Berryology using Wannier interpolation

applied to optics and transport

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Centro de Física de Materiales, San Sebastián, Spain

Wannier Summer School, Trieste, May 2022

What is “Berryology”?

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Let’s search the web...

What is "Berryology"?

Let's search the web...

Berry Science, or Berriology

Posted on September 18, 2012 | 2 Comments

Mmm, mm, good! And they're low carb

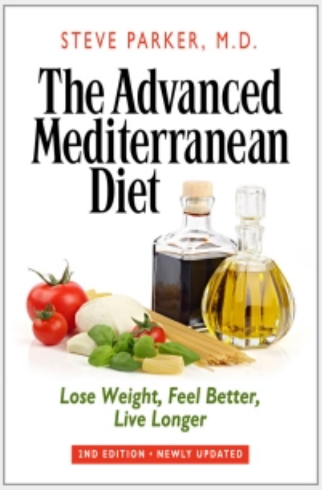
The Mediterranean diet was originally found to be a healthy diet by comparing populations who followed the diet with those who didn't. The result? Mediterranean dieters enjoyed longer lifespans and less heart disease, cancer, strokes, diabetes, and dementia.

Over the last 15 years, researchers have been clarifying exactly how and why this might be the case. A study from Finland is a typical example.

The traditional Mediterranean diet provides an abundance of fresh fruit, including berries. Berries are a rich source of vitamin C and polyphenols, substances with the potential to affect metabolic and disease processes in our bodies.

RSS FEED

RSS - Posts



Click the pic to purchase at Amazon.com. E-book versions also available at Smashwords.com.

$$
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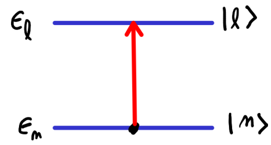
Oscillator strength: $$f^{(a)}_{n\to l} = \frac{2m\omega_{ln}}{\hbar}\left|\langle l|r_a|n\rangle\right|^2 = \frac{2m}{\hbar\omega_{ln}}\left|\langle l|v_a|n\rangle\right|^2$$



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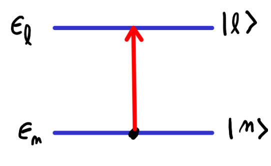
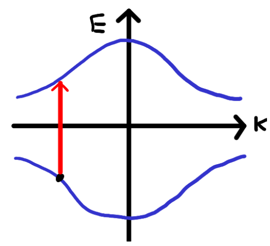


Crystal: $|n\rangle \rightarrow |\psi_{n\mathbf{k}}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u_{n\mathbf{k}}\rangle$



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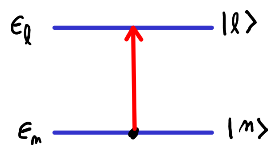

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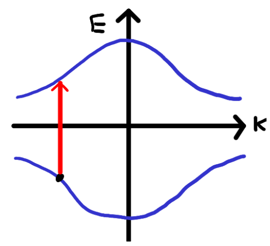

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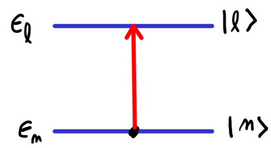

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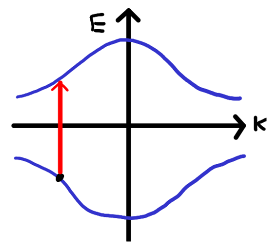

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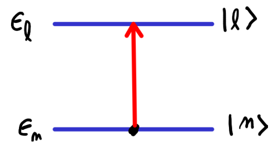

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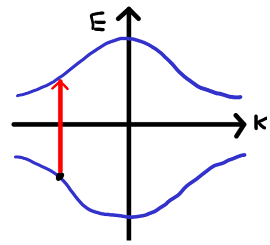

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Interband dipole:

off-diagonal $A^a_{ln\mathbf{k}}$

Dielectric function:

$$\epsilon''_{ab}(\omega) = \frac{\pi e^2}{\hbar} \int_{\mathbf{k}} \sum_{nl} f_{nl} \mathrm{Re}\left(A^a_{nl} A^b_{ln} \right) \delta\left(\omega - \omega_{ln}\right)$$

$f_{nl} = f(\epsilon_{n\mathbf{k}}) - f(\epsilon_{l\mathbf{k}})$

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Shift (photo)current:

$j_a = 2\sigma_{abc}(0;\omega,-\omega)E_b(\omega)E_c(-\omega)$

$$\sigma_{abc}(0;\omega,-\omega) = \frac{\pi e^3}{2\hbar^2} \int_{\mathbf{k}} \sum_{nl} f_{nl} \mathrm{Im}\left[A^b_{ln} A^{c;a}_{nl} + (b \leftrightarrow c) \right] \delta\left(\omega - \omega_{ln}\right)$$

$A^{c;a}_{nl} = \partial_a A^c_{nl} - i\left(A^a_{nn} - A^a_{ll}\right) A^c_{nl}$ ("covariant $\mathbf{k}$ derivative")

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Semiclassical transport:

$$\hbar\dot{\mathbf{r}} = \boldsymbol{\nabla}_{\mathbf{k}}\epsilon - \hbar\dot{\mathbf{k}} \times \boldsymbol{\Omega}$$

$$\hbar\dot{\mathbf{k}} = -e\mathbf{E} - \dot{\mathbf{r}} \times \mathbf{B}$$

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Current:

$$j_a = -e\int_{\mathbf{k}} \dot{r}_a f(\epsilon)$$

Boltzmann:

$$f(\epsilon) = f_0(\epsilon) + \tau e\mathbf{E}\cdot\mathbf{v} f_0'(\epsilon), \quad \text{where } \mathbf{v} = \text{band vel.}$$

$$
\begin{aligned}
j_a &= -e \int_{\mathbf{k}} \left[v_a + (e/\hbar)\Omega_{ab} E_b + \ldots\right] \left[f_0 + \tau e v_c E_c f_0' + \ldots\right] \\
&= \sigma_{ab} E_b + \sigma_{abc} E_b E_c + \ldots
\end{aligned}
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\sigma_{ab} = \underbrace{-e^2\tau \int_{\mathbf{k}} v_a v_b f_0'}_{\sigma_{ab}=\sigma_{ba}} \underbrace{- \frac{e^2}{\hbar} \int_{\mathbf{k}} \Omega_{ab} f_0}_{\sigma_{ab}=-\sigma_{ba}}
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Linear Ohmic + Hall

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\sigma_{abc} &= -\frac{e^3\tau}{\hbar}\int_{\mathbf{k}} \Omega_{ab} v_c f_0' \\
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Nonlinear Hall

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$$= \sigma_{ab} E_b + \sigma_{abc} E_b E_c + \ldots$$

$$\sigma_{ab} = \underbrace{-e^2 \tau \int_{\mathbf{k}} v_a v_b f_0'}_{\sigma_{ab}=\sigma_{ba}} \underbrace{- \frac{e^2}{\hbar} \int_{\mathbf{k}} \Omega_{ab} f_0}_{\sigma_{ab}=-\sigma_{ba}}$$

Linear Ohmic + Hall

Anomalous Hall effects (AHE)

$$\sigma_{abc} = -\frac{e^3 \tau}{\hbar} \int_{\mathbf{k}} \Omega_{ab} v_c f_0'$$
$$= \frac{e^3 \tau}{\hbar^2} \int_{\mathbf{k}} \left(\partial_c \Omega_{ab} \right) f_0 = -\sigma_{bac}$$

Nonlinear Hall

Symmetry constraints on AHE:

Time reversal $\mathcal{T}$	Inversion $\mathcal{I}$	$\mathcal{T} * \mathcal{I}$
$\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k})$	$\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k})$	
$\Omega(\mathbf{k}) = -\Omega(-\mathbf{k})$	$\Omega(\mathbf{k}) = \Omega(-\mathbf{k})$	$\Omega(\mathbf{k}) = 0$
$\int_{\mathbf{k}} \Omega f_0 = 0$	$\int_{\mathbf{k}} \left(\boldsymbol{\nabla}_{\mathbf{k}}\Omega\right) f_0 = 0$	

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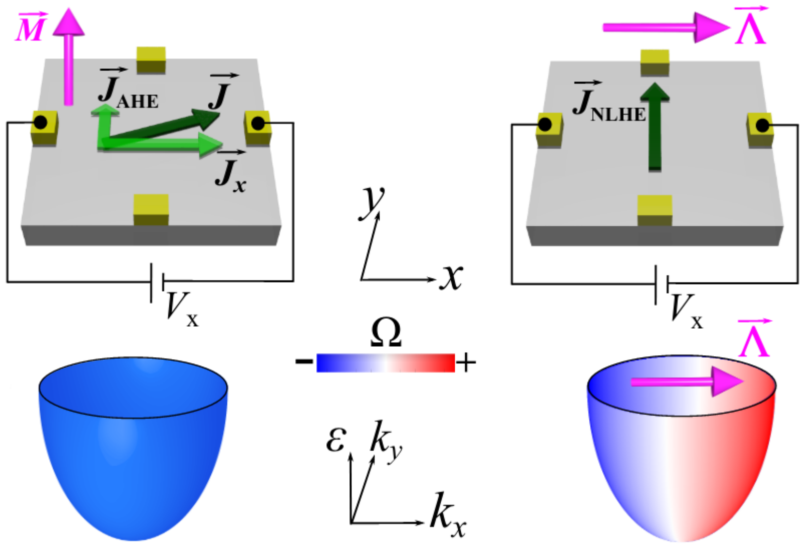
$\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k})$	$\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k})$	
$\Omega(\mathbf{k}) = -\Omega(-\mathbf{k})$	$\Omega(\mathbf{k}) = \Omega(-\mathbf{k})$	$\Omega(\mathbf{k}) = 0$
$\int_{\mathbf{k}} \Omega f_0 = 0$	$\int_{\mathbf{k}} (\boldsymbol{\nabla}_{\mathbf{k}}\Omega)\, f_0 = 0$	

$$\left.\begin{array}{l}\text{Linear}\\ \text{Nonlinear}\end{array}\right\} \text{AHE requires broken} \left\{\begin{array}{l}\text{time reversal}\\ \text{inversion}\end{array}\right.$$

Linear AHE　　　　Nonlinear AHE



$$\int_{\mathbf{k}} \Omega f_0 \neq 0$$

broken time reversal

$$\vec{\Lambda} = \int_{\mathbf{k}} \left(\boldsymbol{\nabla}_{\mathbf{k}} \Omega\right) f_0 \neq 0$$

broken inversion

Nonlinear AHE in bilayer WTe_2: Ma *et al*, Nature **565**, 337 (2019)

Summary so far:

- Optics: need $\epsilon_{n\mathbf{k}}$, $\mathbf{A}_{ln\mathbf{k}}$
- Transport: need $\epsilon_{n\mathbf{k}}$, $\boldsymbol{\nabla}_{\mathbf{k}}\epsilon_{n\mathbf{k}}$, $\boldsymbol{\Omega}_{n\mathbf{k}}$
- Also $\boldsymbol{\nabla}_{\mathbf{k}}\boldsymbol{\Omega}_{n\mathbf{k}}$, etc. at higher orders in $\mathbf{E}$

Such k-space quantities are conveniently evaluated using Wannier interpolation

Wannier interpolation:

Bloch basis functions: $|\psi^{(\mathrm{w})}_{j\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\tau}_j)}|\mathbf{R}j\rangle$, $\boldsymbol{\tau}_j = \langle \mathbf{0}j|\mathbf{r}|\mathbf{0}j\rangle$

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$$H^{(\mathsf{w})}_{ij}(\mathbf{k}) = \frac{1}{N_{\mathsf{cells}}}\langle\psi^{(\mathsf{w})}_{i\mathbf{k}}|H|\psi^{(\mathsf{w})}_{j\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\tau}_j-\boldsymbol{\tau}_i)}\langle\mathbf{0}i|H|\mathbf{R}j\rangle$$

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Diagonalize: $\left[U^\dagger(\mathbf{k})H^{(\mathsf{w})}(\mathbf{k})U(\mathbf{k})\right]_{ln} = \epsilon_{n\mathbf{k}}\delta_{ln}$

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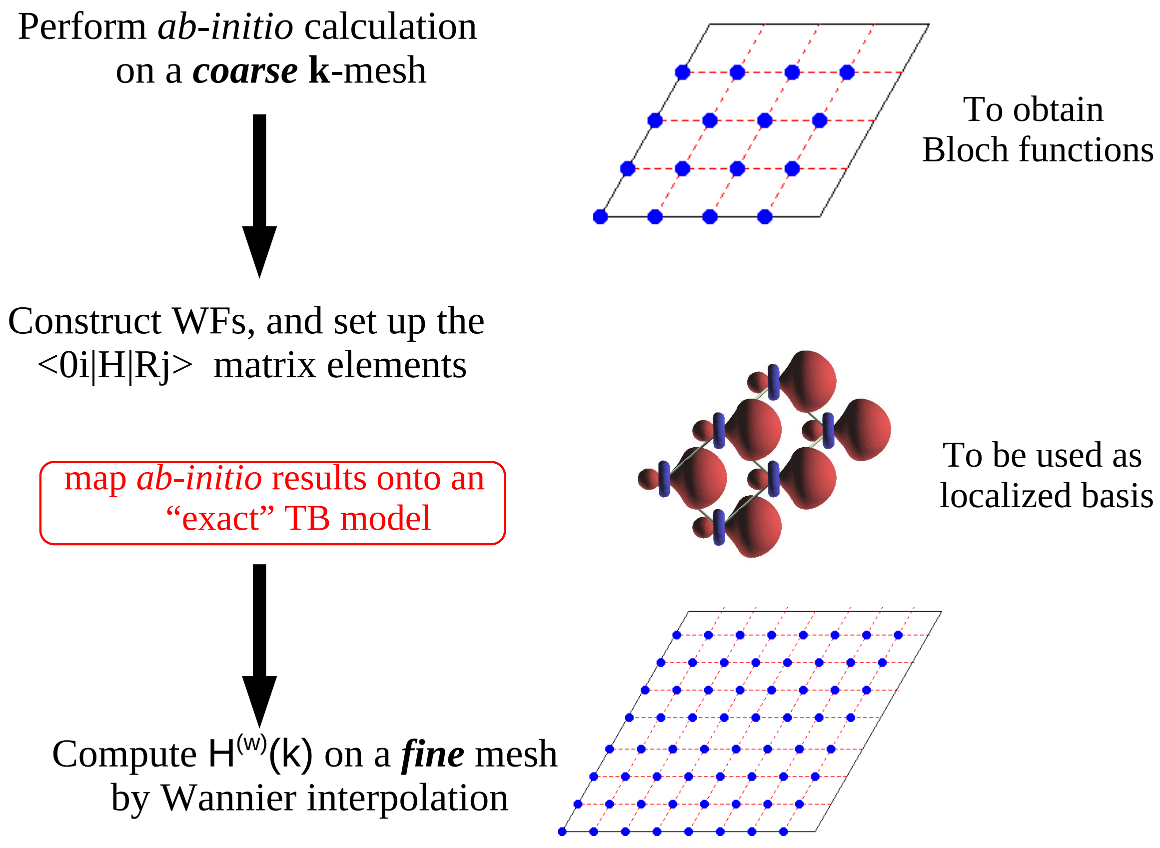
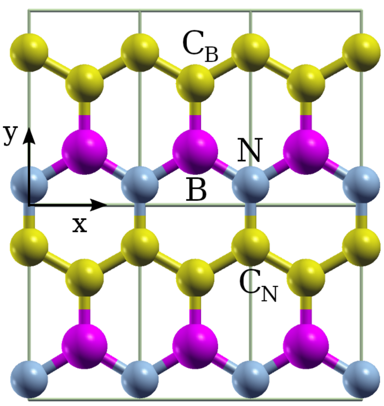
Orthogonal tight-binding (TB), with WFs as basis orbitals

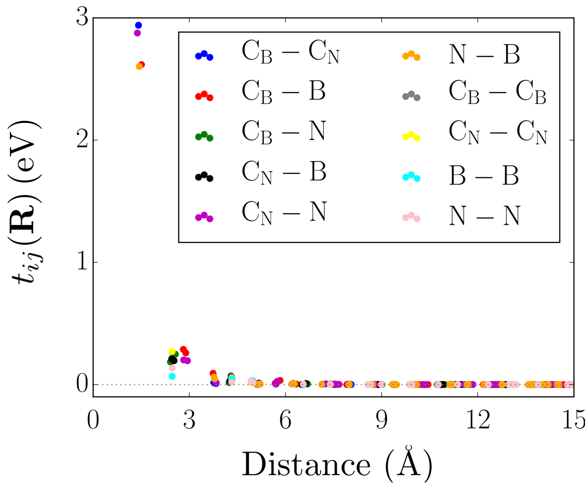
$\langle\mathbf{0}i|H|\mathbf{0}i\rangle$ = on-site energies ϵ_i $\qquad$ $\langle\mathbf{0}i|H|\mathbf{R}j\rangle$ = hoppings $t_{ij}(\mathbf{R})$

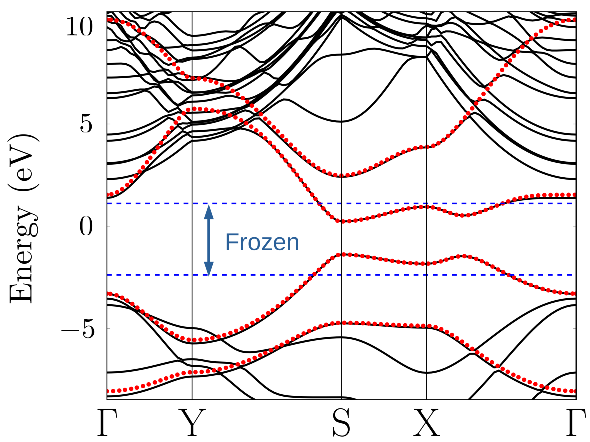


Perform *ab-initio* calculation
on a ***coarse*** **k**-mesh
To obtain
Bloch functions
Construct WFs, and set up the
<0i|H|Rj> matrix elements
map *ab-initio* results onto an
“exact” TB model
To be used as
localized basis
Compute $H^{(w)}(k)$ on a ***fine*** mesh
by Wannier interpolation

Monolayer BC_2N: Ibañez-Azpiroz *et al*, SciPost Phys. **12**, 070 (2022)







One p_z-type WF on each atom

$$U = \begin{array}{c} \begin{array}{ccc} \|1\rangle\!\rangle & \|n\rangle\!\rangle & \|N\rangle\!\rangle \end{array} \\ \left[\begin{array}{c|c|c|c} \quad & \cdots & \cdots & \quad \end{array} \right] \end{array}$$

Columns of $U =$ TB eigenvectors

$|\psi_n\rangle = \sum_j |\psi_j^{(\mathsf{w})}\rangle U_{jn}$ Bloch eigenstates

$$\left[U^\dagger H^{(\mathsf{w})} U\right]_{ln} = \epsilon_n \delta_{ln}$$

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Columns of U = TB eigenvectors

$|\psi_n\rangle = \sum_j |\psi_j^{(\mathsf{w})}\rangle U_{jn}$ Bloch eigenstates

$$\langle\!\langle l \| H^{(\mathsf{w})} \| n \rangle\!\rangle = \epsilon_n \delta_{ln}$$

$$\begin{array}{c} \quad\;\; \|1\rangle\!\rangle \quad\;\; \|n\rangle\!\rangle \quad\;\; \|N\rangle\!\rangle \\ U = \left[\begin{array}{c|c|c|c|c} & & & & \\ & & \cdots & \cdots & \\ & & & & \end{array} \right] \end{array}$$

Columns of U = TB eigenvectors

$|\psi_n\rangle = \sum_j |\psi_j^{(\mathsf{w})}\rangle U_{jn}$ Bloch eigenstates

$$\nabla_{\mathbf{k}} \langle\!\langle l \| H^{(\mathsf{w})} \| n \rangle\!\rangle = \nabla_{\mathbf{k}} \epsilon_n \delta_{ln}$$

- $l \neq n$: $$\boxed{\mathbf{D}_{ln} = \underbrace{\left[U^\dagger \nabla_{\mathbf{k}} U \right]_{ln}}_{\langle\!\langle l \| \nabla_{\mathbf{k}} n \rangle\!\rangle} = \frac{\left[U^\dagger \left(\nabla_{\mathbf{k}} H^{(\mathsf{w})} \right) U \right]_{ln}}{\epsilon_n - \epsilon_l}}$$

$$\nabla_{\mathbf{k}} H_{ij}^{(\mathsf{w})} = \sum_{\mathbf{R}} i(\mathbf{R} + \boldsymbol{\tau}_j - \boldsymbol{\tau}_i) e^{i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\tau}_j-\boldsymbol{\tau}_i)} \langle \mathbf{0}i | H | \mathbf{R}j \rangle$$

Cell-periodic Bloch eigenstates:

$$|u_n\rangle = \sum_j |u_j^{(\mathsf{w})}\rangle U_{jn}$$

$$|u_j^{(\mathsf{w})}\rangle = \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}-\boldsymbol{\tau}_j)}|\mathbf{R}j\rangle$$

$\Rightarrow$ Wavefunction-derived quantities:

- $\mathbf{A}_{ln} = i\langle u_l|\boldsymbol{\nabla}_{\mathbf{k}} u_n\rangle$
- $\boldsymbol{\Omega}_n = \boldsymbol{\nabla}_{\mathbf{k}} \times \mathbf{A}_{nn}$
- $\ldots$

Berry connection:

$$\mathbf{A}_{ln} = i\langle u_l|\boldsymbol{\nabla}_{\mathbf{k}} u_n\rangle \,, \qquad |\boldsymbol{\nabla}_{\mathbf{k}} u_n\rangle = \sum_j \boldsymbol{\nabla}_{\mathbf{k}} \left[|u_j^{(\mathsf{w})}\rangle U_{jn} \right]$$

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$$\boldsymbol{\nabla}_{\mathbf{k}} U = U\mathbf{D} \quad\Rightarrow\quad |\boldsymbol{\nabla}_{\mathbf{k}} u_n\rangle = \textstyle\sum_l |u_l\rangle \mathbf{D}_{ln} + \sum_j |\boldsymbol{\nabla}_{\mathbf{k}} u_j^{(\mathsf{w})}\rangle U_{jn}$$

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$$\boxed{\mathbf{A} = i\mathbf{D} + U^\dagger \mathbf{A}^{(\mathsf{w})} U}$$

$$\mathbf{A}_{ij}^{(\mathsf{w})} = i\langle u_i^{(\mathsf{w})}|\boldsymbol{\nabla}_{\mathbf{k}} u_j^{(\mathsf{w})}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\tau}_j-\boldsymbol{\tau}_i)}\langle \mathbf{0}i|\mathbf{r}-\boldsymbol{\tau}_j|\mathbf{R}j\rangle$$

Berry connection:

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$\langle \mathbf{0}i|\mathbf{r}|\mathbf{0}i\rangle$ = WF centers $\boldsymbol{\tau}_i$

$\langle \mathbf{0}i|\mathbf{r}-\boldsymbol{\tau}_j|\mathbf{R}j\rangle$ = "$\mathbf{r}$ hoppings" $\mathbf{d}_{ij}(\mathbf{R})$

$$\boxed{\mathbf{A} = i\mathbf{D} + U^\dagger \mathbf{A}^{(\mathsf{w})} U}$$

If we discard $\mathbf{r}$ hoppings:

$$\langle \mathbf{0}i|\mathbf{r}|\mathbf{R}j\rangle = \boldsymbol{\tau}_i \delta_{ij} \delta_{\mathbf{R}\mathbf{0}} + \cancelto{0}{\mathbf{d}_{ij}(\mathbf{R})}$$

$$\mathbf{A} = i\mathbf{D} + U^\dagger \cancelto{0}{\mathbf{A}^{(\mathsf{w})}} U$$

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TB approximation

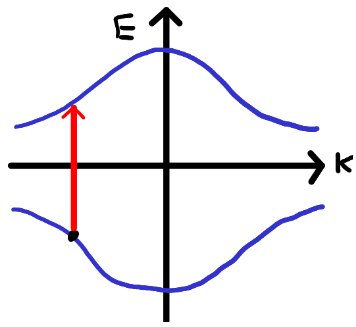
$$\mathbf{A}_{ln} \approx i\langle\!\langle l \| \boldsymbol{\nabla}_{\mathbf{k}} n \rangle\!\rangle$$

Input: ϵ_i, $t_{ij}(\mathbf{R})$, $\boldsymbol{\tau}_i$

(e.g., `PythTB`)

Summary of Wannier interpolation:

Fourier transform and diagonalize small $N \times N$ matrices (N WFs/cell) $\Rightarrow$ **Fast!**



- Energy bands: need $\langle \mathbf{0}i|H|\mathbf{R}j\rangle$
- Optical matrix elements: need $\langle \mathbf{0}i|H|\mathbf{R}j\rangle$ and $\langle \mathbf{0}i|\mathbf{r}|\mathbf{R}j\rangle$

$$\langle \mathbf{0}i|H|\mathbf{R}j\rangle = \epsilon_i \delta_{ij}\delta_{\mathbf{R0}} \; + \; t_{ij}(\mathbf{R})$$

$$\langle \mathbf{0}i|\mathbf{r}|\mathbf{R}j\rangle = \boldsymbol{\tau}_i \delta_{ij}\delta_{\mathbf{R0}} \; + \; \mathbf{d}_{ij}(\mathbf{R})$$

On-site Hoppings

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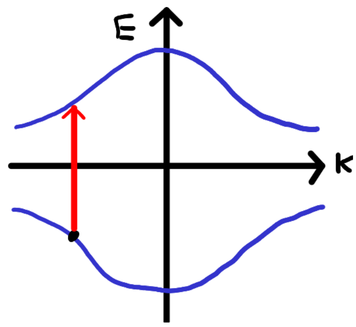

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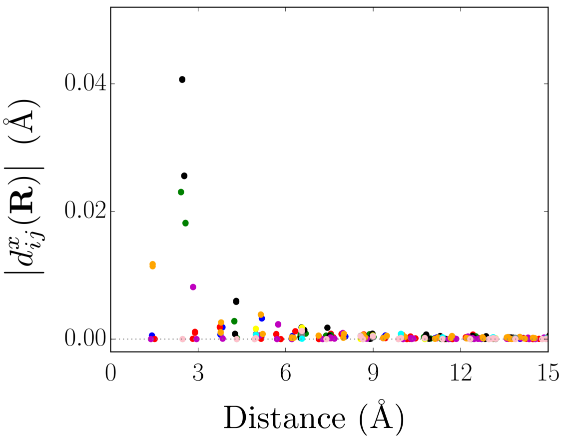
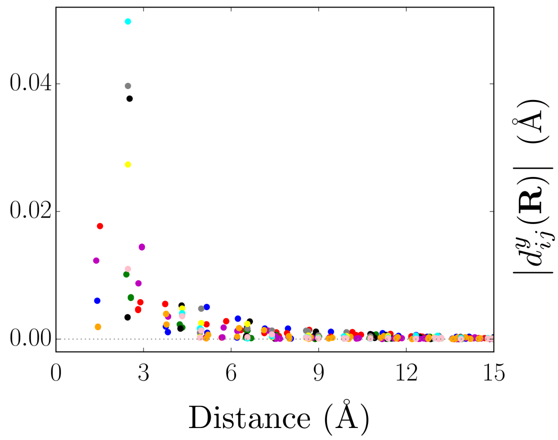
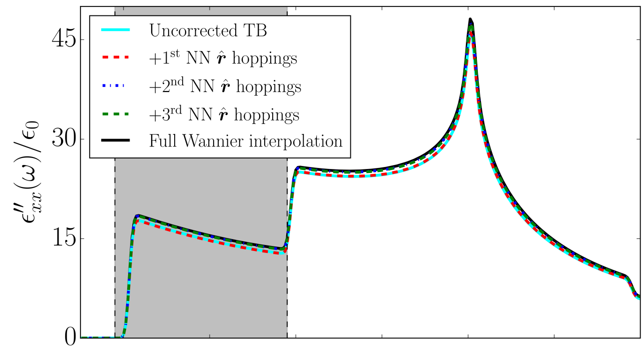
On-site Hoppings

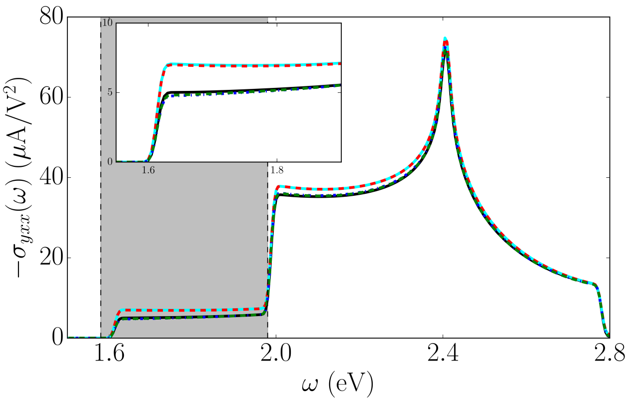
BC_2N







Dielectric fct.



Shift photoconductivity

Ibañez-Azpiroz *et al*, SciPost Phys. **12**, 070 (2022)

Berry curvature:

$\mathbf{k}$-derivatives formula:

$$\boldsymbol{\Omega}_n = \boldsymbol{\nabla}_{\mathbf{k}} \times \mathbf{A}_{nn} = -\mathrm{Im}\langle \boldsymbol{\nabla}_{\mathbf{k}} u_n | \times | \boldsymbol{\nabla}_{\mathbf{k}} u_n \rangle$$

Kubo (sum-over-states) formula:

$$\boldsymbol{\Omega}_n = -\mathrm{Im} \sum_{l \neq n} \frac{\langle u_n | \boldsymbol{\nabla}_{\mathbf{k}} H | u_l \rangle \times \langle u_l | \boldsymbol{\nabla}_{\mathbf{k}} H | u_n \rangle}{(\epsilon_n - \epsilon_l)^2}$$

$\boldsymbol{\Omega}_n \propto (\epsilon_n - \epsilon_l)^{-2}$, reacts strongly to (avoided) crossings

Berry curvature by Wannier interpolation:

$$\mathbf{\Omega}_n = -\mathrm{Im}\langle \boldsymbol{\nabla}_{\mathbf{k}} u_n | \times | \boldsymbol{\nabla}_{\mathbf{k}} u_n \rangle$$

$$|\boldsymbol{\nabla}_{\mathbf{k}} u_n\rangle = \sum_l |u_l\rangle \mathbf{D}_{ln} + \sum_j |\boldsymbol{\nabla}_{\mathbf{k}} u_j^{(\mathrm{w})}\rangle U_{jn}$$

$$\mathbf{\Omega}_n = -\mathrm{Im}\left[\mathbf{D}^\dagger \times \mathbf{D}\right]_{nn} + \text{ (}\mathbf{r}\text{-hopping terms)}$$

Berry curvature by Wannier interpolation:

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If we discard $\mathbf{r}$ hoppings:

TB approximation

$$\mathbf{\Omega}_n \approx -\mathrm{Im}\langle\!\langle \boldsymbol{\nabla}_{\mathbf{k}} n \| \times \| \boldsymbol{\nabla}_{\mathbf{k}} n \rangle\!\rangle$$

Input: ϵ_i, $t_{ij}(\mathbf{R})$, $\boldsymbol{\tau}_i$

Berry curvature:

$$\boldsymbol{\Omega}_n \approx -\mathrm{Im}\left[\mathbf{D}^\dagger \times \mathbf{D}\right]_{nn} \quad \boxed{\text{TB Kubo formula}}$$

$$\mathbf{D}_{ln} = \begin{cases} \frac{\left[U^\dagger\left(\boldsymbol{\nabla}_{\mathbf{k}} H^{(\mathrm{w})}\right)U\right]_{ln}}{\epsilon_n - \epsilon_l}\,, & \text{if } l \neq n \\ 0\,, & \text{if } l = n \end{cases} \qquad \text{(small matrix)}$$

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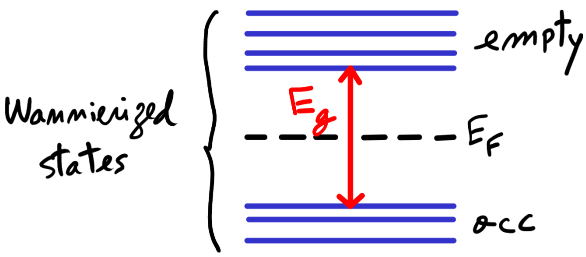
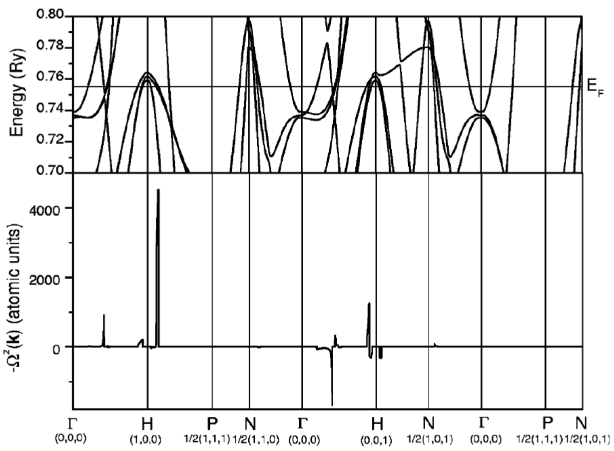


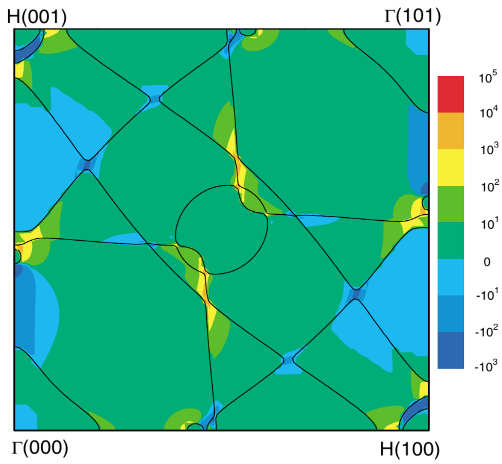
$$\boxed{\Omega_{\text{occ}} = \sum_n^{\text{occ}} \Omega_n \propto E_{\mathrm{g}}^{-2}}$$

- Reacts strongly to small gaps across E_{F}
- Insensitive to crossings among occ. states

Anomalous Hall conductivity (AHC) of bcc Fe:

$$\mathbf{M} \parallel \hat{\mathbf{z}} \qquad \sigma_{xy} = -\frac{e^2}{\hbar}\int_{\mathbf{k}} \Omega^z_{\text{occ}}(\mathbf{k}) \qquad \Omega^z_{\text{occ}} = \sum_n f_0(\epsilon_n)\Omega^z_n$$





Evaluating σ_{xy} requires ultradense, nonuniform BZ sampling

Yao *et al*, Phys. Rev. Lett. **92**, 037204 (2004)

AHC of ferromagnetic metals:

- First evaluated in 2003–2004 from the Kubo formula using "brute-force" *ab initio* methods. **Challenging/expensive!**
- Stimulated development of Wannier interpolation scheme for transport and optics (2006–2007). **k points become cheap!**
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  - Released in `Wannier90` as part of the `postw90` module
- Further Berry-type quantities:
  - Nonlinear AHC
  - Spin Hall conductivity
  - Shift current
  - Orbital magnetization

Recent developments implemented in `Wannier Berri`:

- Mixed fast/slow Fourier transform
- Iterative adaptive refinement of $\mathbf{k}$ mesh
- Efficient scanning of E_F
- Tetrahedron method for BZ integrals
- Symmetrization of matrix elements
- Interpolation of $\boldsymbol{\nabla}_\mathbf{k}\boldsymbol{\Omega}$, $\boldsymbol{\nabla}_\mathbf{k}\mathbf{m}_\mathsf{orb}$, etc.

Tsirkin, npj Comput. Mater. **7**, 33 (2021)