Wannier functions, Modern theory of polarization

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Overview

- Reminder: Bloch functions, periodic boundary condition
- Wannier functions: introduction
- Maximally localized Wannier functions
- Modern theory of polarization
- Polarization and Wannier centers
- Calculation of Berry phase in discrete k space
- Position operator and periodic boundary conditions
- Calculation of Wannier centers in 1D systems

Bloch functions, periodic boundary condition

We want to describe the "bulk" properties of crystalline materials.
In non-interacting approximation:

$$\hat{H} = \sum_{i=1}^{N_e} \left(\frac{\hat{p}_i^2}{2m_e} + U(\mathbf{r}_i) \right)$$

$U(\mathbf{r}) = U(\mathbf{r} + \mathbf{R}_n)$ is lattice-periodic potential, $\mathbf{R}_n$ lattice vector.

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$\Rightarrow$ Hamiltonian is a sum of single-particle Hamiltonians, the solution of this N_e electron problem can be obtained using the solutions of the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m_e} \nabla^2 + U(\mathbf{r}) \right] \Psi_i(\mathbf{r}) = E_i \Psi_i(\mathbf{r})$$

Bloch functions, periodic boundary condition

In order to capture the translational invariance of the bulk, we use use periodic boundary condition $\Rightarrow$ the solutions satisfy (Bloch theorem)

$$\Psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_m) = e^{i\mathbf{k}\cdot\mathbf{R_m}}\Psi_{\mathbf{k}}(\mathbf{r})$$

wavevector $\mathbf{k}$ can take on discrete values in the Brillouin zone

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Equivalent formulation:

$$\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$$

where $u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}_m) = u_{\mathbf{k}}(\mathbf{r})$ lattice periodic and

$$\left[\frac{(\hat{p}+\hbar\mathbf{k})^2}{2m_e} + U(\mathbf{r})\right] u_{n,\mathbf{k}}(\mathbf{r}) = E_{n,\mathbf{k}}u_{n,\mathbf{k}}(\mathbf{r})$$

Bloch functions, periodic boundary condition

For equivalent wavenumber vectors $\mathbf{k}' = \mathbf{k} + \mathbf{G}$ ($\mathbf{G}$ lattice vector of the reciprocal lattice)

$$\Psi_{n,\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) = e^{i(\mathbf{k}'-\mathbf{G})\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}'\cdot\mathbf{r}} u_{n\mathbf{k}'}(\mathbf{r})$$

where $u_{n\mathbf{k}'}(\mathbf{r}) = u_{n\mathbf{k}+\mathbf{G}}(\mathbf{r}) = e^{-i\mathbf{G}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$.

One can also show that $E_{n\mathbf{k}+\mathbf{G}} = E_{n\mathbf{k}}$.

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Wannier functions

Since

$$\Psi_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r}) = e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} u_{n,\mathbf{k}+\mathbf{G}} = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}} = \Psi_{n,\mathbf{k}}(\mathbf{r})$$

for fixed $\mathbf{r}$ the Bloch function $\Psi_{n,\mathbf{k}}(\mathbf{r})$ is periodic in the reciprocal space.

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$\Rightarrow$ it can be expanded into a Fourier series:

$$\Psi_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_j} \Phi_n(\mathbf{r}, \mathbf{R}_j) e^{i\mathbf{k}\cdot\mathbf{R}_j}$$

$\mathbf{R}_j$: Lattice vectors in real space

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$\mathbf{R}_j$: Lattice vectors in real space

Reverse transformation:

$$\Phi_n(\mathbf{r}, \mathbf{R}_j) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in BZ} e^{-i\mathbf{k}\cdot\mathbf{R}_j} \Psi_{n,\mathbf{k}}(\mathbf{r})$$

Wannier functions

$\Phi_n(\mathbf{r}, \mathbf{R}_j)$ is a function of $\mathbf{r} - \mathbf{R}_j$:

$$\begin{aligned}
\Phi_n(\mathbf{r} + \mathbf{R}_n, \mathbf{R}_j + \mathbf{R}_n) &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in Bz} e^{-i\mathbf{k}\cdot(\mathbf{R}_j + \mathbf{R}_n)} \psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}_n) \\
&= \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in BZ} e^{-i\mathbf{k}\cdot(\mathbf{R}_j + \mathbf{R}_n)} e^{i\mathbf{k}\cdot\mathbf{R}_n} \psi_{n\mathbf{k}}(\mathbf{r}) \\
&= \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in BZ} e^{-i\mathbf{k}\cdot\mathbf{R}_j} \psi_{n\mathbf{k}}(\mathbf{r}) \\
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For $\mathbf{R}_n = -\mathbf{R}_j$: $\Phi_n(\mathbf{r}, \mathbf{R}_j) = \Phi_n(\mathbf{r} - \mathbf{R}_j, 0)$ it depends only on $\mathbf{r} - \mathbf{R}_j$

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$$\Phi_n(\mathbf{r} - \mathbf{R}_j, 0) = W_n(\mathbf{r} - \mathbf{R}_j) \text{ are Wannier functions}$$

(See, e.g., Ref[5]).

Wannier functions

Orthonormality and completeness:
Bloch functions:

$$\int \Psi^*_{n,\mathbf{k}}(\mathbf{r})\Psi_{n',\mathbf{k}'}(\mathbf{r})d\mathbf{r} = \delta_{n,n'}\delta_{\mathbf{k},\mathbf{k}'}$$

$$\sum_{n,\mathbf{k}} \Psi^*_{n,\mathbf{k}}(\mathbf{r})\Psi_{n,\mathbf{k}}(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$$

Wannnier functions

$$\int W^*_n(\mathbf{r}-\mathbf{R}_j)W_{n'}(\mathbf{r}-\mathbf{R}_{j'})d\mathbf{r} = \delta_{\mathbf{R}_j,\mathbf{R}_{j'}}\delta_{n,n'}$$

$$\sum_{n,\mathbf{R}_j} W^*_n(\mathbf{r}-\mathbf{R}_j)W_n(\mathbf{r}-\mathbf{R}_{j'}) = \delta(\mathbf{r}-\mathbf{r}')$$

(See, e.g., Ref[5]).

Wannier centers

Define the Wannier center of $W_n(\mathbf{r} - \mathbf{R}_j)$ as

$$\bar{\mathbf{r}}_n^{(j)} = \langle W_n(\mathbf{r} - \mathbf{R}_j)|\mathbf{r}|W_n(\mathbf{r} - \mathbf{R}_j)\rangle$$

In general, a non-trivial question if the the above expectation value is finite in extended systems

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In general, a non-trivial question if the the above expectation value is finite in extended systems $\Rightarrow$ localization properties of Wannier functions

For explicit calculation of the Wannier functions in the SSH model, see Phys. Rev. B **26**, 4269 (2016).

Wannier centers in the Rice-Mele model

Consider the Rice-Mele model (N site long, periodic boundary condition)
Bloch functions: $|\Psi_n(k)\rangle = |k\rangle \otimes |u_n(k)\rangle$

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Position operator:

$$\hat{x} = \sum_{m=1}^{N} m \left(|m, A\rangle\langle m, A| + |m, B\rangle\langle m, B| \right)$$

m: unit cell index; A, B, site index in a unit cell

Wannier centers in the Rice-Mele model

$$
\begin{aligned}
\hat{x}W_n(j) &= \hat{x}\frac{1}{\sqrt{N}}\sum_{k_x} e^{-ijk_x}|\Psi_n(k_x)\rangle \\
&= \frac{1}{\sqrt{N}}\sum_{k_x} e^{-ijk_x}\hat{x}\frac{1}{\sqrt{N}}\sum_{l}^{N} e^{ilk_x}|l\rangle \otimes |u_n(k_x)\rangle \\
&= \frac{1}{N}\sum_{k_x} e^{-ijk_x}\sum_{m} m e^{imk_x}|m\rangle \otimes |u_n(k_x)\rangle
\end{aligned}
$$

Wannier centers in the Rice-Mele model

For $N \to \infty$ k_x continous, use partial integration:

$$\begin{aligned}
\hat{x} W_n(j) &= \frac{1}{2\pi} \int_0^{2\pi} dk_x e^{-ijk_x} \sum_m m e^{imk_x} |m\rangle \otimes |u_n(k_x)\rangle \\
&= \frac{1}{2\pi}(-i) \int_0^{2\pi} dk_x \frac{\partial}{\partial k_x} \sum_m e^{i(m-j)k_x} |m\rangle \otimes |u_n(k_x)\rangle \\
&+ \frac{1}{2\pi} \int_0^{2\pi} dk_x \, j \, e^{-ijk_x} \sum_m |m\rangle \otimes |u_n(k_x)\rangle \\
&+ \frac{i}{2\pi} \int_0^{2\pi} dk_x \sum_m |m\rangle \otimes \frac{\partial}{\partial k_x} |u_n(k_x)\rangle
\end{aligned}$$

Wannier centers in the Rice-Mele model

This can be simplified:

$$\begin{aligned}
\hat{x} W_n(j) &= \left(\frac{-i}{2\pi} \sum_m e^{i(m-j)k_x} |m\rangle \otimes |u_n(k_x)\rangle \right) \Bigg|_0^{2\pi} \\
&+ \frac{j}{2\pi} \int_0^{2\pi} dk_x e^{-ijk_x} \sum_m |m\rangle \otimes |u_n(k_x)\rangle \\
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&+ \frac{j}{2\pi} \int_0^{2\pi} dk_x e^{-ijk_x} \sum_m |m\rangle \otimes |u_n(k_x)\rangle = j \cdot W_n(j) \\
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\end{aligned}$$

One finds:

$$\langle W_n(j)|\hat{x}|W_n(j)\rangle = \frac{i}{2\pi} \int_0^{2\pi} dk_x \langle u_n(k_x)|\partial_{k_x}|u_n(k_x)\rangle + j$$

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$$+ \frac{j}{2\pi} \int_0^{2\pi} dk_x e^{-ijk_x} \sum_m |m\rangle \otimes |u_n(k_x)\rangle = j \cdot W_n(j)$$

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$\Rightarrow$ can be expressed in terms of Berry-phase (Zak's phase)

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$\Rightarrow$ Wannier centers are equally spaced

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Maximally localized Warnier functions

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Maximally localized generalized Wannier functions for composite energy bands

Nicola Marzari and David Vanderbilt
Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08855-0849
(Received 10 July 1997)

We discuss a method for determining the optimally localized set of generalized Wannier functions associated with a set of Bloch bands in a crystalline solid. By ''generalized Wannier functions'' we mean a set of localized orthonormal orbitals spanning the same space as the specified set of Bloch bands. Although we minimize a functional that represents the total spread $\Sigma_n \langle r^2 \rangle_n - \langle \mathbf{r} \rangle_n^2$ of the Wannier functions in real space, our method proceeds directly from the Bloch functions as represented on a mesh of k points, and carries out the minimization in a space of unitary matrices $U_{mn}^{(\mathbf{k})}$ describing the rotation among the Bloch bands at each k point. The method is thus suitable for use in connection with conventional electronic-structure codes. The procedure also returns the total electric polarization as well as the location of each Wannier center. Sample results for Si, GaAs, molecular C_2H_4, and LiCl will be presented. [S0163-1829(97)02944-5]

Figure: Phys Rev B **56**, 12847 (1997).

Maximally localized Warnier functions

Gauge freedom in choosing the Bloch orbitals: $\Psi_{n\mathbf{k}}(\mathbf{r}) \rightarrow e^{i\phi_n(\mathbf{k})}\Psi_{n\mathbf{k}}(\mathbf{r})$ $[u_{n\mathbf{k}}(\mathbf{r}) \rightarrow e^{i\phi_n(\mathbf{k})}u_{n\mathbf{k}}(\mathbf{r})]$ describes the same electron density

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$\Rightarrow$ Wannier functions are not unique!

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$\rightarrow$ not sufficient to consider isolated bands $\rightarrow$ consider a set of J bands (composite bands)

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If there are band degeneracies for some $\mathbf{k}$ (symmetries, e.g., time reversal):
$\rightarrow$ not sufficient to consider isolated bands $\rightarrow$ consider a set of J bands (composite bands)
A more general $U(J)$ gauge freedom:

$$u_{n\mathbf{k}}(\mathbf{r}) \rightarrow \sum_p U^{(\mathbf{k})}_{pn} u_{p\mathbf{k}}(\mathbf{r})$$

Maximally localized Warnier functions (MLWF)

Define for the Wannier functions at the origin $\mathbf{R}_j = 0$ the following:

1. Wannier center $\bar{\mathbf{r}}_n = \langle W_n(\mathbf{r})|\mathbf{r}|W_n(\mathbf{r})\rangle$
2. second moment $\langle r^2\rangle_n = \langle W_n(\mathbf{r})|r^2|W_n(\mathbf{r})\rangle$

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A measure of the spread (delocalization) of the Wannier functions:

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

One can then try to minimize Ω with respect to the unitary transformations $U_{pn}^{(\mathbf{k})} \Rightarrow$ Maximally localized Wannier functions (MLWF)

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This approach can be used to obtain MLWFs from DFT calculations in plane-wave basis.

Maximally localized Warnier functions (MLWF)

One can decompose $\Omega = \Omega_1 + \Omega_2$, where

$$\Omega_1 = \sum_n \left[\langle r^2 \rangle_n - \sum_{\mathbf{R},m} |\langle \mathbf{R}m|\mathbf{r}|\mathbf{0}n\rangle|^2 \right]$$

$$\Omega_2 = \sum_n \sum_{\mathbf{R}m \neq \mathbf{0}n} |\langle \mathbf{R}m|\mathbf{r}|\mathbf{0}n\rangle|^2$$

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$$\Omega_1 = \sum_n \left[\langle r^2 \rangle_n - \sum_{\mathbf{R},m} |\langle \mathbf{R}m|\mathbf{r}|\mathbf{0}n\rangle|^2 \right]$$

$$\Omega_2 = \sum_n \sum_{\mathbf{R}m \neq \mathbf{0}n} |\langle \mathbf{R}m|\mathbf{r}|\mathbf{0}n\rangle|^2$$

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$\Rightarrow$ minimalization of Ω means minimalization of Ω_2

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Argument does not work in 3D, because $P\,\hat{x}\,P$, $P\,\hat{y}\,P$, $P\,\hat{z}\,P$ do not commmute

Summary I

- bulk properties of materials $\rightarrow$ periodic boundary conditions $\rightarrow$ Bloch functions
- alternative description: Wannier functions
- Wannier-centers (expectation value of the position operator): in Rice-Mele model $\rightarrow$ Berry-phase
- Maximally localized Wannier functions: in 1D eigenfunctions of the projected position operator $P\hat{x}P$

Overview

- Reminder: Bloch functions, periodic boundary condition
- Wannier functions: introduction
- Maximally localized Wannier functions
- Modern theory of polarization
- Polarization and Wannier centers
- Calculation of Berry phase in discrete k space
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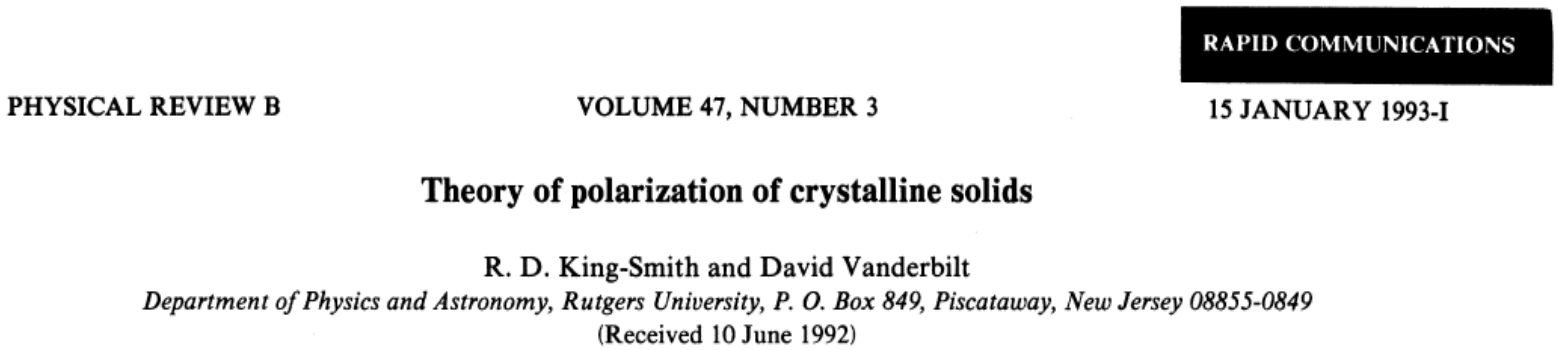
Modern theory of polarization



RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 47, NUMBER 3 15 JANUARY 1993-I

Theory of polarization of crystalline solids

R. D. King-Smith and David Vanderbilt
Department of Physics and Astronomy, Rutgers University, P. O. Box 849, Piscataway, New Jersey 08855-0849
(Received 10 June 1992)

Theory of Polarization: A Modern Approach

Raffaele Resta[1] and David Vanderbilt[2]

Figure: Theory of Polarization: A Modern Approach," in *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)

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Macroscopic polarization **P**: fundamental concept in the phenomenological description of dielectrics

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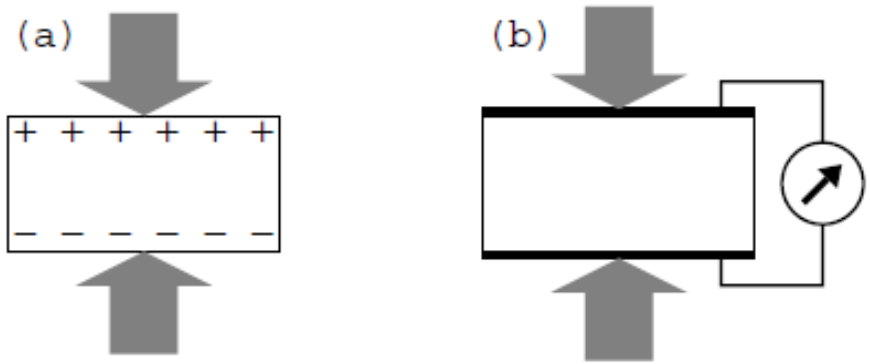

Figure: Pieozoelectricity: surface or bulk effect? (Figure from Ref[4]).

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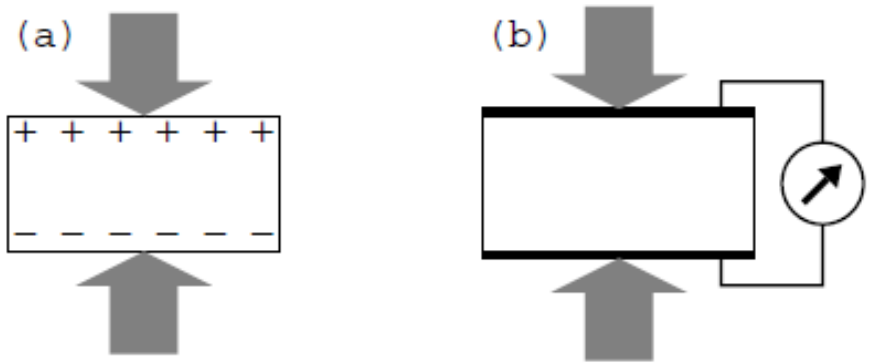

Figure: Pieozoelectricity: surface or bulk effect? (Figure from Ref[4]).

While the crystal is strained, a transient electrical current flows through the sample

Modern theory of polarization

Fundamental relation: the change in polarization $\mathbf{P}$ is accompanied with a transient current $\mathbf{j}(t)$ flowing through the sample:

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Assumptions:

- system remains insulating for all values of λ
- system bulk retains crystalline periodicity for all λ

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$$\left[\frac{(\hat{p} + \hbar\mathbf{k})^2}{2m_e} + U^{(\lambda)}(\mathbf{r})\right] u_{n,\mathbf{k}}^{(\lambda)}(\mathbf{r}) = E_{n,\mathbf{k}}^{(\lambda)} u_{n,\mathbf{k}}^{(\lambda)}(\mathbf{r})$$

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Adiabatic change: the current $\mathbf{j}^{(\lambda)}$ can be calculated using adiabatic perturbation theory

For a adiabatically changing time periodic 1D lattice $[H(k,t) = H(k,t+T)]$ this is done in Chapter 5 of the Lecture Notes (Ref[7])

The same steps can be done here: $t \to \lambda$, λ does not need be periodic

Formal description of the theory: current $\mathbf{j}^{(\lambda)}$

Current from a single filled band n:

$$\frac{d\mathbf{P}_n^{(\lambda)}}{d\lambda} = \mathbf{j}_n^{(\lambda)} = \frac{-ie}{(2\pi)^3} \int_{BZ} d\mathbf{k} [\langle \partial_{\mathbf{k}} u_{n,\mathbf{k}}^{(\lambda)} | \partial_\lambda u_{n,\mathbf{k}}^{(\lambda)} \rangle - \langle \partial_\lambda u_{n,\mathbf{k}}^{(\lambda)} | \partial_{\mathbf{k}} u_{n,\mathbf{k}}^{(\lambda)} \rangle]$$

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Total change in polarization ($\rightarrow$ number of pumped particles):

$$\Delta\mathbf{P} = \frac{-ie}{(2\pi)^3}\sum_{n=1}^{N}\int_{BZ} d\mathbf{k}\int_0^\lambda d\lambda[\langle\partial_{\mathbf{k}} u_{n,\mathbf{k}}^{(\lambda)}|\partial_\lambda u_{n,\mathbf{k}}^{(\lambda)}\rangle - \langle\partial_\lambda u_{n,\mathbf{k}}^{(\lambda)}|\partial_{\mathbf{k}} u_{n,\mathbf{k}}^{(\lambda)}\rangle]$$

N: number of filled bands

Polarization as Berry phase

For simplicity, consider a 1D system:

$$\Delta P = \frac{-ie}{(2\pi)} \sum_{n=1}^{N} \int_{BZ} dk \int_{0}^{\lambda} d\lambda [\langle \partial_k u_{n,k}^{(\lambda)} | \partial_\lambda u_{n,k}^{(\lambda)} \rangle - \langle \partial_\lambda u_{n,k}^{(\lambda)} | \partial_k u_{n,k}^{(\lambda)} \rangle]$$

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- partial integration with respect to λ
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Note: the total electrical polarization of any material has an ionic contribution as well (but this will not be important in the discussion of topological properties)

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In 3D: $\tilde{\mathbf{P}}_n = \mathbf{P}_n + \frac{e\mathbf{R}}{V_{cell}}$, $\mathbf{R}$ a lattice vector.

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Polarization $\sim$ sum of the Wannier centers of the occupied bands (for one given R_m)

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$$\Delta \mathbf{P}_{cyc} = \oint_0^1 d\lambda \frac{d\mathbf{P}}{d\lambda}$$

The Wannier center must return to their initial location at the end of the cyclic evolution. But this is possible in two different ways:

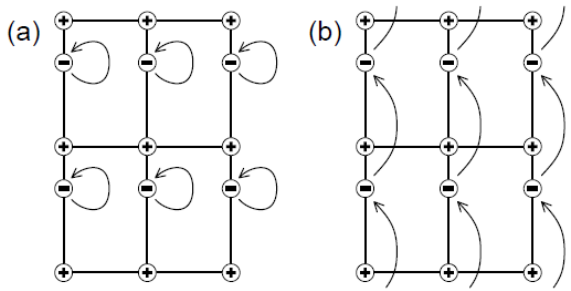

Figure: Fig.10 of "Theory of Polarization: A Modern Approach"

Tracking the Wannier centers in the Rice-Mele model

In the case of Rice-Mele model, $\lambda = t$ time, $\Rightarrow$ the adiabatic charge pumping can be visualized by tracking the Wannier centers:

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$$\langle W_n^{(t)}(j)|\hat{x}|W_n^{(t)}(j)\rangle = \frac{i}{2\pi}\int_0^{2\pi} dk_x \langle u_n^{(t)}(k_x)|\partial_{k_x}|u_n^{(t)}(k_x)\rangle + j$$

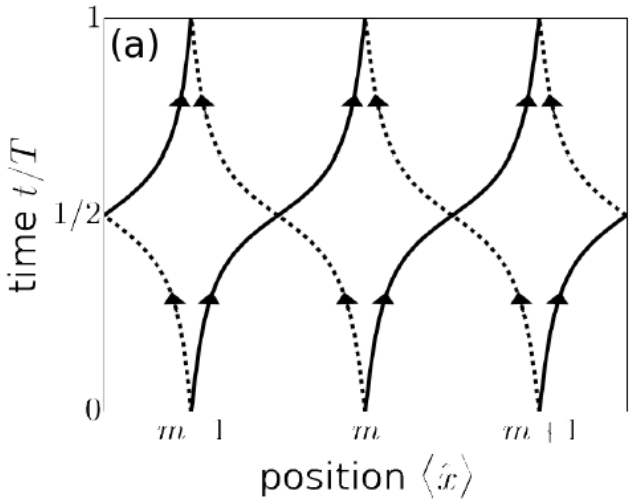

Figure: Figure 4.5(a) of the Lecture Notes. Time evolution of the Wannnier centers of the bands. Solid line: valence band, dashed line: conduction band. The Chern number is 1.

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Polarization as Berry phase: calculation in discrete **k**-space

We only consider the 1D case
$P_n^{(\lambda)} = \frac{e}{2\pi}\Phi_n^{(\lambda)}$; L length of sample

$$\Phi_n^{(\lambda)} = -\mathrm{Im}\int_{\mathrm{BZ}} \mathrm{dk}\langle \mathrm{u}_{\mathrm{n,k}}^{(\lambda)}|\partial_{\mathrm{k}}|\mathrm{u}_{\mathrm{n,k}}^{(\lambda)}\rangle$$

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Typically, we need to calculate this on a discrete grid of k-points

$$\int dk\langle u_{n,k}|\partial_k u_{n,k}\rangle dk \rightarrow \sum_{k_j} dk\langle u_{n,k}|\partial_k u_{n,k}\rangle|_{k=k_j}$$

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$$u_{n,k+dk} \approx u_{n,k} + \partial_k u_{n,k}\, dk$$

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$$\ln[\langle u_{n,k}|u_{n,k+dk}\rangle] = \ln[1 + \langle u_{n,k}|\partial_k u_{n,k}\rangle dk] \approx \langle u_{n,k}|\partial_k u_{n,k}\rangle dk$$

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Can be considered a "1D Wilson loop" for a single non-degenerate band

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A subtle issue: position operator and periodic boundary conditions

In 1D the eigenfunctions of the operator $P\hat{x}P$, where P is a projector onto a set of bands, yields a localized set of Wannier functions.
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$\Rightarrow$ We need to find a "periodic" form of $P\hat{x}P$

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Raffaele Resta [3]: if periodic boundary conditions are used, expectation values that involve the operator $\hat{x}$ should be calculated using the unitary operator

$$\hat{X} = e^{i\frac{2\pi}{L}\hat{x}}$$

L: imposed periodicity in the system

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$\Rightarrow$ to obtain well-localized Wannier functions while using periodic boundary conditions: find the eigenfunction(s) of

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Note: in general $\hat{X}_P$ is not a Hermitian operator, only for $L \to \infty$

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$P\hat{X}P$ operator in 1D lattice system

For a 1D system consisting of M unit cells:

$$\hat{x} = \sum_{m=1}^{M} \sum_{\alpha} R_m |m, \alpha\rangle\langle m, \alpha|$$

α band index, R_m labels the mth unit cell

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$$\Rightarrow \hat{X} = \sum_{m=1}^{M} \sum_{\alpha} e^{i\delta_k R_m} |m, \alpha\rangle\langle m, \alpha| \qquad \delta_k = \frac{2\pi}{Ma}$$

a: lattice constant

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&= \frac{1}{M}\langle u(k')|u(k)\rangle \sum_{m=1}^{M} e^{i(k+\delta_k-k')R_m} \\
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$$\Rightarrow \hat{X}_P = \sum_{k,k'} |\Psi_{k'}\rangle\langle\Psi_{k'}|\hat{X}|\Psi_k\rangle\langle\Psi_k| = \sum_{k} \langle u(k+\delta_k)|u(k)\rangle |\Psi_{k+\delta_k}\rangle\langle\Psi_k|$$

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Note, we used that $\langle u(k_2)|u(k_1)\rangle$, $\langle u(k_3)|u(k_2)\rangle$ etc are complex numbers $\rightarrow$ they commmute

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Note: since $\hat{X}_P$ is not Hermitian, the eigenvectors are not orthogonal in general, only in the $M \to \infty$ limit (we will actually not need the eigenstates)

Wannier centers and the eigenvalues of $P\hat{X}P$

Remember from earlier:

1) polarization of a single filled band in a 1D lattice $\sim \bar{x}_j$ Wannier centers, $\bar{x}_j = \langle W(j)|x|W(j)\rangle$, j is unit cell index

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If there are M unit cells, k is discretized as $k_m = \frac{2\pi}{Ma} m$

$\Rightarrow$ The Wannier centers $\bar{x}_m$ can be obtained from λ_m as

$$\bar{x}_m = \frac{M}{2\pi} \mathrm{Im} \ln[\lambda_m] = \frac{\theta}{2\pi} + m = \frac{\mathrm{Im} \ln[w]}{2\pi} + m$$