \frac{1}{V_{\text{cell}}} \int_{\text{cell}} \rho(\mathbf{r}) \mathbf{r} d^3r$$

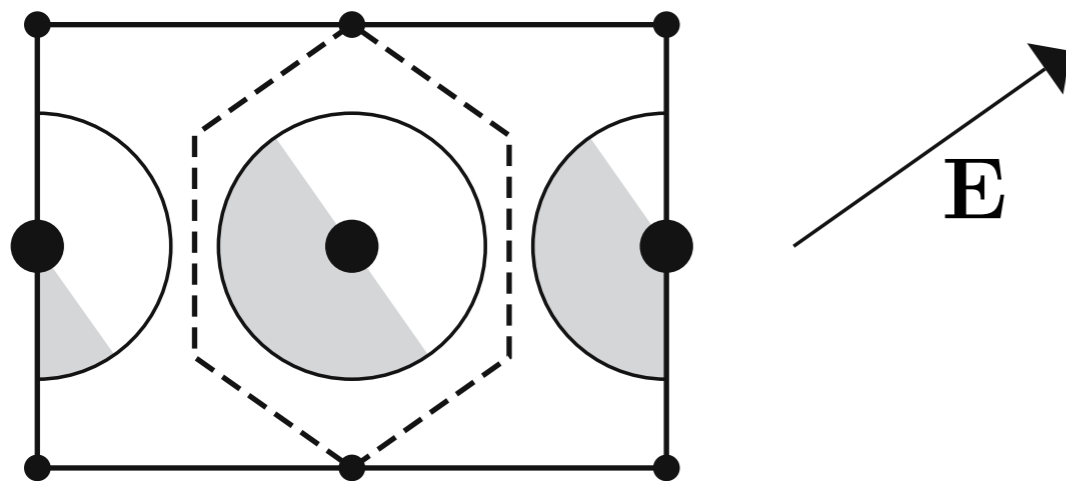
Charge density is not sufficient to calculate the polarization*

*R. Martin, Phys. Rev. B 9, 1998 (1974)

Classical theory of macroscopic polarization

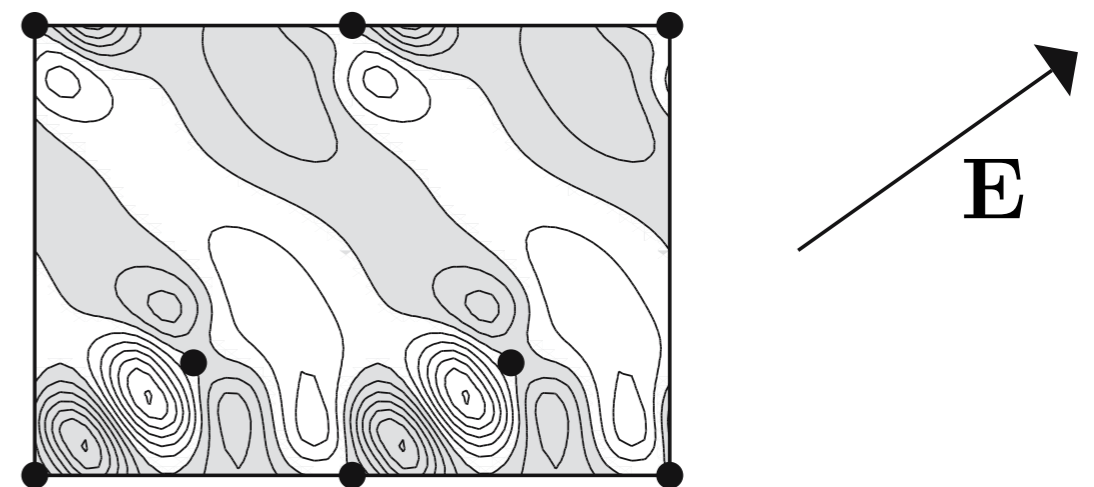
Classical theory presupposes a solid to be a collection of polarizable units

Clausius-Mossotti picture



Anions and cations separated by empty interstitial regions

Real materials



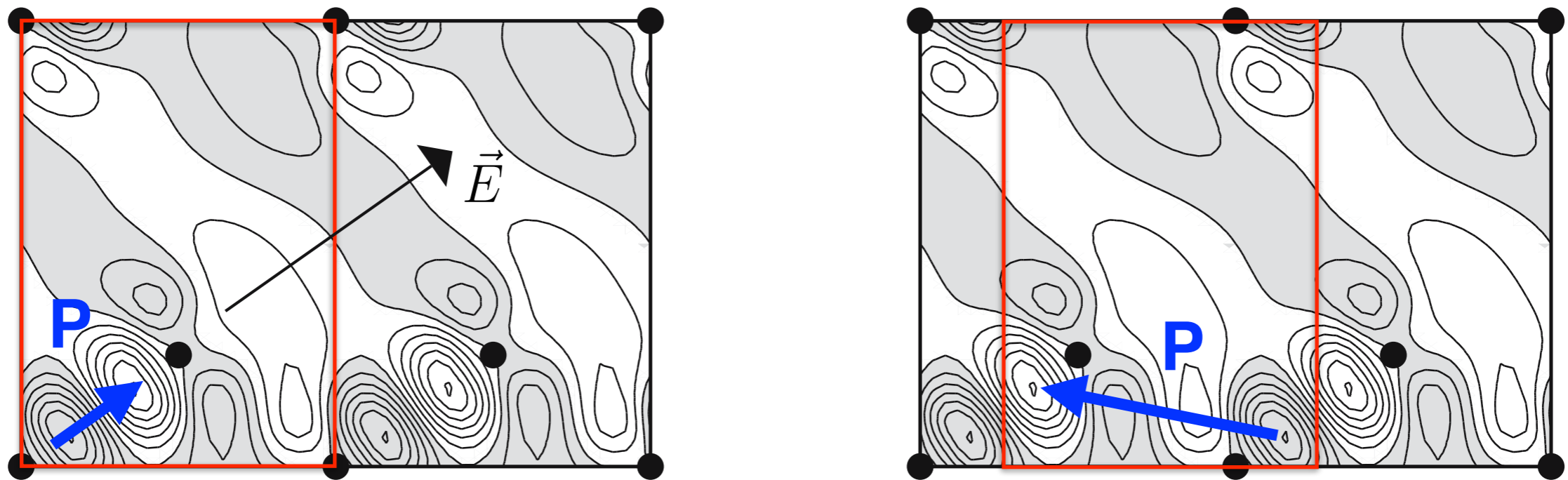
Induced charge density of Si in (110) plane; \mathbf{E} in (111) direction

Fundamental problem with the classical theory

“the [charge density in a solid] ... cannot be unambiguously decomposed into [localized] contributions.”

Incorrect definition of the macroscopic bulk polarization:

$$\mathbf{P}_{\text{macro}} \neq \frac{1}{V_{\text{cell}}} \int_{\text{cell}} \rho(\mathbf{r}) \mathbf{r} d^3r$$



shaded regions = regions of negative induced charge density

Definition of macroscopic polarization

Experiments actually measure changes in the polarization when some parameter λ changes adiabatically

$$\Delta \mathbf{P}_{\text{macro}} = \int_{t_1}^{t_2} \frac{\partial \mathbf{P}_{\text{macro}}}{\partial \lambda} \dot{\lambda} dt$$

Therefore, Resta proposed the definition

$$\Delta \mathbf{P} = \int_{t_1}^{t_2} dt \frac{1}{V_{\text{cell}}} \int_{\text{cell}} d^3 r \mathbf{j}(\mathbf{r}t)$$

Properties:

- (i) intensive bulk quantity, insensitive to surface
- (ii) has nothing to do with the charge density
- (iii) depends on quantum mechanical phases through \mathbf{j}

Role of the electronic current

Maxwell's equations in matter

$$\nabla \cdot \mathbf{D} = \rho_f$$

$$\nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}$$

constitutive relations

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$$

$$\mathbf{H} = \frac{1}{\mu_0} \mathbf{B} + \mathbf{M}$$

$$\nabla \times \left(\frac{1}{\mu_0} \mathbf{B} + \mathbf{M} \right) = \mathbf{J}_{tot} - \mathbf{J}_b + \frac{\partial}{\partial t} (\epsilon_0 \mathbf{E} + \mathbf{P})$$

$$- \left[\nabla \times \frac{1}{\mu_0} \mathbf{B} = \mathbf{J}_{tot} + \frac{\partial}{\partial t} \epsilon_0 \mathbf{E} \right]$$

$$\mathbf{J}_{tot} = \mathbf{J}_f + \mathbf{J}_b$$

\mathbf{J}_f = free current

\mathbf{J}_b = bound current

\mathbf{M} = magnetization

$$\nabla \times \mathbf{M} = -\mathbf{J}_b + \frac{\partial \mathbf{P}}{\partial t}$$

Change in macroscopic polarization

$$\frac{\partial \mathbf{P}(\mathbf{r})}{\partial t} = \mathbf{J}_b(\mathbf{r}) + \nabla \times \mathbf{M}(\mathbf{r})$$

$$\begin{aligned} \Delta \mathbf{P}_{\text{macro}} &\equiv \int_{t_1}^{t_2} \frac{1}{V_{\text{cell}}} \int_{\text{cell}} d^3 r \frac{\partial \mathbf{P}(\mathbf{r})}{\partial t} \\ &= \int_{t_1}^{t_2} \frac{1}{V_{\text{cell}}} \int_{\text{cell}} d^3 r \mathbf{J}_b(\mathbf{r}) + \int_{t_1}^{t_2} \frac{1}{V_{\text{cell}}} \int_{\text{cell}} d^3 r \nabla \times \mathbf{M}(\mathbf{r}) \\ &= \int_{t_1}^{t_2} \frac{1}{V_{\text{cell}}} \int_{\text{cell}} d^3 r \mathbf{J}_b(\mathbf{r}) + \int_{t_1}^{t_2} \frac{1}{V_{\text{cell}}} \int_{\partial(\text{cell})} d\mathbf{S} \times \mathbf{M}(\mathbf{r}) \end{aligned}$$

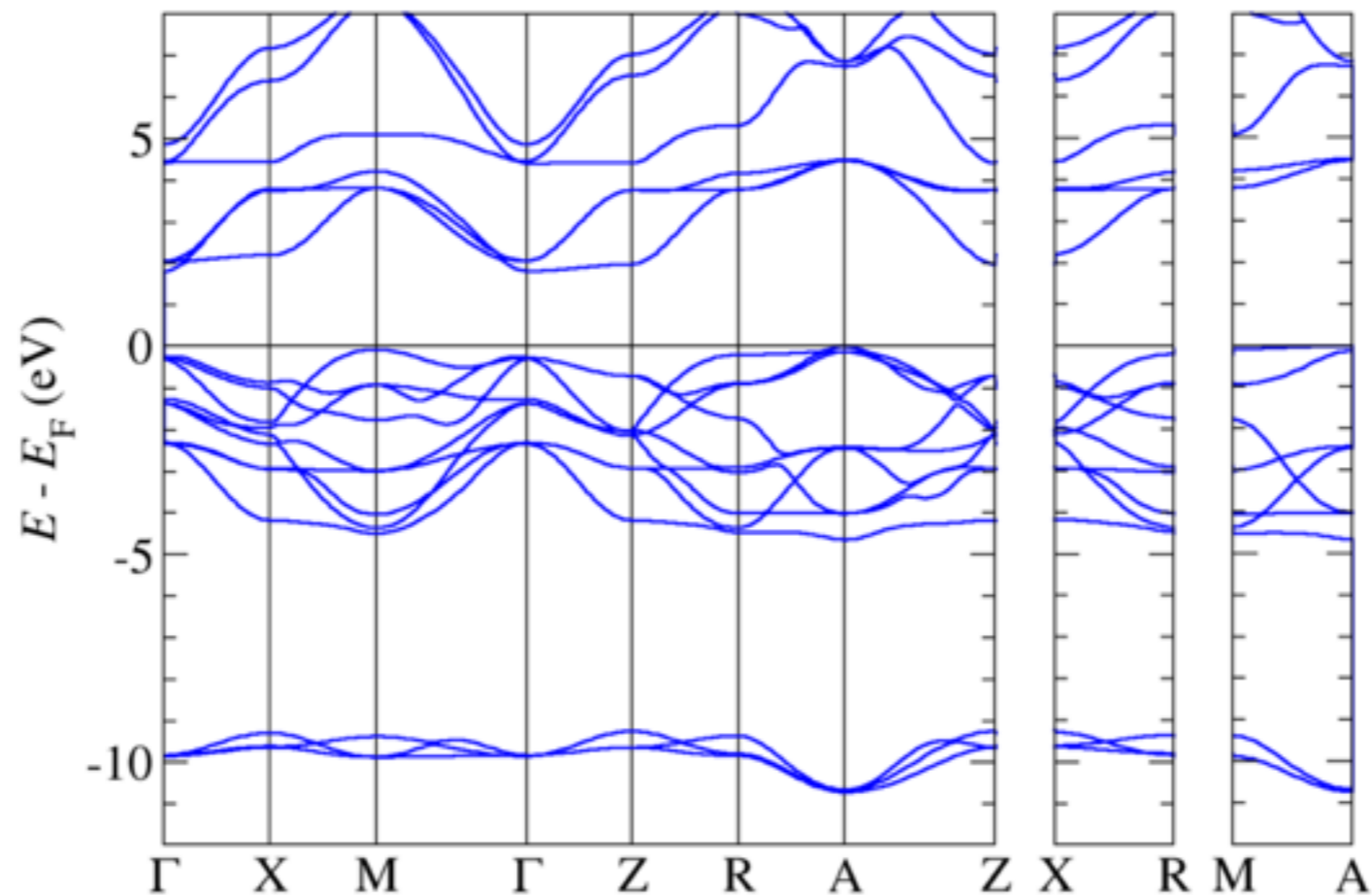
vanishes due to
periodicity of $\mathbf{M}(\mathbf{r})$

$$\Rightarrow \Delta \mathbf{P}_{\text{macro}} = \int_{t_1}^{t_2} \frac{1}{V_{\text{cell}}} \int_{\text{cell}} d^3 r \mathbf{j}(\mathbf{r})$$

$[\mathbf{j}(\mathbf{r}) = \mathbf{J}_b(\mathbf{r})]$ (ions give addl. contribution)

Geometric phase formula: mean-field case

Kohn-Sham electronic band structure of BaTiO₃



$$\left[\frac{\mathbf{p}^2}{2m} + v_{\text{ext}}(\mathbf{r}) + v_h(\mathbf{r}) + v_{xc}(\mathbf{r}) \right] \psi_{n\mathbf{k}}(\mathbf{r}) = \epsilon_{n\mathbf{k}} \psi_{n\mathbf{k}}(\mathbf{r}) \quad \text{Kohn-Sham equations}$$

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) = \text{Bloch function for band } n \text{ and wavevector } \mathbf{k}$$

Geometric phase formula: mean-field case

To first order in $\dot{\lambda}$, time dependent perturbation theory gives

$$|\delta\psi_{n\mathbf{k}}\rangle = i\hbar\dot{\lambda} \sum_{m \neq n} \frac{\langle \psi_{m\mathbf{k}} | \partial_{\lambda} \psi_{n\mathbf{k}} \rangle}{\epsilon_{m\mathbf{k}} - \epsilon_{n\mathbf{k}}} |\psi_{m\mathbf{k}}\rangle$$

Induced current from the n^{th} occupied band is

$$\mathbf{j}_n = \frac{i\hbar e \dot{\lambda}}{m} \sum_{m \neq n} \int \frac{d^3 k}{(2\pi)^3} \frac{\langle \psi_{n\mathbf{k}} | \hat{\mathbf{P}} | \psi_{m\mathbf{k}} \rangle \langle \psi_{m\mathbf{k}} | \partial_{\lambda} \psi_{n\mathbf{k}} \rangle}{\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}}} + c.c.$$

After some manipulation

$$\frac{d\mathbf{P}}{dt} = -e\dot{\lambda} \sum_n^{\text{occ}} \int \frac{d^3 k}{(2\pi)^3} 2\text{Im} \langle \nabla_{\mathbf{k}} u_{n\mathbf{k}} | \partial_{\lambda} u_{n\mathbf{k}} \rangle$$

Geometric phase formula: mean-field case

$$\Delta \mathbf{P} = -e \int_0^1 d\lambda \int_{BZ} \frac{d^3 k}{(2\pi)^3} B_{\mathbf{k}\lambda}$$

with the Berry curvature

$$B_{\mathbf{k}\lambda} = 2\text{Im} \sum_n \langle \nabla_{\mathbf{k}} u_{n\mathbf{k}} | \partial_\lambda u_{n\mathbf{k}} \rangle,$$

To calculate $\Delta P_\alpha = \frac{1}{2\pi} \Delta \mathbf{P} \cdot \mathbf{G}_\alpha$ along a given lattice vector \mathbf{R}_α , define, e.g.,

$$\Delta P_3 = -\frac{e}{2\pi} \sum_n^{\text{occ}} \int \frac{dk_1 dk_2}{(2\pi i)^2} \underbrace{\int_0^{|\mathbf{G}_3|} i \langle u_{n\mathbf{k}} | \partial_{k_3} u_{n\mathbf{k}} \rangle dk_3}_{\gamma(k_1, k_2, \lambda)} \Bigg|_{\lambda=0}^{\lambda=1}$$

Geometric phase formula: mean-field case

$$\gamma = \sum_n^{\text{occ}} \int i \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle d^3 k \text{ is a gauge-invariant quantity modulo } 2\pi$$

gauge transformation

$$|u_{n\mathbf{k}}\rangle \rightarrow |\tilde{u}_{n\mathbf{k}}\rangle = e^{-i\lambda(k_\alpha)} |u_{n\mathbf{k}}\rangle \quad \gamma \rightarrow \tilde{\gamma} = \gamma + \int_0^{2\pi/a} \frac{\partial \lambda}{\partial k_\alpha} dk_\alpha$$
$$= \gamma + 2\pi m$$

$$\mathbf{P} = -\frac{e}{2\pi} \sum_n^{\text{occ}} \int i \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle d^3 k \quad \text{defines the polarization modulo a } \textit{polarization quantum}$$

Polarization quantum $\mathbf{P}_{\text{quant}} = \frac{e\mathbf{R}}{V_{\text{cell}}}$, \mathbf{R} = lattice vector

Wannier function centers

Defining Wannier functions as

$$w_n(\mathbf{r} - \mathbf{R}) = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{BZ} d^3k e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})} u_{n\mathbf{k}}(\mathbf{r})$$

and using

$$u_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})} w_n(\mathbf{r} - \mathbf{R})$$

one finds

$$\langle w_{n\mathbf{R}} | \mathbf{r} | w_{n\mathbf{R}} \rangle = \frac{V_{\text{cell}}}{(2\pi)^3} \int i \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle d^3k$$

Hence

$$\mathbf{P} = -\frac{e}{V_{\text{cell}}} \sum_n \langle w_{n\mathbf{R}} | \mathbf{r} | w_{n\mathbf{R}} \rangle$$

Limitations of the mean-field formula

When using the Kohn-Sham Bloch orbitals $|\psi_{n\mathbf{k}}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u_{n\mathbf{k}}\rangle$, the mean-field formula

$$\mathbf{P} = -\frac{e}{2\pi} \sum_n \int i \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} u_{n\mathbf{k}} \rangle d^3k$$

is not guaranteed to give the correct macroscopic polarization even when the exact v_{xc} is used.

It is not valid for insulating materials for which the Kohn-Sham band structure is metallic,* e.g. Mott insulators, and can be expected to have significant errors in strongly-correlated materials.

Density-polarization functional theory, where the exchange-correlation functional depends on the macroscopic polarization in addition to the density, has been proposed to overcome this issue.*

*Gonze, Ghosez & Godby, Phys. Rev. Lett. 74, 4035 (1995); *ibid.* 78, 294 (1997)

Geometric phase formula: interacting case

$$\hat{H} = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m} + \hat{V}_{ee} + \hat{V}_{\text{ext}}(\lambda)$$

Based on Thouless's charge pumping formula,* Ortiz and Martin proposed†

$$\Delta P = -e \lim_{\substack{N, L \rightarrow \infty \\ N/L = \text{const.}}} \int_0^1 d\lambda \int_0^{2\pi/L} \frac{dk}{2\pi} 2\text{Im} \langle \partial_k \Phi | \partial_\lambda \Phi \rangle,$$

where $\Phi(r_1\sigma_1, \dots, r_N\sigma_N)$ is the ground state of the “twisted” Hamiltonian

$$\hat{H}_k = \sum_{i=1}^N \frac{(\hat{p}_i + \hbar k)^2}{2m} + \hat{V}_{ee} + \hat{V}_{\text{ext}}(\lambda).$$

$|\Phi\rangle$ is related to the ground state of the original Hamiltonian via

$$\Phi(r_1\sigma_1, \dots, r_N\sigma_N) = e^{-ik(r_1 + \dots + r_N)} \Psi(r_1\sigma_1, \dots, r_N\sigma_N).$$

*D. J. Thouless, PRB 27, 6083 (1983); Q. Niu and D. J. Thouless, J. Phys. A: Math. Gen. 17, 2453 (1984).

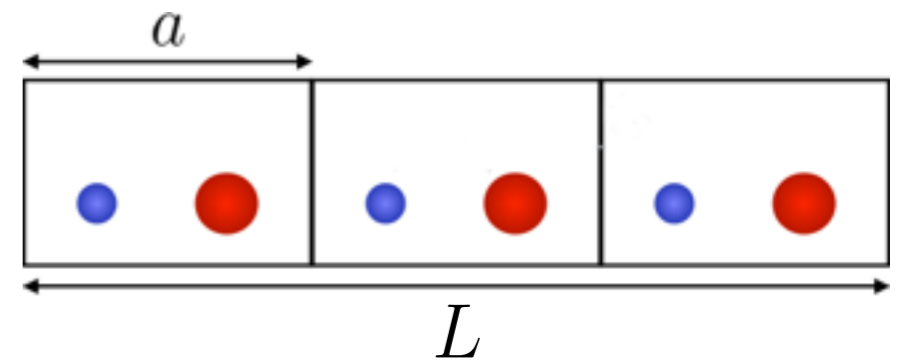
†G. Ortiz and R. M. Martin, PRB 49, 14202 (1994).

Geometric phase formula: interacting case

$$\begin{aligned}\Delta P &= -\frac{e}{2\pi} \lim_{\substack{N, L \rightarrow \infty \\ N/L = \text{const.}}} \int_0^{2\pi/L} i \langle \Phi | \partial_k \Phi \rangle dk \Big|_{\lambda=0}^{\lambda=1} \\ &= -\frac{e}{2\pi} [\gamma(\lambda = 1) - \gamma(\lambda = 0)]\end{aligned}$$

N = number of electrons

$L = Ma =$ length of supercell, $M =$ integer



Twisted boundary conditions

$$\Psi(r_1, \dots, r_i + L, \dots, r_N) = e^{ikL} \Psi(r_1, \dots, r_i, \dots, r_N)$$

Reduced geometric phase formula

$$\Delta \mathbf{P}_{red} = -e \int_0^1 d\lambda \int_{BZ} \frac{d^3 k}{(2\pi)^3} 2\text{Im} \sum_{n=1}^{\infty} \langle \nabla_{\mathbf{k}} v_{n\mathbf{k}} | \partial_{\lambda} v_{n\mathbf{k}} \rangle$$

$$\Delta P_3 = -\frac{e}{(2\pi)^3} \sum_{n=1}^{\infty} \int dk_1 dk_2 \int_0^{|\mathbf{G}_3|} i \langle v_{n\mathbf{k}} | \partial_{k_3} v_{n\mathbf{k}} \rangle dk_3 \Big|_{\lambda=0}^{\lambda=1}$$

natural orbital geometric phases^{*} $\gamma_n = \int_{BZ} \frac{d^3 k}{(2\pi)^3} i \langle v_{n\mathbf{k}} | \partial_{k_3} v_{n\mathbf{k}} \rangle$

natural Bloch orbitals[†]

$$\psi_{n\mathbf{k}}(\mathbf{r}) = v_{n\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}}$$

$$v_{n\mathbf{k}}(\mathbf{r}) = \sqrt{f_{n\mathbf{k}}} e^{-i\zeta_{n\mathbf{k}}} \phi_{n\mathbf{k}}(\mathbf{r})$$

$\phi_{n\mathbf{k}}(\mathbf{r}) =$ natural orbital

$f_{n\mathbf{k}} =$ occupation number

$\zeta_{n\mathbf{k}} =$ phase variable from higher-order reduced density matrices^{*#}

^{*}RR & Pankratov, PRA 81, 042519 (2010); PRA 83, 052510 (2011);

RR PRA 86, 022117 (2012)

[†]RR & Gross, arxiv:1709.03372

[#]Related work for molecules by Giesbertz Gritsenko Baerends PRL 105, 013002 (2010)

Reduced geometric phase formula

$$\Delta P_{red} = -\frac{e}{2\pi} \sum_{n=1}^{\infty} \int_{BZ} i \langle \chi_{nk} | \partial_k \chi_{nk} \rangle dk \Big|_{\lambda=0}^{\lambda=1}$$

One-body reduced density matrix

$$\rho_1(r\sigma, r'\sigma') = \sum_{\sigma_2 \dots \sigma_N} \int \Psi(r\sigma, r_2\sigma_2, \dots, r_N\sigma_N) \Psi^*(r'\sigma', r_2\sigma_2, \dots, r_N\sigma_N) dr_2 \dots dr_N$$

$$\sum_{\sigma'} \int \rho_1(r\sigma, r'\sigma') \psi_{nk}(r'\sigma') dr' = f_{nk} \psi_{nk}(r\sigma) \quad \frac{\partial E(\{f_{nk}, \phi_{nk}, \zeta_{nk}, \beta_{nk}\})}{\partial \zeta_{nk}} = 0$$

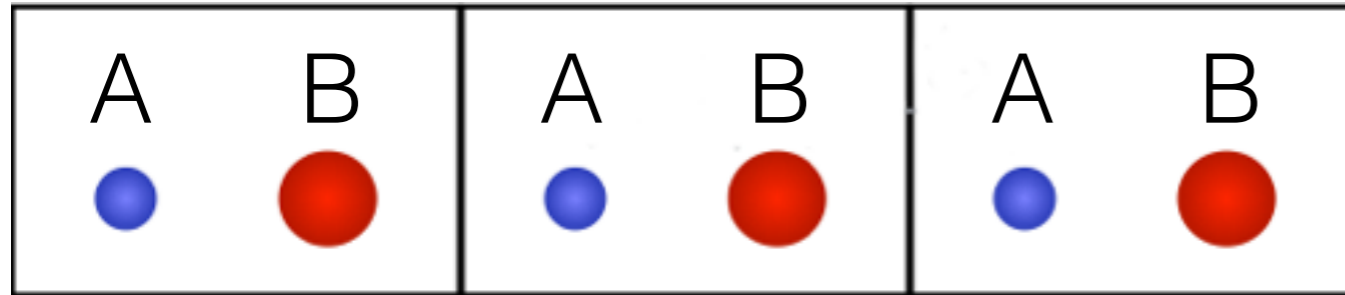
Properties:

- (i) approximates the Ortiz-Martin formula
- (ii) accounts for quantum fluctuations through the f_{nk}
- (iii) reduces to King-Smith-Vanderbilt in noninteracting limit
- (iv) exact in certain cases

Rice-Mele-Hubbard model

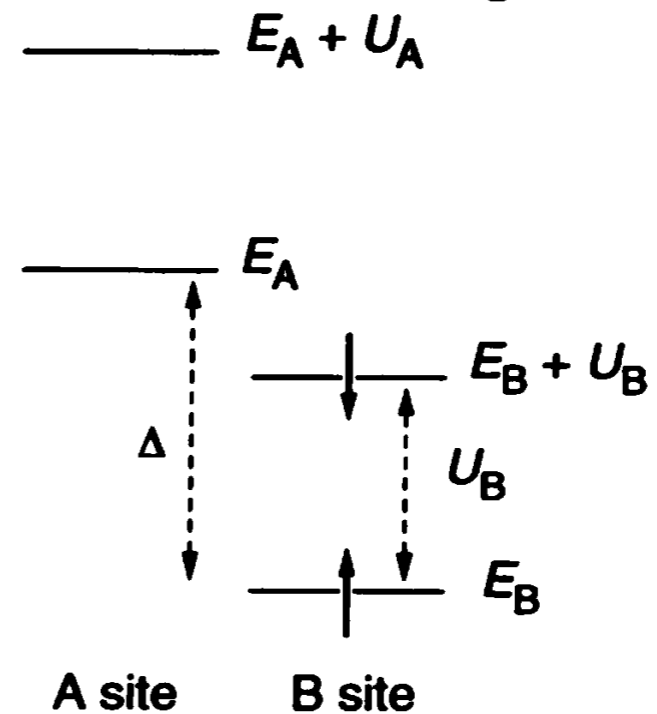
$$\Delta P = -\frac{e}{2\pi} \lim_{\substack{N, L \rightarrow \infty \\ N/L = \text{const.}}} \int_0^{2\pi/L} i \langle \Phi | \partial_k \Phi \rangle dk \Big|_{\lambda=0}^{\lambda=1}$$

Applications to the *band insulator* - *Mott insulator* transition in the Rice-Mele-Hubbard model in 1D and 2D.*

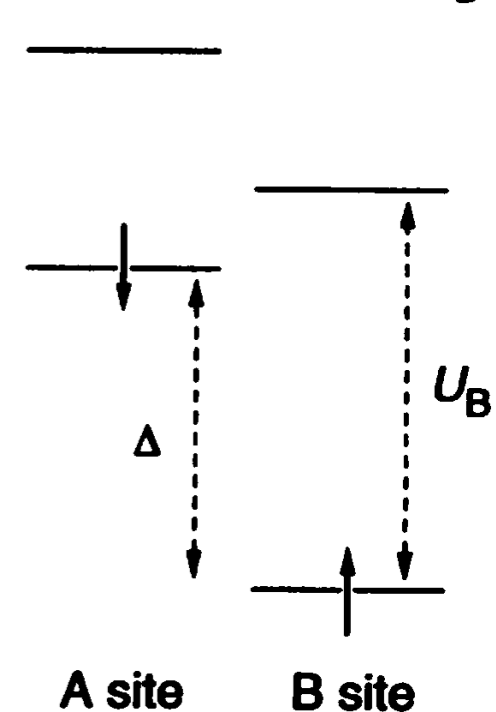


● = cation, e.g. Mg
● = anion, e.g. O

Ionic insulator ($\Delta > U_B$)



Mott insulator ($\Delta < U_B$)



*R. Resta and S. Sorella, PRL 74, 4738 (1995);

G. Ortiz, P. Ordejon, R. M. Martin and G. Chiappe, PRB 54, 13515 (1996);

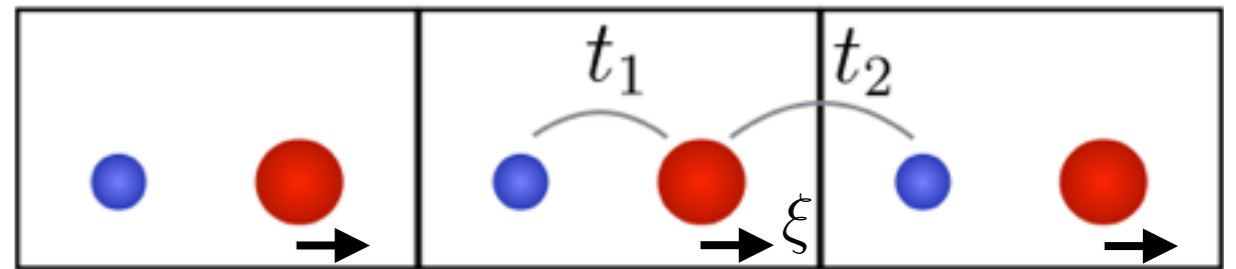
N. Gidopoulos, S. Sorella and E. Tosatti, Eur. Phys. J. B 14, 217 (2000).

Diagram from T. Egami, S. Ishihara and M. Tachiki, Science 261, 1307 (1993); PRB 49, 8944 (1994).

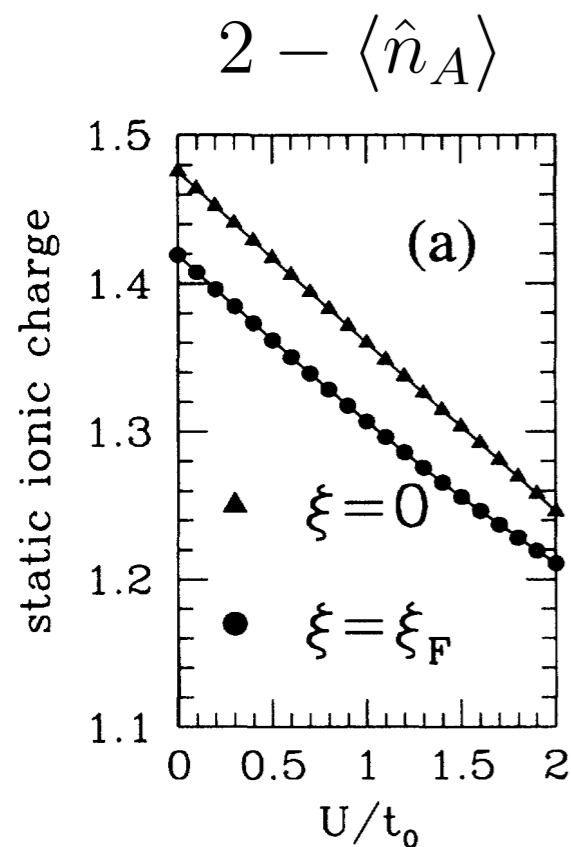
Rice-Mele-Hubbard model

$$\hat{H} = \sum_{n\sigma} \left[\epsilon_n c_{n\sigma}^\dagger c_{n\sigma} + t_{nn+1} (c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma}) + U c_{n\uparrow}^\dagger c_{n\uparrow} c_{n\downarrow}^\dagger c_{n\downarrow} \right]$$

$$\begin{aligned} \epsilon_{2n} &= -\Delta & t_1 &= t_0 - \alpha\xi \\ \epsilon_{2n+1} &= +\Delta & t_2 &= t_0 + \alpha\xi \end{aligned}$$

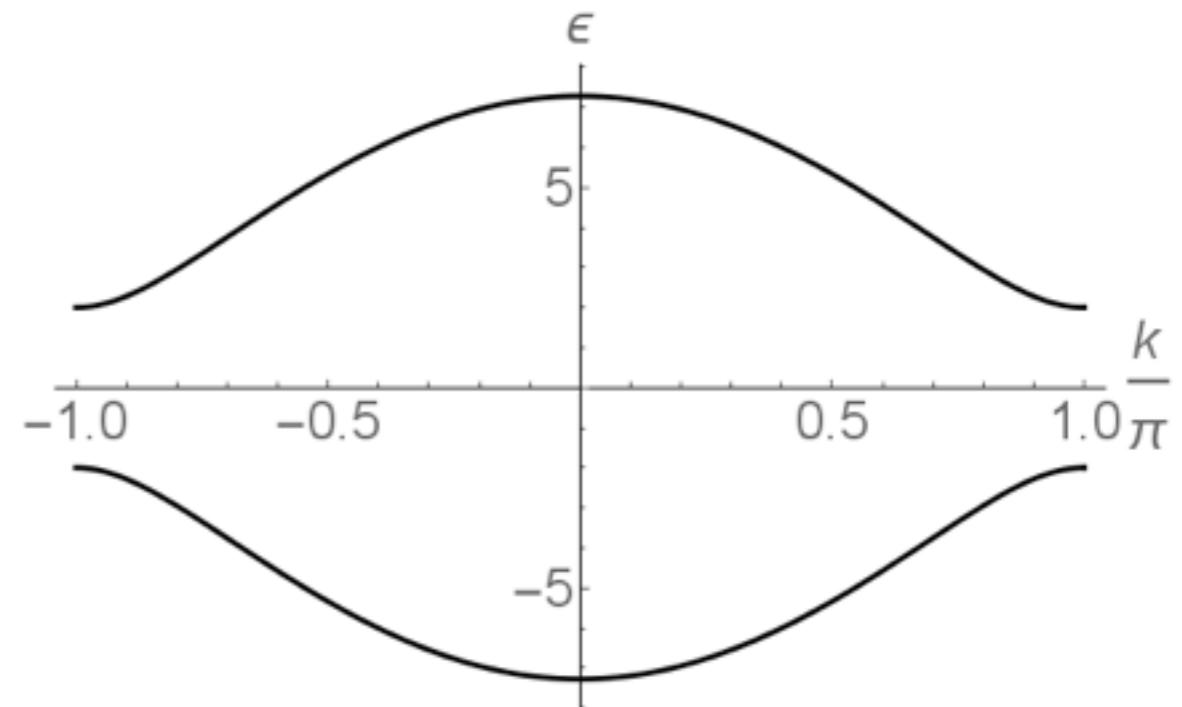


ξ = displacement of B sublattice



$$\begin{aligned} \Delta &= 2.0 \text{ eV} \\ t_0 &= 3.5 \text{ eV} \\ \alpha &= 20 \text{ eV}/a \\ \xi_F &= 0.05a \end{aligned}$$

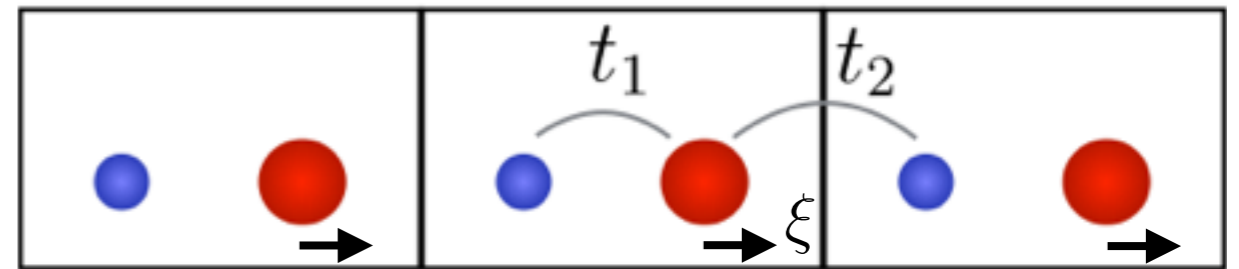
Bands for $U = 0$



Rice-Mele-Hubbard model

$$\hat{H} = \sum_{n\sigma} \left[\epsilon_n c_{n\sigma}^\dagger c_{n\sigma} + t_{nn+1} (c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma}) + U c_{n\uparrow}^\dagger c_{n\uparrow} c_{n\downarrow}^\dagger c_{n\downarrow} \right]$$

$$\begin{aligned} \epsilon_{2n} &= -\Delta & t_1 &= t_0 - \alpha\xi \\ \epsilon_{2n+1} &= +\Delta & t_2 &= t_0 + \alpha\xi \end{aligned}$$

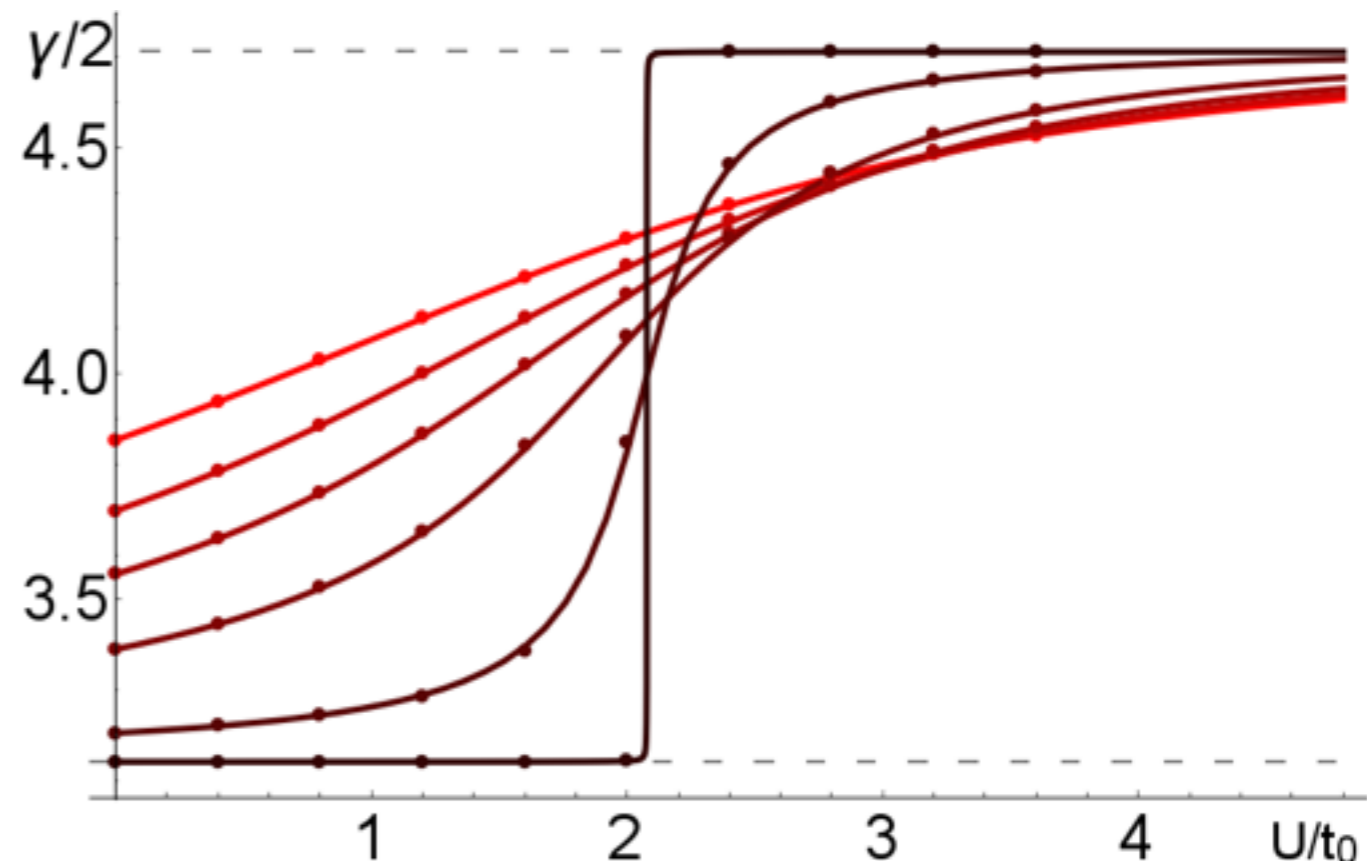


ξ = displacement of B sublattice

$$\mathbf{P} = -\frac{e}{2\pi} \gamma(\xi)$$

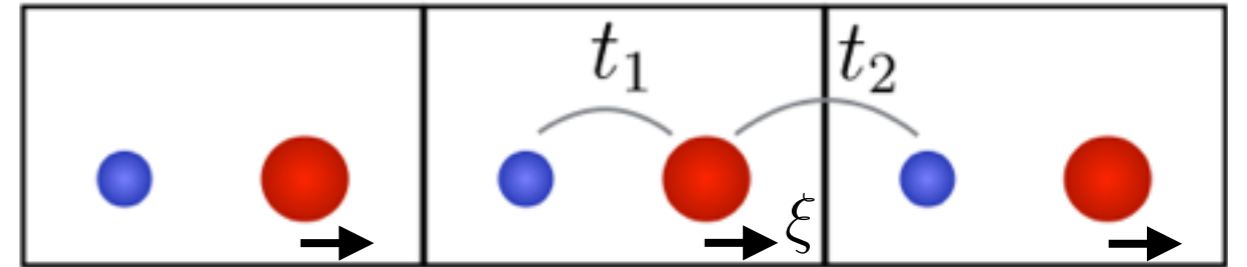
$$\gamma(\xi) = \int_0^{2\pi/L} i \langle \Phi | \partial_k \Phi \rangle dk$$

$\gamma(\xi)$ is an order parameter for the band insulator-Mott insulator transition



Average Born charge $\langle Z^*(\xi) \rangle$

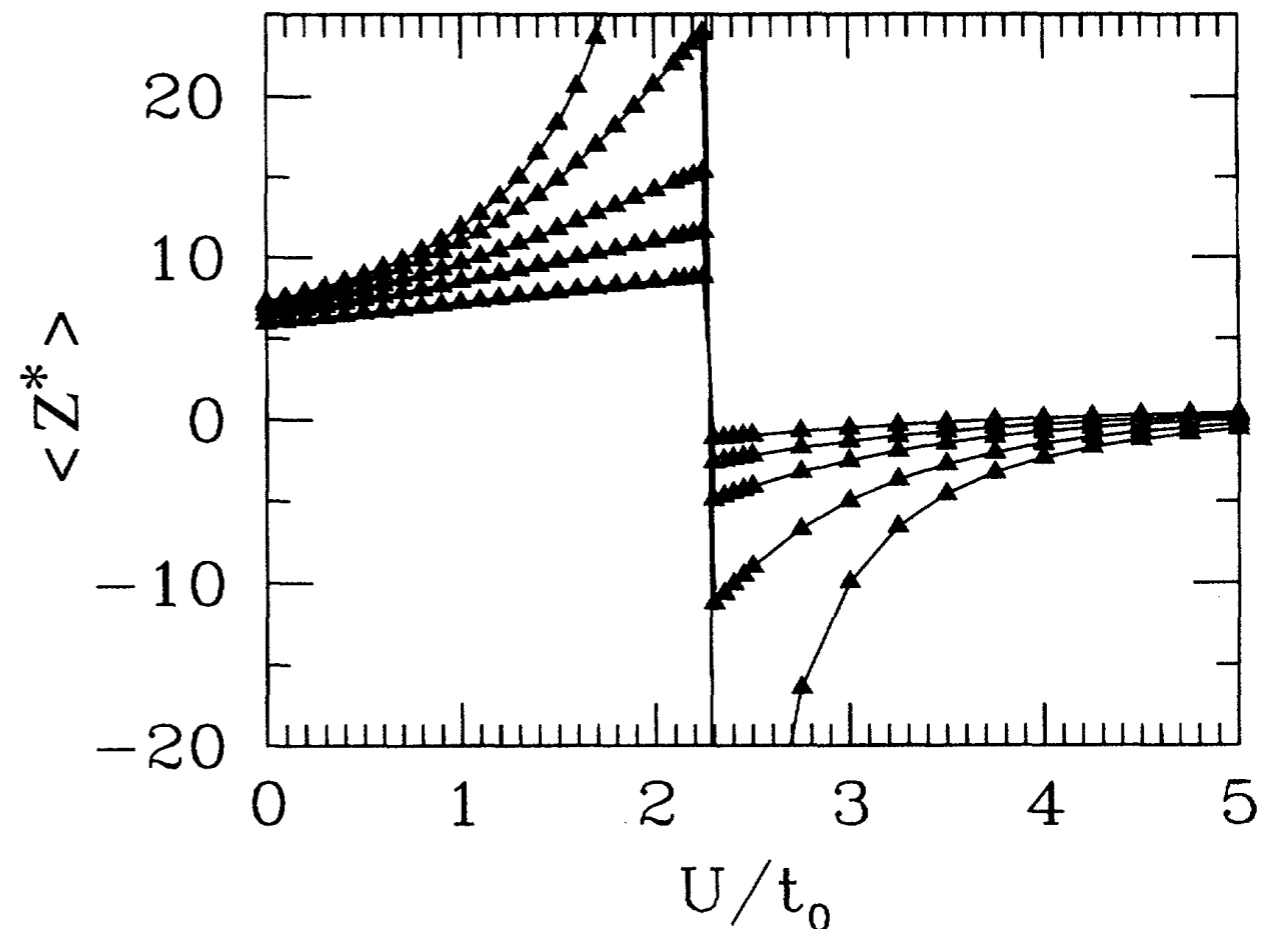
$$\Delta P(\xi_1, \xi_2, \dots) = e \sum_s \langle Z_s^*(\xi_s) \rangle \xi_s$$



ξ = displacement of B sublattice

Definition of Born charge

$$\langle Z^*(\xi) \rangle = \frac{\Delta P(\xi)}{\xi}$$



$\xi = (0.05, 0.035, 0.0245, 0.0140, 0.0035)$

Summary

- Charge density does not uniquely determine the macroscopic polarization in infinite crystals (periodic boundary conditions)
- Macroscopic polarization is related to the adiabatic current flowing through a unit cell and can be expressed as a geometric phase
- Mean-field formula gives the polarization as the geometric phase of the Kohn-Sham Bloch functions across the Brillouin zone
- Interacting formula gives the polarization as the geometric phase of the many-body wavefunction w.r.t. twisted boundary conditions
- Reduced geometric phase formula simplifies the full interacting formula, while retaining the most important correlation effects