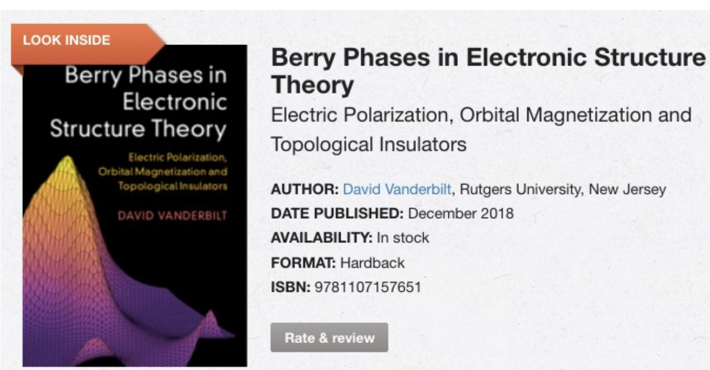
Wannier functions, electric polarization, orbital magnetoelectric coupling, and axion electrodynamics



David Vanderbilt
Rutgers University

Slides available at https://is.gd/inFID2

RUTGERS

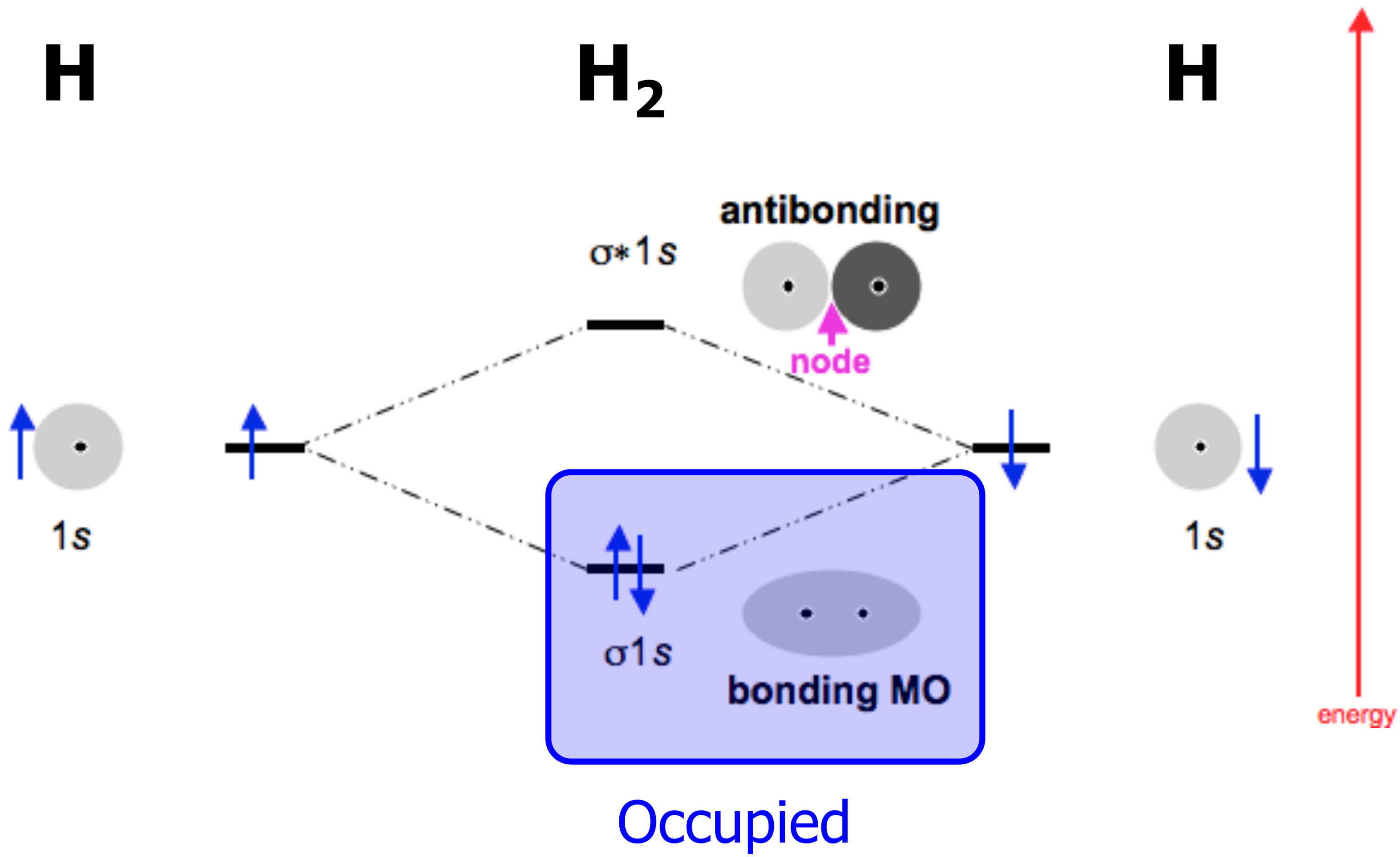
NSF DMR-1408838

QMS23, August 21-25, 2023

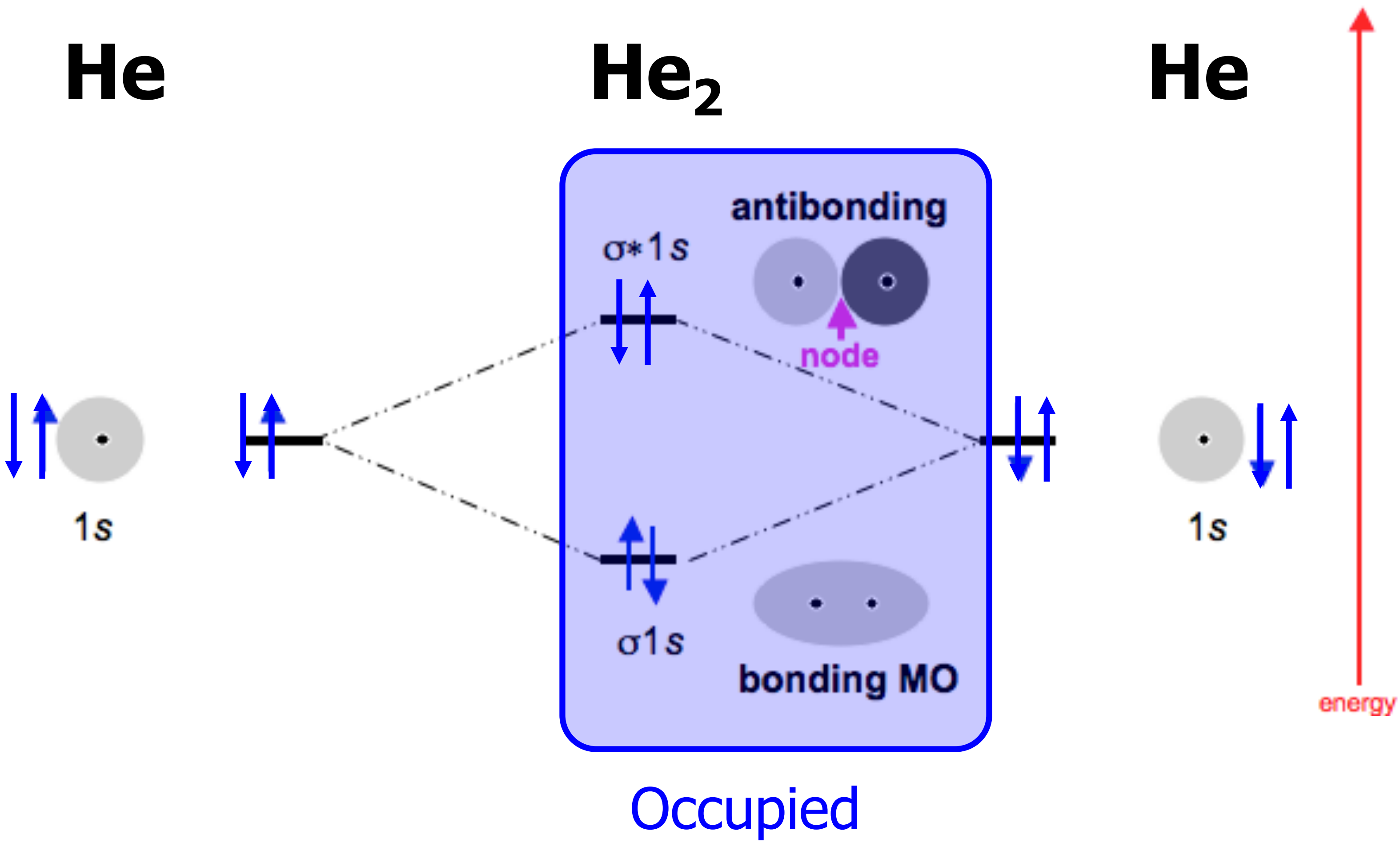
Outline

- Wannier functions for occupied subspace
  - Electric polarization
  - Topological obstruction
- Wannier functions as a basis
  - Wannier interpolation
- Orbital magnetoelectric coupling
  - Axion electrodynamics

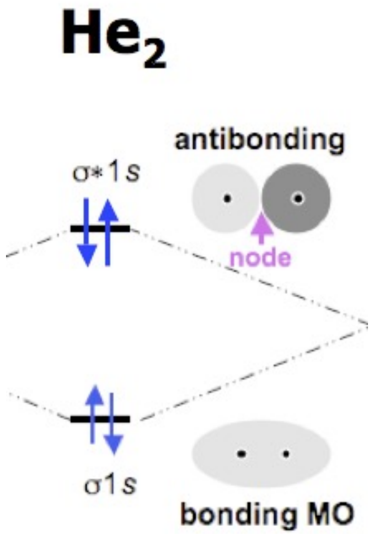
H_2 molecule

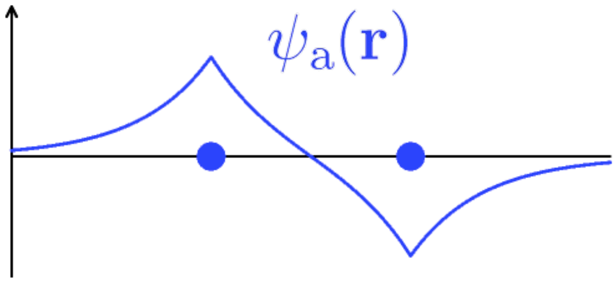

H
H_2
H
antibonding
σ*1s
node
1s
1s
σ1s
bonding MO
energy
Occupied

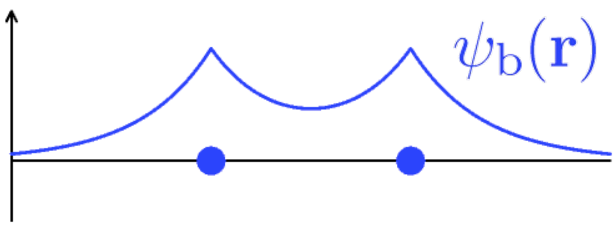
He_2 molecule



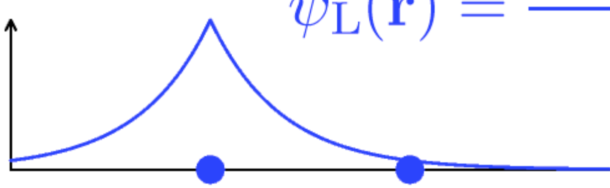
He_2 molecule



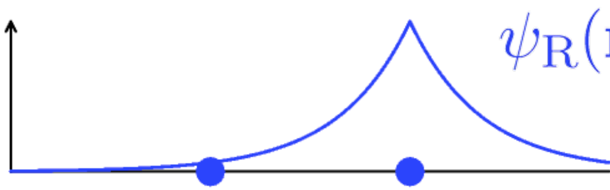




$$\psi_{\mathrm{L}}(\mathbf{r}) = \frac{\psi_{\mathrm{a}}(\mathbf{r}) + \psi_{\mathrm{b}}(\mathbf{r})}{\sqrt{2}}$$



$$\psi_{\mathrm{R}}(\mathbf{r}) = \frac{\psi_{\mathrm{a}}(\mathbf{r}) - \psi_{\mathrm{b}}(\mathbf{r})}{\sqrt{2}}$$



Construction of LMOs

Given a set of occupied states $|\Psi_n\rangle$, $n = \{1,N\}$

Find unitary transformation to $|\phi_j\rangle$, $j = \{1,N\}$

$$|\phi_j\rangle = \sum_n U_{nj}\,|\psi_n\rangle$$

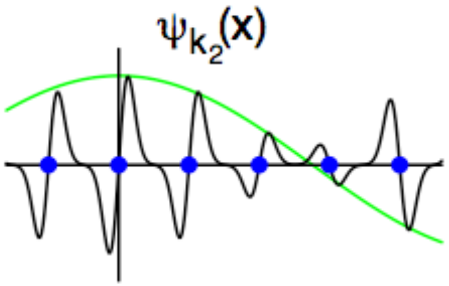
such that the $|\phi_j\rangle$ are maximally localized.

Foster-Boys criterion: Minimize

$$\Omega = \sum_j \left[\langle\phi_j|r^2|\phi_j\rangle - |\langle\phi_j|\mathbf{r}|\phi_j\rangle|^2\right]$$

Apply Foster-Boys criterion for crystalline solids?

Problem: $\langle\psi_{nk}|x|\psi_{nk}\rangle$ and $\langle\psi_{nk}|x^2|\psi_{nk}\rangle$ are ill defined!



Maximally localized Wannier functions

N. Marzari and D. Vanderbilt, "Maximally localized generalized Wannier functions for composite energy bands," Phys. Rev. B 56, 12847 (1997). (*journal link*, *local copy*)

I. Souza, N. Marzari, and D. Vanderbilt, "Maximally-localized Wannier functions for entangled energy bands," Phys. Rev. B 65, 035109 (2002). (*journal link*, *local copy*)

N. Marzari, A.A. Mostofi, J.R. Yates, I. Souza, and D. Vanderbilt, "Maximally localized Wannier functions: Theory and applications," Rev. Mod. Phys. 84, 1419 (2012). (*journal link*, *local copy*)

WANNIER90 https://wannier.org

A.A. Mostofi, Y.S. Lee, I. Souza, D. Vanderbilt, and N. Marzari, "Wannier90: A tool for obtaining maximally-localized Wannier functions from energy bands," Comput. Phys. Commun. 178, 685 (2008). (*journal link*, *local preprint*)

A.A. Mostofi, J.R. Yates, G. Pizzi, Y.S. Lee, I. Souza, D. Vanderbilt, and N. Marzari, "An updated version of Wannier90: A tool for obtaining maximally-localized Wannier functions from energy bands," Comput. Phys. Commun. 185, 2309 (2014). (*journal link*, *local copy*)

G. Pizzi, V. Vitale, R. Arita, S. Blügel, F. Freimuth, G. Géranton, M. Gibertini, D. Gresch, C. Johnson, T. Koretsune, J. Ibañez-Azpiroz, H. Lee, D. Marchand, A. Marrazzo, Y. Mokrousov, J.I. Mustafa, Y. Nohara, Y. Nomura, L. Paulatto, S Poncé, T. Ponweiser, J. Qiao, F. Thöle, S. Tsirkin, M. Wierzbowska, N. Marzari, D. Vanderbilt, I. Souza, A.A. Mostofi, and J.R. Yates, "Wannier90 as a community code: New features and applications," J. Phys. Cond. Matt. 32, 165902 (2020). (*journal link*)

Maximally localized Wannier functions

H eigenstates (Bloch)

$$|\widetilde{\psi}_{j\mathbf{k}}\rangle = \sum_n U_{nj}(\mathbf{k})\, |\psi_{n\mathbf{k}}\rangle$$

Pseudo-Bloch
(smooth in k)

Variable unitary matrices

$$|w_{\mathbf{R},n}\rangle = \frac{V}{(2\pi)^3} \int_{\mathrm{BZ}} d^3k\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, |\widetilde{\psi}_{n\mathbf{k}}\rangle$$

Wannier functions
(LMO's)

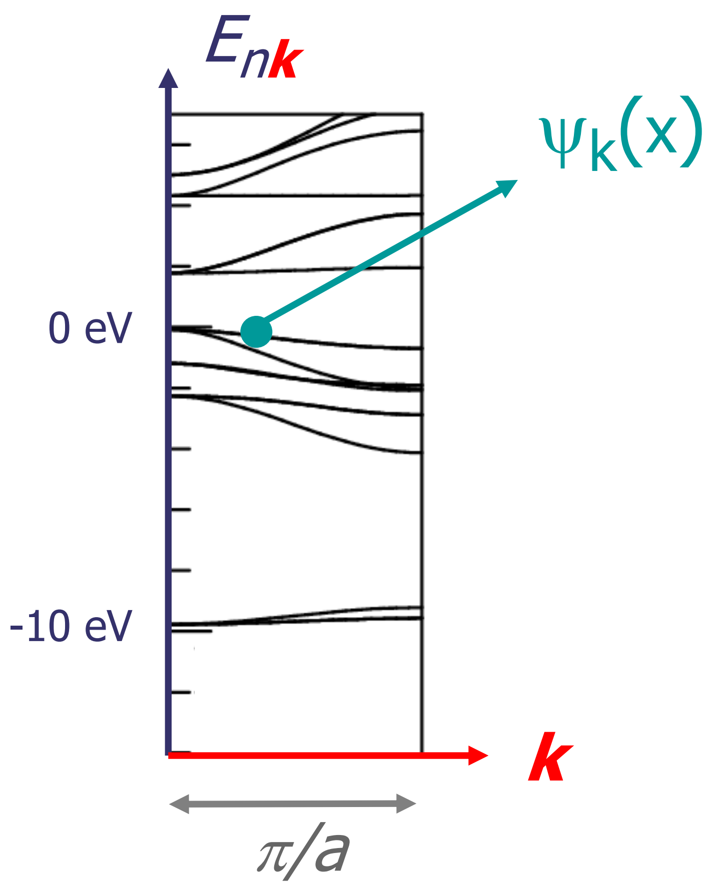
Wannier functions
in home unit cell

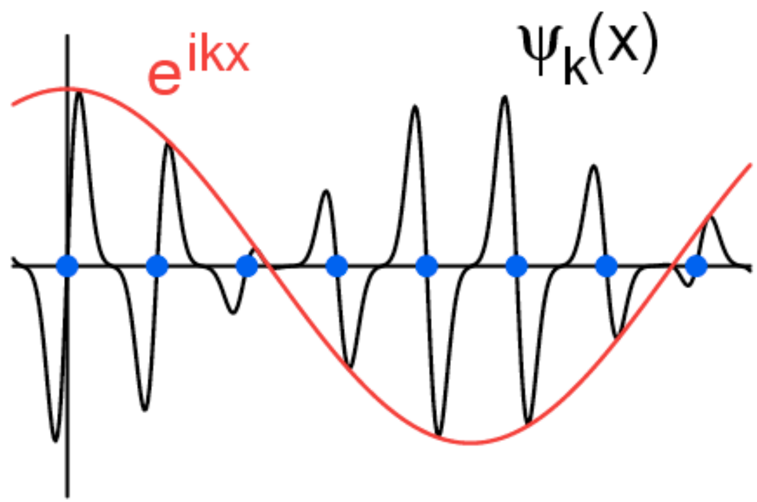
$$|w_n\rangle = |w_{0,n}\rangle$$

Minimize $\Omega = \sum_n \left[\langle w_n | r^2 | w_n \rangle - |\langle w_n | \mathbf{r} | w_n \rangle|^2 \right]$

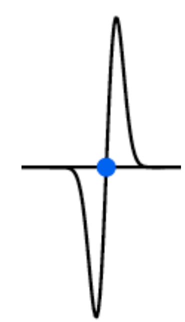
Bloch states

Bloch wavefunction





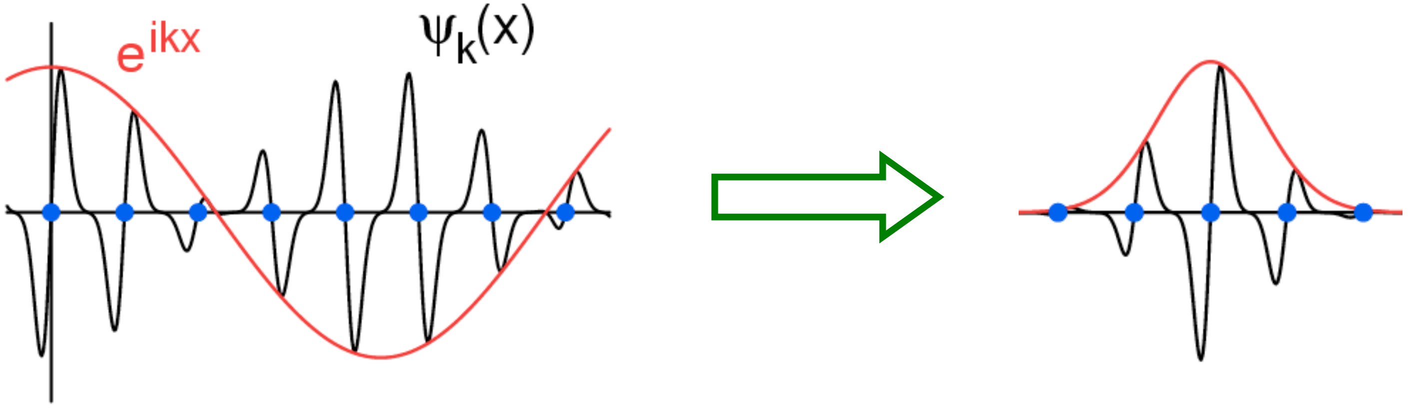
Ingredient:
Atomic
wavefunction



Tutorial on Wannier functions

Choose Wannier functions as

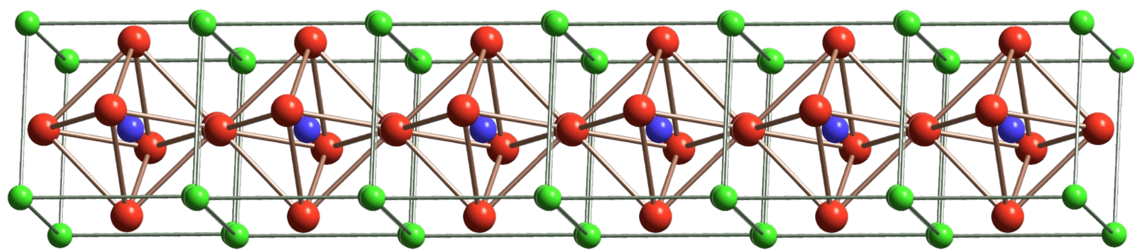
$$w_n(\mathbf{r}-\mathbf{R}) = \int_{BZ} \psi_{n\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$



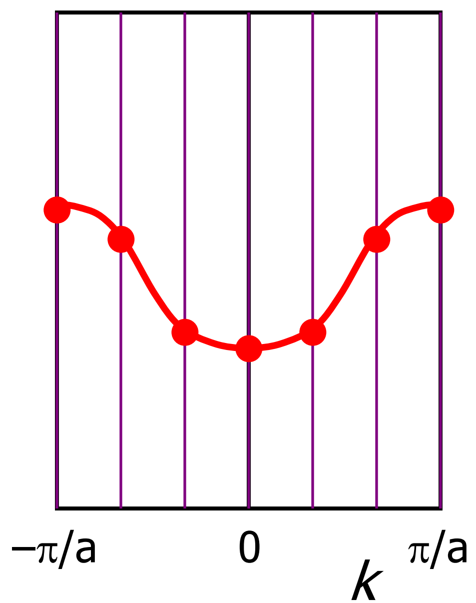
Form wave-packet = "Wannier function"

Tutorial on Wannier functions

Crystal in real space:

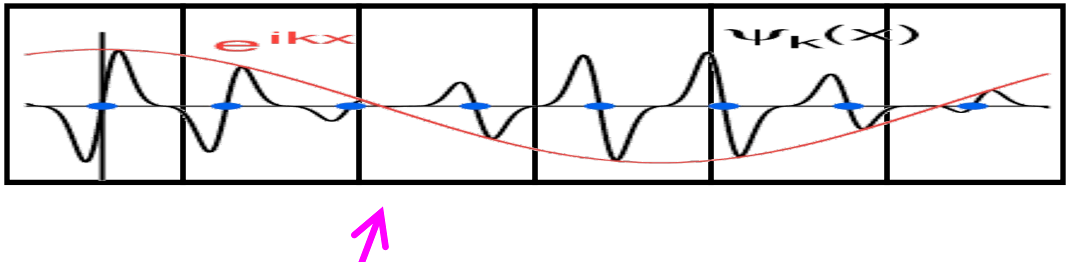


Brillouin zone in reciprocal space:

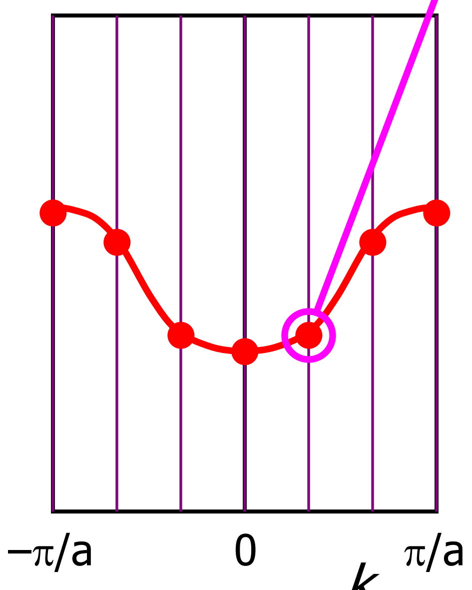


Tutorial on Wannier functions

Crystal in real space:

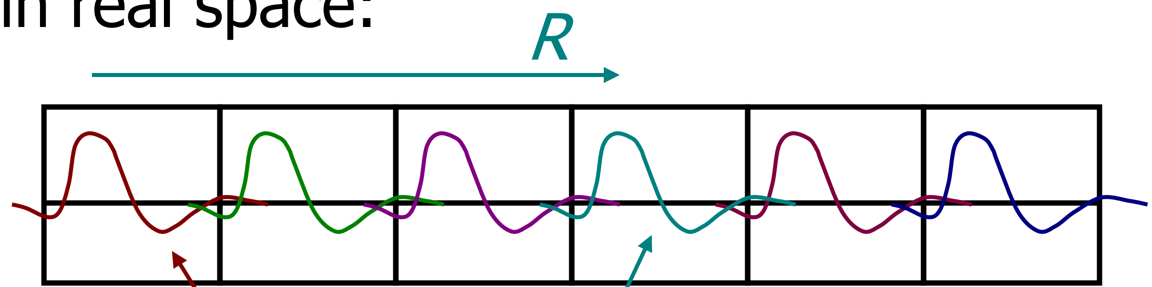


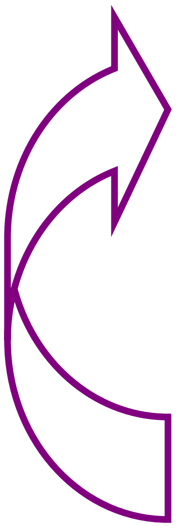
Brillouin zone in reciprocal space:



Tutorial on Wannier functions

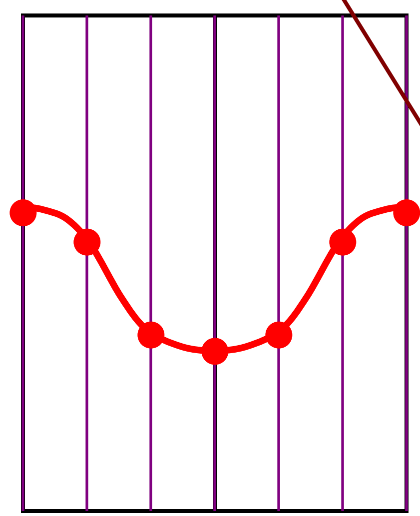
Crystal in real space:





Unitary transformation

Brillouin zone in reciprocal space:

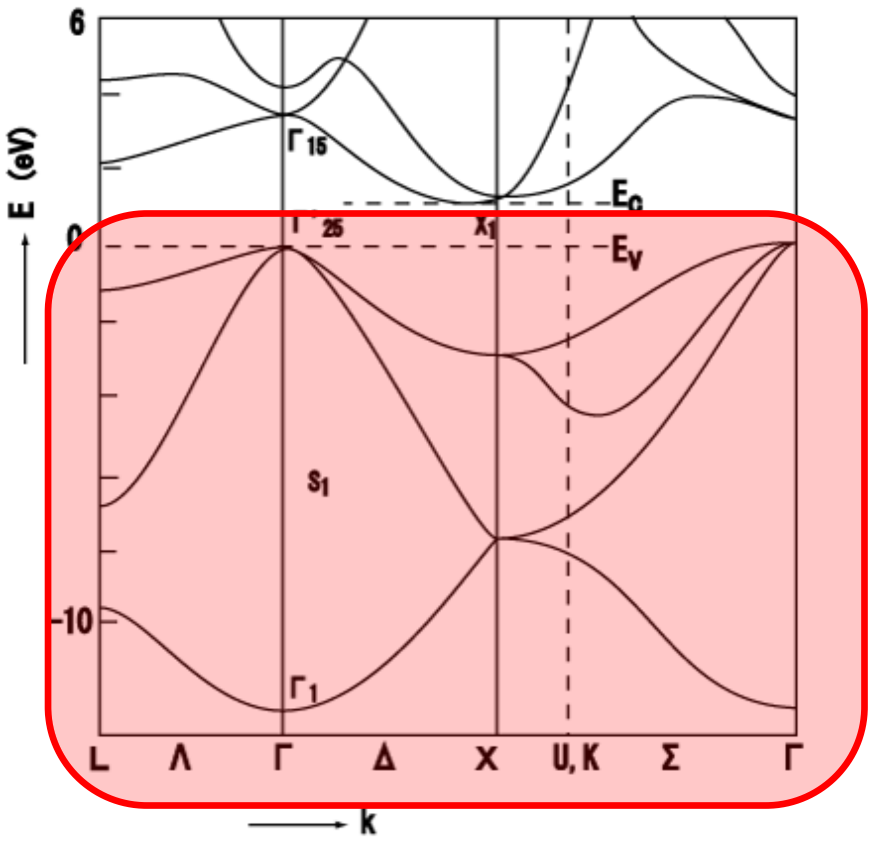


$$w_{\mathbf{R}}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

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

Four occupied bands

Si



Four occupied bands

Expect four WFs per cell

Multiband Wannier construction

H eigenstates (Bloch)

$$|\widetilde{\psi}_{j\mathbf{k}}\rangle = \sum_n U_{nj}(\mathbf{k})\,|\psi_{n\mathbf{k}}\rangle$$

Pseudo-Bloch (smooth in k)

Variable unitary matrices

$$|w_{\mathbf{R},n}\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\, e^{-i\mathbf{k}\cdot\mathbf{R}}\,|\widetilde{\psi}_{n\mathbf{k}}\rangle$$

Wannier functions (LMO's)

Wannier functions in home unit cell $\rightarrow$ $|w_n\rangle = |w_{0,n}\rangle$

Minimize $\Omega = \sum_n \left[\langle w_n|r^2|w_n\rangle - |\langle w_n|\mathbf{r}|w_n\rangle|^2\right]$

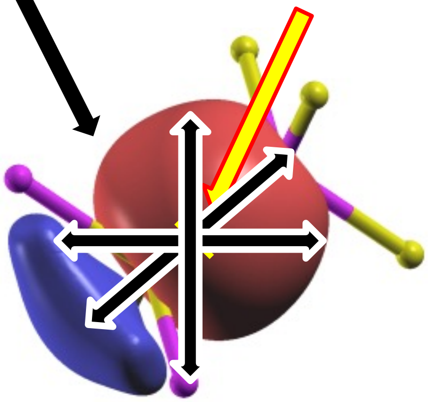
Minimize spread relative to center

Choose unitary matrices to minimize quadratic spread

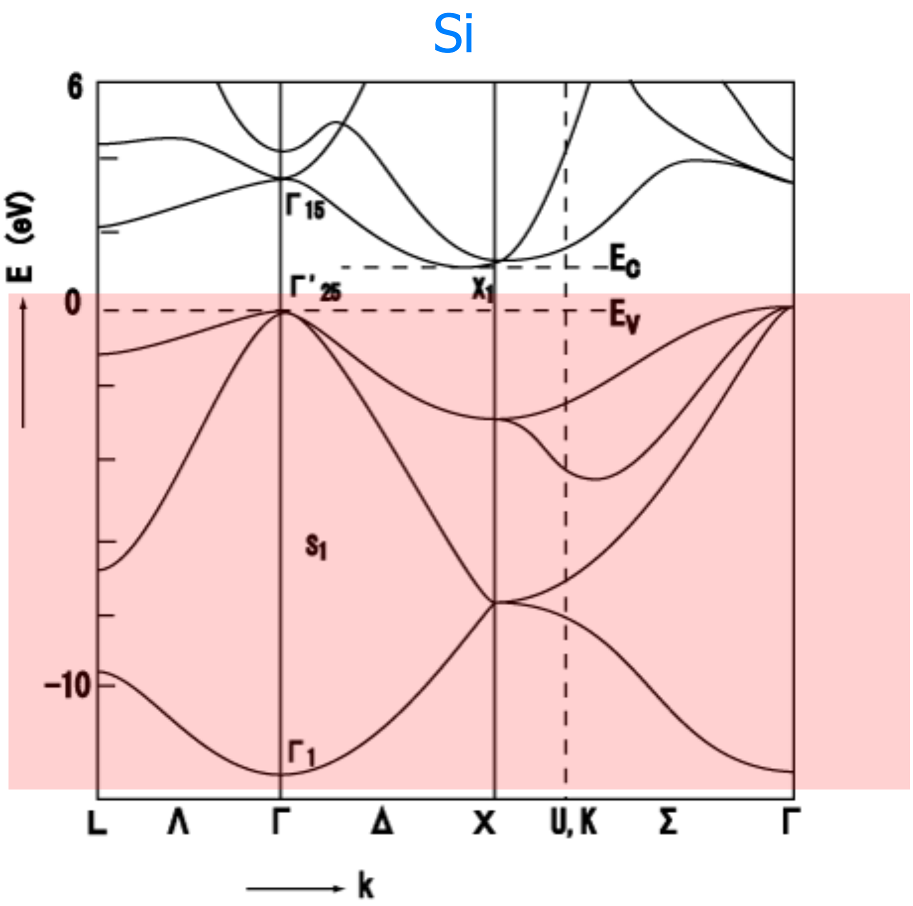
$$\Omega = \sum_n \left[\langle r^2 \rangle_n - \langle \mathbf{r} \rangle_n^2 \right]$$

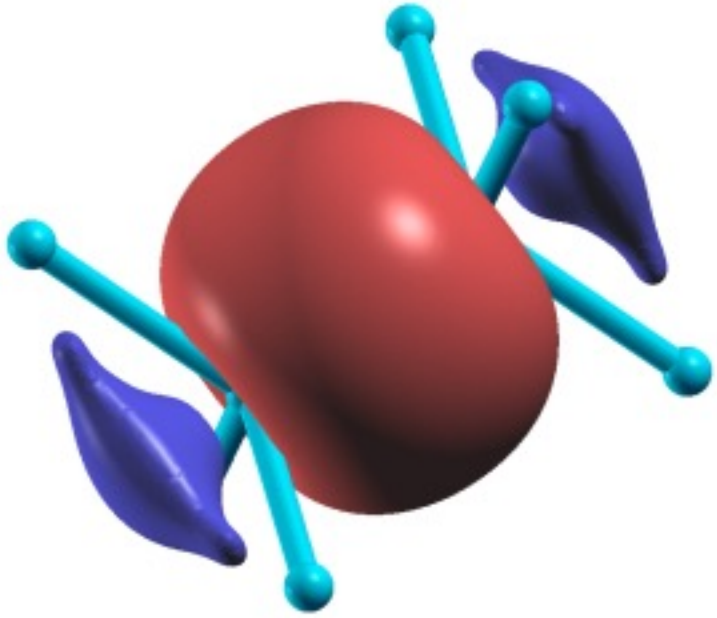
where

$$\langle r^2 \rangle_n = \langle w_n | r^2 | w_n \rangle \ , \quad \langle \mathbf{r} \rangle_n = \langle w_n | \mathbf{r} | w_n \rangle \ .$$



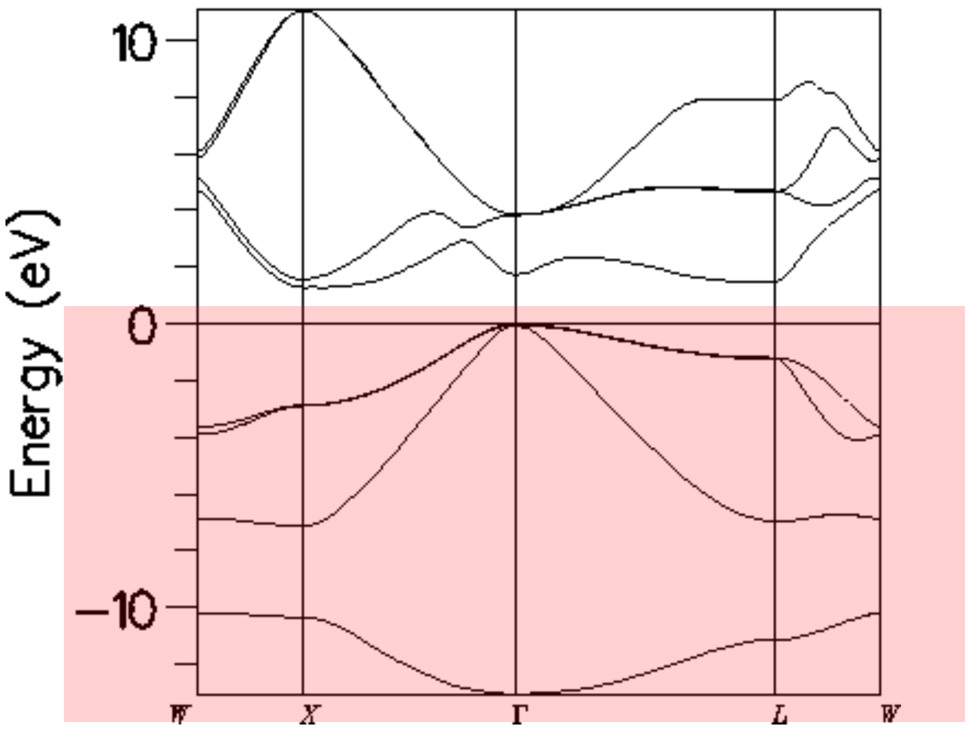
Wannier functions: Si

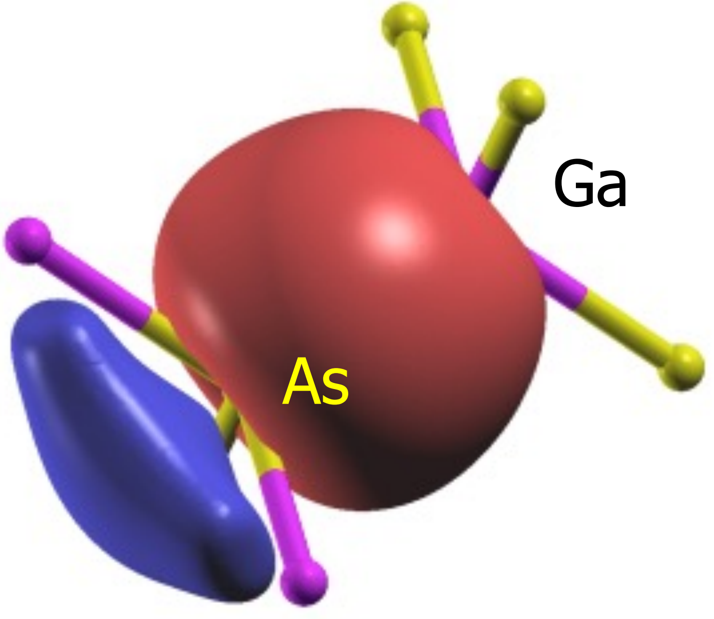




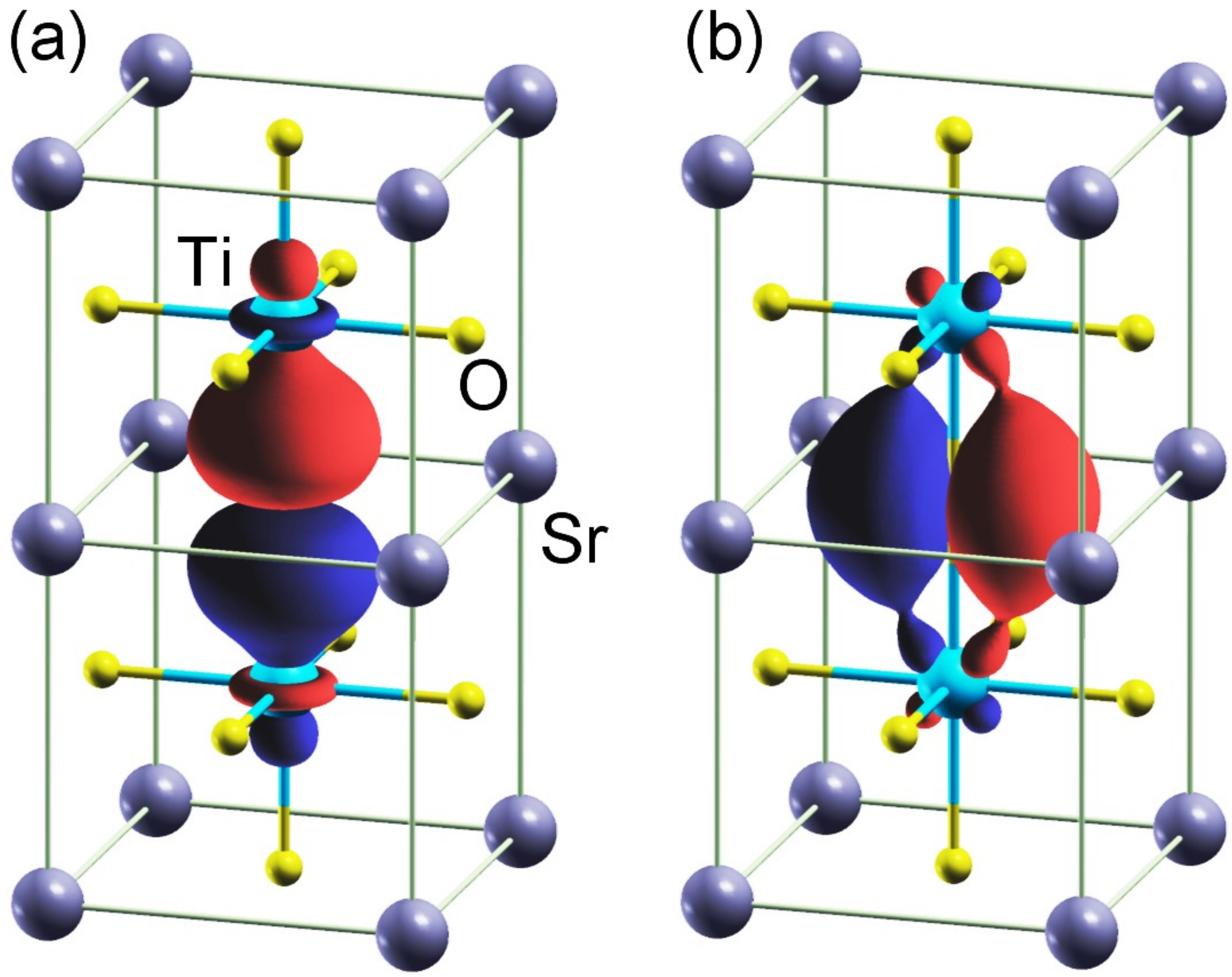
Wannier functions: GaAs

GaAs

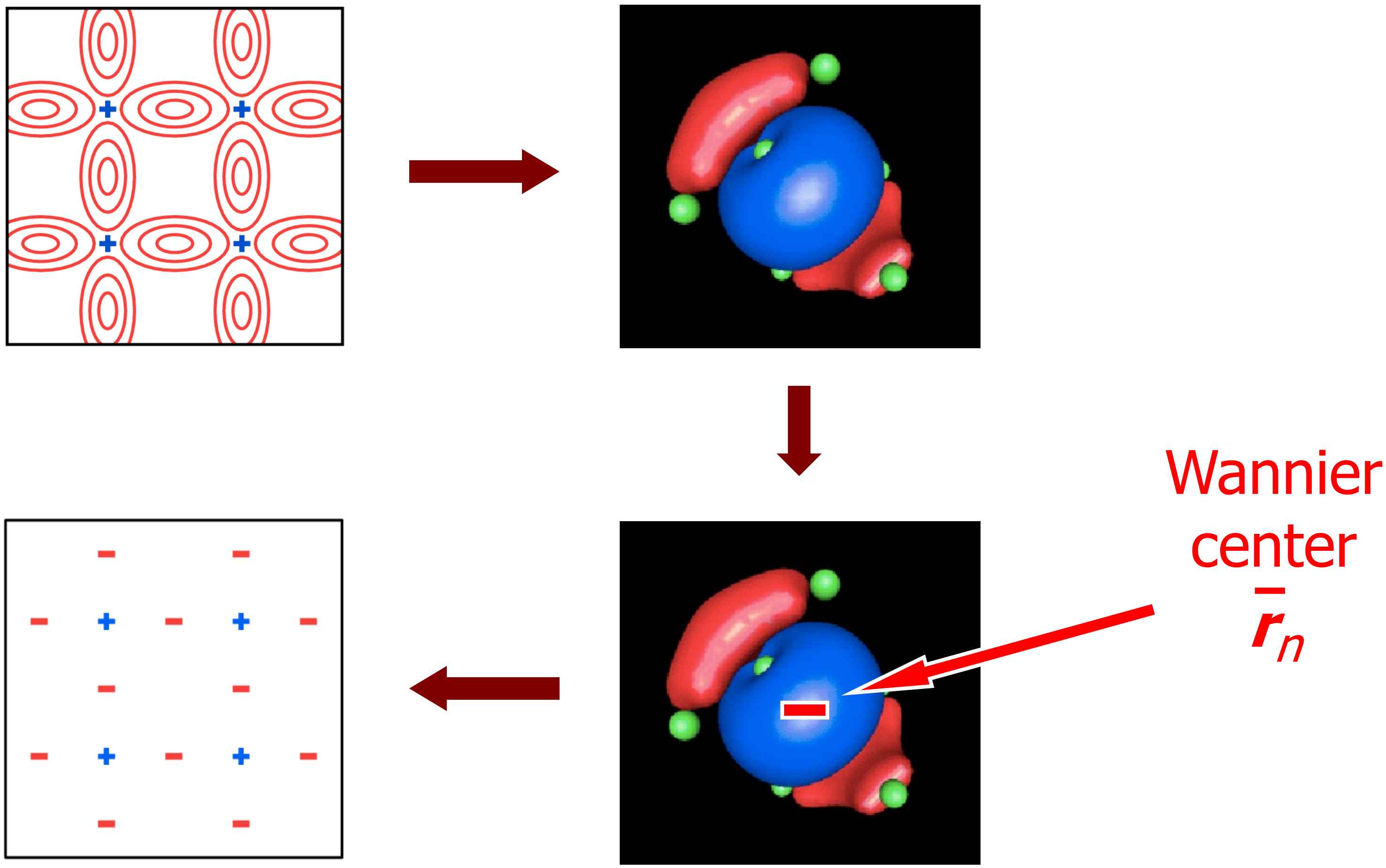




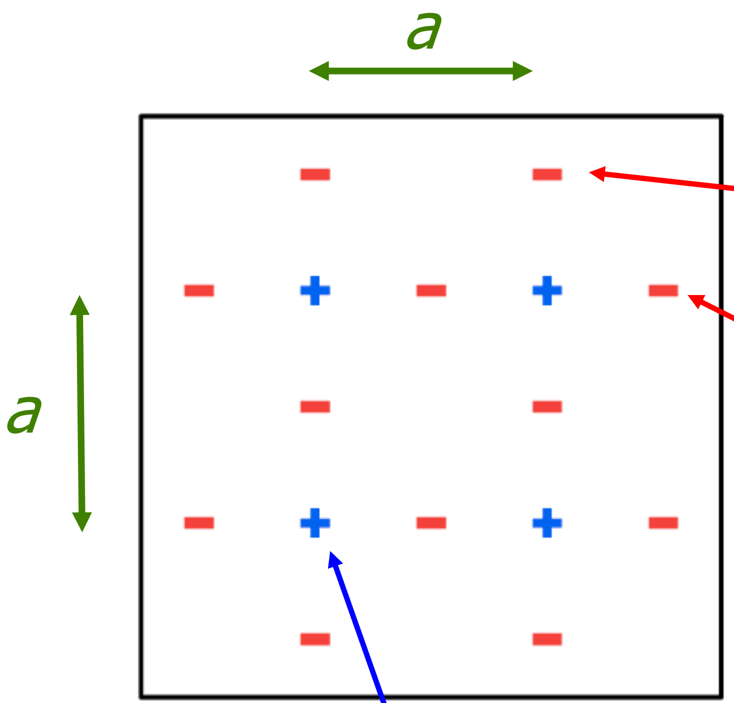
WFs in $SrTiO_3$



Mapping to Wannier centers



Mapping to Wannier centers



Wannier center
of band 1
(charge -2e)

Wannier center
of band 2
(charge -2e)

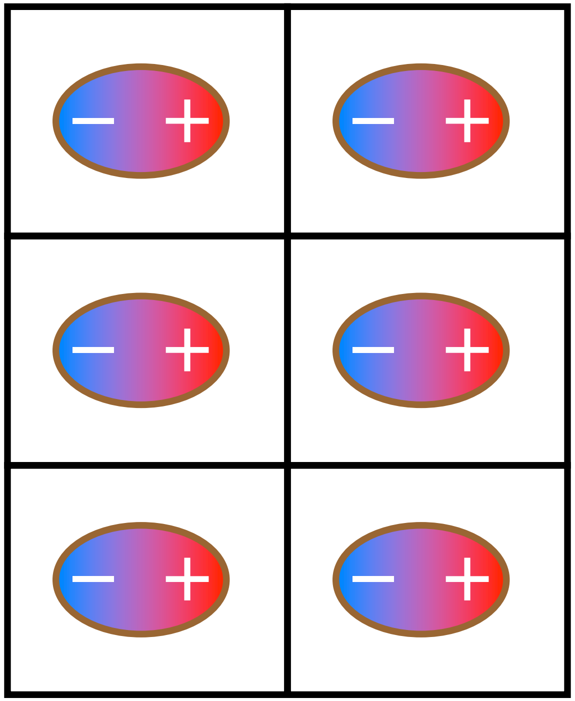
Location of ion
(nucleus)
(charge +4e)

Electric polarization ***P*** of the crystal can be deduced from pictures like this

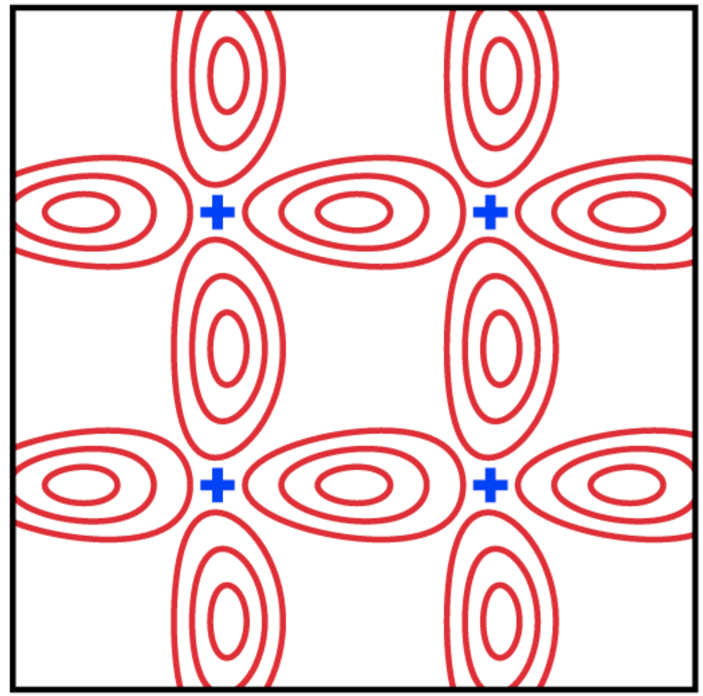
Outline

- Wannier functions for occupied subspace
  - **Electric polarization**
  - Topological obstruction
- Wannier functions as a basis
  - Wannier interpolation
- Orbital magnetoelectric coupling
  - Axion electrodynamics

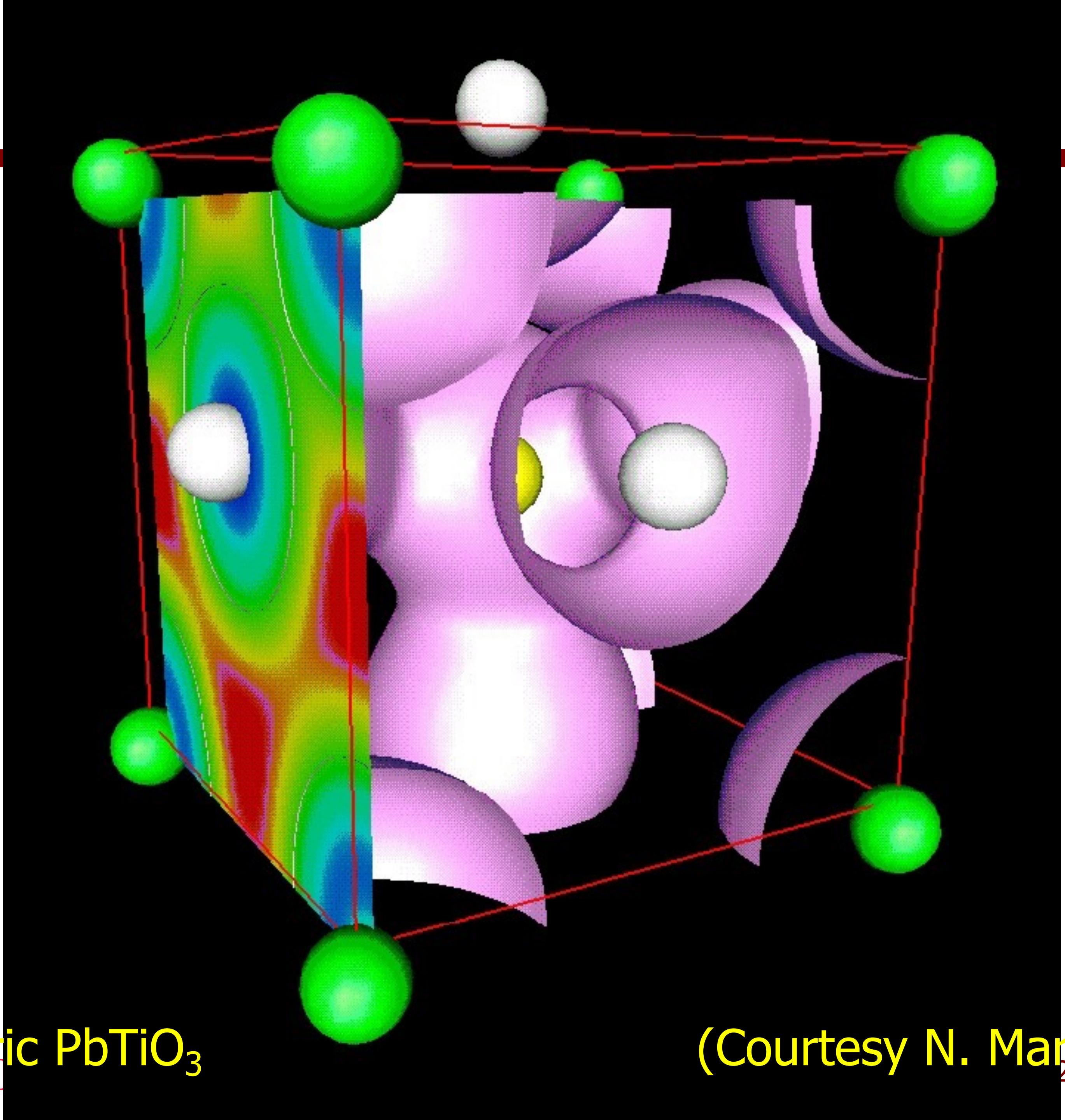
The Problem: Polarization



Textbook illustration

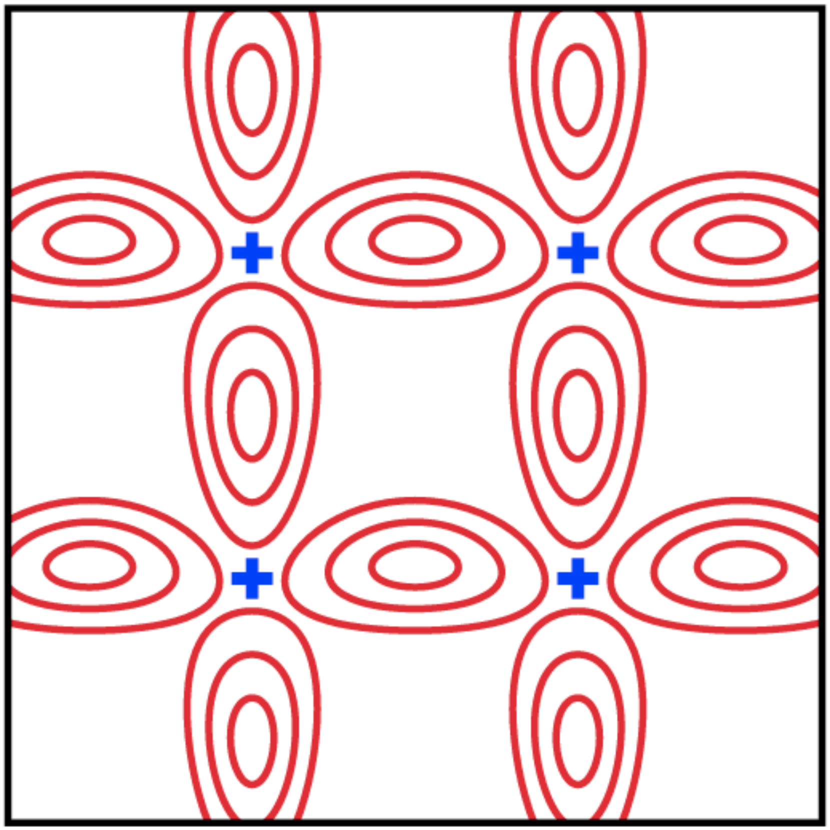


More realistic picture

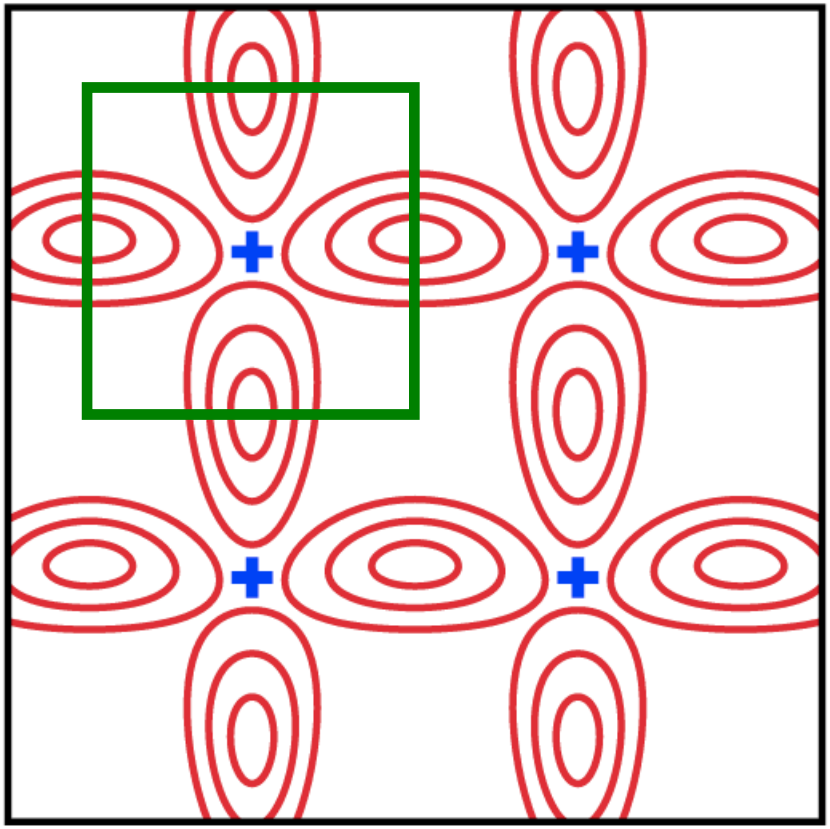


Ferroelectric $PbTiO_3$ (Courtesy N. Marzari)

$P = d_{cell} / V_{cell}$?



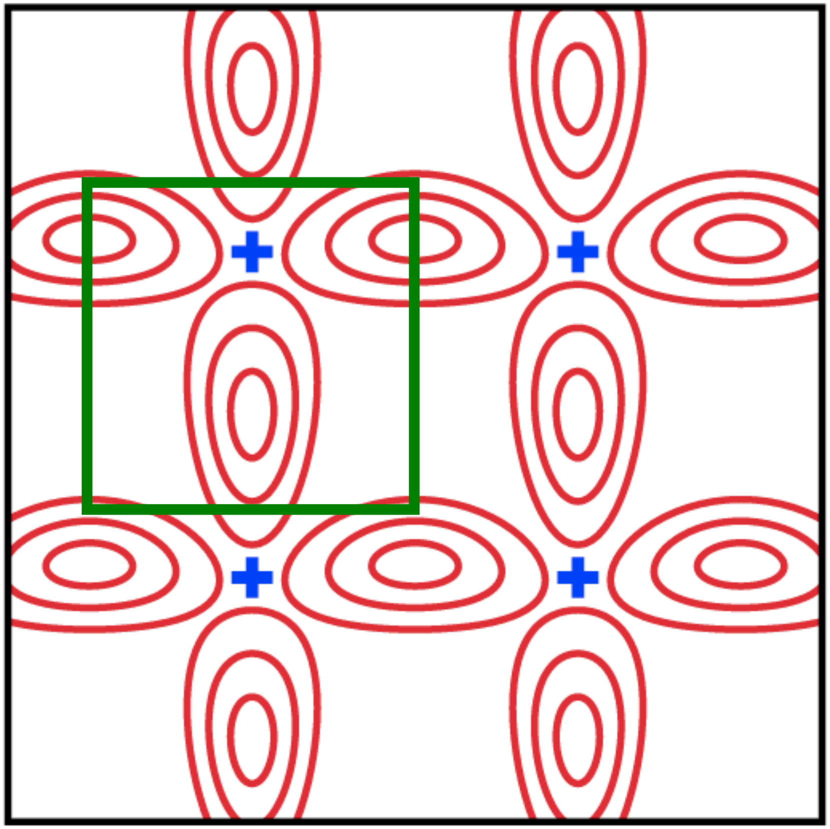
$\boldsymbol{P} = \boldsymbol{d}_{cell} \,/\, V_{cell}$?



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

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

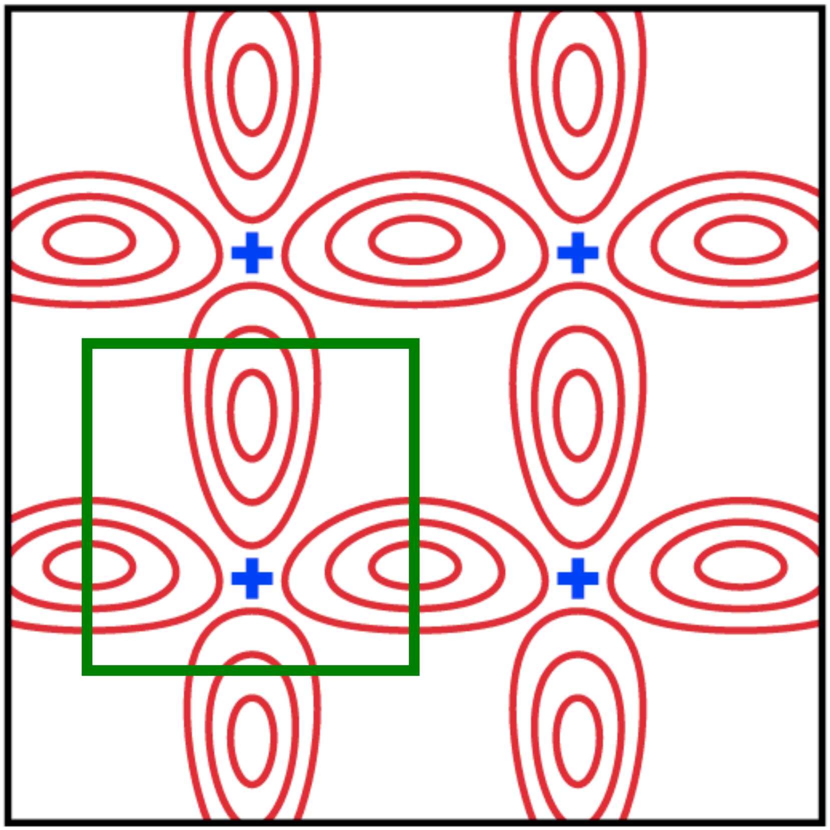
$\boldsymbol{P} = \boldsymbol{d}_{cell} \,/\, V_{cell}$?



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

$\boldsymbol{d}_{cell} =$ ⬆

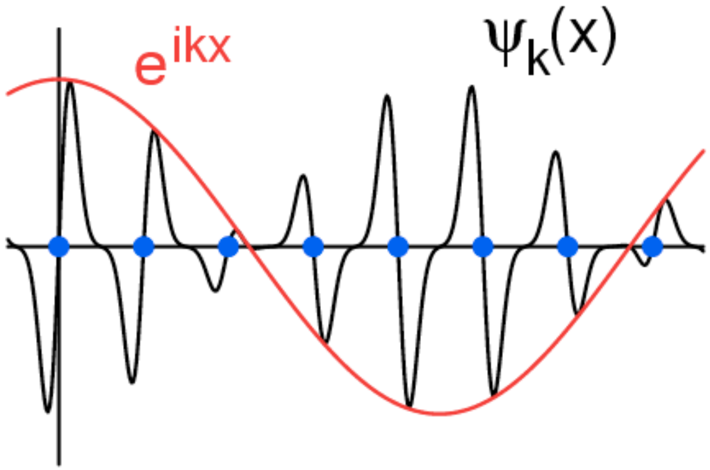
$\boldsymbol{P} = \boldsymbol{d}_{cell} \,/\, V_{cell}$?

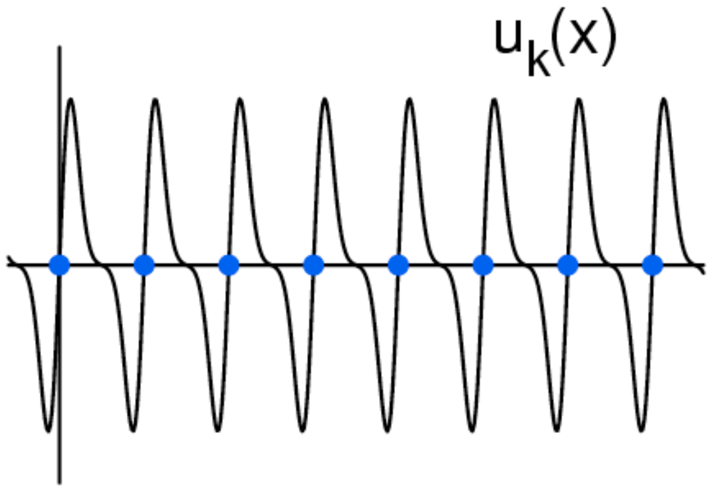


$$\boldsymbol{d}_{\mathrm{cell}} = \int_{\mathrm{cell}} \boldsymbol{r}\, \rho(\boldsymbol{r})\, d^3 r$$

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

Review: Bloch's Theorem





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

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

Theory of electric polarization

$$\boldsymbol{P} \propto \Sigma_{nk} \langle \psi_{nk} | \boldsymbol{r} | \psi_{nk} \rangle \ ?$$ Ill-defined…

Recall that in quantum mechanics

$$\boldsymbol{p} \rightarrow -i\hbar \nabla_{\boldsymbol{r}}$$

so it is plausible that

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

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

But also ill-defined

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

Theory of electric polarization

Resta, 1992:

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

King-Smith and Vanderbilt, 1993:

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

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

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

Simplify: 1 band, 1D

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

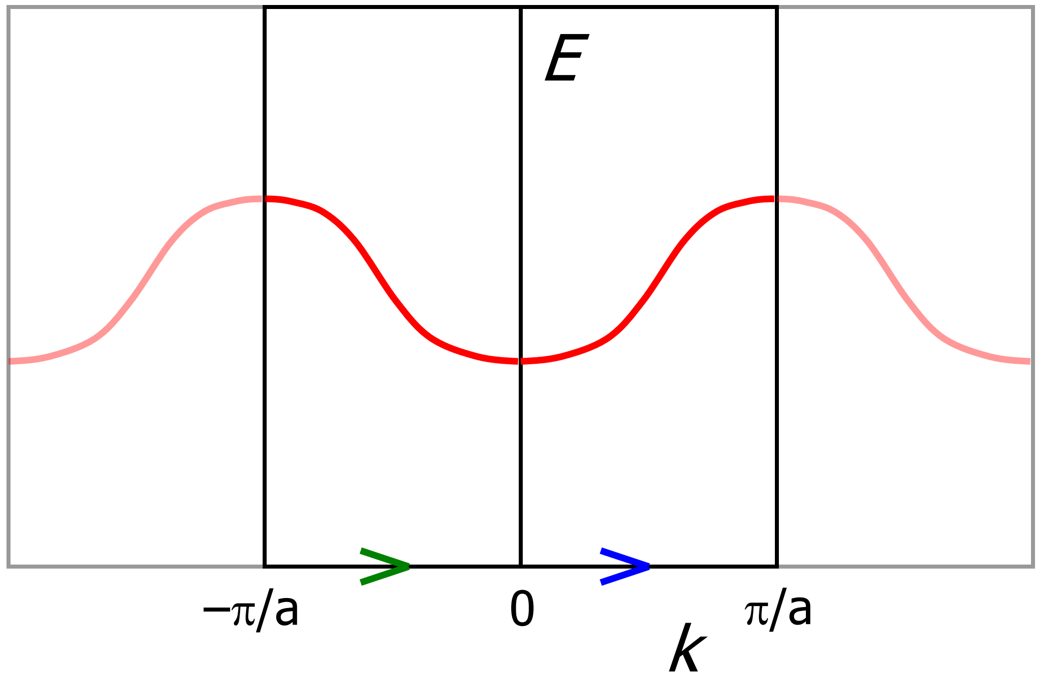
Heuristically, $x \Leftrightarrow i\dfrac{d}{dk}$ (Compare $p \Leftrightarrow -i\hbar\dfrac{d}{dx}$)

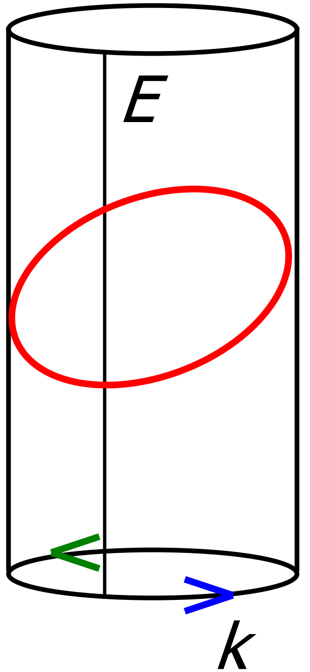
$$\mathbf{P} = -e\,\frac{\phi}{2\pi} \quad \text{where} \quad \phi = i \oint_C dk \, \langle u_{\mathbf{k}} | \tfrac{d}{dk} | u_{\mathbf{k}} \rangle$$

What is this?

Simplify: 1 band, 1D

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





Simplify: 1 band, 1D

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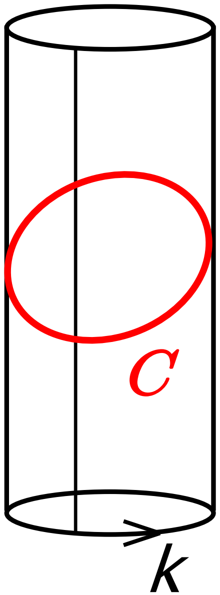
Heuristically, $x \Leftrightarrow i\dfrac{d}{dk}$ (Compare $p \Leftrightarrow -i\hbar\dfrac{d}{dx}$)

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



This is a Berry phase!

Relation to Wannier functions

Centers of Wannier functions:

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

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

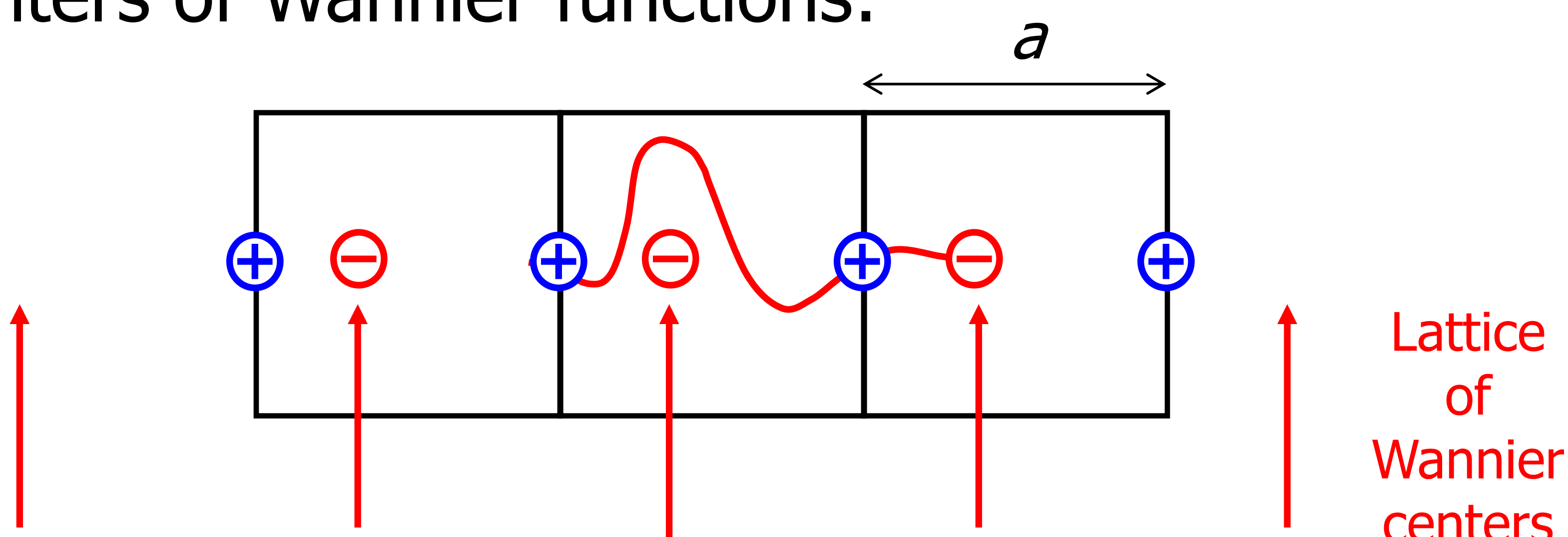
$$\mathbf{r}\,|\, w_0\rangle = \frac{V}{(2\pi)^3} \int_{\mathrm{BZ}} d\mathbf{k}\; \left(-\, i\nabla_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{r}} \right) |u_{\mathbf{k}}\rangle$$

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

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

Berry phases $\leftrightarrow$ Wannier centers

Centers of Wannier functions:

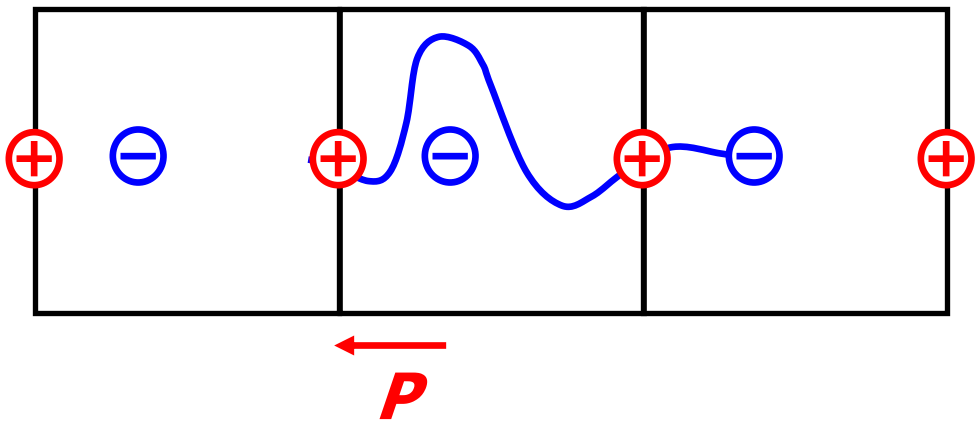


$$\langle w_n|x|w_n\rangle = \langle w_n|x|w_n\rangle \; _{nk}|\, i\frac{d}{dk}\,|u_{nk}\rangle\, dk$$

$$\langle w_n|x|w_n\rangle = \frac{a}{2\pi}\,\phi_n$$

Polarization $\leftrightarrow$ Wannier centers

Centers of Wannier functions:

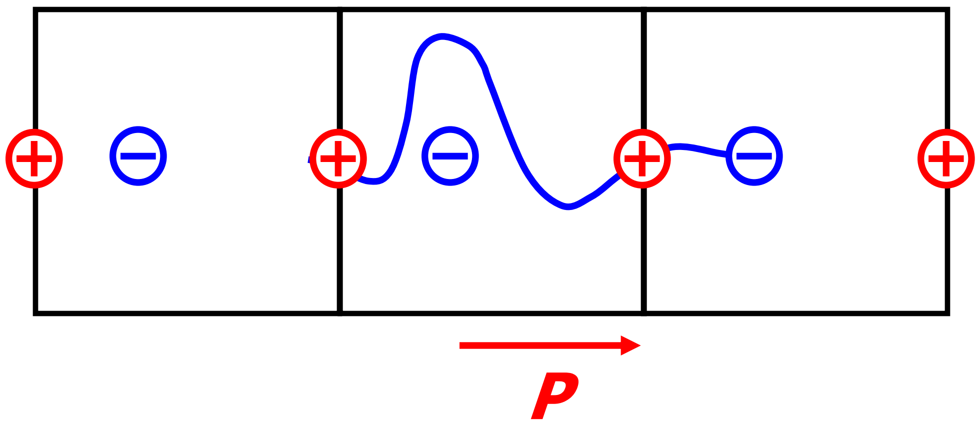


$$\boxed{\mathbf{P} = \frac{ie}{(2\pi)^3} \sum_n \int_{\mathrm{BZ}} d^3k \, \langle u_{nk} | \nabla_{\mathbf{k}} | u_{nk} \rangle}$$

as before !!

Polarization ↔ Wannier centers

Centers of Wannier functions:

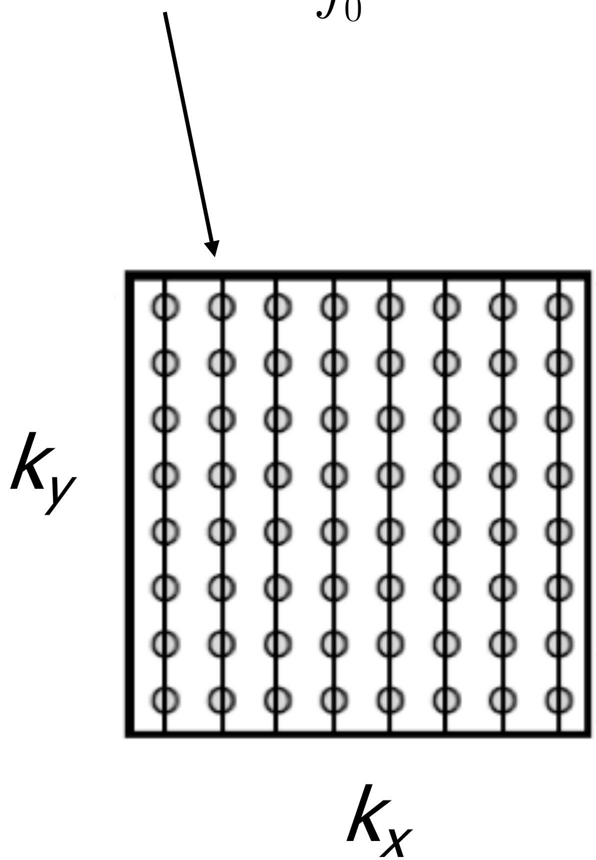


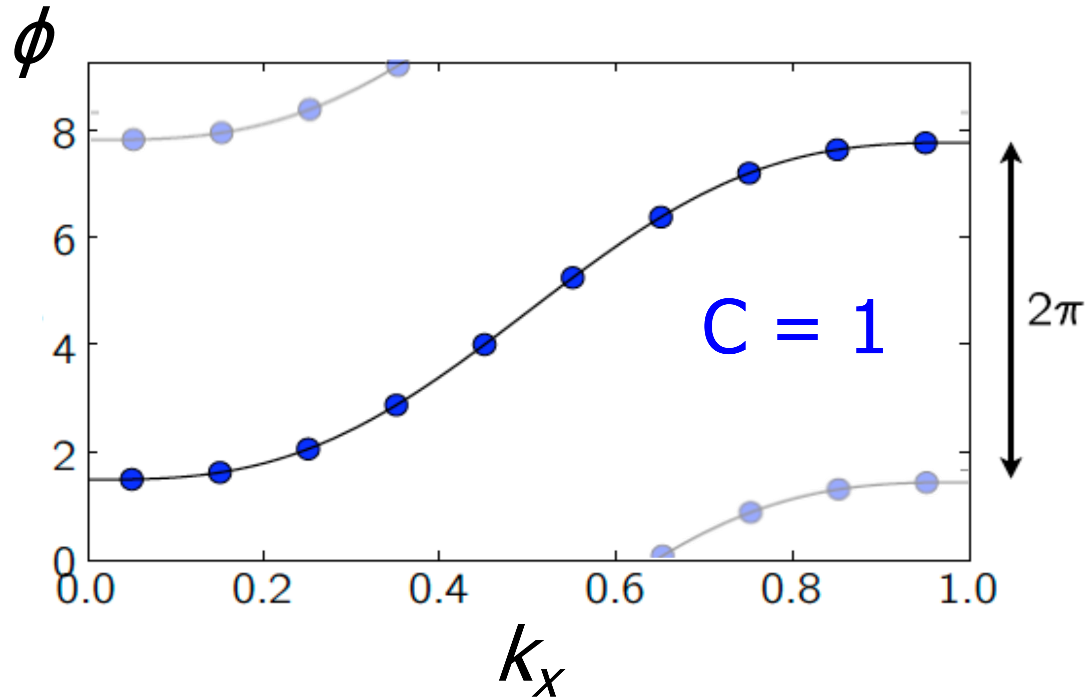
$$\boxed{\mathbf{P} = \frac{ie}{(2\pi)^3} \sum_n \int_{\mathrm{BZ}} d^3k \, \langle u_{nk} | \nabla_{\mathbf{k}} | u_{nk} \rangle}$$

as before !!

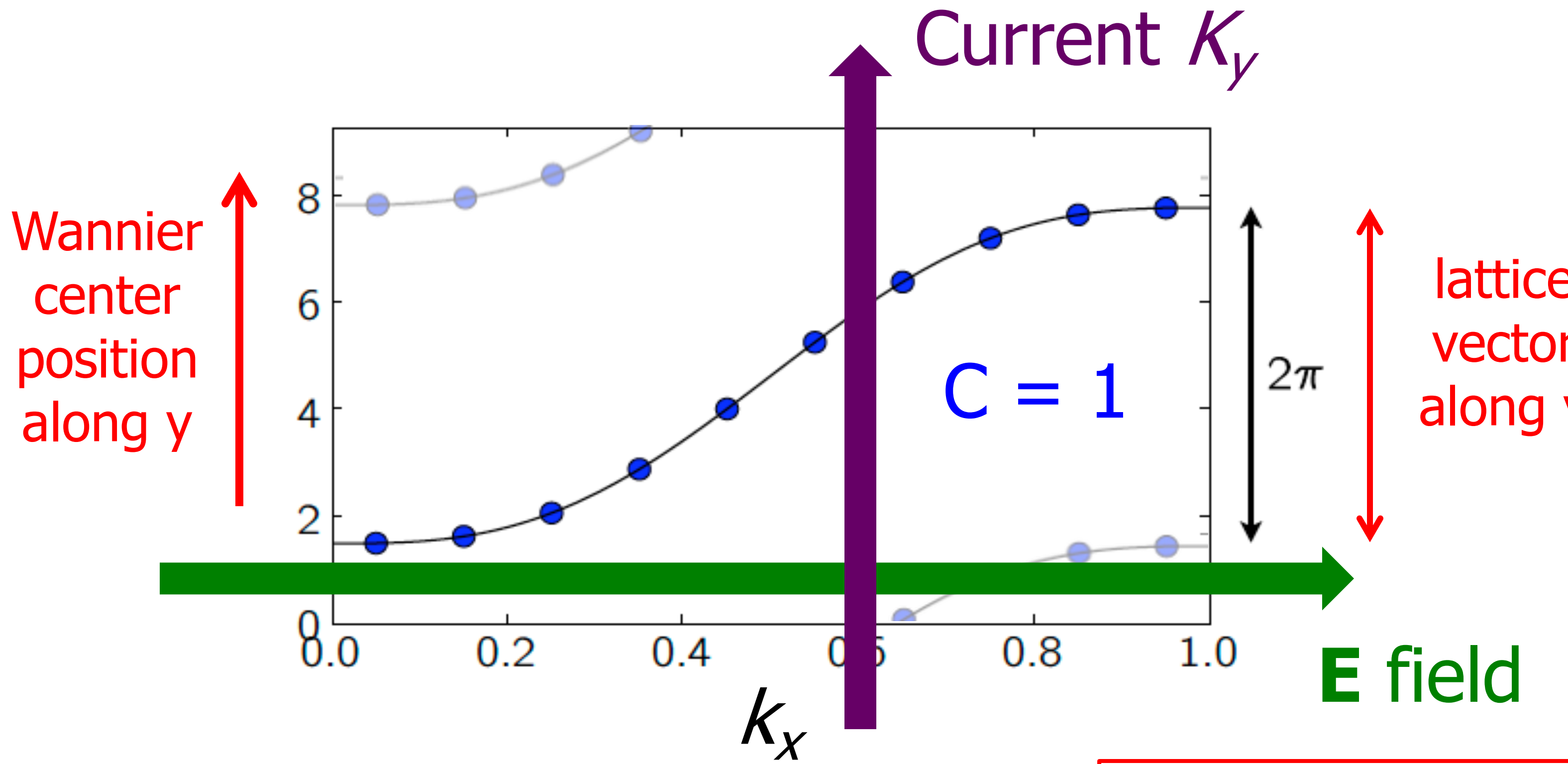
Reprise: Quantum anomalous Hall

$$\phi_y(k_x) = \int_0^{2\pi/b} dk_y \; A_y(k_x, k_y)$$





Reprise: Quantum anomalous Hall



$$\sigma_{yx} = \frac{e^2}{h} C$$

Outline

- Wannier functions for occupied subspace
  - Electric polarization
  - **Topological obstruction**
- Wannier functions as a basis
  - Wannier interpolation
- Orbital magnetoelectric coupling
  - Axion electrodynamics

Maximally localized Wannier functions

H eigenstates (Bloch)

$$|\widetilde{\psi}_{j\mathbf{k}}\rangle = \sum_n U_{nj}(\mathbf{k})\,|\psi_{n\mathbf{k}}\rangle$$

Pseudo-Bloch (smooth in k)

Variable unitary matrices

$$|w_{\mathbf{R},n}\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\, e^{-i\mathbf{k}\cdot\mathbf{R}}\,|\widetilde{\psi}_{n\mathbf{k}}\rangle$$

Wannier functions (LMO's)

Wannier functions in home unit cell $\rightarrow$ $|w_n\rangle = |w_{0,n}\rangle$

Minimize $\Omega = \sum_n \left[\langle w_n|r^2|w_n\rangle - |\langle w_n|\mathbf{r}|w_n\rangle|^2\right]$

Maximally localized Wannier functions

H eigenstates (Bloch)

$$|\widetilde{\psi}_{j\mathbf{k}}\rangle = \sum_n U_{nj}(\mathbf{k})\,|\psi_{n\mathbf{k}}\rangle$$

Pseudo-Bloch (smooth in k)

For topological states, it may be impossible to choose such unitary matrices

$$|w_{\mathbf{R},n}\rangle = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\, e^{-i\mathbf{k}\cdot\mathbf{R}}\,|\widetilde{\psi}_{n\mathbf{k}}\rangle$$

Wannier functions (LMO's)

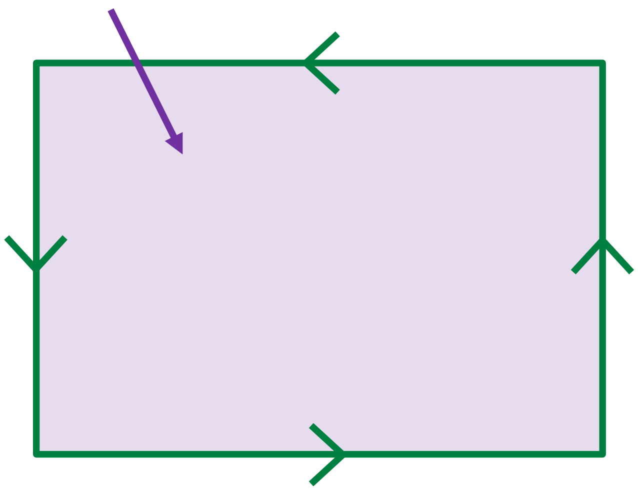
Wannier functions in home unit cell $\rightarrow$ $|w_n\rangle = |w_{0,n}\rangle$

Minimize $\Omega = \sum_n \left[\langle w_n|r^2|w_n\rangle - |\langle w_n|\mathbf{r}|w_n\rangle|^2\right]$

Example: 2D QAH insulator

Berry potential ("gauge field") $\mathbf{A}(\mathbf{k}) = \langle u_{n\mathbf{k}} | i\nabla_{\mathbf{k}} | u_{n\mathbf{k}} \rangle$

$\mathbf{A}(\mathbf{k})$ smooth and continuous



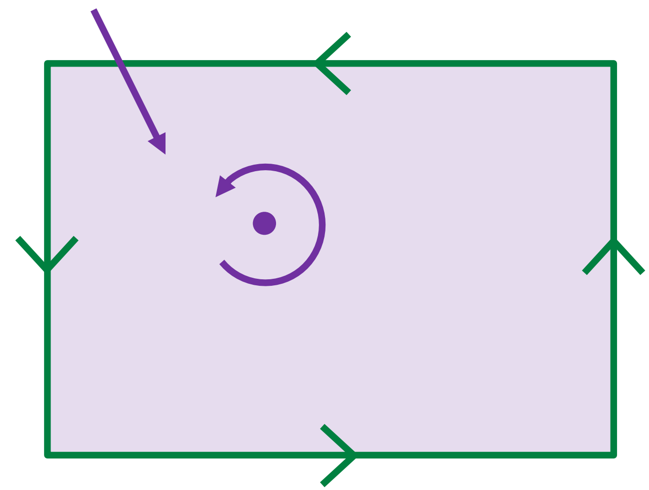
Boundary Berry phase = 2π

Not a periodic gauge

Cannot construct WFS

OR

$\mathbf{A}(\mathbf{k})$ has vortex in interior



Boundary Berry phase = 0

Not a smooth gauge

Cannot construct WFs

Topological obstruction

<u>Conclusion</u>

- Exponentially localized Wannier functions do not exist for QAH insulator

<u>Other examples</u>

- For TR-invariant strong topological insulator (e.g., Bi_2Se_3), it is not possible to choose WFs in a way that respects TR symmetry
- For crystalline topological insulators, it is not possible to choose WFs that respect the crystalline symmetries

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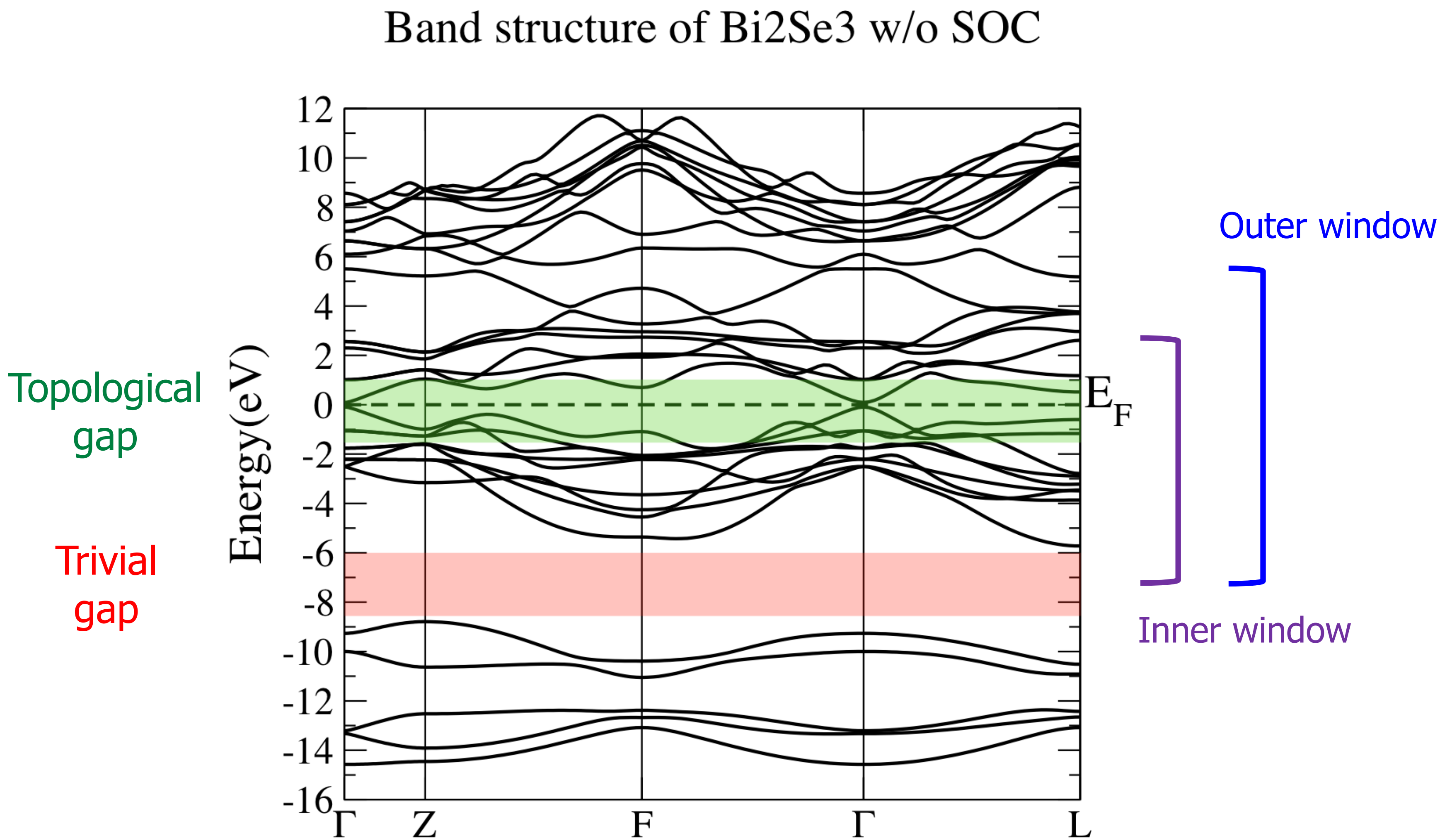
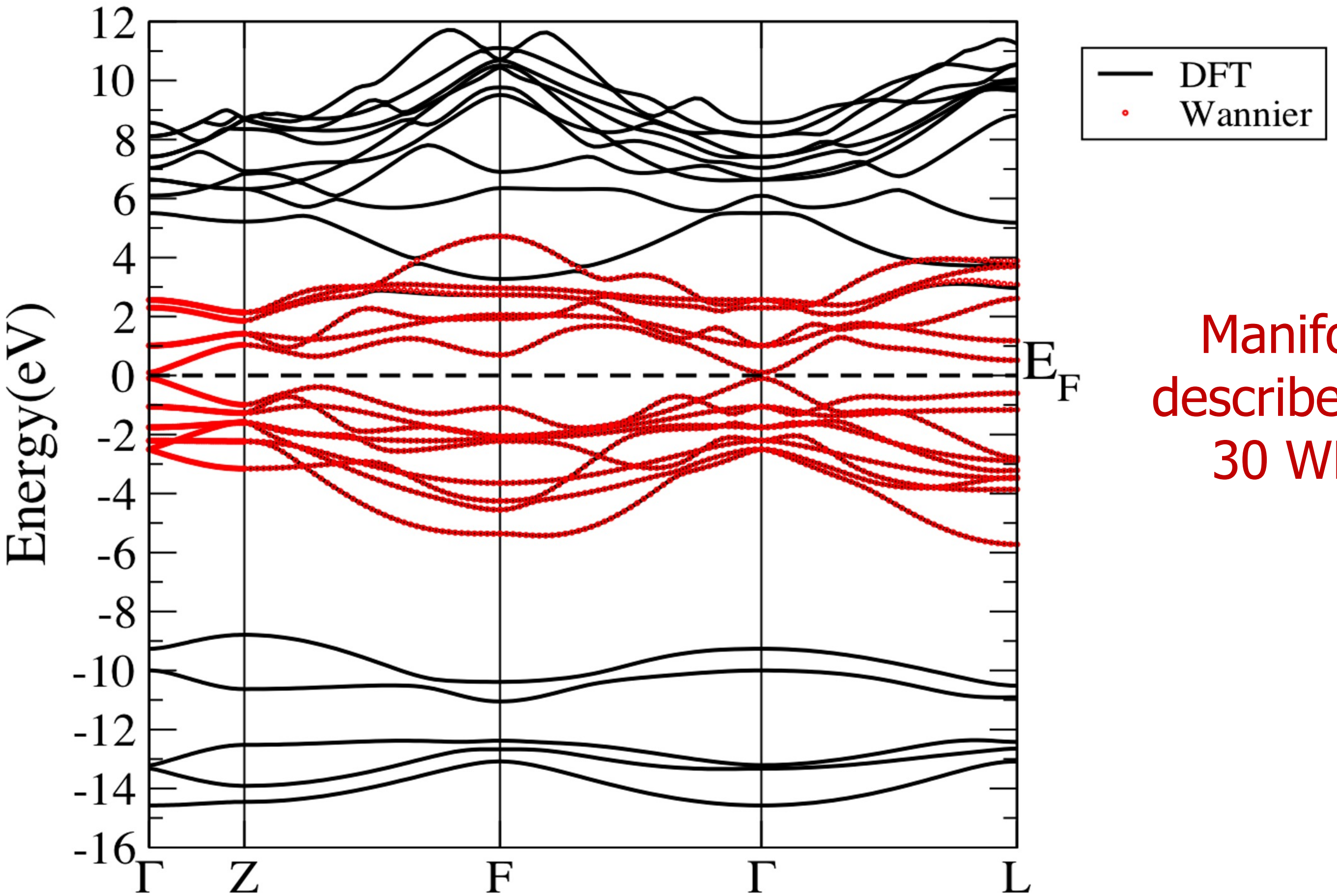
Wannier disentangling



From WannierTools Documentation

Wannier disentangling

Band structure of Bi2Se3 w/o SOC



Manifold described by 30 WFs

Wannier interpolation

- Setup N x N x N supercell
- Compute

$$\langle w_{0n}|H|w_{Rm}\rangle$$
$$\langle w_{0n}|x|w_{Rm}\rangle$$
$$\langle w_{0n}|y|w_{Rm}\rangle$$
$$\langle w_{0n}|z|w_{Rm}\rangle$$

- Up to some radius r_{cut} , $r_{cut} < Na/2$
- Solve this "tight binding" model

Wannier interpolation

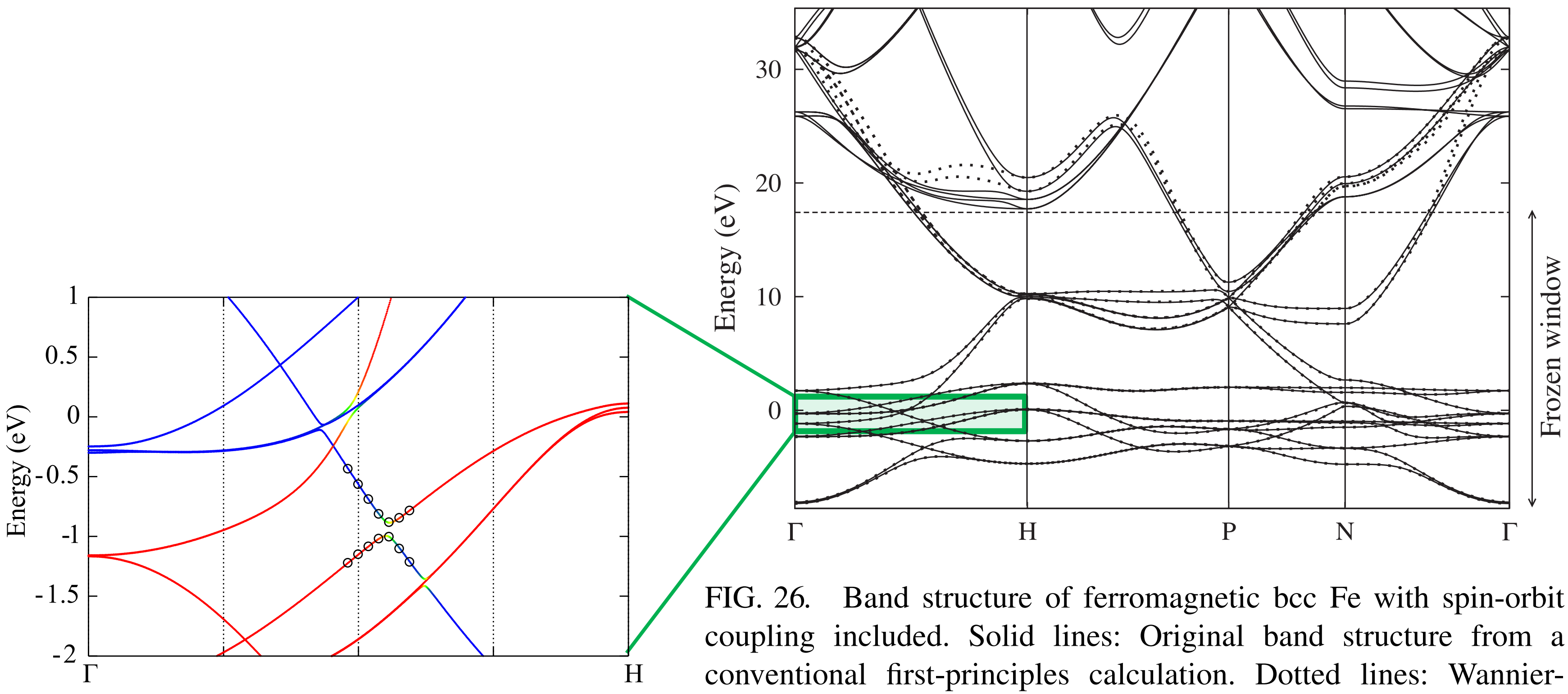


FIG. 26. Band structure of ferromagnetic bcc Fe with spin-orbit coupling included. Solid lines: Original band structure from a conventional first-principles calculation. Dotted lines: Wannier-interpolated band structure. The zero of energy is the Fermi level. From Wang *et al.*, 2006.

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Dropped for time

- ~~**Orbital magnetoelectric coupling**~~
  - **Axion electrodynamics**

Theory of magnetoelectric axion angle θ

"geometrical" = "axion" = "Chern-Simons" piece

$$\boxed{\alpha_{ij} = \frac{e^2}{h}\frac{\theta}{2\pi}\delta_{ij}}$$

(***E*•*B*** term in Lagrangian)

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

Berry connection $A_{a,nm} = i\,\langle u_{n\mathbf{k}}|\partial_a|u_{m\mathbf{k}}\rangle$

*Qi, Hughes and Zhang, PRB **78**, 195424 (2008)*
*Essin, Moore and Vanderbilt, PRL **120**, 146805 (2009)*

Axion electrodynamics

Maxwell equations:

$$\nabla \cdot \mathcal{E} = 4\pi \left(\rho_{\mathrm{f}} + \rho_{\mathrm{b}}\right)$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathcal{E} = -\frac{1}{c}\,\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\left(\mathbf{J}_{\mathrm{f}} + \mathbf{J}_{\mathrm{b}} + \mathbf{J}_{\mathrm{p}}\right) + \frac{1}{c}\,\frac{\partial \mathcal{E}}{\partial t}$$

$$\boxed{\begin{aligned} \rho_{\mathrm{b}} &= -\nabla \cdot \mathbf{P}\,, \\ \mathbf{J}_{\mathrm{b}} &= \nabla \times \mathbf{M}\,, \\ \mathbf{J}_{\mathrm{p}} &= \frac{\partial \mathbf{P}}{\partial t} \end{aligned}}$$

Separate out magnetoelectric part:

$$\mathbf{P} = \mathbf{P}_0 + \alpha\,\mathbf{B}\,,$$

$$\mathbf{M} = \mathbf{M}_0 + \alpha\,\mathcal{E}\,,$$

Axion electrodynamics

Maxwell equations:

$$\nabla \cdot \mathcal{E} = 4\pi \left(\rho_{\mathrm{f}} + \tilde{\rho}_{\mathrm{b}} - (\nabla\alpha)\cdot\mathbf{B}\right)$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathcal{E} = -\frac{1}{c}\,\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\left(\mathbf{J}_{\mathrm{f}} + \tilde{\mathbf{J}}_{\mathrm{b}} + \tilde{\mathbf{J}}_{\mathrm{p}} + c\,(\nabla\alpha)\times\mathcal{E} + \frac{\partial\alpha}{\partial t}\mathbf{B}\right) + \frac{1}{c}\,\frac{\partial\mathcal{E}}{\partial t}$$

$$\boxed{\begin{aligned} \tilde{\rho}_{\mathrm{b}} &= -\nabla\cdot\mathbf{P}_0 \\ \tilde{\mathbf{J}}_{\mathrm{b}} &= \nabla\times\mathbf{M}_0 \\ \tilde{\mathbf{J}}_{\mathrm{p}} &= \partial\mathbf{P}_0/\partial t \end{aligned}}$$

Separate out magnetoelectric part:

$$\mathbf{P} = \mathbf{P}_0 + \alpha\,\mathbf{B}\,,$$

$$\mathbf{M} = \mathbf{M}_0 + \alpha\,\mathcal{E}\,,$$

Axion electrodynamics

Maxwell equations:

$$\nabla \cdot \mathcal{E} = 4\pi \left(\rho_{\mathrm{f}} + \tilde{\rho}_{\mathrm{b}} - (\nabla\alpha) \cdot \mathbf{B}\right)$$

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$$\nabla \times \mathcal{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\left(\mathbf{J}_{\mathrm{f}} + \tilde{\mathbf{J}}_{\mathrm{b}} + \tilde{\mathbf{J}}_{\mathrm{p}} + c\,(\nabla\alpha) \times \mathcal{E} + \frac{\partial \alpha}{\partial t}\mathbf{B}\right) + \frac{1}{c}\frac{\partial \mathcal{E}}{\partial t}$$

In absence of **B**

$$\boxed{\begin{aligned} \tilde{\rho}_{\mathrm{b}} &= -\nabla \cdot \mathbf{P}_0 \\ \tilde{\mathbf{J}}_{\mathrm{b}} &= \nabla \times \mathbf{M}_0 \\ \tilde{\mathbf{J}}_{\mathrm{p}} &= \partial \mathbf{P}_0/\partial t \end{aligned}}$$

$$\boxed{\alpha(\mathbf{r}, t) = \frac{e^2}{2\pi hc}\,\theta(\mathbf{r}, t)}$$

Only spatial and time derivatives of θ enter field equations !

Axion electrodynamics

Equations of motion of fields

$$\boxed{\alpha(\mathbf{r},t) = \frac{e^2}{2\pi hc}\,\theta(\mathbf{r},t)}$$

$$\nabla \cdot \mathcal{E} = 4\pi\left(\rho_{\mathrm{f}} + \tilde{\rho}_{\mathrm{b}} - (\nabla\alpha)\cdot\mathbf{B}\right)$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathcal{E} = -\frac{1}{c}\,\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \frac{4\pi}{c}\left(\mathbf{J}_{\mathrm{f}} + \tilde{\mathbf{J}}_{\mathrm{b}} + \tilde{\mathbf{J}}_{\mathrm{p}} + c\,(\nabla\alpha)\times\mathcal{E} + \frac{\partial\alpha}{\partial t}\mathbf{B}\right) + \frac{1}{c}\,\frac{\partial \mathcal{E}}{\partial t}$$

Equations of motion of electrons

$$\left(1 + \frac{e}{\hbar c}\mathbf{B}\cdot\mathbf{\Omega}\right)\dot{\mathbf{r}} = \mathbf{v}_{\mathrm{g}} + \frac{e}{\hbar}\,\mathcal{E}\times\mathbf{\Omega} + \frac{e}{\hbar c}\,(\mathbf{v}_{\mathrm{g}}\cdot\mathbf{\Omega})\,\mathbf{B}\,,$$

$$\left(1 + \frac{e}{\hbar c}\mathbf{B}\cdot\mathbf{\Omega}\right)\dot{\mathbf{k}} = -\frac{e}{\hbar}\mathcal{E} - \frac{e}{\hbar c}\mathbf{v}_{\mathrm{g}}\times\mathbf{B} - \frac{e^2}{\hbar^2 c}\,(\mathcal{E}\cdot\mathbf{B})\,\mathbf{\Omega}\,.$$

Summary

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Slides available at https://is.gd/inFID2