Synopsis of the geometrical observables in condensed matter

(partitioned in two classes)

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Outline

1. Generalities
2. Class I observables: Bulk value defined modulo 2π
3. Class II observables: Exempt from 2π ambiguity
4. Local nature of class II observables
   - Anomalous Hall conductivity and orbital magnetization
   - SWM sum rule vs. local density of states
5. Beyond band-structure theory

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5 Beyond band-structure theory

Metric, connection, curvature

- $|\Psi_{\boldsymbol{\kappa}}\rangle$ a **differentiable** function of $\boldsymbol{\kappa}$

- Quantum metric $g_{\alpha\beta}(\boldsymbol{\kappa})$:

$$D^2_{\boldsymbol{\kappa},\boldsymbol{\kappa}+d\boldsymbol{\kappa}} = g_{\alpha\beta}(\boldsymbol{\kappa}) d\kappa_\alpha d\kappa_\beta$$ **gauge-invariant**

- Berry connection $\mathcal{A}_\alpha(\boldsymbol{\kappa})$:

$$\varphi_{\boldsymbol{\kappa},\boldsymbol{\kappa}+d\boldsymbol{\kappa}} = \mathcal{A}_\alpha(\boldsymbol{\kappa}) d\kappa_\alpha$$ **gauge-dependent**

- Berry curvature $\Omega_{\alpha\beta}(\boldsymbol{\kappa})$ (curl of the connection):

$$\Omega_{\alpha\beta}(\boldsymbol{\kappa}) d\kappa_\alpha d\kappa_\beta = [\partial_{\kappa_\alpha} \mathcal{A}_\beta(\boldsymbol{\kappa}) - \partial_{\kappa_\beta} \mathcal{A}_\alpha(\boldsymbol{\kappa})] d\kappa_\alpha d\kappa_\beta$$

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Metric, connection, curvature

- Quantum metric:

$$D^2_{\boldsymbol{\kappa},\boldsymbol{\kappa}+d\boldsymbol{\kappa}} = g_{\alpha\beta}(\boldsymbol{\kappa})d\kappa_\alpha d\kappa_\beta \qquad \textbf{2-form}$$

- Berry connection:

$$\varphi_{\boldsymbol{\kappa},\boldsymbol{\kappa}+d\boldsymbol{\kappa}} = \mathcal{A}_\alpha(\boldsymbol{\kappa})d\kappa_\alpha \qquad \textbf{1-form}$$

- Berry curvature:

$$\Omega_{\alpha\beta}(\boldsymbol{\kappa})d\kappa_\alpha d\kappa_\beta = [\partial_{\kappa_\alpha}\mathcal{A}_\beta(\boldsymbol{\kappa}) - \partial_{\kappa_\beta}\mathcal{A}_\alpha(\boldsymbol{\kappa})]d\kappa_\alpha d\kappa_\beta$$

2-form

Metric, connection, curvature

- Quantum metric **2-form**:

$$g_{\alpha\beta}(\boldsymbol{\kappa}) = \text{Re}\,\langle \partial_{\kappa_\alpha}\Psi_{\boldsymbol{\kappa}}|\partial_{\kappa_\beta}\Psi_{\boldsymbol{\kappa}}\rangle - \langle \partial_{\kappa_\alpha}\Psi_{\boldsymbol{\kappa}}|\Psi_{\boldsymbol{\kappa}}\rangle\langle \Psi_{\boldsymbol{\kappa}}|\partial_{\kappa_\beta}\Psi_{\boldsymbol{\kappa}}\rangle$$

- Berry connection **(1-form)**:

$$\mathcal{A}_\alpha(\boldsymbol{\kappa}) = i\langle \Psi_{\boldsymbol{\kappa}}|\partial_{\kappa_\alpha}\Psi_{\boldsymbol{\kappa}}\rangle$$

- Berry curvature **(2-form)**:

$$\Omega_{\alpha\beta}(\boldsymbol{\kappa}) = -2\,\text{Im}\,\langle \partial_{\kappa_\alpha}\Psi_{\boldsymbol{\kappa}}|\partial_{\kappa_\beta}\Psi_{\boldsymbol{\kappa}}\rangle$$

- Metric-curvature tensor **(2-form)**:

$$\mathcal{F}_{\alpha\beta}(\boldsymbol{\kappa}) = g_{\alpha\beta}(\boldsymbol{\kappa}) - \frac{i}{2}\Omega_{\alpha\beta}(\boldsymbol{\kappa})$$

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More general "geometrical" forms

- So far, the only entries have been the state vectors

- A typical more general "geometrical" 2-form:

$$\langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | (H_{\boldsymbol{\kappa}} - E_{\boldsymbol{\kappa}}) | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle$$

- Besides the state vectors, the Hamiltonian $H_{\boldsymbol{\kappa}}$ is the **sole** legal ingredient

- Why the combination $(H_{\boldsymbol{\kappa}} - E_{\boldsymbol{\kappa}})$?

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Identifying κ with $\mathbf{k}$, many-band case

- Berry connection **(insulators only)**:

$$\mathcal{A}_\alpha(\mathbf{k}) = i \sum_{j=1}^{n_b} \langle u_{j\mathbf{k}} | \partial_{k_\alpha} u_{j\mathbf{k}} \rangle$$

- Metric-curvature tensor **(including metals)**:

$$\begin{aligned} \mathcal{F}_{\alpha\beta}(\mathbf{k}) &= \sum_{\epsilon_{j\mathbf{k}} \le \mu} \langle \partial_{k_\alpha} u_{j\mathbf{k}} | \partial_{k_\beta} u_{j\mathbf{k}} \rangle \\ &- \sum_{\epsilon_{j\mathbf{k}}, \epsilon_{j'\mathbf{k}} \le \mu} \langle \partial_{k_\alpha} u_{j\mathbf{k}} | u_{j'\mathbf{k}} \rangle \, \langle u_{j'\mathbf{k}} | \partial_{k_\beta} u_{j\mathbf{k}} \rangle \end{aligned}$$

P and **M** could not be more different!

$$P_\alpha^{(\mathrm{el})} = -2ie\sum_{j=1}^{n_\mathrm{b}}\int_{\mathrm{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\langle u_{j\mathbf{k}}|\partial_{k_\alpha}u_{j\mathbf{k}}\rangle = -2e\int_{\mathrm{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\mathcal{A}_\alpha(\mathbf{k})$$

$$M_\gamma = -\frac{ie}{2\hbar c}\varepsilon_{\gamma\alpha\beta}\sum_{\varepsilon_{j\mathbf{k}}<\mu}\int_{\mathrm{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\langle\partial_{k_\alpha}u_{j\mathbf{k}}|\left(H_\mathbf{k}+\epsilon_{j\mathbf{k}}-2\mu\right)|\partial_{k_\beta}u_{j\mathbf{k}}\rangle$$

- **Polarization**
  - Insulators only
  - Gauge-dependent integrand
  - Integral of a 1-form
  - At bare bones, **P** is 1-dimensional
  - Bulk **P** multiple valued
  - Tinkering with the boundaries can alter **P**
- **Orbital Magnetization**
  - Insulators and metals
  - Gauge-invariant integrand
  - Integral of a 2-form
  - At bare bones, **M** is 2-dimensional
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- **Polarization:** **prototipe of class I**
  - Insulators only
  - Gauge-dependent integrand
  - Integral of a 1-form
  - At bare bones, **P** is 1-dimensional
  - Bulk **P** multiple valued
  - Tinkering with the boundaries can alter **P**
- **Orbital Magnetization:** **prototipe of class II**
  - Insulators and metals
  - Gauge-invariant integrand
  - Integral of a 2-form
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  - **M** is single-valued
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Message from modern differential geometry (& algebraic topology)

Results due to Pontryagin, Cartan, Weyl, Chern, Simons....
($\simeq$ first half of 20th century)

- Features in **odd** vs. **even** dimension are quite different
- $2n$-forms and $(2n-1)$-forms behave in quite different ways
- Chern forms, and the (topological) Chern number only exists in dimension $2n$
- Chern-Simons forms are instead $(2n-1)$-forms

- The Berry connection entering the P in $1d$ formula is a Chern-Simons 1-form
- Does any Chern-Simons 3-form have physical meaning?

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The polarization "quantum"

D. Vanderbilt and R. D. King-Smith, Phys. Rev. B **48**, 4442 (1993)

- Bulk polarization **P** is a **lattice**, not a **vector!**
- The value of **P** remains ambiguous until the sample **termination** is specified

- For a 1d system polarization is defined **modulo** e

$$P = \frac{e}{2\pi}\gamma, \quad \text{the Berry phase } \gamma \text{ is defined modulo } 2\pi$$

- In a centrosymmetric polymer $P = -P$:
  - either $P = 0$ mod e
  - or $P = e/2$ mod e

- Kind of obvious if one adopts the "single-point Berry phase" viewpoint!

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NonAbelian connection and curvature

- Insulators only
- NonAbelian connection **matrix**:

$$\mathcal{A}_{\alpha,jj'}(\mathbf{k}) = i\langle u_{j\mathbf{k}}|\partial_{k_\alpha} u_{j'\mathbf{k}}\rangle$$

- NonAbelian curvature **matrix**:

$$\begin{aligned}\Omega_{\alpha\beta,jj'}(\mathbf{k}) &= \partial_{k_\alpha}\mathcal{A}_{\beta,jj'}(\mathbf{k}) - \partial_{k_\beta}\mathcal{A}_{\alpha,jj'}(\mathbf{k}) \\ &= i(\,\langle\partial_{k_\alpha} u_{j\mathbf{k}}|\partial_{k_\beta} u_{j'\mathbf{k}}\rangle - \langle\partial_{k_\beta} u_{j\mathbf{k}}|\partial_{k_\alpha} u_{j\mathbf{k}}\rangle\,)\end{aligned}$$

Chern-Simons 1-form & 3-form

- $1d$ BZ integral of the Chern-Simons 1-form:

$$\gamma^{(el)} = \int_{\mathrm{BZ}} dk_x \,\mathrm{tr}\, \{\mathcal{A}_x(k_x)\}$$ (**physical meaning: polarization**)

- $3d$ BZ integral of the Chern-Simons 3-form:

$$\theta = -\frac{1}{4\pi}\varepsilon_{\alpha\gamma\beta}\int_{\mathrm{BZ}} d\mathbf{k}\,\mathrm{tr}\,\left\{\mathcal{A}_\alpha(\mathbf{k})\partial_{k_\beta}\mathcal{A}_\gamma(\mathbf{k}) - \frac{2i}{3}\mathcal{A}_\alpha(\mathbf{k})\mathcal{A}_\beta(\mathbf{k})\mathcal{A}_\gamma(\mathbf{k})\right\}$$

  - Formula taken from the **mathematical literature**
  - θ gauge-invariant modulo 2π
  - Does θ have any **physical meaning**?
  - **Yes:** "Axion" term in magnetoelectric response (X.-L. Qi, T.L.Hughes, & S.-C. Zhang, PRB 2008)

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Class I observables: γ and θ defined modulo 2π

Chern-Simons 1-form	Polarization (insulators only)
Chern-Simons 3-form	Axion term in magnetoelectrics (insulators only)

$$\langle \mathcal{O} \rangle = \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \, \mathfrak{f}(\mathbf{k})$$

- Integrand $\mathfrak{f}(\mathbf{k})$ is **gauge-dependent**
- Bulk $\langle \mathcal{O} \rangle$ defined modulo 2π (in dimensionless units)
- For a bounded sample $\langle \mathcal{O} \rangle$ depends on termination
- In presence of some “protecting” symmetry both γ and θ are $\mathbb{Z}_2$ topological invariants

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Common features

Time-reversal odd	Time-reversal even
Anomalous Hall conductivity	Souza-Wilkens-Martin sum rule
Magneto-optical sum rule	**??**
Orbital magnetization	Drude weight

$$\langle \mathcal{O} \rangle = \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \, \mathfrak{f}_{\alpha\beta}(\mathbf{k})$$

- Integrand $\mathfrak{f}_{\alpha\beta}(\mathbf{k})$ **gauge-independent**
- **No** modulo 2π ambiguity
- For a bounded sample $\langle \mathcal{O} \rangle$ **independent of termination**
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- All of them admit a **local** representation

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Synoptic table of class II observables

Time-reversal odd (antisymmetric 2-forms)	**Time-reversal even** (symmetric 2-forms)
Anomalous Hall conductivity metals and insulators	Souza-Wilkens-Martin sum rule insulators only
Magneto-optical sum rule metals and insulators	**??**
Orbital magnetization metals and insulators	Drude weight metals only

- On the same row: **k**-integral of the same $\mathfrak{f}_{\alpha\beta}(\mathbf{k})$
  - Left: **Imaginary antisymmetric** term
  - Right **Real symmetric** term
- Two are **sum rules**: why?
  The Souza-Wilkens-Martin sum rule:
  - Measures the WFs gauge-invariant quadratic spread
  - Diverges in all metals

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Observables cast as gauge-invariant in form

- Band projector (gauge-invariant):

$$\mathcal{P}_{\mathbf{k}} = \sum_{\epsilon_{j\mathbf{k}} \leq \mu} |u_{j\mathbf{k}}\rangle\langle u_{j\mathbf{k}}|$$

- The integrand $\mathfrak{f}_{\alpha\beta}(\mathbf{k})$, being gauge-invariant, is expressible in terms of **k**-derivatives of $\mathcal{P}_{\mathbf{k}}$
- **All class II observables** are rooted in a 2-form
- Common entry in $\mathfrak{f}_{\alpha\beta}(\mathbf{k})$ in all cases:

Products of the kind: $(\partial_{k_\alpha} \mathcal{P}_{\mathbf{k}})(\partial_{k_\beta} \mathcal{P}_{\mathbf{k}})$

T-odd class II observables

- Defined in the same way in **insulators and metals**

- Anomalous Hall conductivity:

$$\text{Re}\ \sigma^{(-)}_{\alpha\beta}(0) = -\frac{ie^2}{\hbar}\int_{\text{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\text{Tr}_{\text{cell}}\{\mathcal{P}_{\mathbf{k}}\left[\partial_{k_\alpha}\mathcal{P}_{\mathbf{k}}, \partial_{k_\beta}\mathcal{P}_{\mathbf{k}}\right]\}$$

- Magneto-optical sum rule:

$$\text{Im}\int_0^\infty d\omega\ \sigma^{(-)}_{\alpha\beta}(\omega) = \frac{i\pi e^2}{2\hbar^2}\int_{\text{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\text{Tr}_{\text{cell}}\{(\mathcal{H}_{\mathbf{k}}-\mu)[\partial_{k_\alpha}\mathcal{P}_{\mathbf{k}}, \partial_{k_\beta}\mathcal{P}_{\mathbf{k}}]\}$$

- Orbital Magnetization:

$$\mathbf{M} = \frac{ie}{2\hbar c}\int_{\text{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\text{Tr}_{\text{cell}}\{|\mathcal{H}_{\mathbf{k}} - \mu|\nabla_{\mathbf{k}}\mathcal{P}_{\mathbf{k}} \times \nabla_{\mathbf{k}}\mathcal{P}_{\mathbf{k}}\}$$

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Role of the Fermi surface

- Band projector and its derivative:

$$\mathcal{P}_{\mathbf{k}} = \sum_j \theta(\mu - \epsilon_{j\mathbf{k}}) \, |u_{j\mathbf{k}}\rangle\langle u_{j\mathbf{k}}|$$

$$\begin{aligned} \partial_{\mathbf{k}} \mathcal{P}_{\mathbf{k}} &= -\sum_j \delta(\mu - \epsilon_{j\mathbf{k}}) \, (\partial_{\mathbf{k}} \epsilon_{j\mathbf{k}}) \, |u_{j\mathbf{k}}\rangle\langle u_{j\mathbf{k}}| \\ &+ \sum_j \theta(\mu - \epsilon_{j\mathbf{k}}) \, (|u_{j\mathbf{k}}\rangle\langle \partial_{\mathbf{k}} u_{j\mathbf{k}}| + |u_{j\mathbf{k}}\rangle\langle \partial_{\mathbf{k}} u_{j\mathbf{k}}|) \end{aligned}$$

- δ-like singularity **only for metals**
- δ-term annihilated by antisymmetrization **in T-odd cases**
- Metallic δ-term does contribute **in T-even cases**

T-evenclass II observables

- Souza-Wilkens-Martin sum rule **in insulators**:

$$\int_0^\infty \frac{d\omega}{\omega} \mathrm{Re}\, \sigma^{(+)}_{\alpha\beta}(\omega) = \frac{\pi e^2}{\hbar} \mathrm{Re} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \mathrm{Tr}_{\mathrm{cell}}\{\mathcal{P}_{\mathbf{k}}\,(\partial_{k_\alpha}\mathcal{P}_{\mathbf{k}})(\partial_{k_\beta}\mathcal{P}_{\mathbf{k}})\}$$

- What about **metals**?

- Drude weight:

$$D_{\alpha\beta} = \frac{\pi e^2 n}{m}\delta_{\alpha\beta} - \frac{2\pi e^2}{\hbar^2} \mathrm{Re} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \mathrm{Tr}_{\mathrm{cell}}\{|\mathcal{H}_{\mathbf{k}} - \mu|(\partial_{k_\alpha}\mathcal{P}_{\mathbf{k}})(\partial_{k_\beta}\mathcal{P}_{\mathbf{k}})\}$$

- $D_{\alpha\beta} = 0$ in insulators;
  in metals use the **regular** term only in $\partial_{k_\alpha}\mathcal{P}_{\mathbf{k}}$.

T-evenclass II observables

- Souza-Wilkens-Martin sum rule **in insulators**:

$$\int_0^\infty \frac{d\omega}{\omega} \mathrm{Re}\ \sigma^{(+)}_{\alpha\beta}(\omega) = \frac{\pi e^2}{\hbar} \mathrm{Re} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \mathrm{Tr}_{\mathrm{cell}}\{\mathcal{P}_{\mathbf{k}}\, (\,\partial_{k_\alpha} \mathcal{P}_{\mathbf{k}})(\partial_{k_\beta} \mathcal{P}_{\mathbf{k}})\}$$

- What about **metals**?

- Drude weight:

$$\begin{aligned} D_{\alpha\beta} &= \frac{\pi e^2 n}{m} \delta_{\alpha\beta} \\ &- \frac{2\pi e^2}{\hbar^2} \mathrm{Re} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \mathrm{Tr}_{\mathrm{cell}}\{|\mathcal{H}_{\mathbf{k}} - \mu|(\partial_{k_\alpha} \mathcal{P}_{\mathbf{k}})(\partial_{k_\beta} \mathcal{P}_{\mathbf{k}})\} \end{aligned}$$

- $D_{\alpha\beta} = 0$ in insulators;
  in metals use the **regular** term only in $\partial_{k_\alpha} \mathcal{P}_{\mathbf{k}}$.

Outline

1 Generalities

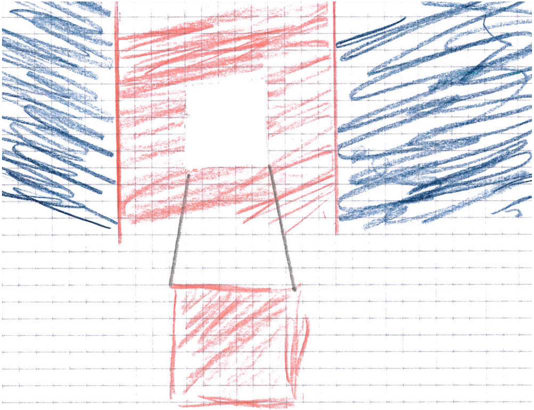
2 Class I observables: Bulk value defined modulo 2π

3 Class II observables: Exempt from 2π ambiguity

4 Local nature of class II observables
- Anomalous Hall conductivity and orbital magnetization
- SWM sum rule vs. local density of states

5 Beyond band-structure theory

Kohn's "nearsightedness" principle (1996)



- W. Kohn: "The principle applies to the one particle density matrix but not to individual eigenfunctions"

- Expressions in terms of $\mathcal{P}$ both in **k**-space and in **r**-space

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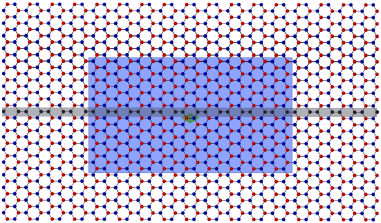
Densities in Haldanium flakes



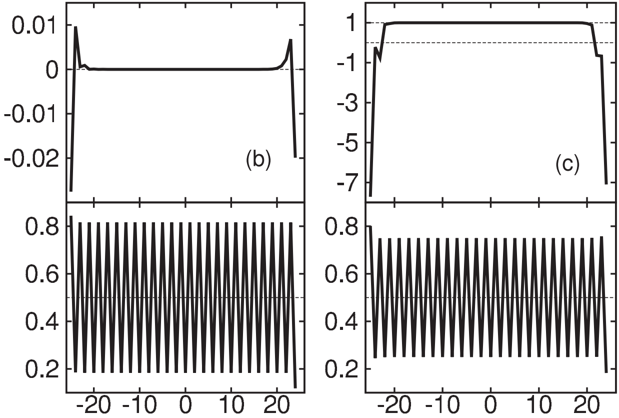
- Tensor fields in **r**-space:

$$\mathfrak{F}_{\alpha\beta}(\mathbf{r}) = \text{Im} \langle \mathbf{r}| \, \mathcal{P} \, [r_\alpha, \mathcal{P}] \, [r_\beta, \mathcal{P}] \, |\mathbf{r}\rangle$$

$$\mathfrak{M}_{\alpha\beta}(\mathbf{r}) = \text{Im} \langle \mathbf{r}| \, |\mathcal{H} - \mu| \, [r_\alpha, \mathcal{P}] \, [r_\beta, \mathcal{P}] \, |\mathbf{r}\rangle.$$

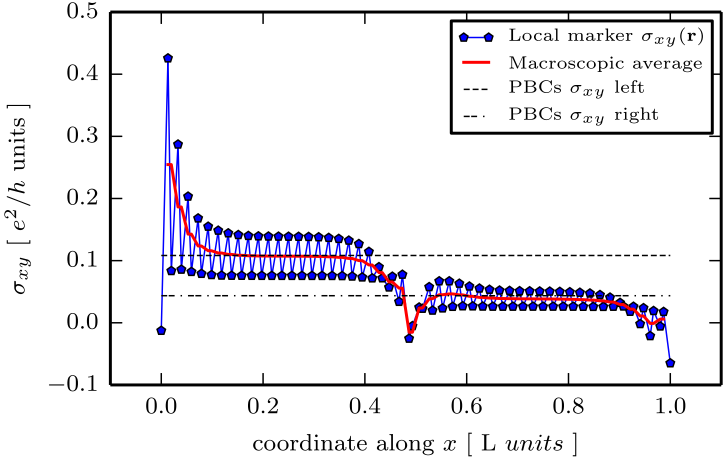
- $\mathfrak{F}_{\alpha\beta}(\mathbf{r})$ and $\mathfrak{M}_{\alpha\beta}(\mathbf{r})$ are **“densities”** well defined even for disordered and/or inhomogeneous bounded samples

QAHC in Haldanium flakes at half filling



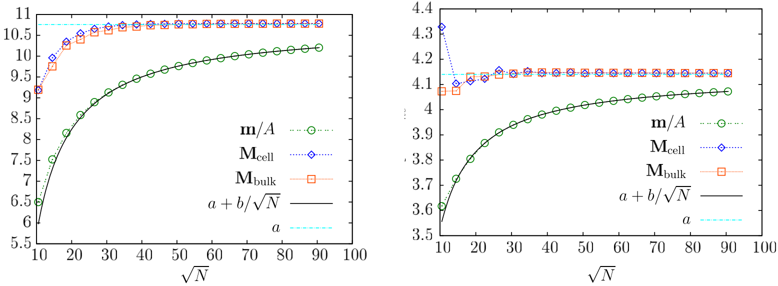
- Topological "density" $\mathfrak{F}_{\alpha\beta}(\mathbf{r})$ along the central line(top)
- Site occupancy (bottom)

AHC in Haldanium metal/metal heterojunctions



Geometrical “density” $\mathfrak{F}_{\alpha\beta}(\mathbf{r})$

Orbital magnetization in insulators and metals



Insulator Metal

- **$1/L$ convergence with size:** $\frac{1}{2cV} \int d\mathbf{r}\, \mathbf{r} \times \mathbf{j}^{(\text{micro})}(\mathbf{r})$
- **Much better convergence:** $\frac{e}{2\hbar c} \varepsilon_{\gamma\alpha\beta} \mathrm{Tr}_V \{\mathfrak{M}_{\alpha\beta}\}$

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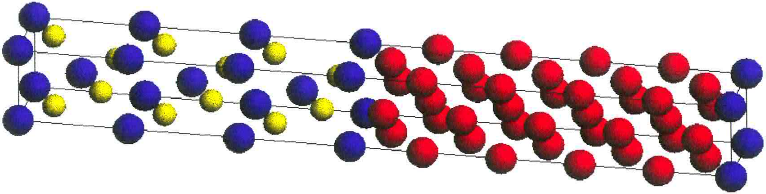
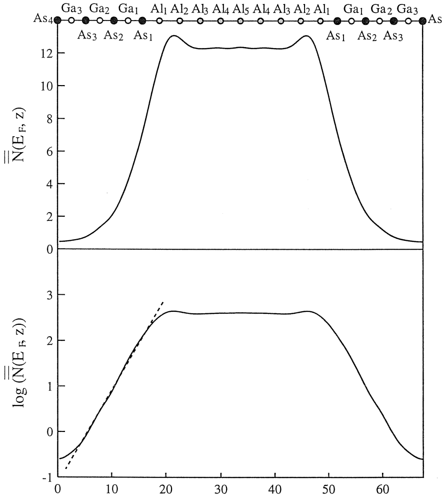
A metal-semiconductor heterojunction



- (001)Al/GaAs heterojunction
- The **local density of states** at the Fermi level is the obvious marker to discriminate insulating vs. metallic regions

Local density of states at the Fermi level



LDOS (macroscopic average) at the Fermi level

Notice the evanescent states

The problem

- The local density of states at the Fermi level cannot work for Anderson insulators: **gapless**

- The OBCs quantum metric
  - Diverges in all metals
  - Converge to a finite value in all insulators
  - It can probe a inhomogeneous system **locally**

Tight binding 1d binary crystal

$$H = \sum_j (\epsilon_j |j\rangle\langle j| - t\,|j+1\rangle\langle j| - t\,|j\rangle\langle j+1| \,)$$

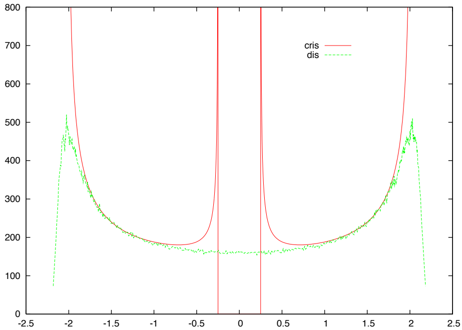
Diagonal disorder: t fixed, $\epsilon_b - \epsilon_a = \Delta$ fixed

Crystalline case:
ABABABABABABABABABABABABABABABABABAB............

Disordered case:
ABAABABBABABBAABABABBABAABABBABABBAA ....

Random choice with equal probability, average over many replicas.

Density of states

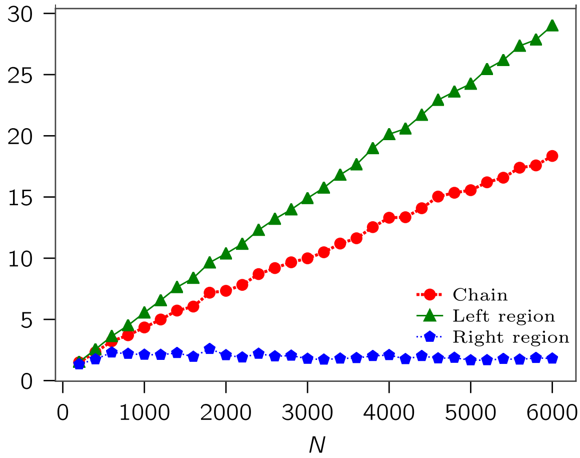


- At half filling both (crystalline and disordered) are insulating
- At any other filling the crystalline is conducting and the disordered is insulating.

Simulations for 1d heterojunctions

A. Marrazzo and R. Resta, Phys. Rev. Lett. **122**, 166602 (2019)

Local Souza-Wilkens-Martin sum rule.



Left half-chain: Metal

Right half-chain: Anderson insulator

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Formulæ for correlated & disordered systems (in a different Hilbert space)

Chern-Simons 1-form	Polarization **yes**
Chern-Simons 3-form	Axion term in magnetoelectrics **no**

Time-reversal odd (antisymmetric 2-forms)	**Time-reversal even** (symmetric 2-forms)
Anomalous Hall conductivity **yes** (insulators)	Souza-Wilkens-Martin sum rule **yes**
Magneto-optical sum rule **yes**	Drude weight **yes**
Orbital magnetization **no**	**???**