Modern theory of ferroelectrics

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Outline

- Modern theory of polarization
  - What is the problem?
  - Berry phase formulation
  - Wannier center formulation
- Effective Hamiltonian approach
- Theory of flexoelectricity
- Summary and prospects

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Density-functional theory

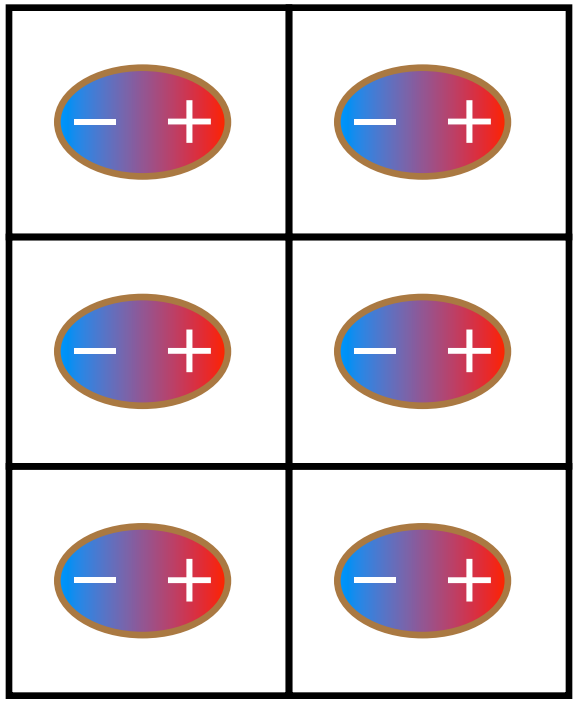
Calculates with pretty good accuracy:

- Energies
- Forces
- Relaxed structures
- Phonons
- Etc.

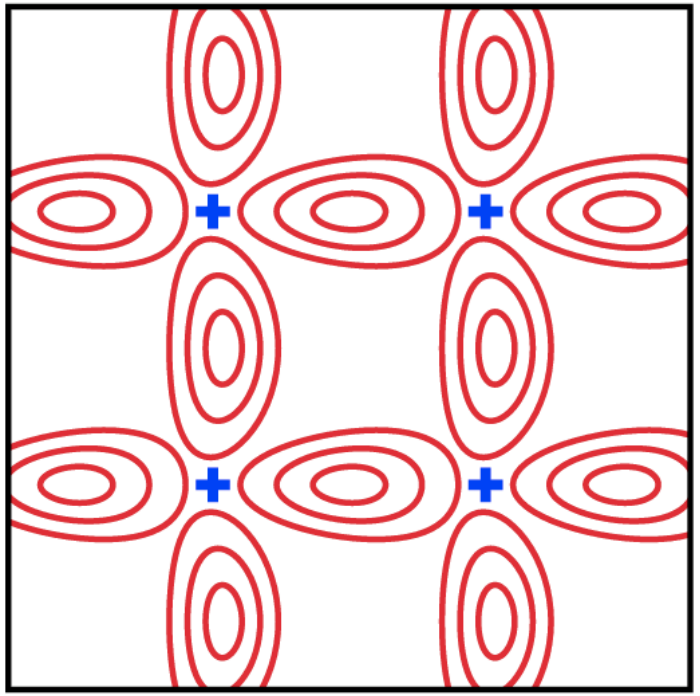
Now implemented in “standard” packages including:

- ABINIT (Belgium; open source)
- Quantum Espresso (Italy; open source)
- VASP (Austria; licensed)

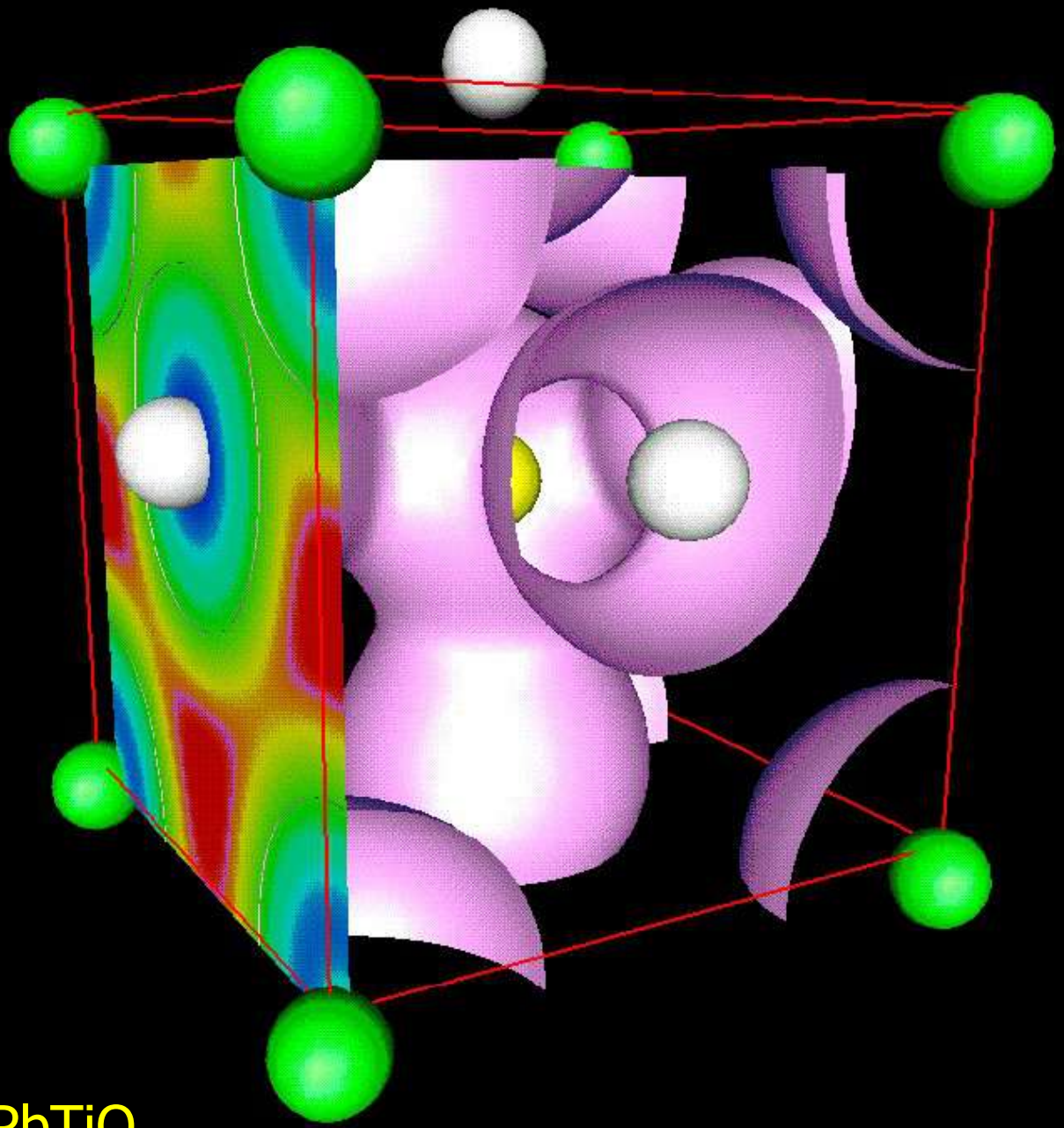
The Problem: Polarization



Textbook illustration

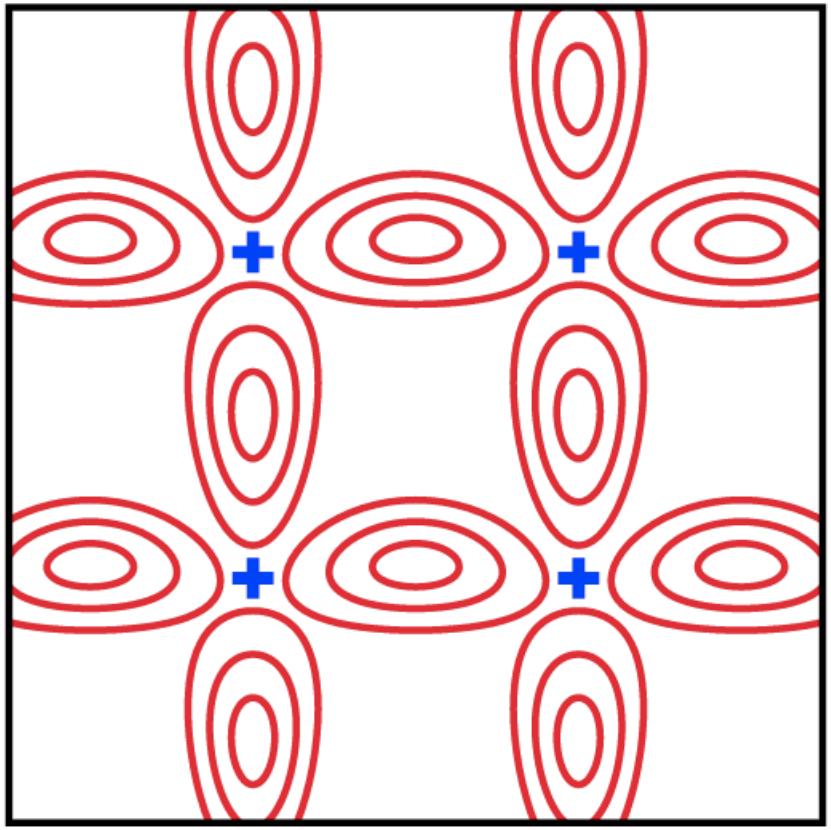


More realistic picture

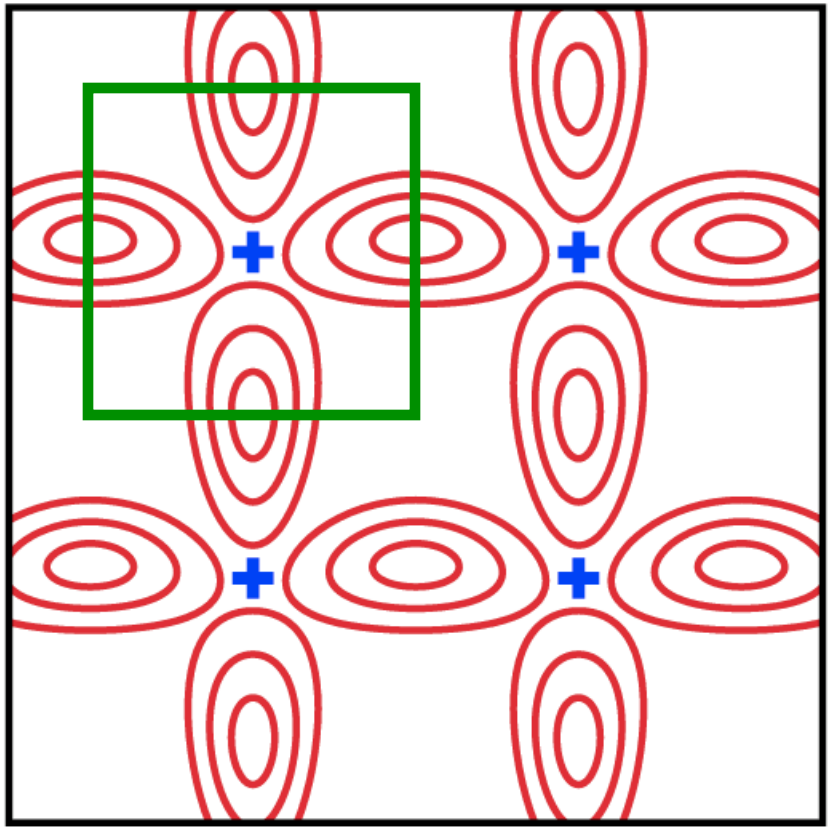


Ferroelectric $PbTiO_3$

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



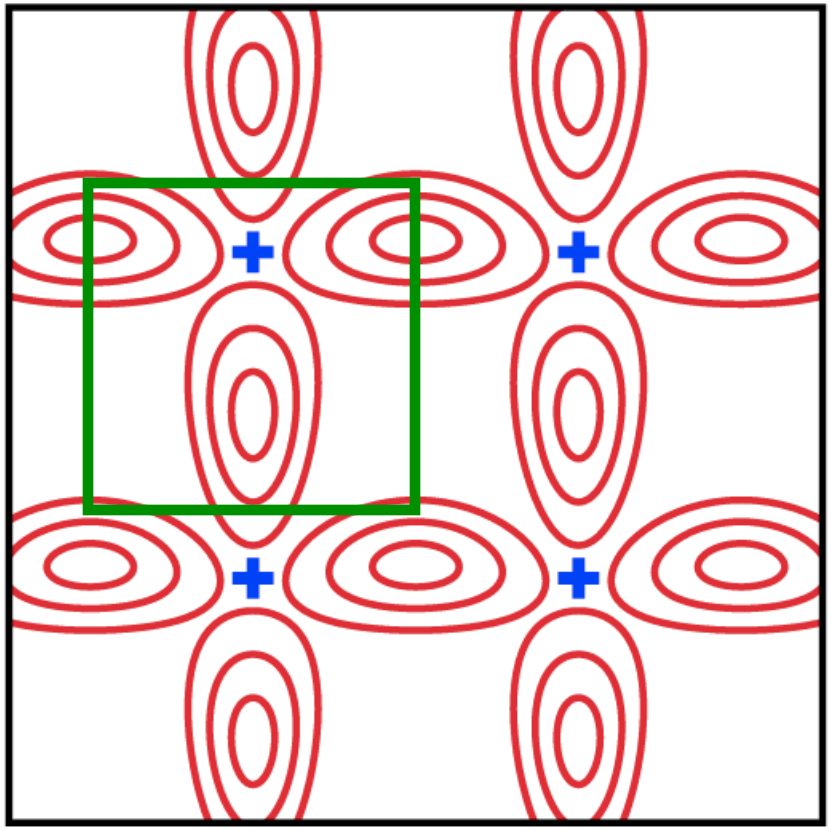
$\boldsymbol{P} = \boldsymbol{d}_{cell} / V_{cell}$?



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

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

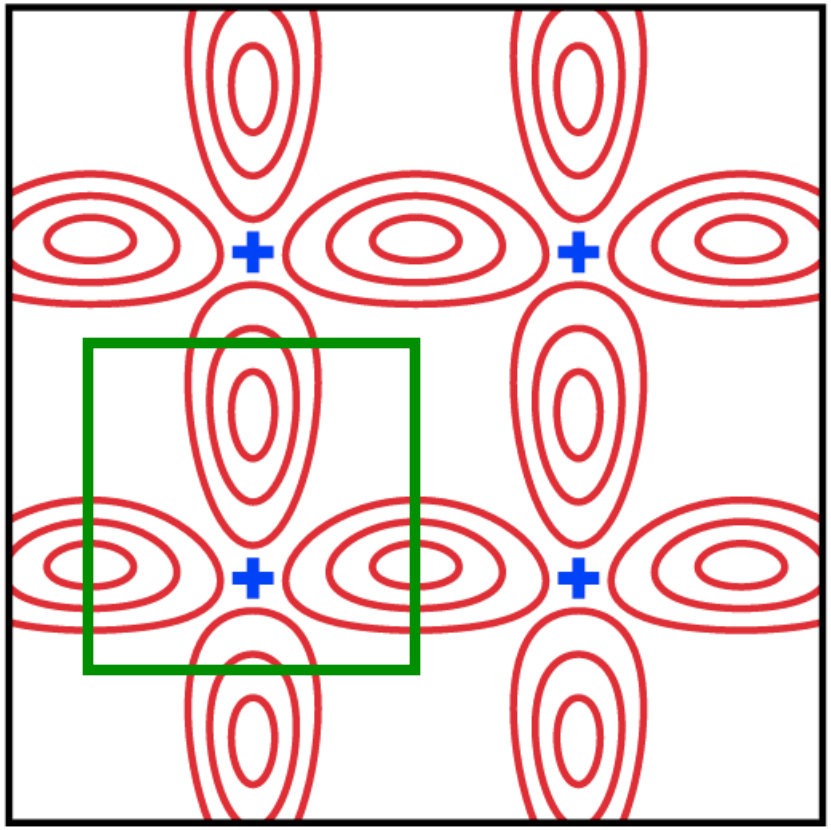
$\boldsymbol{P} = \boldsymbol{d}_{cell} / V_{cell}$?



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

$\boldsymbol{d}_{cell} =$ 

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



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

$\boldsymbol{d}_{cell} =$ 

The Problem: Polarization

Conclusion:

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

Heart of the problem: $\boldsymbol{r}\,\rho(\boldsymbol{r})$ is not a periodic function!

Theory of electric polarization

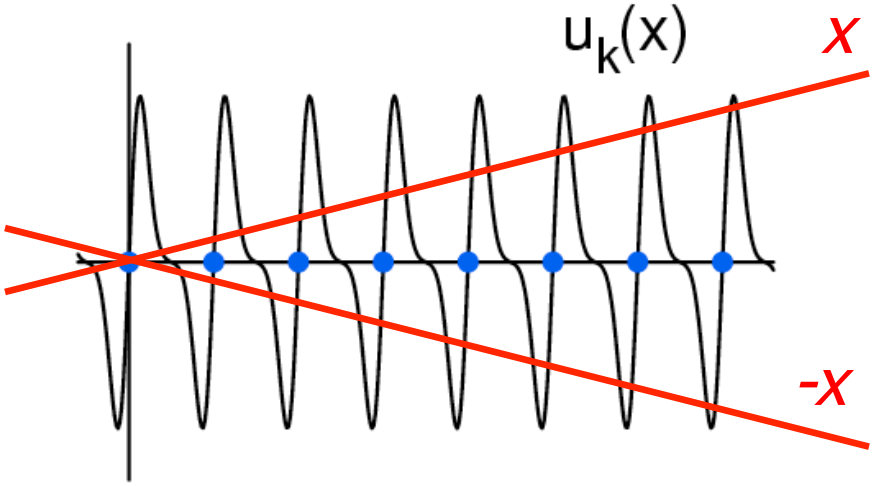
Need to go beyond $\rho(\boldsymbol{r})$;
use wavefunctions?

$$\boldsymbol{P} \propto \Sigma_{nk} \langle \psi_{nk} | \boldsymbol{r} | \psi_{nk} \rangle \, ?$$

Theory of electric polarization

$\boldsymbol{P} \propto \Sigma_{nk} \langle \psi_{nk} | \boldsymbol{r} | \psi_{nk} \rangle$?

$$\langle \psi_k | x | \psi_k \rangle = \int_{-\infty}^{\infty} x \, |u_k(x)|^2 \, dx$$



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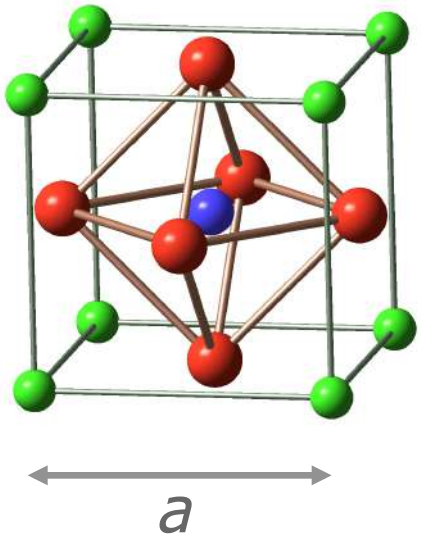
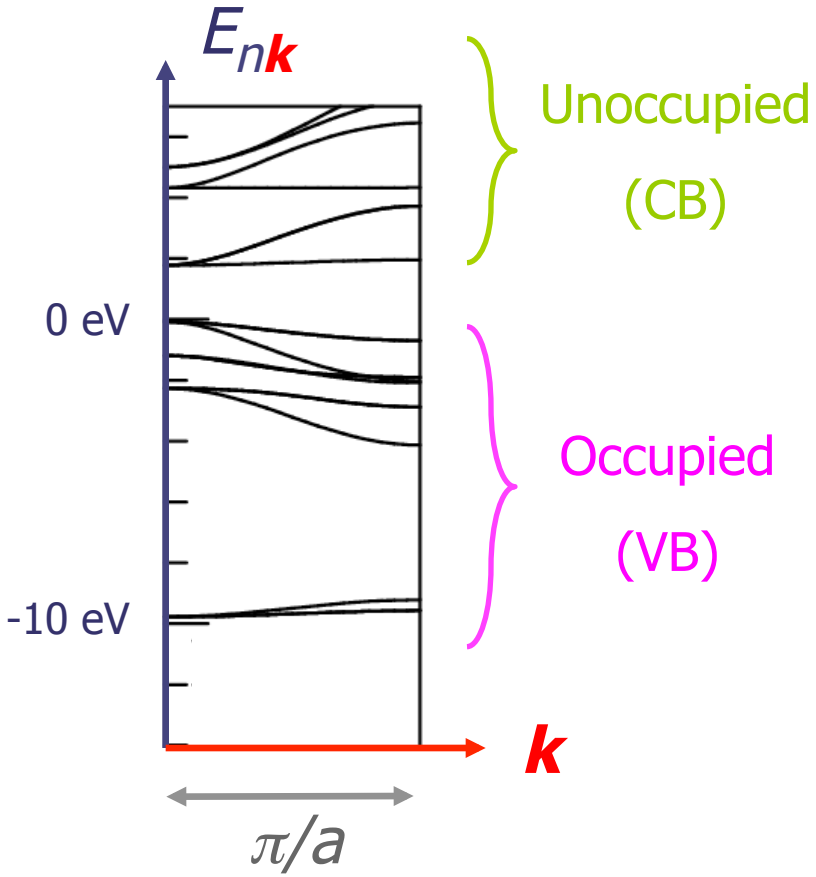
Review: Bloch's Theorem

Real space



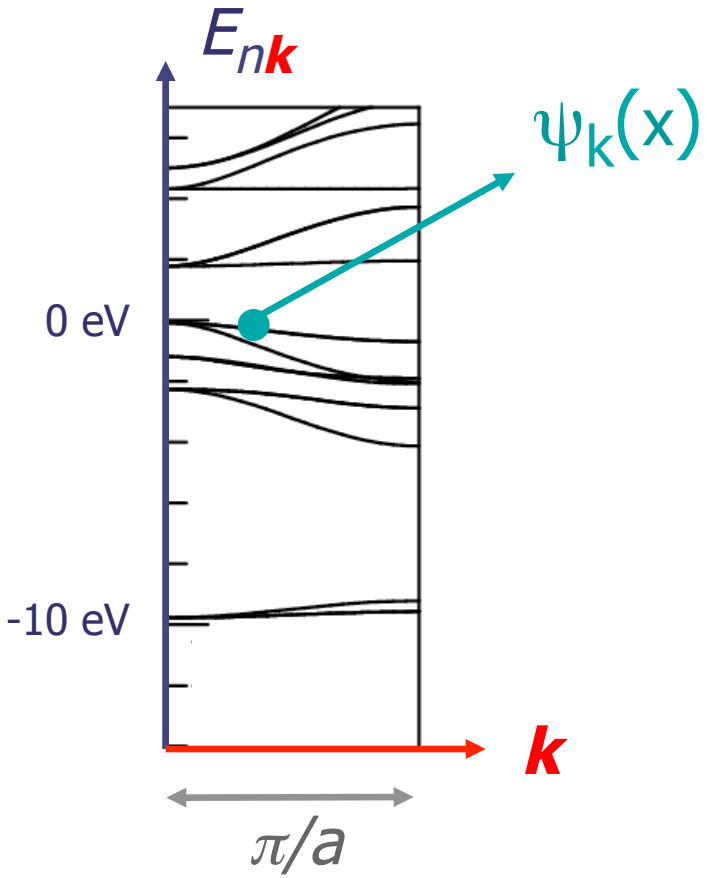
$BaTiO_3$

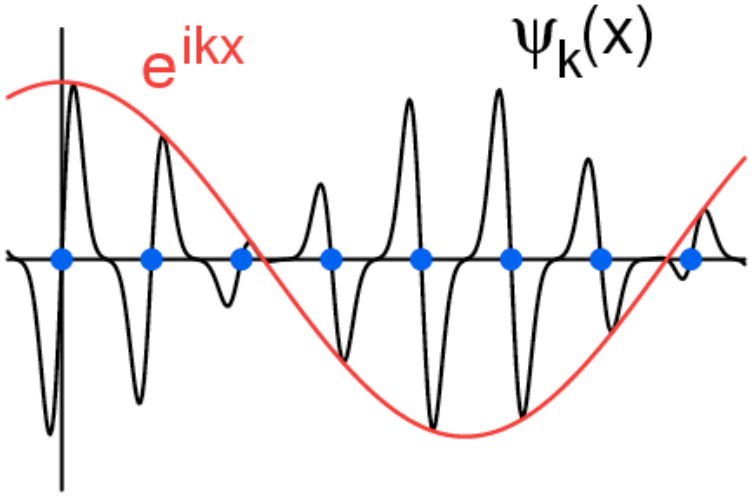
Reciprocal space



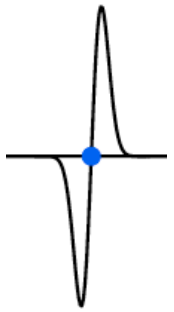
Review: Bloch's Theorem

Bloch wavefunction

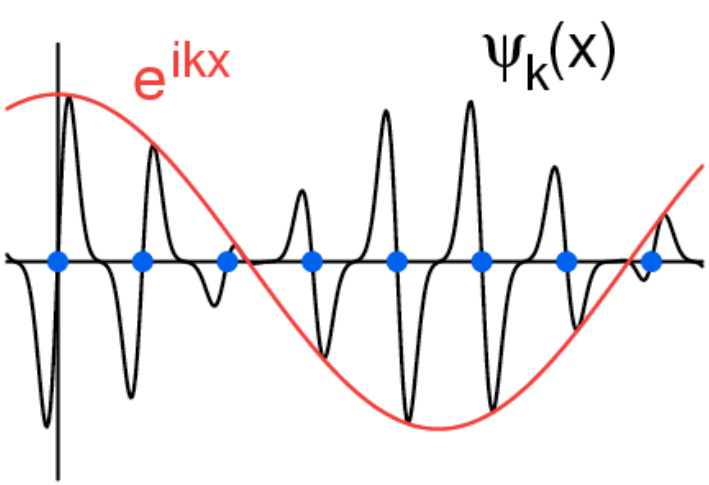


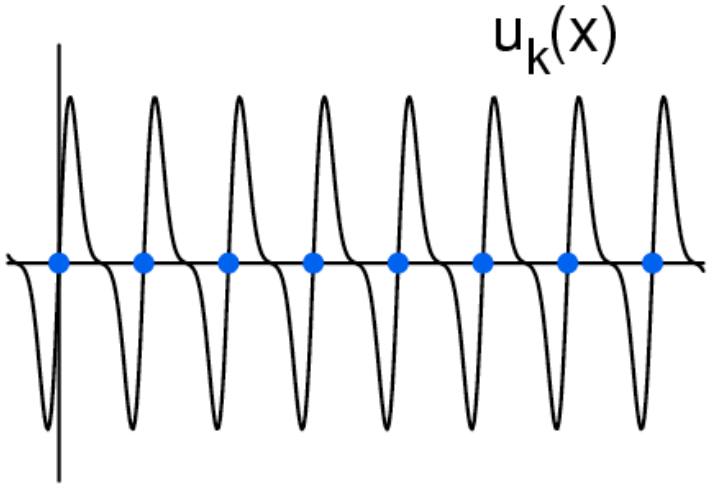


Ingredient:
Atomic
wavefunction



Review: Bloch's Theorem



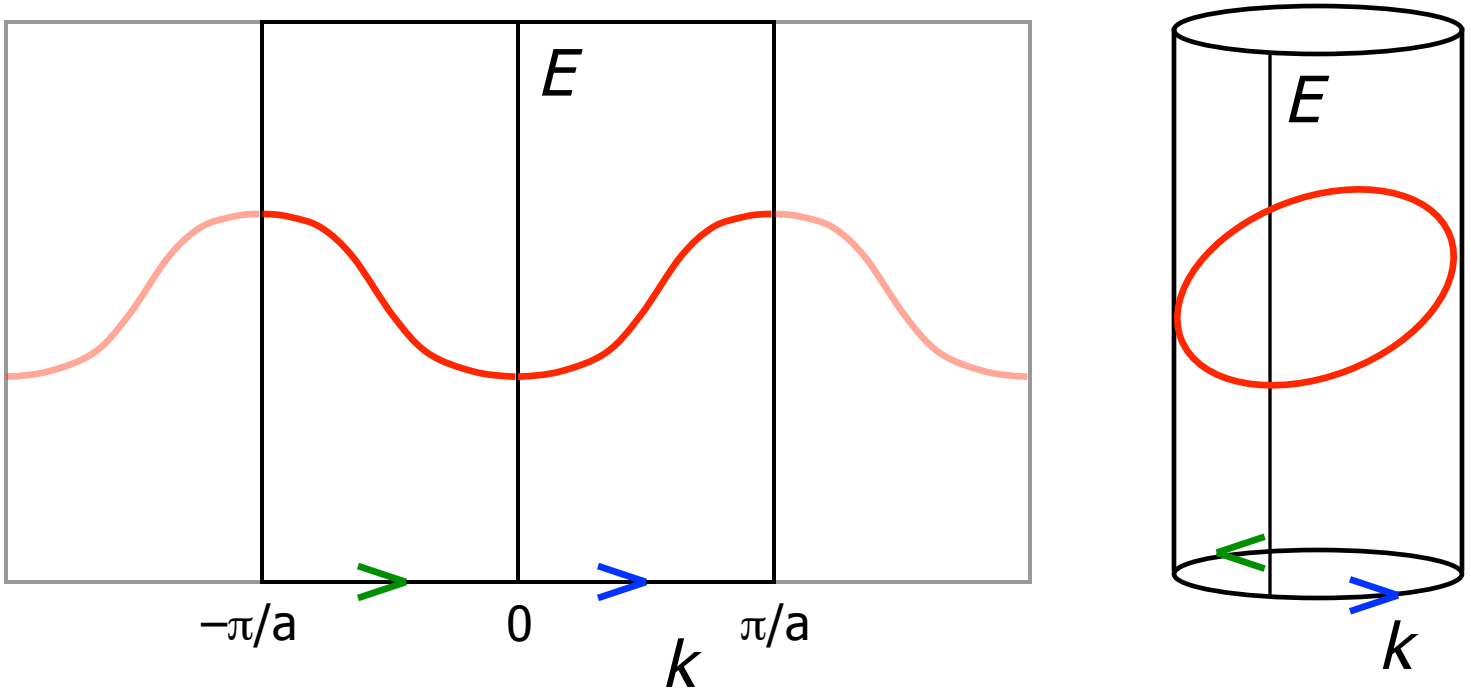


Define the cell-periodic Bloch function $u_k(x)$:

$$u_k(x) = e^{-ikx}\psi_k(x)$$

Review: Bloch's Theorem

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



Theory of electric polarization

$\boldsymbol{P} \propto \Sigma_{nk} \langle \psi_{nk} | \boldsymbol{r} | \psi_{nk} \rangle$? No.

$\boldsymbol{P} \propto \Sigma_{nk} \langle u_{nk} | i\nabla_{\boldsymbol{k}} | u_{nk} \rangle$?

Recall that in quantum mechanics,

$\boldsymbol{p} \rightarrow -i\hbar\nabla$

So it is plausible that

$\boldsymbol{r} \rightarrow i\nabla_{\boldsymbol{k}}$

"Modern Theory of Polarization" (1993)

Use the current

$$\frac{d\mathbf{P}}{dt} = \frac{1}{V}\int_V d^3r\ \mathbf{j}(\mathbf{r})$$

instead of the density

$$\mathbf{P} = \frac{1}{V}\int_V d^3r\ \mathbf{r}\,\rho(\mathbf{r})$$

since $\mathbf{j}(\mathbf{r})$ is periodic but $\mathbf{r}\,\rho(\mathbf{r})$ is not.

Resta, 1992:

$$\Delta\mathbf{P} = \int \left(\frac{d\mathbf{P}}{dt}\right)\ dt$$

"Modern Theory of Polarization" (1993)

Resta, 1992:

$$\Delta\mathbf{P} = \int \left(\frac{d\mathbf{P}}{dt}\right) dt$$

King-Smith and Vanderbilt, 1993:

$$\Delta\mathbf{P} = \mathbf{P}(t_2) - \mathbf{P}(t_1) \qquad \text{where}$$

$$\mathbf{P} = \frac{ie}{(2\pi)^3} \sum_n \int_{\mathrm{BZ}} d^3k \, \langle u_{nk} | \, \nabla_{\mathbf{k}} \, | u_{nk} \rangle$$

where $\psi_{nk}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \, u_{nk}(\mathbf{r})$

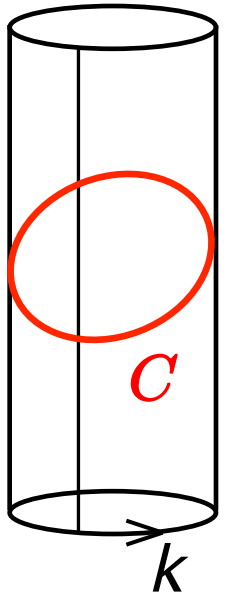
Simplify: 1 band, 1D

$$\mathbf{P} = \frac{-e}{2\pi} \int_{\mathrm{BZ}} dk \, \langle u_{\mathbf{k}} | i \tfrac{d}{dk} | u_{\mathbf{k}} \rangle$$

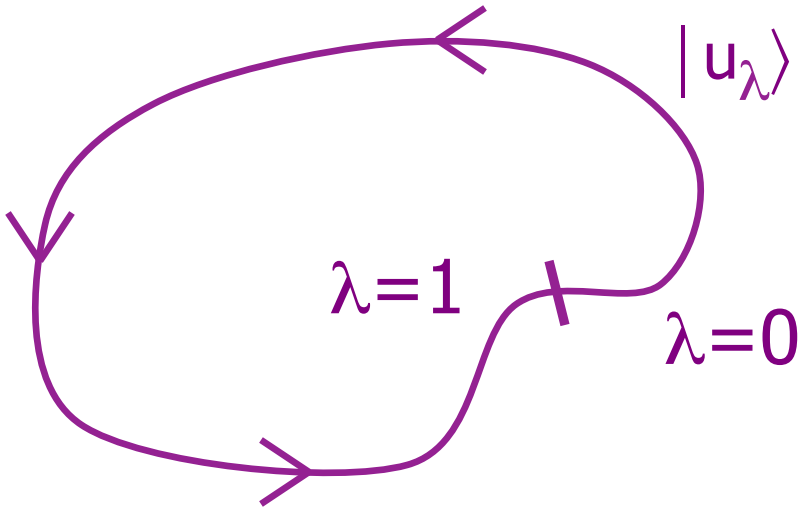
Heuristically, $x \Leftrightarrow i\frac{d}{dk}$ (Compare $p \Leftrightarrow -i\hbar\frac{d}{dx}$)

$$\mathbf{P} = -e\,\frac{\phi}{2\pi} \quad \text{where} \quad \boxed{\phi = i \oint_C dk \, \langle u_{\mathbf{k}} | \, \tfrac{d}{dk} \, | u_{\mathbf{k}} \rangle}$$

This is a Berry phase!



Tutorial on Berry phases



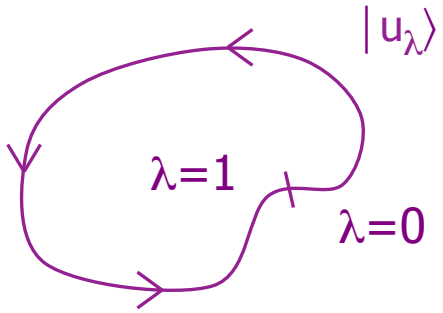
$$\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{du_\lambda}{d\lambda} \rangle$$

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

ϕ is well-defined modulo 2π

$\Rightarrow$ ϕ is a phase.

Proof:



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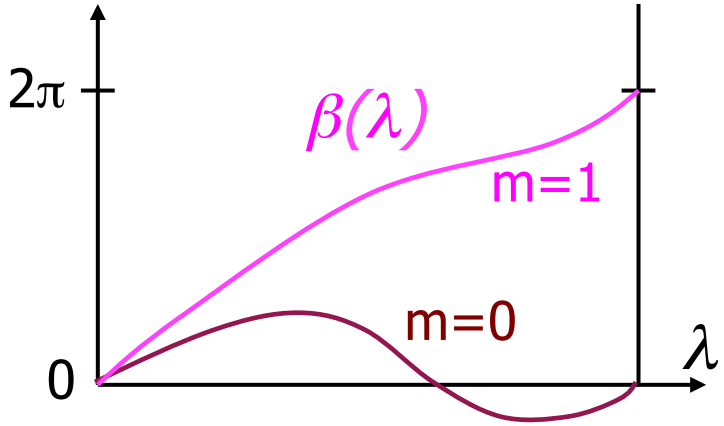


Let:

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

Proof:

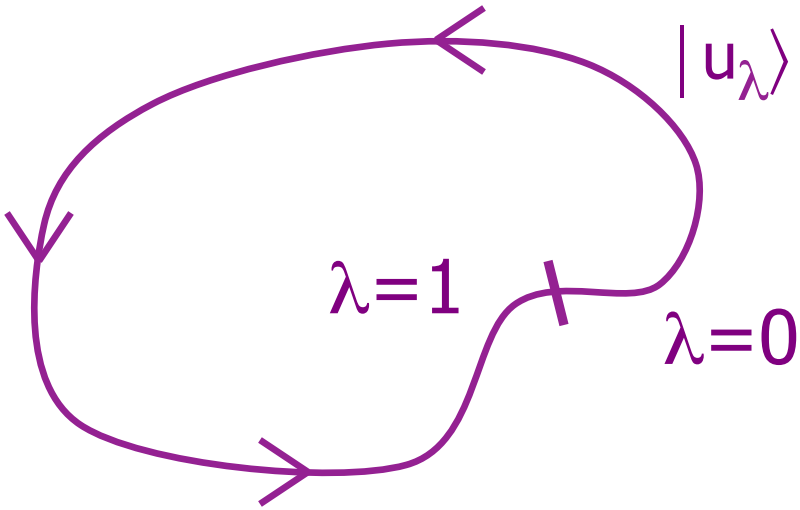
$$\widetilde{\phi} = -\mathrm{Im} \oint d\lambda \, \langle \widetilde{u}_\lambda | \, \frac{d}{d\lambda} \, | \widetilde{u}_\lambda \rangle$$

$$= -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \, e^{i\beta(\lambda)} \, \frac{d}{d\lambda} \left(e^{-i\beta(\lambda)} \, | u_\lambda \rangle \right)$$

$$= -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \, \frac{d}{d\lambda} \, | u_\lambda \rangle + \oint d\lambda \, \langle u_\lambda | u_\lambda \rangle \left(\frac{d\beta}{d\lambda} \right)$$

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

Tutorial on Berry phases



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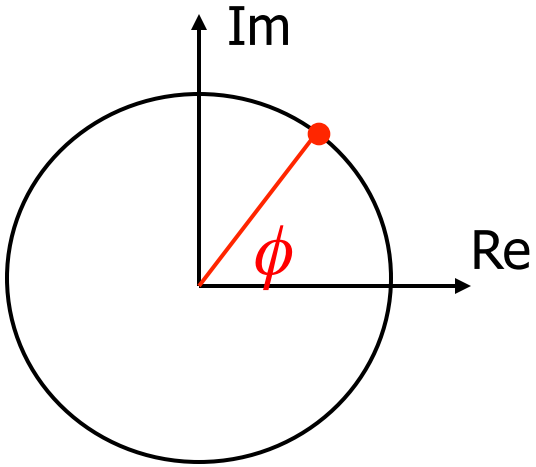
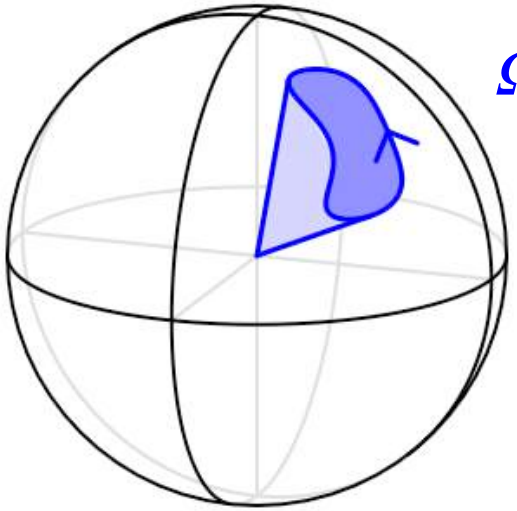
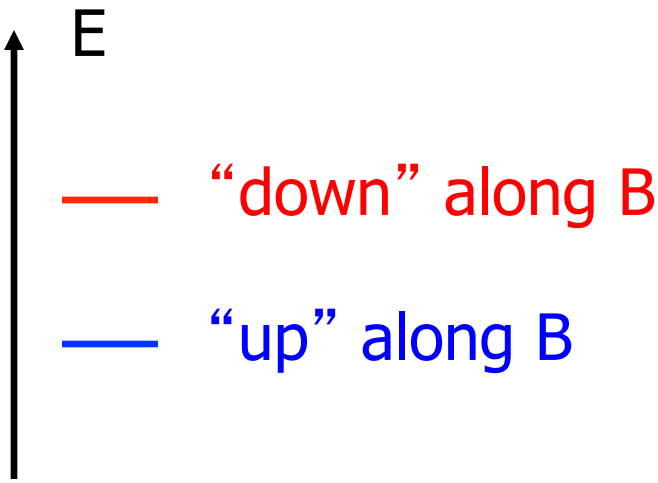


Tutorial on Berry phases

Famous example: Spinor in magnetic field



Ω = solid angle



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

$\phi = \Omega/2$

Simplify: 1 band, 1D

$$\mathbf{P} = \frac{-e}{2\pi} \int_{\mathrm{BZ}} dk \, \langle u_{\mathbf{k}} | i \tfrac{d}{dk} | u_{\mathbf{k}} \rangle$$

Heuristically, $x \Leftrightarrow i\frac{d}{dk}$ (Compare $p \Leftrightarrow -i\hbar\frac{d}{dx}$)

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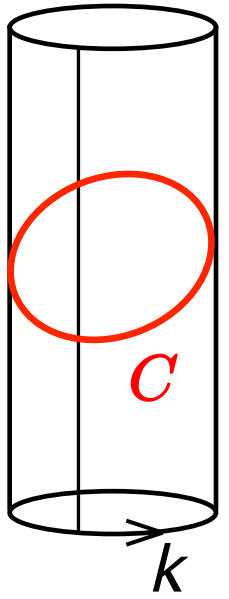
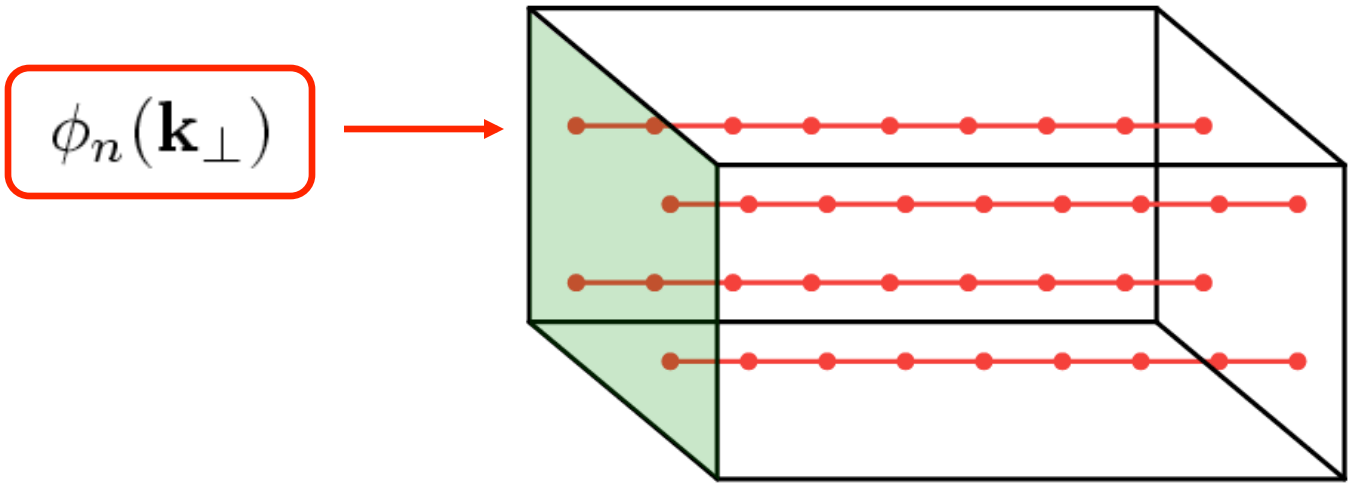


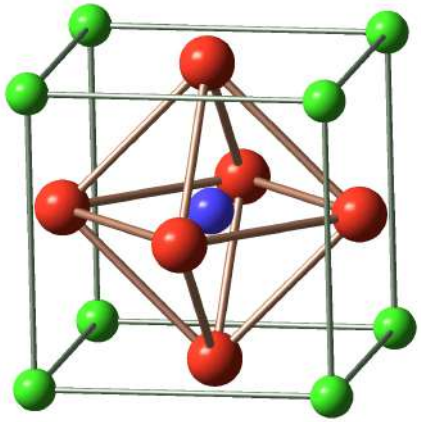
Discretized formula in 3D



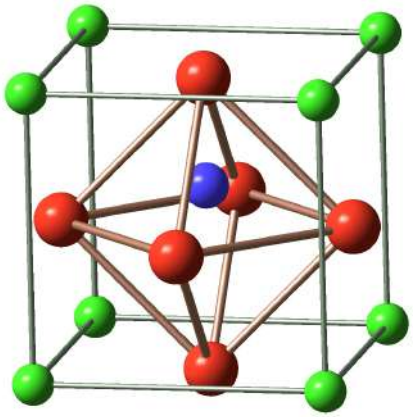
$$\mathbf{P}_n = \frac{1}{2\pi}\frac{e}{\Omega}\sum_j \phi_{n,j}\,\mathbf{R}_j \quad \text{where} \quad \phi_{n,j} = \frac{1}{N_{\mathbf{k}_\perp}}\sum_{\mathbf{k}_\perp}\phi_n(\mathbf{k}_\perp)$$

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

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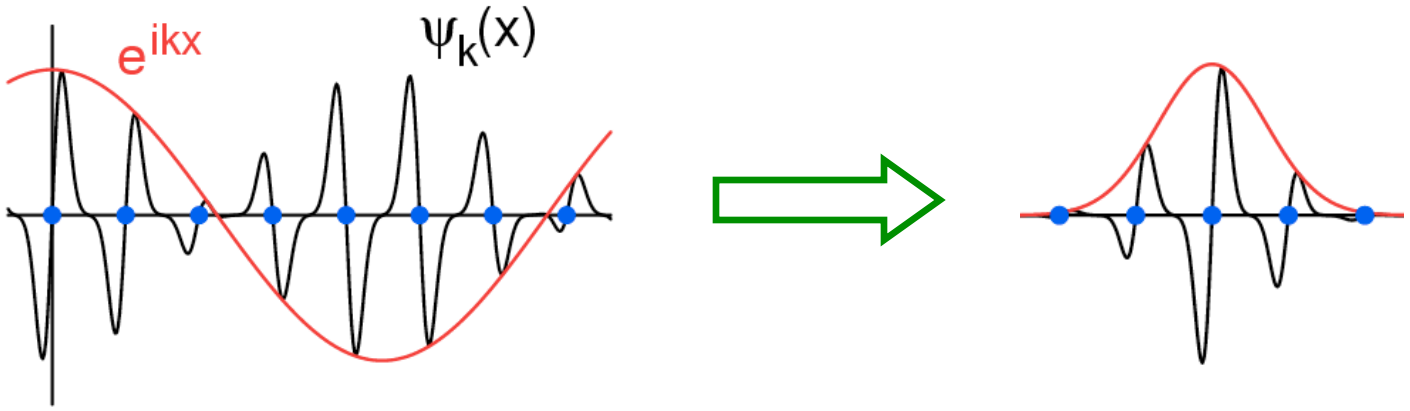
Tutorial on Wannier functions

Choose Wannier functions as

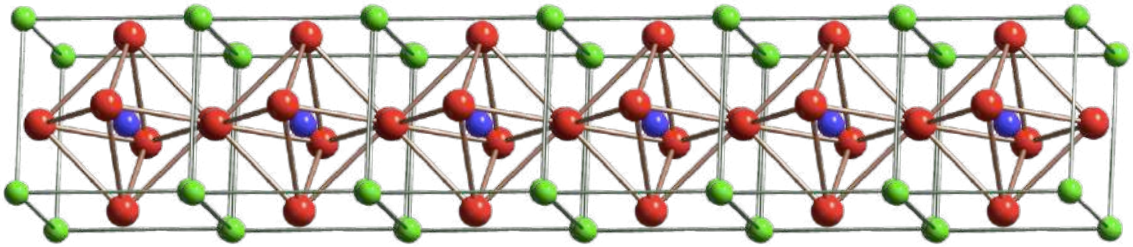
$$w_n(\mathbf{r}-\mathbf{R}) = \int_{BZ} \psi_{n\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$



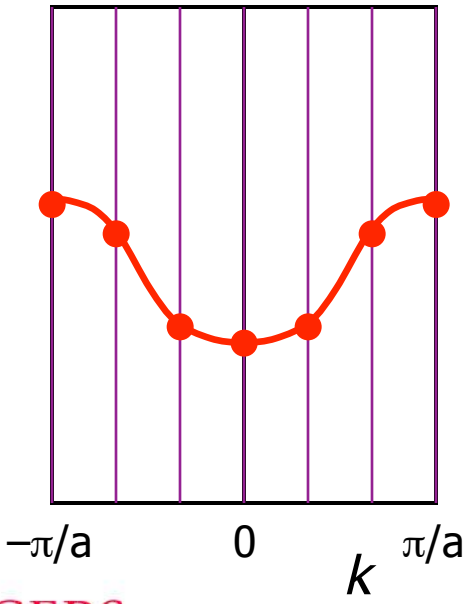
Form wave-packet = "Wannier function"

Tutorial on Wannier functions

Crystal in real space:



Brillouin zone in reciprocal space:



Tutorial on Wannier functions

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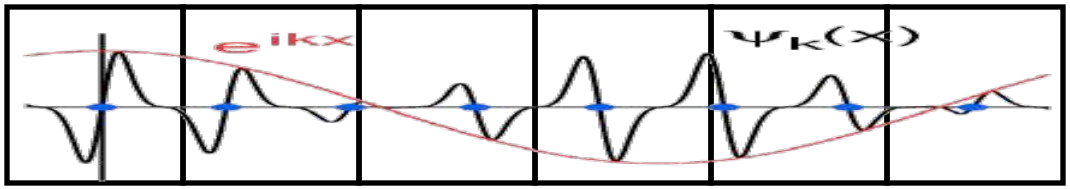

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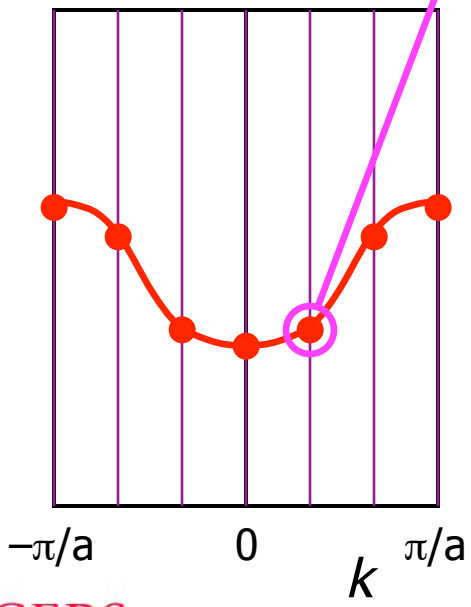

Tutorial on Wannier functions

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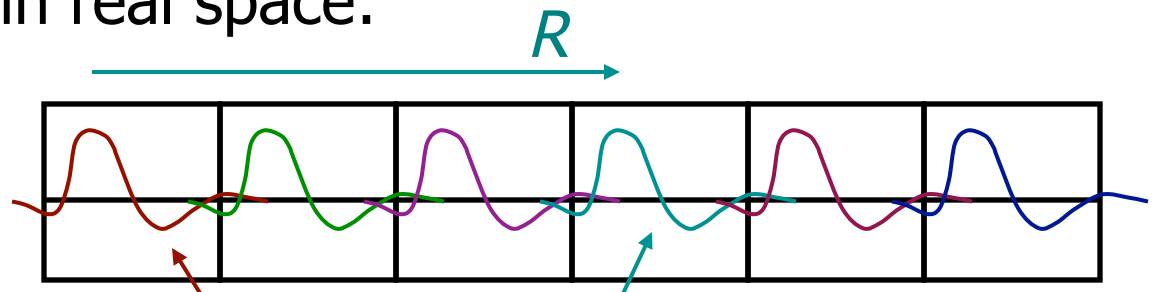

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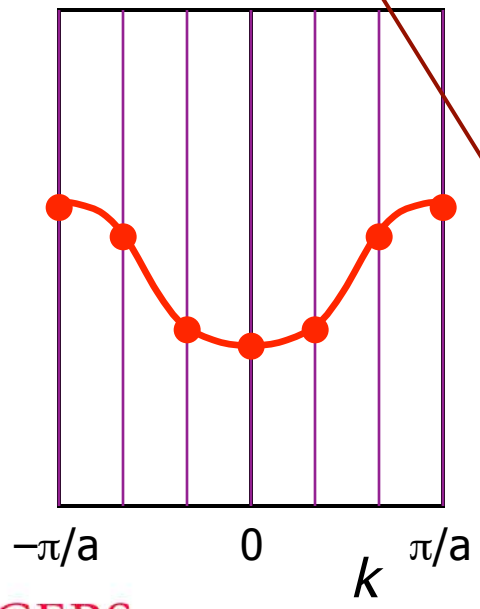


$$w_{\mathbf{R}}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

$$w_0(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{k}$$

Unitary transformation

Tutorial on Wannier functions

Centers of Wannier functions:

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

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

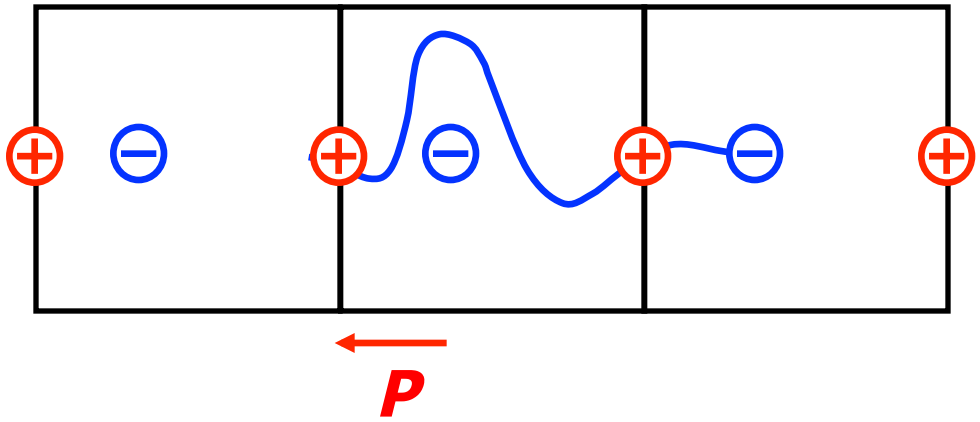
$$\mathbf{r}\,|\, w_0\rangle = \frac{V}{(2\pi)^3} \int_{\mathrm{BZ}} d\mathbf{k}\; (\; -i\nabla_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{r}}\,)\, |u_{\mathbf{k}}\rangle$$

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

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

Polarization ↔ Wannier centers

Centers of Wannier functions:

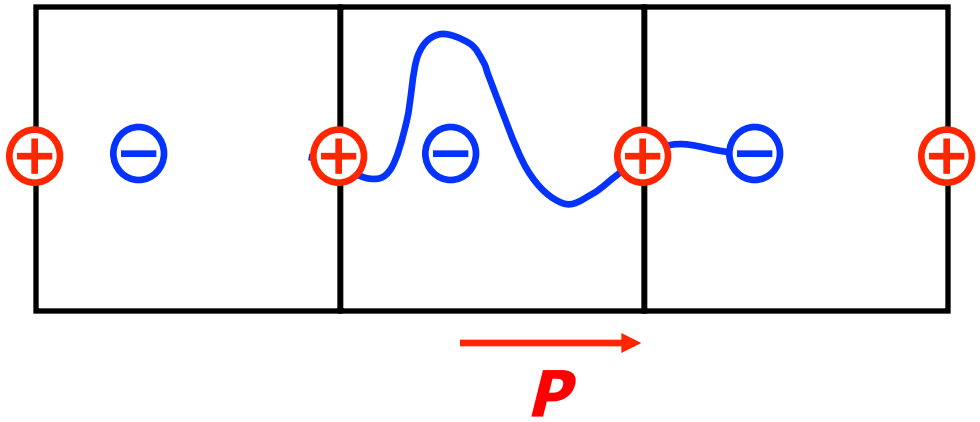


$$\mathrm{P} = \frac{ie}{(2\pi)^3} \sum_n \int_{\mathrm{BZ}} d^3k \, \langle u_{nk} | \, \nabla_{\mathrm{k}} \, | u_{nk} \rangle$$

as before !!

Polarization ↔ Wannier centers

Centers of Wannier functions:



$$\mathrm{P} = \frac{ie}{(2\pi)^3} \sum_n \int_{\mathrm{BZ}} d^3k \, \langle u_{nk} | \, \nabla_{\mathrm{k}} \, | u_{nk} \rangle$$

as before !!

Outline

- Modern theory of polarization
  - What is the problem?
  - Berry phase formulation
  - Wannier center formulation
- Effective Hamiltonian approach
- Theory of flexoelectricity
- Summary and prospects

References

REVIEWS OF MODERN PHYSICS

Macroscopic polarization in crystalline dielectrics: the geometric phase approach

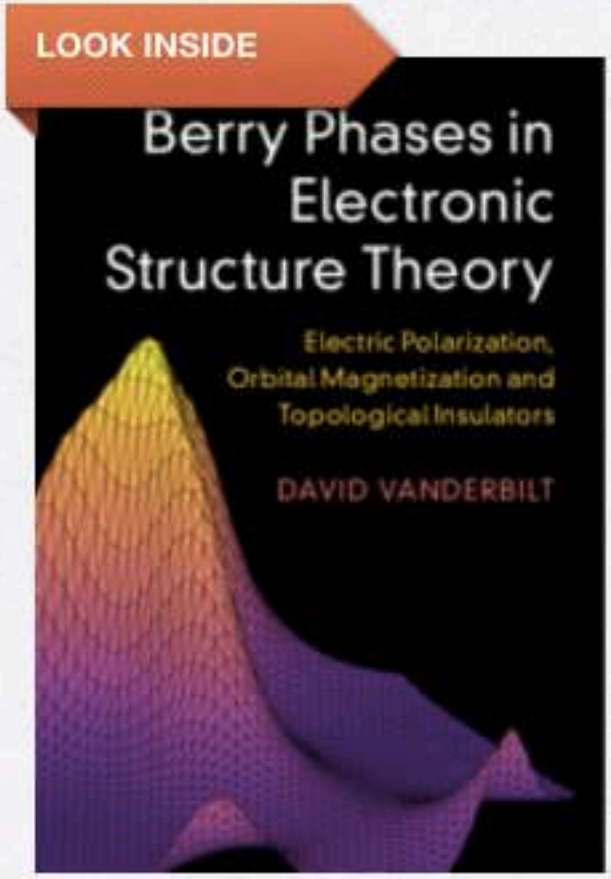
Raffaele Resta

Rev. Mod. Phys. **66**, 899 – Published 1 July 1994

182. 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)*

198. 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)*

Recently published



Berry Phases in Electronic Structure Theory

Electric Polarization, Orbital Magnetization and Topological Insulators

AUTHOR: David Vanderbilt, Rutgers University, New Jersey

DATE PUBLISHED: December 2018

AVAILABILITY: In stock

FORMAT: Hardback

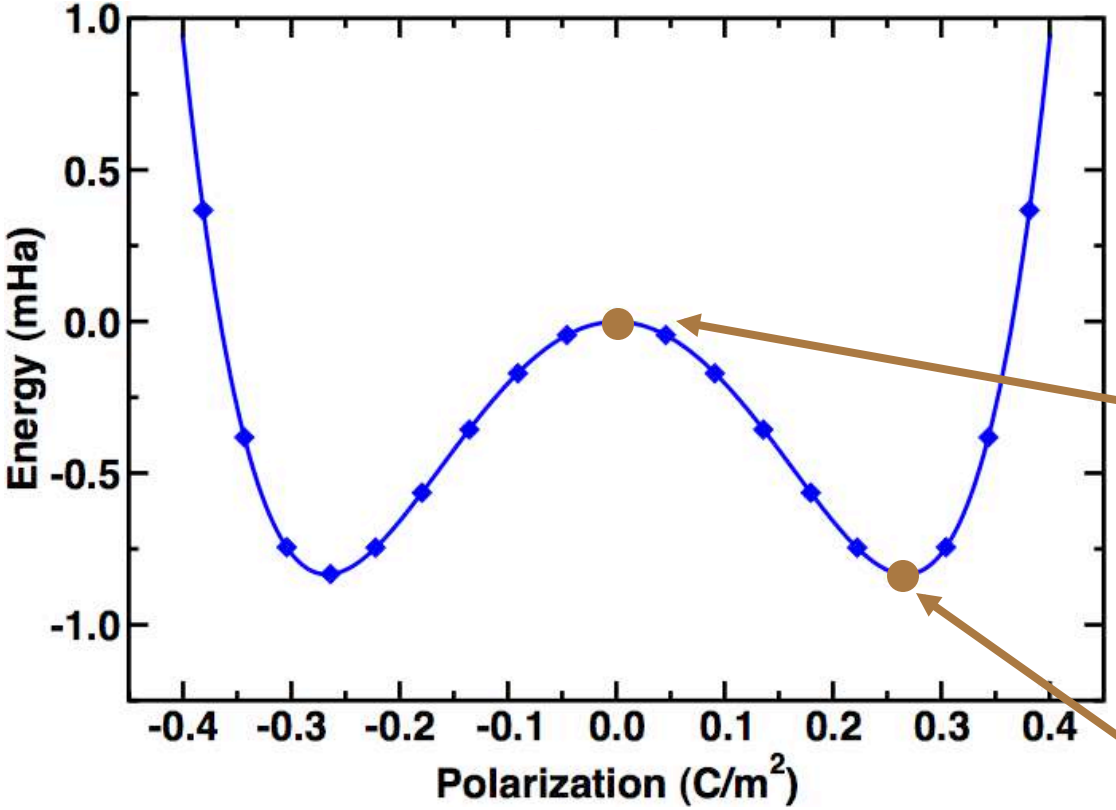
ISBN: 9781107157651

Rate & review

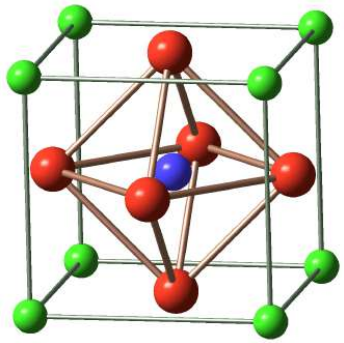
Outline

- Modern theory of polarization
  - What is the problem?
  - Berry phase formulation
  - Wannier center formulation
- Effective Hamiltonian approach
- Theory of flexoelectricity
- Summary and prospects

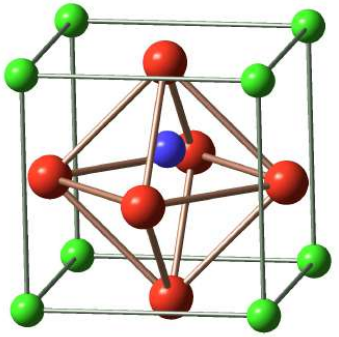
Energy vs. Polarization



$BaTiO_3$

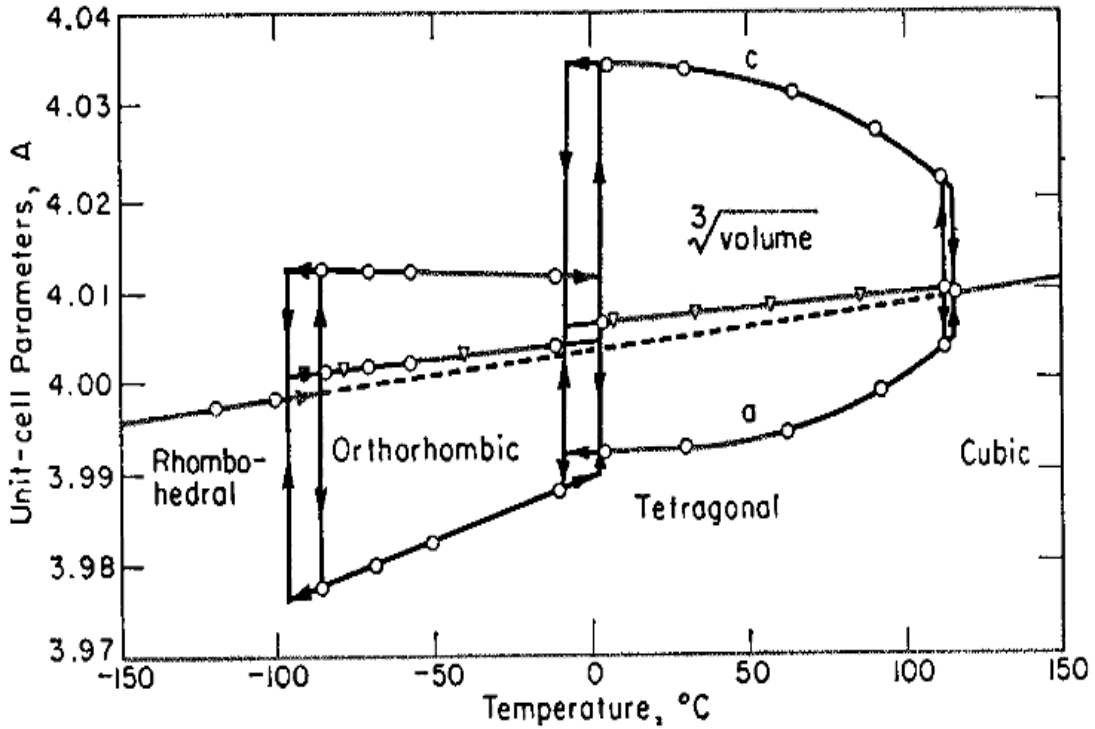


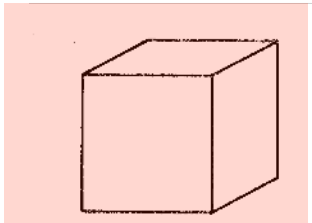
Paraelectric

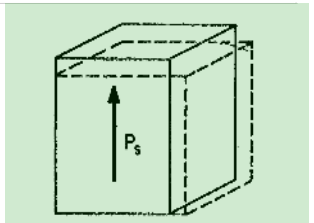


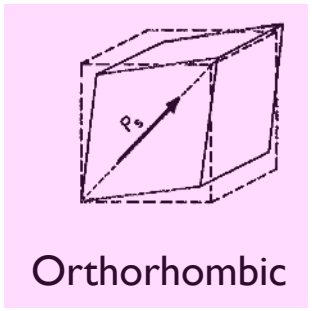
Ferroelectric

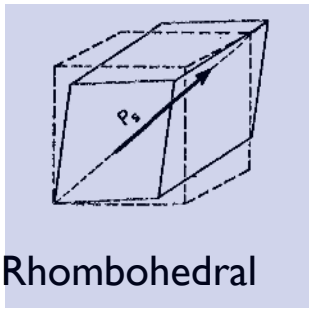
Structural phase transitions in $BaTiO_3$











P ∥ (111)
Rhomb

P ∥ (011)
Orth

P ∥ (001)
Tetrag

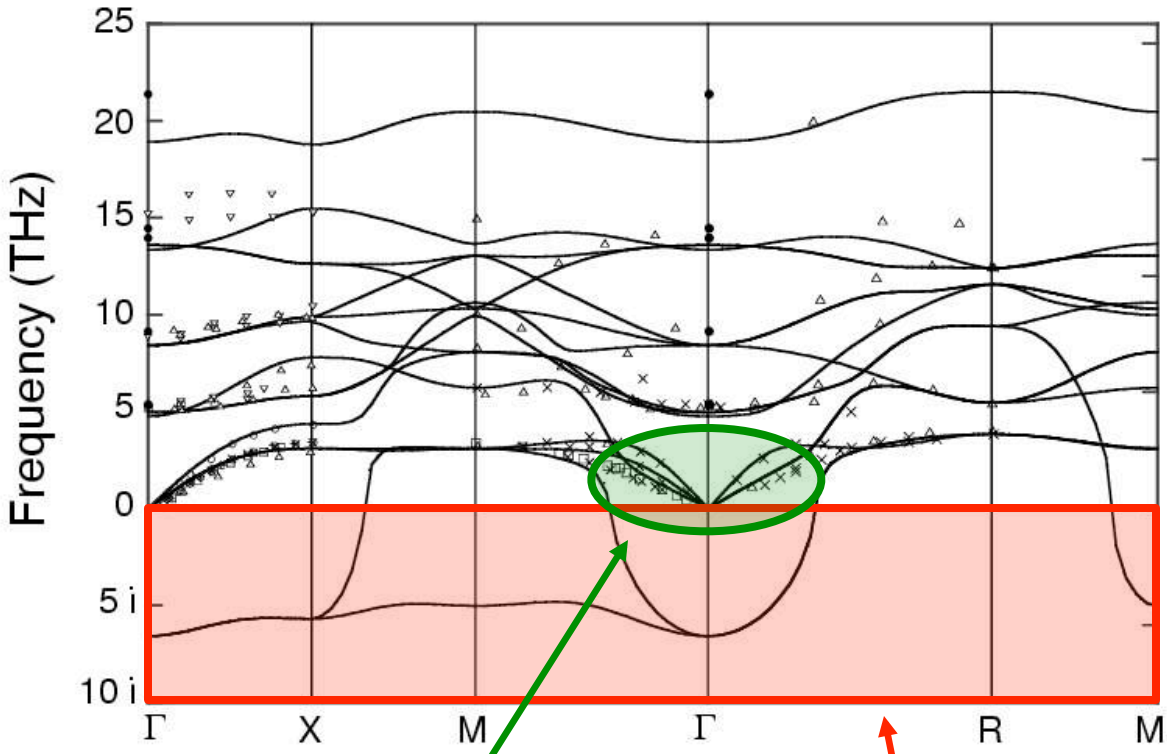
P = 0
Cubic

Effective Hamiltonian Theory

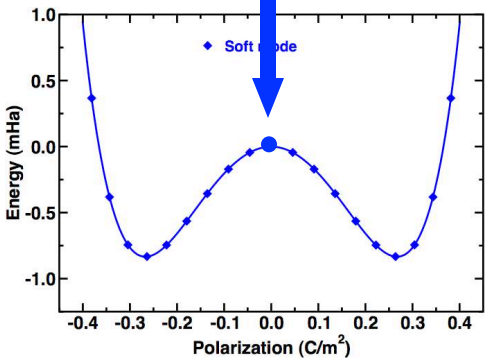
- Define reduced set of structural degrees of freedom
- Write expansion of energy in these variables
- Obtain expansion coefficients
  - From ab-initio calculations
  - No experimental input(*)
- Compute properties as a function of T:
  - Structural phase transitions
  - Dielectric, piezoelectric properties

(*) We cheat a little: Lattice constant

Phonons of cubic $BaTiO_3$ (Ghosez thesis)

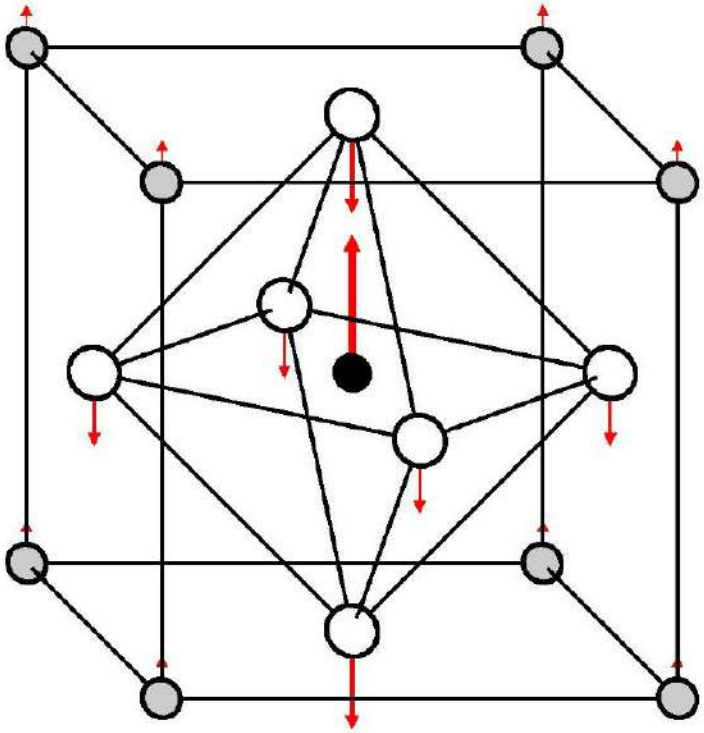


Evaluate here



Acoustic branches

Unstable phonon branches



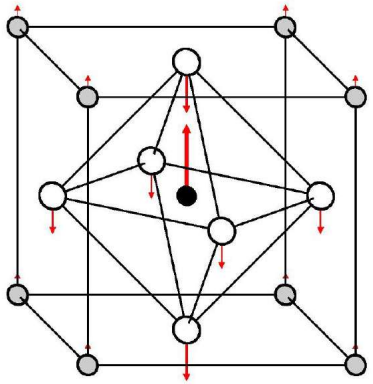
$\{u_i\}$

Local mode defined
in terms of
soft mode eigenvector
in high-symmetry
cubic structure

Relevant low-energy degrees of freedom

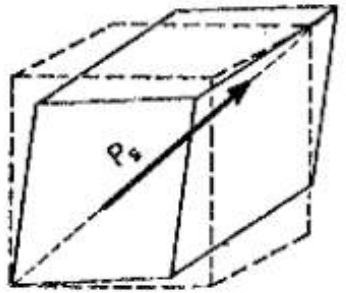
- Amplitude **u** of soft mode

u

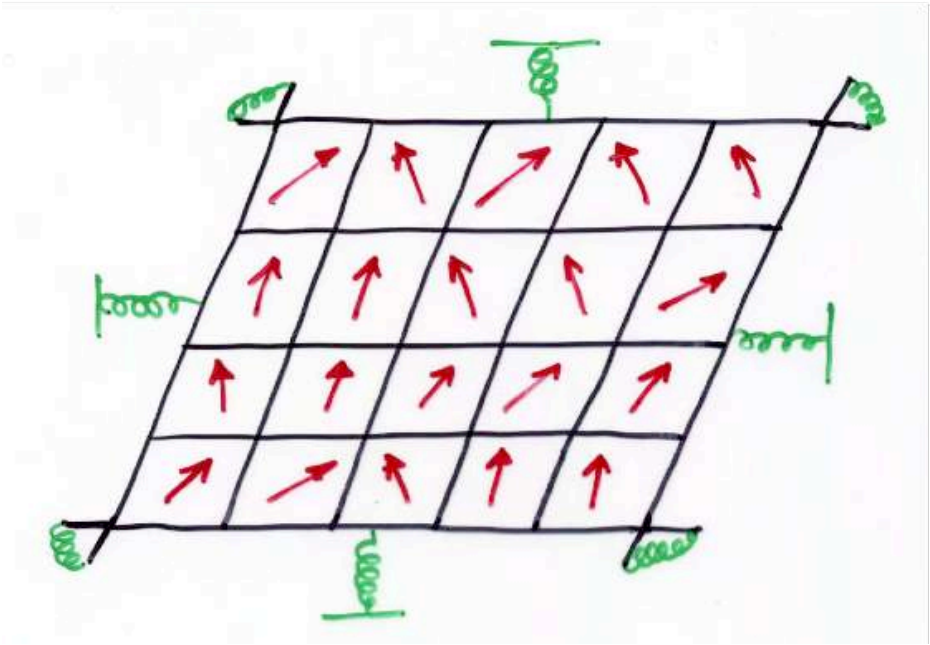


- Acoustic modes near q=0: strain **η**

η



3+3 coords/cell instead of 15



Model system with local modes and strains

$\{u_i\}$ $\{\eta_l\}$

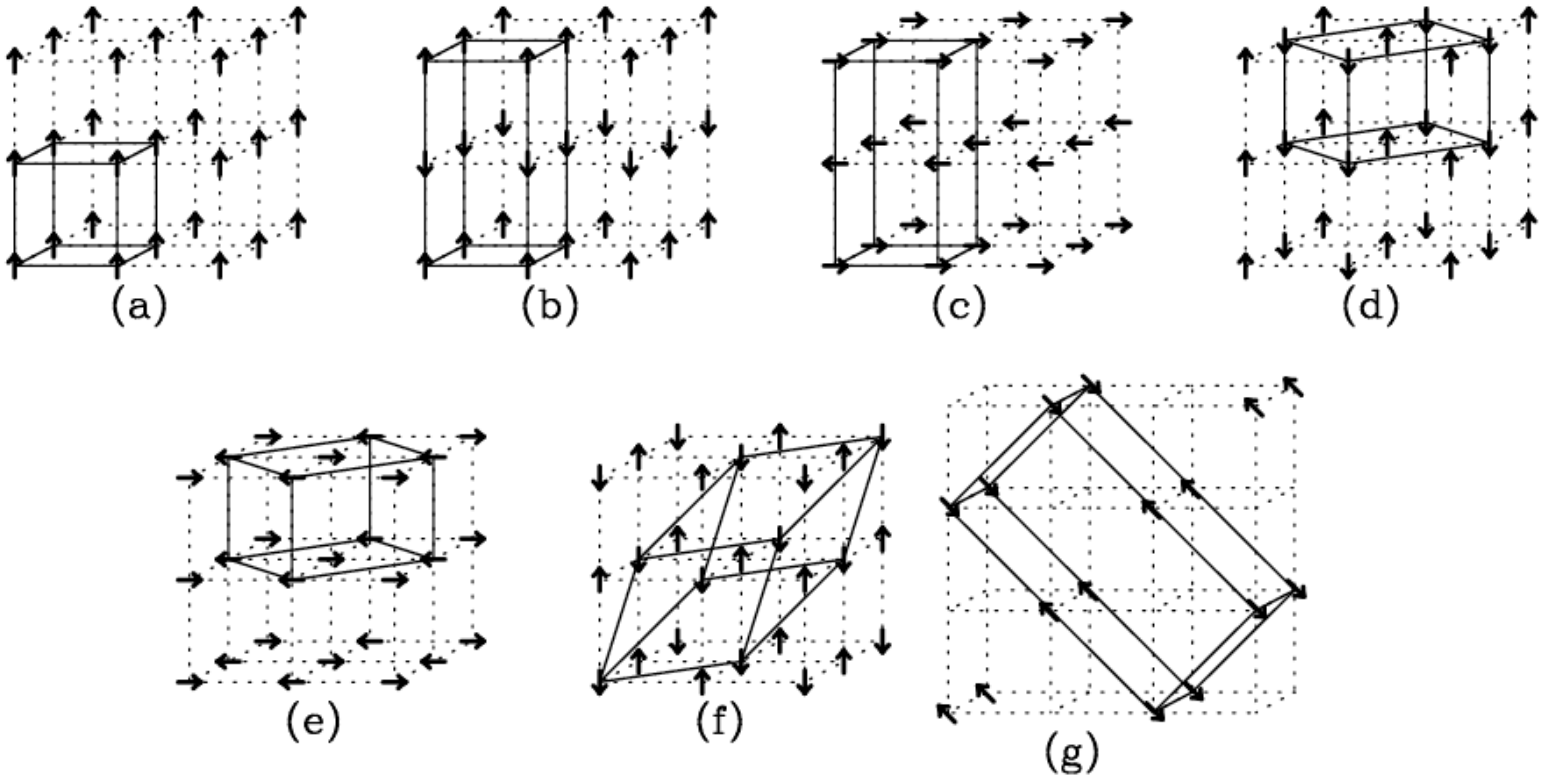
Effective Hamiltonian

Model for the energy landscape
in terms of the reduced set
of degrees of freedom:

$$E^{\mathrm{tot}} = E^{\mathrm{self}}(\{\mathbf{u}\}) + E^{\mathrm{dpl}}(\{\mathbf{u}\}) + E^{\mathrm{short}}(\{\mathbf{u}\})$$

$$+ E^{\mathrm{elas}}(\{\eta_l\}) + E^{\mathrm{int}}(\{\mathbf{u}\}, \{\eta_l\})$$

DFT calculations for database of distorted structures

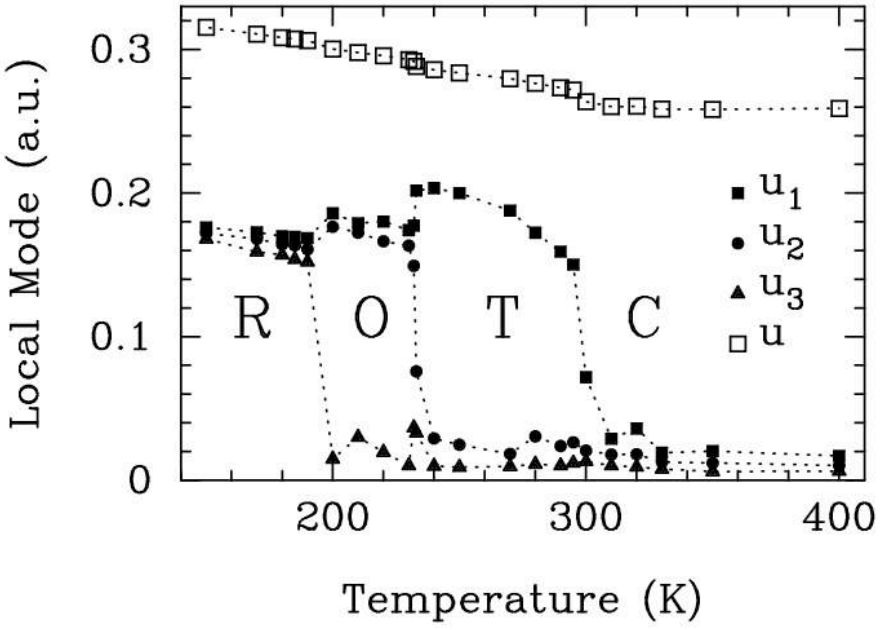


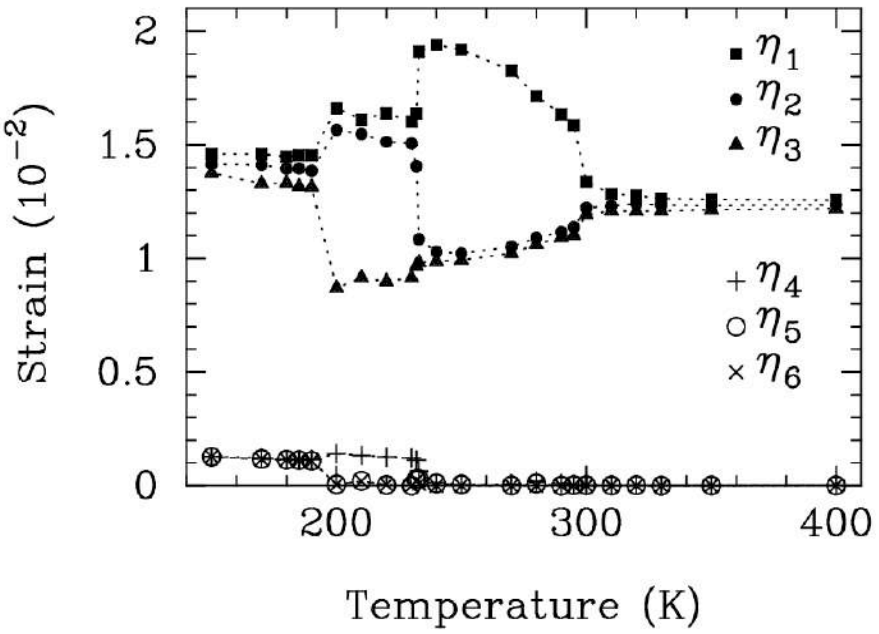
Obtain expansion parameters

Effective Hamiltonian Theory

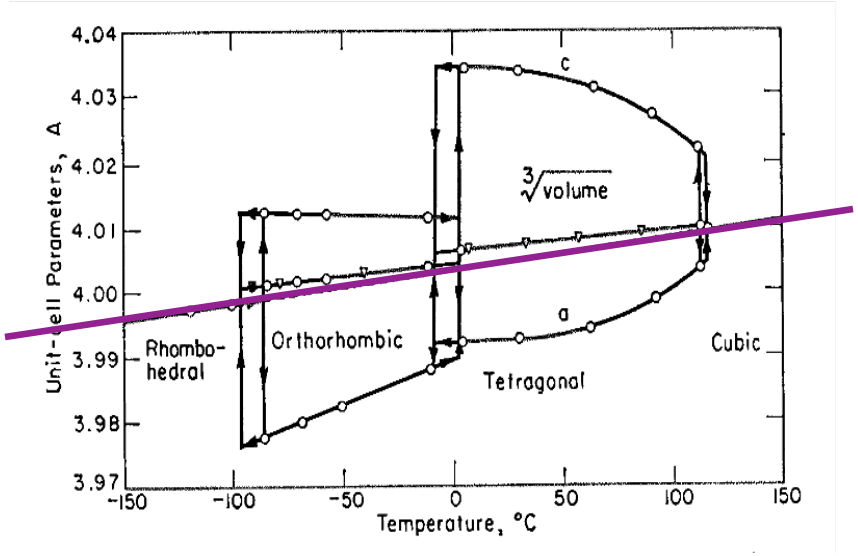
- Model has about 20 parameters
- Fit them from first-principles calculations
- Then use in statistical simulations
  - Sample with Metropolis algorithm
  - Typically 12x12x12 primitive cells
  - Typically 10^5 Monte Carlo sweeps
  - Obtain statistical averages

Results for $BaTiO_3$

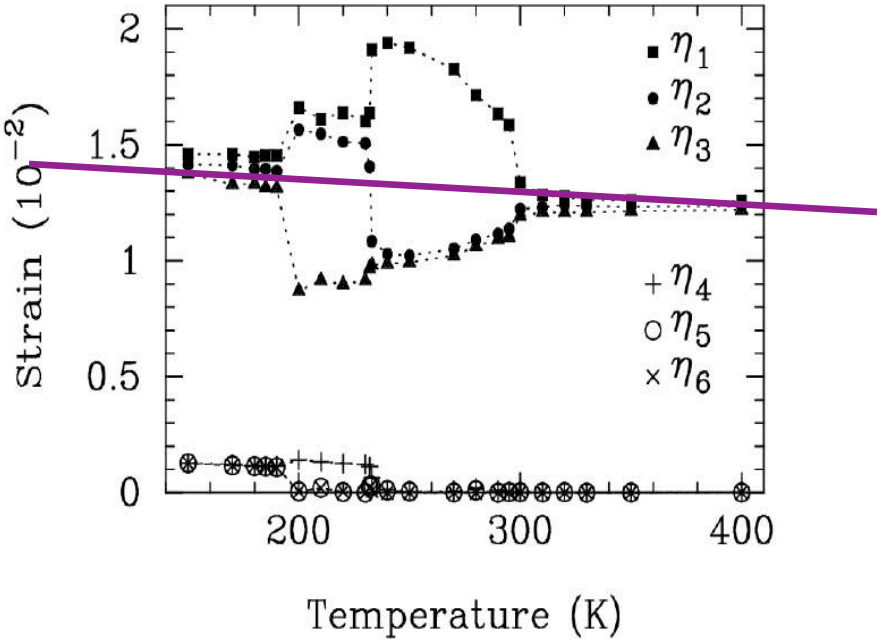




(Zhong, Vanderbilt, and Rabe, 1995)



Experiment



Theory

- Tc's off by ~100K
- But sequence correct
- Note that we miss thermal expansion

All-atom simulation approaches

Journal of Physics: Condensed Matter

PAPER

First-principles model potentials for lattice-dynamical studies: general methodology and example of application to ferroic perovskite oxides

Jacek C Wojdeł[1], Patrick Hermet[2,3], Mathias P Ljungberg[1], Philippe Ghosez[2] and Jorge Íñiguez[1]

Published 5 July 2013 • 2013 IOP Publishing Ltd

Journal of Physics: Condensed Matter, Volume 25, Number 30

PHYSICAL REVIEW B

covering condensed matter and materials physics

Highlights Recent Accepted Authors Referees Search Pre

Reinterpretation of the bond-valence model with bond-order formalism: An improved bond-valence-based interatomic potential for $PbTiO_3$

Shi Liu, Ilya Grinberg, Hiroyuki Takenaka, and Andrew M. Rappe

Phys. Rev. B **88**, 104102 – Published 6 September 2013

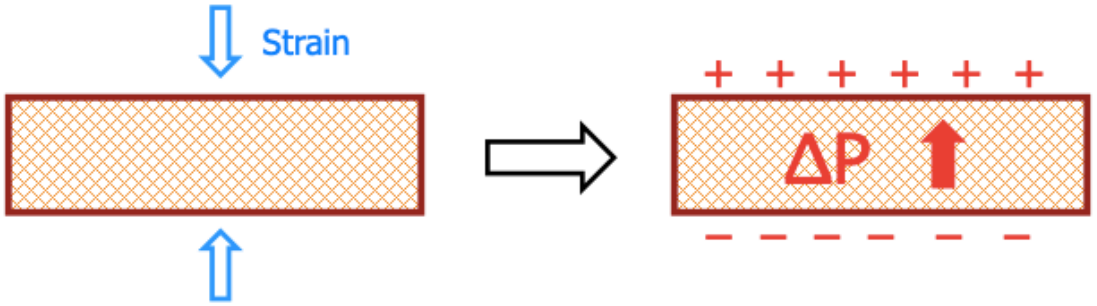
Outline

- Modern theory of polarization
  - What is the problem?
  - Berry phase formulation
  - Wannier center formulation
- Effective Hamiltonian approach
- Theory of flexoelectricity
- Summary and prospects

Theory of Piezoelectricity

Xifan Wu

Don Hamann



This is relatively easy:

- Apply small homogenous strain η
- Re-relax atomic coordinates
- Compute P before and after
- Obtain $dP/d\eta \approx \Delta P/\Delta\eta$

Or, can be done by "linear response"

- No finite differences needed

See ABINIT *Anaddb* package

X. Wu, D. Vanderbilt, and D.R. Hamann, "Systematic treatment of displacements, strains and electric fields in density-functional perturbation theory," Phys. Rev. B 72, 035105 (2005).

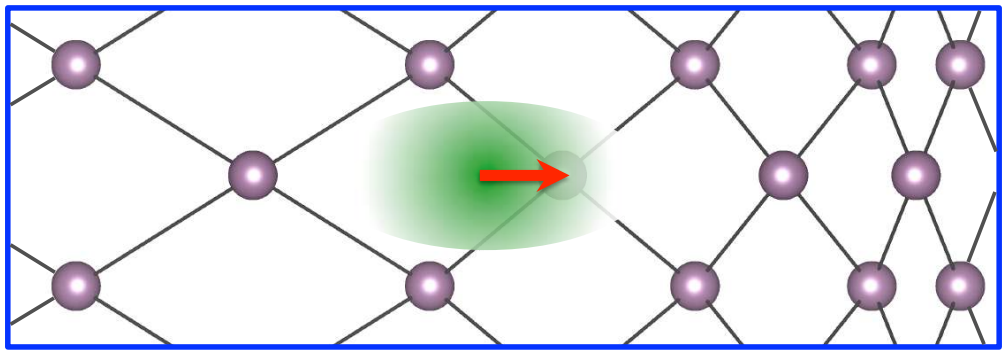
Jiawang Hong

Cyrus Dreyer

Max Stengel

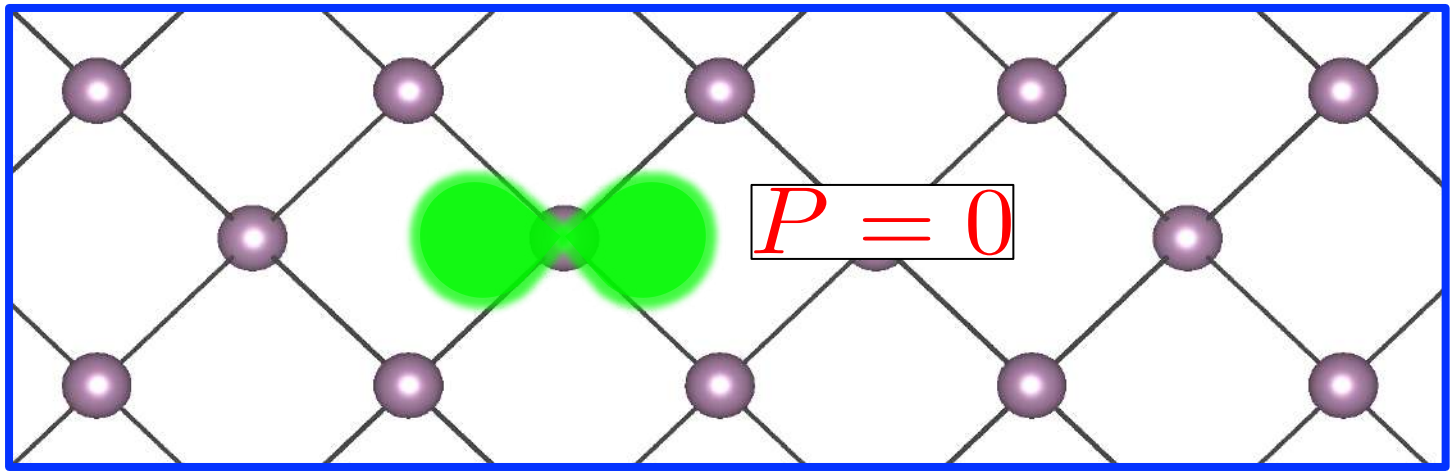
Andrea Schiaffino

Theory of Flexoelectricity

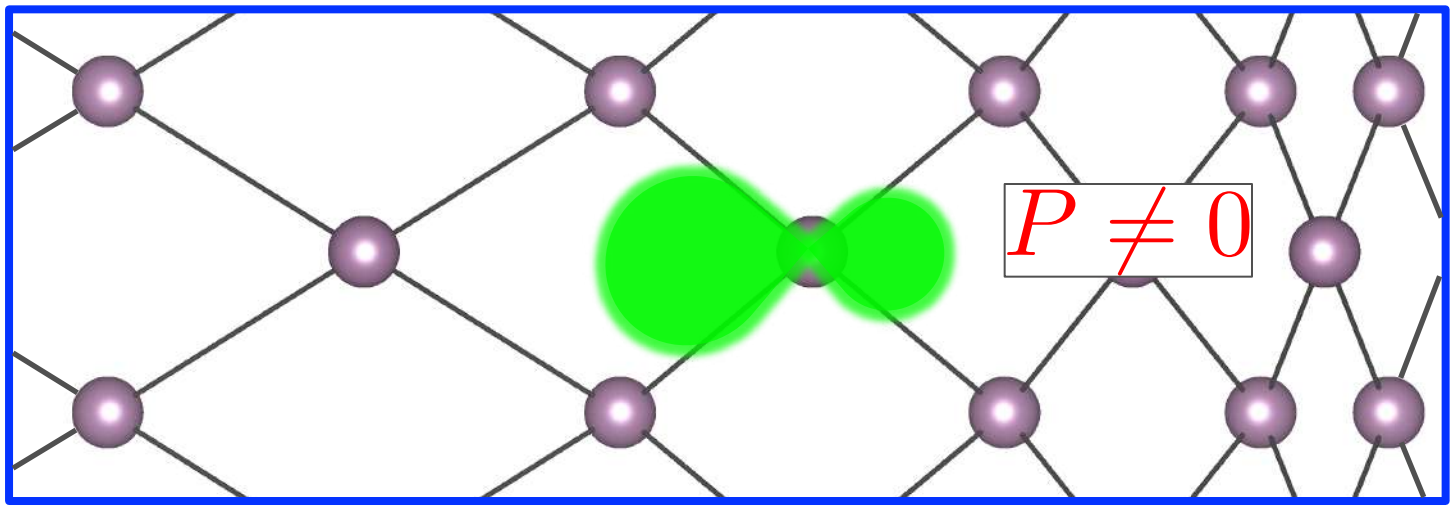


Polarization response to a strain gradient !

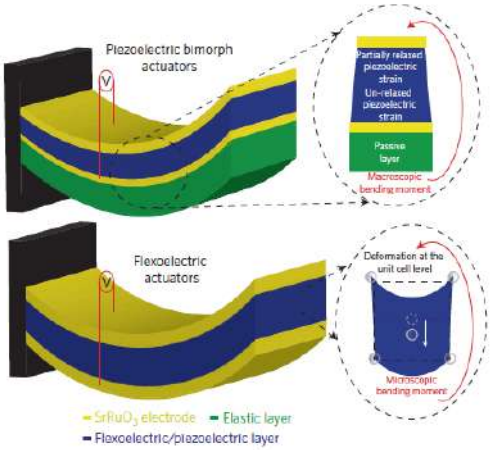
Unstrained crystal:



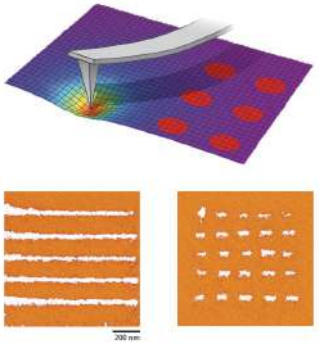
Apply strain **gradient**:



Possibility of novel devices

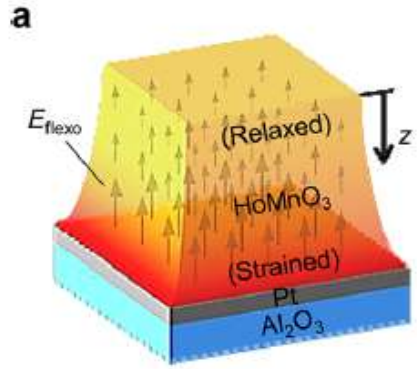


U.K. Bhaskar, *et al.*, Nat. Nano **11**, 263 (2016)

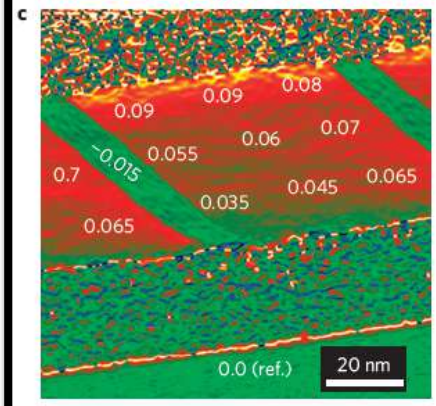


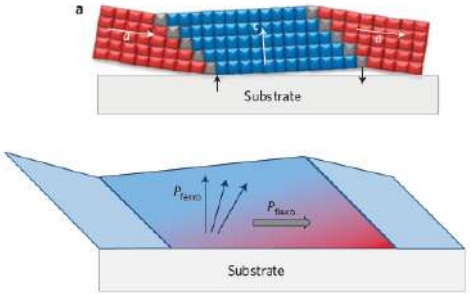
H. Lu, *et al.*, Science 336, 59 (2012)

Affects properties of nanoscale devices



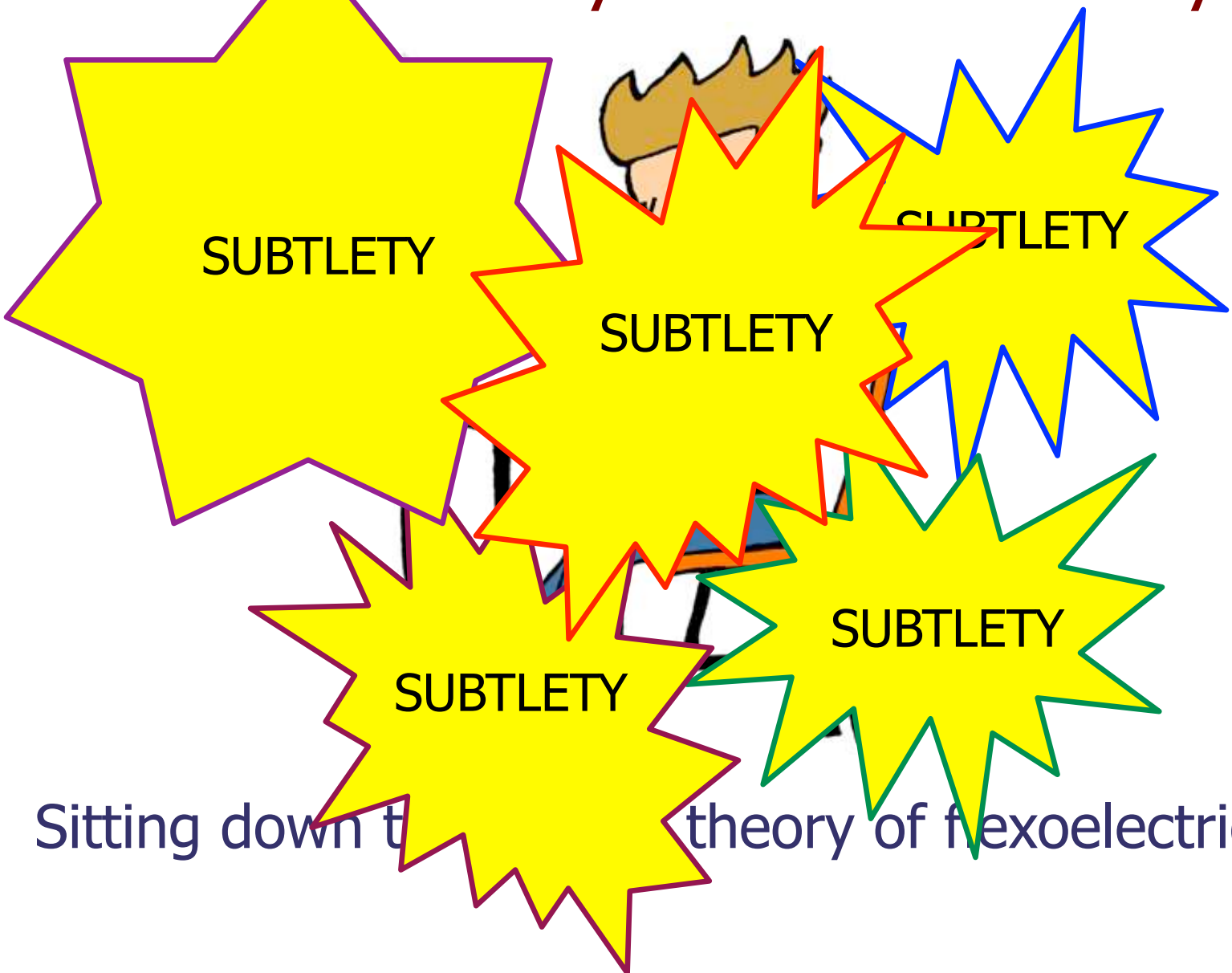
D. Lee, *et al.*, Nano Lett. **12**, 6436 (2012).





G. Catalan, *et al.,* Nat. Mater. 10, 963 (2011).

Theory of flexoelectricity



Sitting down t theory of flexoelectricity...

Flexoelectricity: History of our publications

J. Hong and D. Vanderbilt, "First-principles theory of frozen-ion flexoelectricity," Phys. Rev. B 84, 180101 (2011). *(journal link, local copy)*

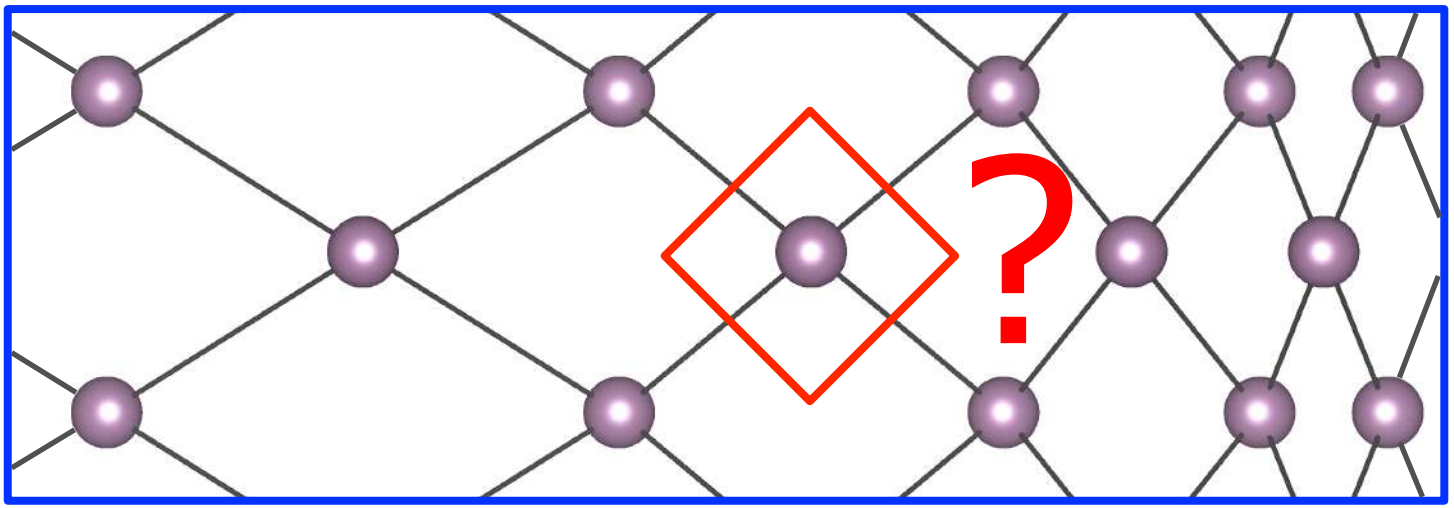
J. Hong and D. Vanderbilt, "First-principles theory and calculation of flexoelectricity," Phys. Rev. B 88, 174107 (2013). *(journal link, local copy)*

M. Stengel and D. Vanderbilt, "First-principles theory of flexoelectricity," in *Flexoelectricity in Solids: From Theory to Applications*, A.K. Tagantsev and P. Yudin, eds. (World Scientific, Singapore, 2016), Chapter 2, pp. 31-110. *(local preprint)*

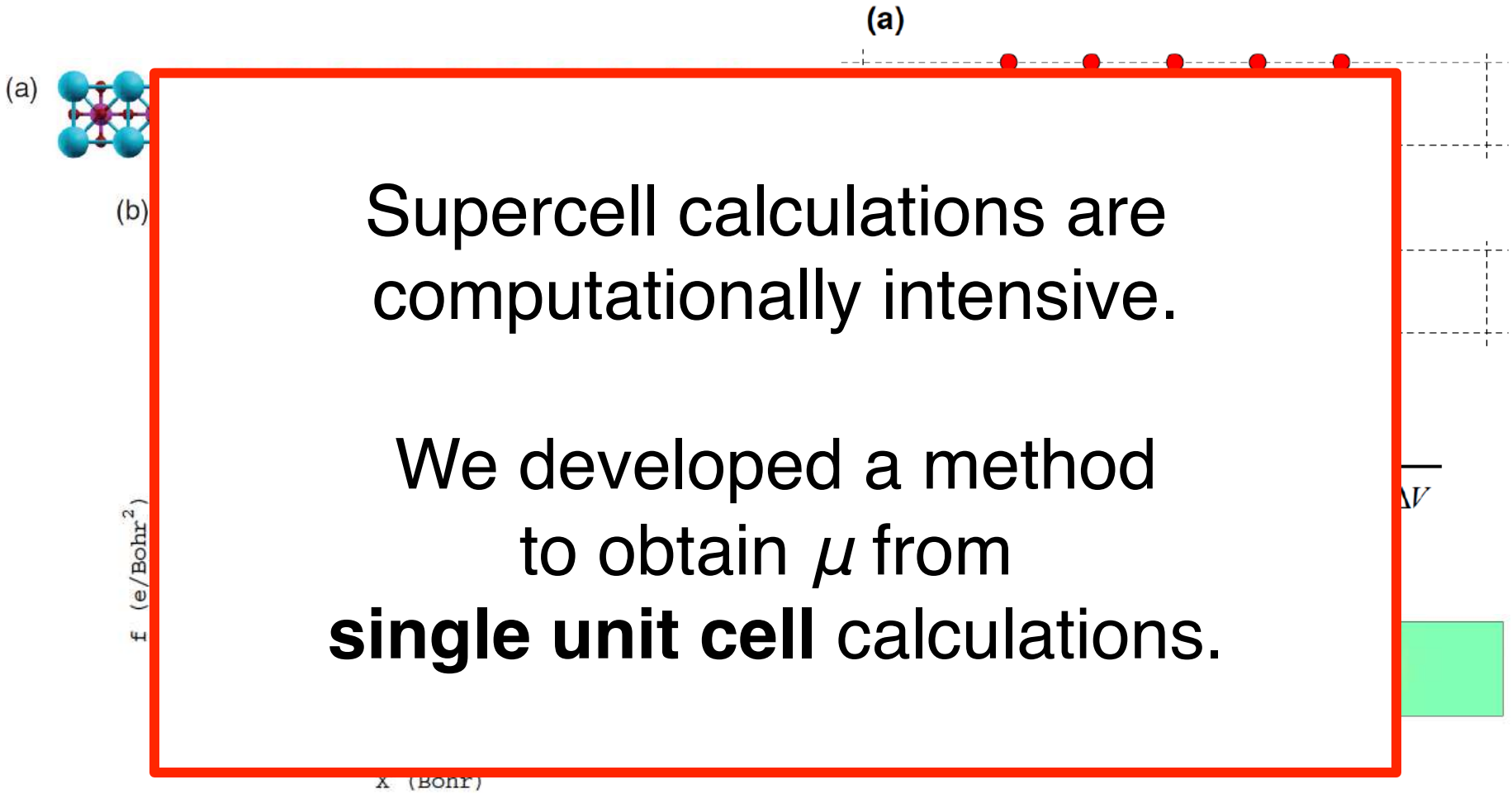
C. Dreyer, M. Stengel, and D. Vanderbilt, "Current-density implementation for calculating flexoelectric coefficients," Phys. Rev. B 98, 075153 (2018). *(journal link, local copy)*

A. Schiaffino, C.E. Dreyer, D. Vanderbilt, and M. Stengel, "Metric-wave approach to flexoelectricity within density-functional perturbation theory," Phys. Rev. B 99, 085107 (2019). *(journal link, local copy)*

How to model a strain gradient in a bulk material?



Previous implementations for calculating μ required supercells



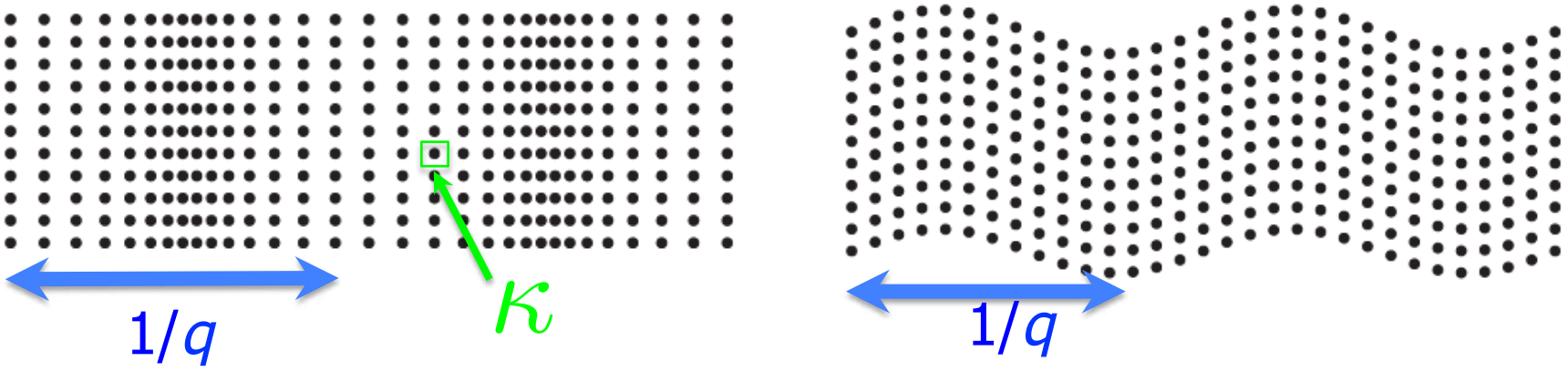
Supercell calculations are computationally intensive.

We developed a method to obtain μ from **single unit cell** calculations.

J. Hong and D. Vanderbilt, Phys. Rev. B **88**, 174107 (2013).

M. Stengel, Phys. Rev. B, **90**, 201112, (2014).

Long wavelength acoustic phonon



- Displacement of atom κ:

$$\mathbf{u}_\kappa = \boldsymbol{\lambda}_\kappa^{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}_\kappa}$$

phase

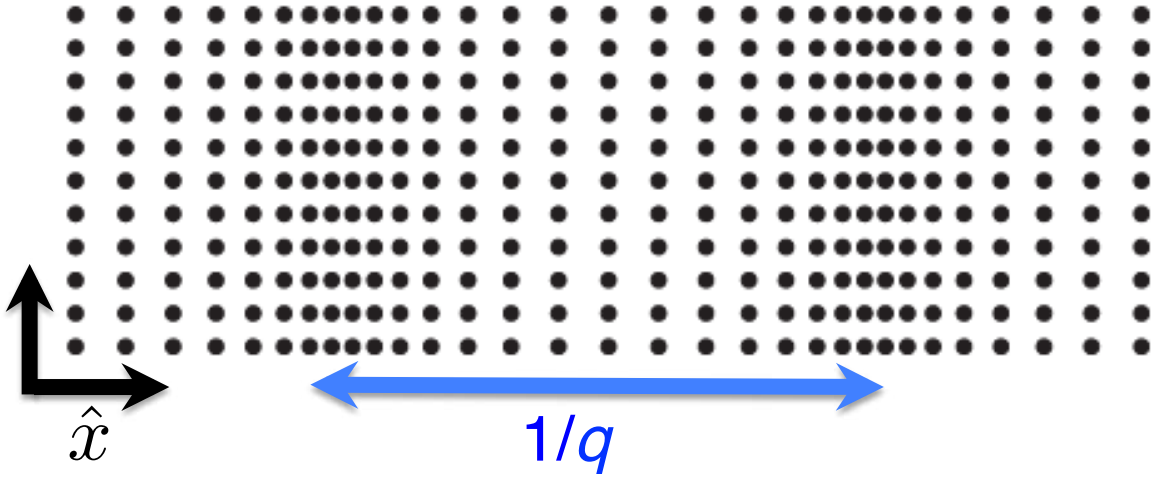
- Polarization response:

Cell periodic response

$$\frac{\partial \mathbf{P}_\kappa(\mathbf{r})}{\partial \boldsymbol{\lambda}_\kappa^{\mathbf{q}}} = \mathbf{P}_\kappa^{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}$$

phase

Long-wavelength expansion of cell-periodic polarization



$$P^{\mathbf{q}}_{x,x} = P^{(\mathbf{q}=0)}_{x,x} - iq_x \left.\frac{\partial P^{\mathbf{q}}_{x,x}}{\partial q_x}\right|_{\mathbf{q}=0} - \frac{q_x^2}{2} \left.\frac{\partial^2 P^{\mathbf{q}}_{x,x}}{\partial q_x^2}\right|_{\mathbf{q}=0} + \cdots$$

Born effective charge

Piezoelectric response

Flexoelectric response

M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford Univ. Press, Oxford, 1954)
R. M. Martin, Phys. Rev. B 5,1607 (1972)
M. Stengel, Phys. Rev. B 88, 174106 (2013

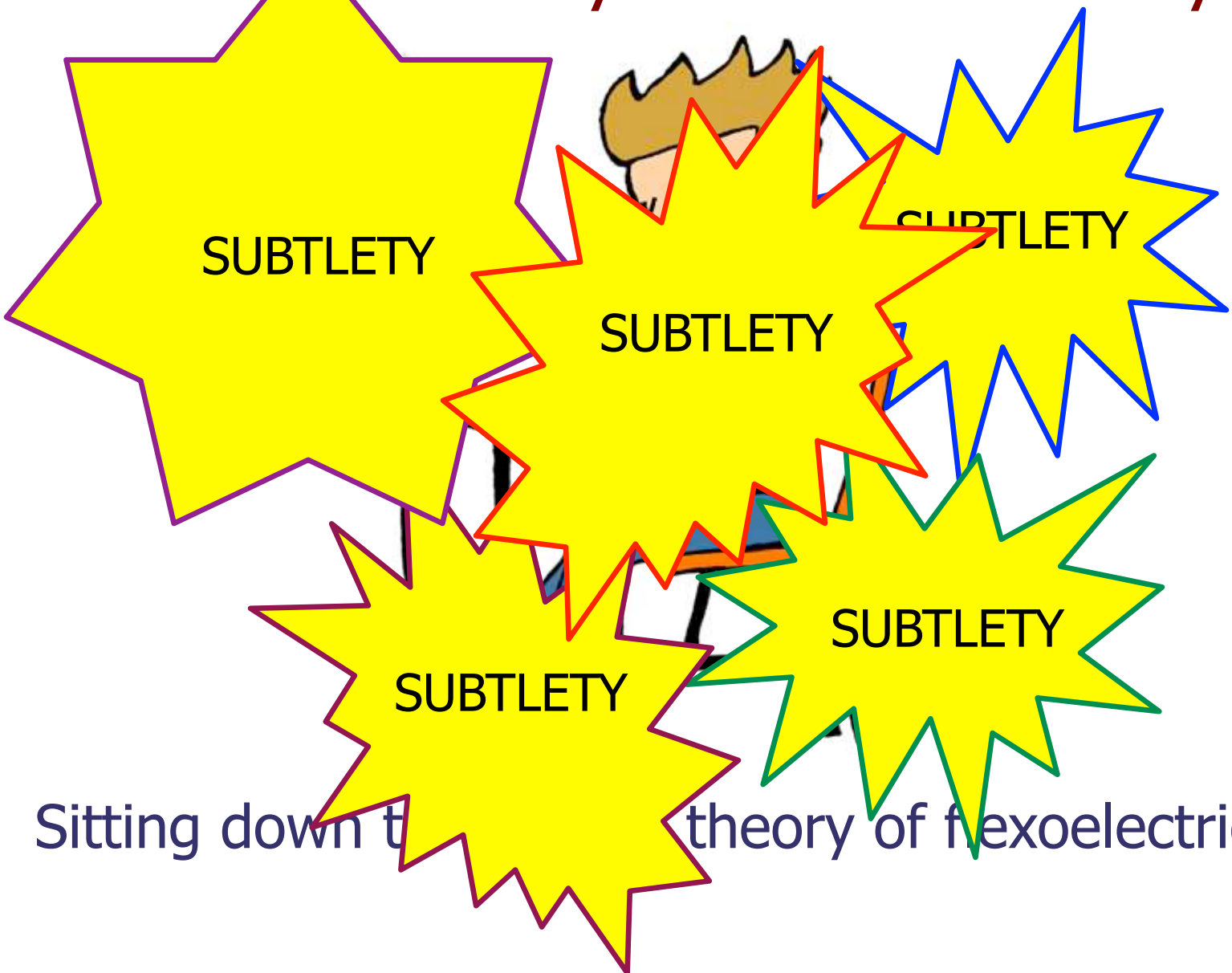
Summary of Approach

- Treat gradient as long-wavelength acoustic phonon
- Second order term in long-wavelength expansion of ***P***

$$\mu^{\mathrm{CI}}_{\alpha\beta,\gamma\delta} = -\frac{1}{2}\frac{\partial^2 P^{\mathbf{q}}_{\alpha,\beta}}{\partial q_\gamma \partial q_\delta}\bigg|_{\mathbf{q}=0}$$

Phonon wavevector

Theory of flexoelectricity



Sitting down t theory of flexoelectricity...

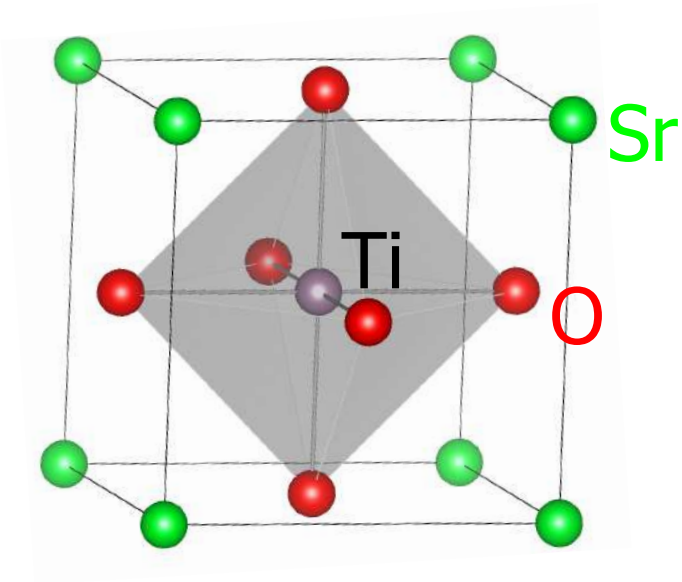
Additional subtleties

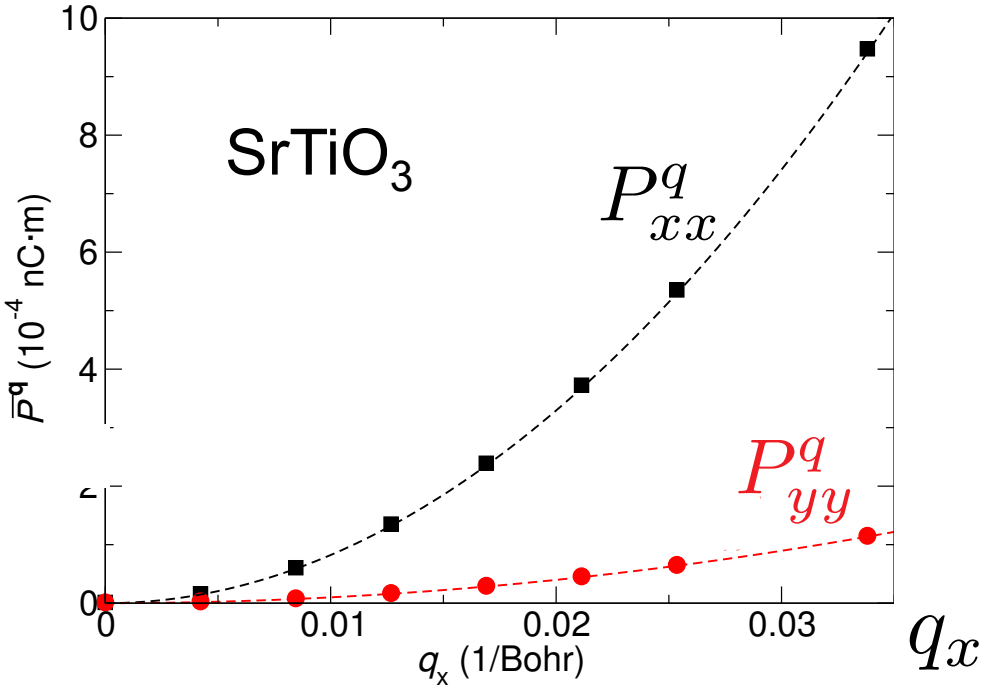
- Calculate *current* response to phonon

$$\mathbf{J}(\mathbf{r},t) = \frac{\partial \mathbf{P}(\mathbf{r},t)}{\partial t}$$

- Define current with *nonlocal pseudopotentials*
- Inhomogeneous deformations involve *rotations*
  - Subtract off *"diamagnetic"* response
  - Via *"metric implementation"*
- Include *internal strain* contributions
- Include *surface* contributions

Example: Frozen-ion μ for $SrTiO_3$

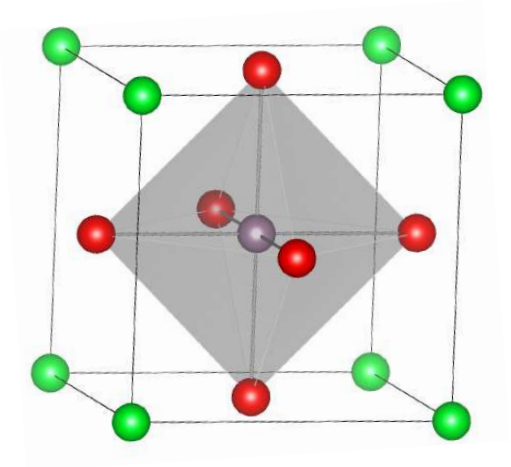




$\mu_{xx,xx}$	$\mu_{xx,yy}$	$\mu_{xy,xy}$
-0.87 $(-0.9^a, -0.88^b)$	-0.84 (-0.83^b)	$-0.08(-0.08^b)$

(a) J. Hong and D. Vanderbilt, PRB 88, 174107 (2013)
(b) M. Stengel, PRB, 90, 201112, (2014)

Cubic oxides



	$\mu_{xx,xx}$	$\mu_{xx,yy}$	$\mu_{xy,xy}$
$SrTiO_3$	-0.87 $(-0.9^a, -0.88^b)$	-0.84 (-0.83^b)	$-0.08(-0.08^b)$
$BaTiO_3$	-1.01 (-1.1^a)	-1.03	-0.07
$SrZrO_3$	-0.61	-0.57	-0.05
$PbTiO_3$	-1.35 (-1.5^a)	-1.35	-0.1
MgO	-0.28 (-0.3^a)	-0.29	-0.07

(a) J. Hong and D. Vanderbilt, PRB 88, 174107 (2013)
(b) M. Stengel, PRB, 90, 201112, (2014)

Next:
Materials physics of flexoelectricity

- Flexoelectricity in different materials classes?
  - How to enhance flexoelectric coefficients?
  - Or, how to suppress them?
- Disseminate our codes

Summary

- Modern theory of polarization
  - What is the problem?
  - Berry phase formulation
  - Wannier center formulation
- Effective Hamiltonian approach
- Theory of flexoelectricity