Theory of the insulating state: Part 2

Raffaele Resta

Trieste, 2020

Outline

1. The insulating state within PBCs
   - λ^2 in band insulators
   - Mott metal-insulator transition
   - Insulator-insulator transition (Mott-like)
2. Conductivity and Drude weight
3. Quantum geometry within OBCs
   - λ^2 in bounded samples
   - Model Anderson insulator in 1d
   - Anderson metal-insulator transition in 3d

Outline

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Wannier functions, one dimension, single band

- $L \to \infty$, q continuous:

$$X_\ell = \ell a \qquad |w_\ell\rangle = \frac{a}{2\pi} \int_{\mathrm{BZ}} dq \, \mathrm{e}^{iqX_\ell} \, |\psi_q\rangle$$

- $L = Ma$ finite, q_j discrete:

$$|w_\ell\rangle = \frac{1}{M} \sum_{j=1}^{M} \mathrm{e}^{iq_j X_\ell} \, |\psi_{q_j}\rangle$$

- **Caveat:** Gauge arbitrariness in $|\psi_{q_j}\rangle$

Invariance of the many-body ground state

- So far, we have written $|\Psi_0\rangle$ an N-particle Slater determinant of Bloch orbitals.
- Any determinant is invariant for unitary transformation of the vectors (orbitals) within the occupied manifold.
- We transform the **Bloch** (delocalized) orbitals into **Wannier** (localized) orbitals.
- In the **insulating case**:
  - The occupied manifold is the whole band: $|\Psi_0\rangle$ is invariant by such unitary transformation.
  - $|\Psi_0\rangle$ can be **equivalently** written as an N-particle Slater determinant of **Wannier** orbitals.
- What about the **metallic** case?

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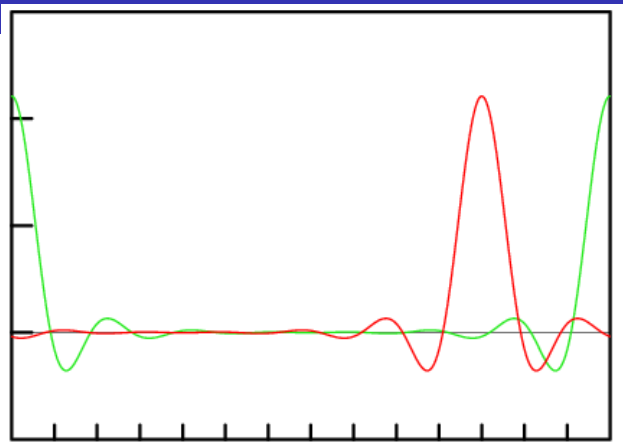
Invariance of the many-body ground state (cont'd)



- Finite L
  - In this drawing, again $L = Ma$, with $M = 14$:
  - Slater determinant built with M occupied Wannier orbitals $w_n(x)$.

- Infinite L $\quad (M \to \infty)$

$$|w_\ell\rangle = \frac{a}{2\pi} \int_{\mathrm{BZ}} dq \, \mathrm{e}^{iqX_\ell} \, |\psi_q\rangle$$

$$\int_{-\infty}^{\infty} dx \, |\langle x|w_\ell\rangle|^2 = 1 \qquad \textbf{finite!}$$

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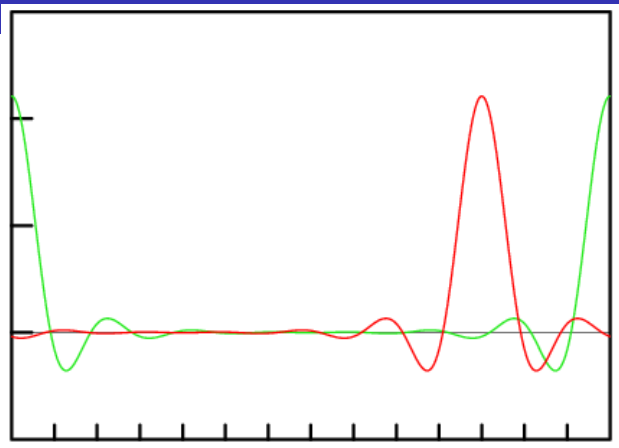

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Maximally localized Wannier functions

- With the **optimal** choice of the gauge:

$$|\langle x|w_\ell\rangle| \to 0 \qquad \textbf{exponentially} \text{ for } x \to \pm\infty$$

$$\langle w_n|x^2|w_n\rangle - |\langle w_n|x|w_n\rangle|^2 \qquad \textbf{minimum}$$

- The minimum "quadratic spread" is equal to the RS λ^2
- The spread diverges in the metallic case.
- **Caveat:** In $3d$ there are some complications: Marzari-Vanderbilt MLWFs (1997).

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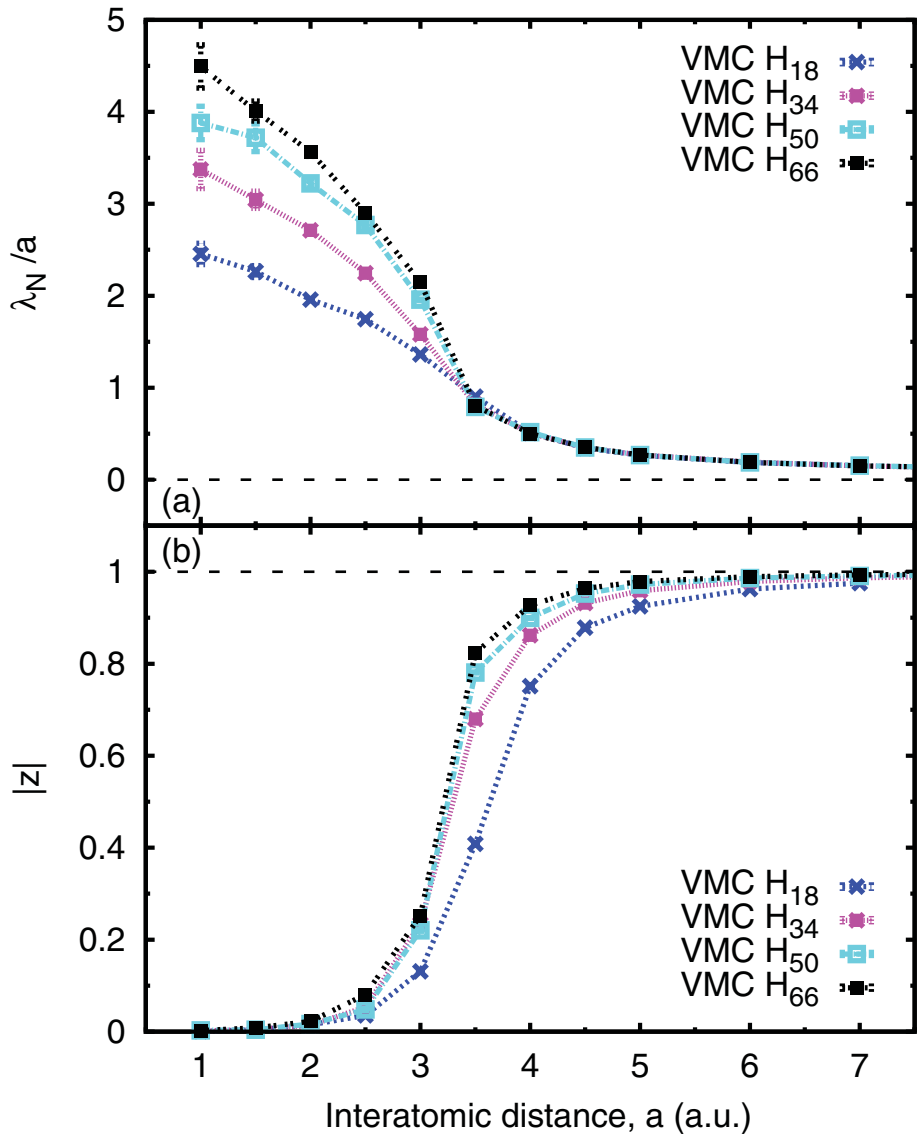
Implementation: Mott transition in H_N chains

Stella, Attaccalite, Sorella & Rubio, PRB 2011



localization length

(tensor in 3d)

$$\lambda_N^2 = -\frac{1}{N}\left(\frac{L}{2\pi}\right)^2 \ln |\mathfrak{z}_N|^2$$

Transition: $\simeq$ 3.5 bohr

Outline

Model $1d$ ionic crystal

$$\gamma = \mathrm{Im}\ \ln\ \langle\Psi_0|e^{i\frac{2\pi}{L}\left(\sum_\ell Z_\ell X_\ell - 2\sum_j x_j\right)}|\Psi_0\rangle = \pi \pmod{2\pi}$$

- $\mathbb{Z}_2$-odd: $P = e/2 \mod e$
- Tight-binding Hamiltonian:

$$H = \sum_j [\ (-1)^j \Delta\ |j\rangle\langle j| - t\,|j+1\rangle\langle j| - t\,|j\rangle\langle j+1|\ ]$$

- In second quantization notations:

$$H = \sum_j [\ (-1)^j \Delta\ c_j^\dagger c_j - t\ c_j^\dagger c_{j+1} - t\ c_{j+1}^\dagger c_j\ ]$$

$$\epsilon(k) = \pm\sqrt{\Delta^2 + 4t^2 \cos^2 ka/2}$$

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Model $1d$ ionic crystal

- Band structure:

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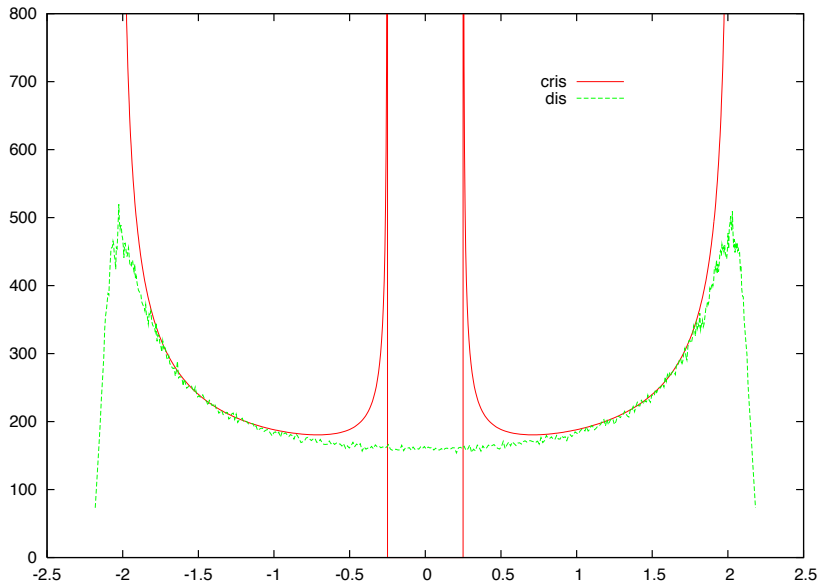
- Insulator at half filling
- Density of states $\mathcal{D}(\epsilon)d\epsilon$: **Red plot**



Tight binding 1d binary crystal again

- Introducing spin:

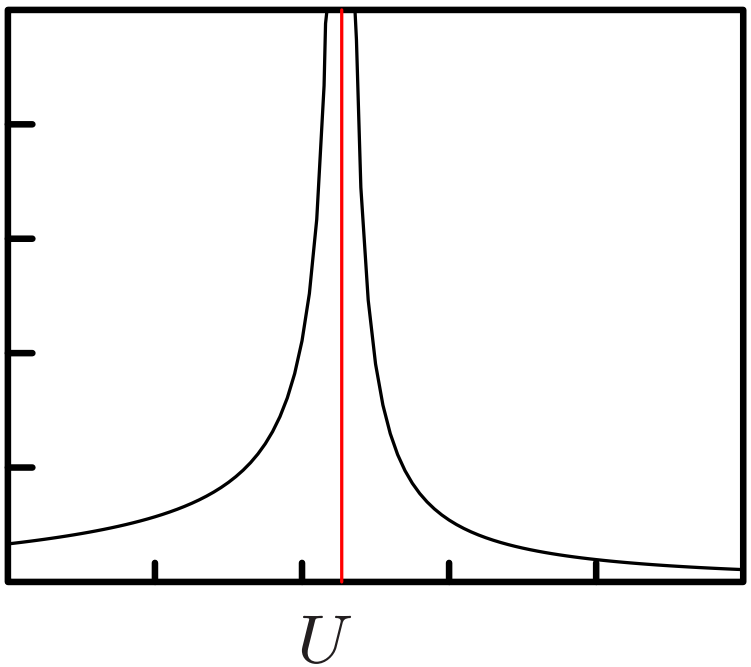
$$H = \sum_{j\sigma} [\ (-1)^j \Delta\ c^\dagger_{j\sigma} c_{j\sigma} - t(c^\dagger_{j\sigma} c_{j+1\sigma} + \text{H.c.})\ ]$$

- Introducing Hubbard on-site repulsion:

$$H = \sum_{j\sigma} [\ (-1)^j \Delta\ c^\dagger_{j\sigma} c_{j\sigma} - t(c^\dagger_{j\sigma} c_{j+1\sigma} + \text{H.c.})] + U \sum_j n_{j\uparrow} n_{j\downarrow}.$$

Monitoring the insulator-insulator transition

- Plot of λ^2 at half filling:



- **Metallic** only for a special U value
- On the left it is a **band-like insulator**
- On the right it is a **Mott-like insulator**
- What happens for $t = 0$?

Outline

Longitudinal conductivity (zero T)

$$\begin{aligned}\sigma^{(+)}_{\alpha\beta}(\omega) &= D_{\alpha\beta}\left[\delta(\omega)+\frac{i}{\pi\omega}\right]+\sigma^{(\text{regular})}_{\alpha\beta}(\omega)\\ &= \sigma^{(\text{Drude})}_{\alpha\beta}(\omega)+\sigma^{(\text{regular})}_{\alpha\beta}(\omega)\end{aligned}$$

- Both terms obtain from Kubo formulas
  (may include disorder & correlation, but **not** dissipation)
- The Drude weight $D_{\alpha\beta}$ is actually a **ground-state** property:
  it measures the (inverse) inertia of the many-electron system
  in the adiabatic limit

- The insulating state requires **both**:
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Drude weight according to Kohn (1964)

- Hamiltonian with a "flux" (a gauge transformation):

$$\hat{H}(\boldsymbol{\kappa}) = \frac{1}{2m} \sum_{i=1}^{N} |\mathbf{p_i} + \hbar\boldsymbol{\kappa}|^2 + \widehat{\mathbf{V}}$$

- Thermodynamic limit **after** taking derivatives
- PBCs violate gauge invariance in the conventional sense: E_0 **does** depend on $\boldsymbol{\kappa}$.

- Drude weight

$$D_{\alpha\beta} = \frac{\pi e^2}{\hbar^2 L^d} \left. \frac{\partial^2 E_0(\boldsymbol{\kappa})}{\partial \kappa_\alpha \partial \kappa_\beta} \right|_{\boldsymbol{\kappa}=0}$$

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Why RS discriminate insulators from metals

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- It **does not** obey PBCs
- Except for a commensurate $\boldsymbol{\kappa}_0$
- Does $|\tilde{\Psi}_0(\boldsymbol{\kappa}_0)\rangle$ coincide with the genuine $|\Psi_0(\boldsymbol{\kappa}_0)\rangle$?
  - **Yes** (modulo a phase) if $D = 0$
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Kohn's Hamiltonian within OBCs

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$$\hat{H}(\boldsymbol{\kappa}) = \frac{1}{2m}\sum_{i=1}^{N} |\mathbf{p_i} + \hbar\boldsymbol{\kappa}|^2 + \widehat{\mathbf{V}}$$

- Within OBCs:
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Many-body quantum metric within OBCs

- Quantum metric tensor (derivatives taken at $\boldsymbol{\kappa} = 0$))

$$\tilde{g}_{\alpha\beta} = \frac{1}{N}\left(\text{Re } \langle \partial_{\kappa_\alpha} \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle - \langle \partial_{\kappa_\alpha} \Psi_0 | \Psi_0 \rangle \langle \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle \right)$$

- Intensive ground state property, gauge-invariant (dimensions: squared length)

- **Basic tenet of the modern theory:**
  The OBCs metric $\tilde{g}_{\alpha\beta}$ in the thermodynamic limit
  - Diverges in all metals
  - Converges in all insulators
  - In the isotropic case $\tilde{g}_{xx}$ converges to λ^2.

Many-body quantum metric within OBCs

$$
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&= \frac{1}{N}\left(\langle \Psi_0 | \hat{r}_\alpha \hat{r}_\beta \Psi_0 \rangle - \langle \Psi_0 | \hat{r}_\alpha | \Psi_0 \rangle \langle \Psi_0 | \hat{r}_\beta \Psi_0 \rangle \right) \\
&= \frac{1}{2N} \int d\mathbf{r} d\mathbf{r}' \, (\mathbf{r} - \mathbf{r}')_\alpha (\mathbf{r} - \mathbf{r}')_\beta [\, n(\mathbf{r}) n(\mathbf{r}') - n^{(2)}(\mathbf{r}, \mathbf{r}') \,]
\end{aligned}
$$

- Exchange-correlation hole (integrates to -1):

$$
n_{xc}(\mathbf{r}, \mathbf{r}') = n^{(2)}(\mathbf{r}, \mathbf{r}') - n(\mathbf{r}) n(\mathbf{r}')
$$

- $\tilde{g}_{\alpha\beta}$ is the second moment of the XC hole, averaged over the sample

Special case: independent electrons

- Isotropic system in dimension d:

$$\tilde{g}_{xx} = \lambda^2 = \frac{1}{2Nd} \int d\mathbf{r} d\mathbf{r}' \, |\mathbf{r} - \mathbf{r}'|^2 [\, n(\mathbf{r}) n(\mathbf{r}') - n^{(2)}(\mathbf{r}, \mathbf{r}') \,]$$

- **Independent electrons:** $n^{(2)}(\mathbf{r}, \mathbf{r}')$ is a function of $\langle \mathbf{r} | \, \mathcal{P} \, | \mathbf{r}' \rangle$:

$$\begin{aligned} n(\mathbf{r}) n(\mathbf{r}') - n^{(2)}(\mathbf{r}, \mathbf{r}') &= 2 \, |\langle \mathbf{r} | \, \mathcal{P} \, | \mathbf{r}' \rangle|^2 \qquad \text{(spinful)} \\ &= |\langle \mathbf{r} | \, \mathcal{P} \, | \mathbf{r}' \rangle|^2 \qquad \text{(spinless)} \end{aligned}$$

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Tight binding 1d binary crystal

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

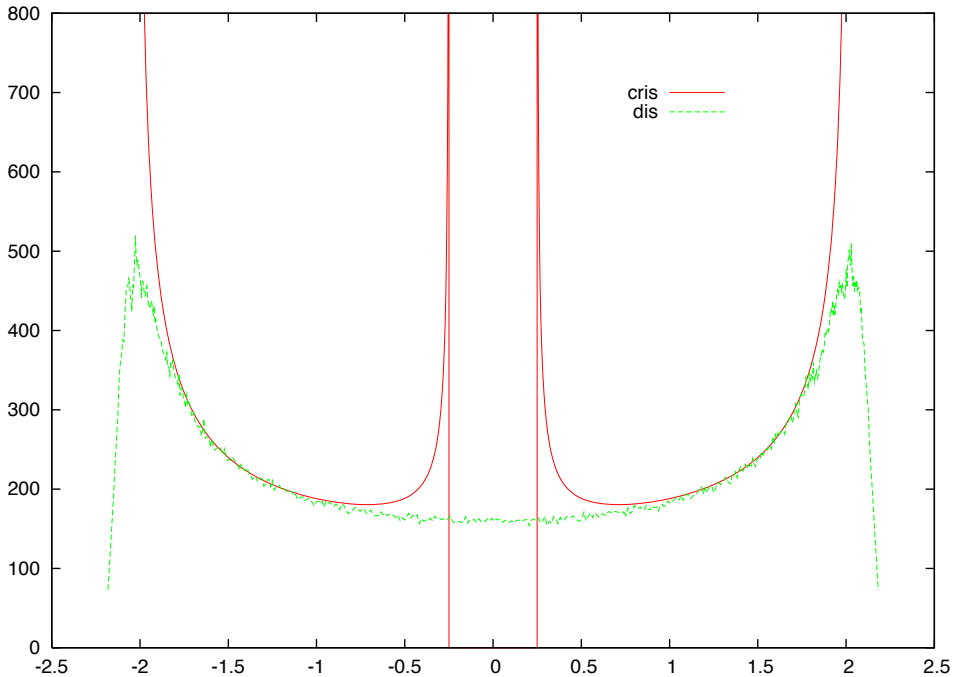
Diagonal disorder: t fixed, $\epsilon_b - \epsilon_a = 2\Delta$ fixed

Crystalline case: $\epsilon_j = (-1)^j \Delta$
ABABABABABABABABABABABABABABABABAB.....

Disordered case: random choice of ± 1 factors
ABAABABBABABBAABABABBABAABABBABABBAA .....

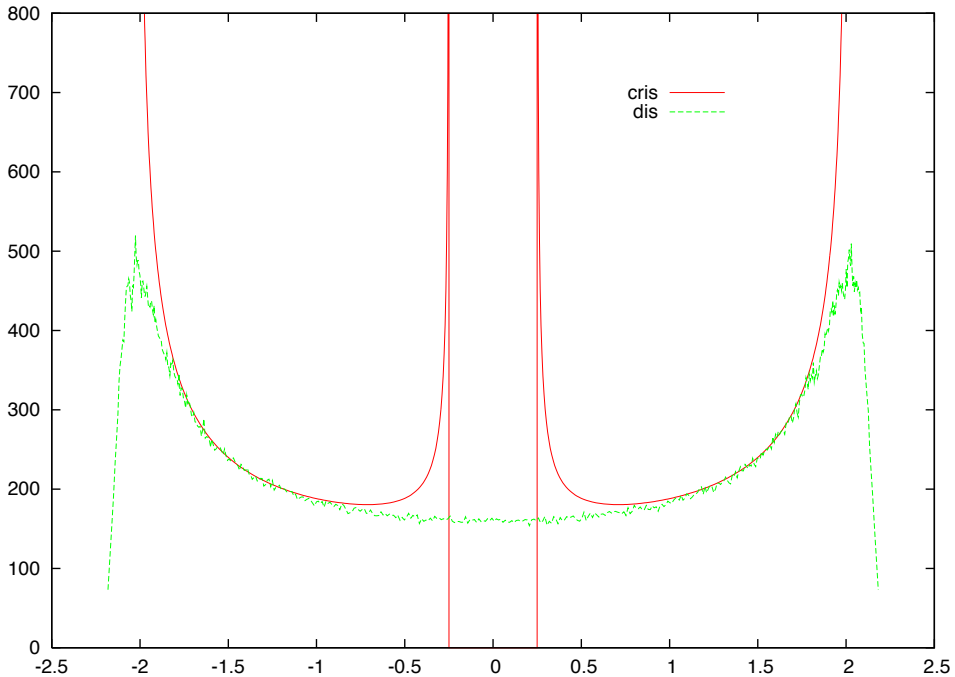
Random choice with equal probability, average over many replicas.

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.
- What about $\tilde{g}$ (a.k.a. λ^2)?

Density of states



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Results of the simulations
(5000 sites, 1000 replicas, 1/2 & 1/4 filling)

$$\tilde{g} = \frac{1}{2N} \int dx dx' \, (x - x')^2 |\langle x| \, \mathcal{P} \, |x'\rangle|^2 = \frac{a^2}{2N} \sum_{\ell,\ell'=1}^{N} P^2_{\ell\ell'} (\ell - \ell')^2$$

- In the crystalline case $\tilde{g}$ converges to a finite limit for 1/2 filling, diverges for 1/4 (as expected).
- In the disordered case $\tilde{g}$ always converge (to a very similar value for the two cases).
- The disordered case $\tilde{g}$ is about 20 times larger than the crystalline one. Why?
- The insulating mechanism (band vs. Anderson) is quite different, despite the very similar Hamiltonian.

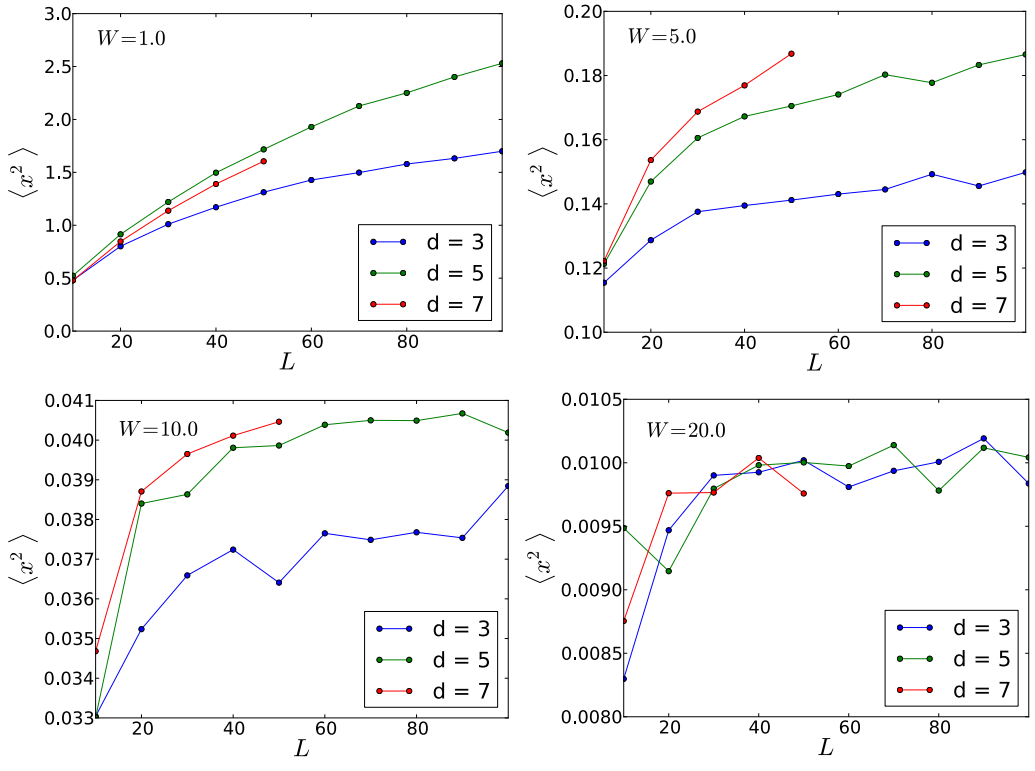
Outline

The benchmark model 3d system

- Need a 3d system to observe the **M-I transition**
- A standard 3d tight-binding Hamiltonian is known from previous literature to undergo the transition at $W_c = 8.25$ (W is the amount of tunable disorder, in appropriate units)
- In our (and others') simulations:
  - Computational samples are long rods of square section
  - Results are averaged over several disorder realizations
- The novelty here: use our marker to detect the transition **in the ground state**

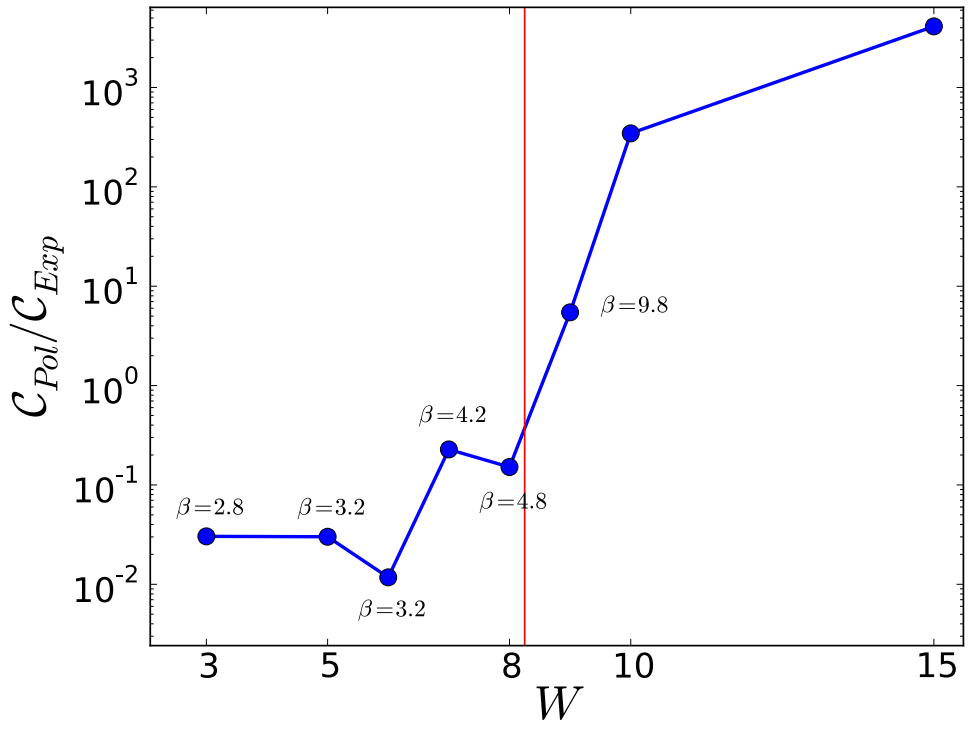
Anderson transition as a ground-state property

T. Olsen, R. Resta, and I. Souza, Phys. Rev. B **95**, 045109 (2017)



Localization length $\lambda = \sqrt{\tilde{g}_{\alpha\alpha}}$ as a function of rod length L
(average over 100 disorder realizations)

A smarter way to estimate W_c (by Thomas Olsen)



Our best estimate: $W_c = 8.5$

We are probing "the organization" of the electrons in their **ground state**

Summary

- Phenomenology:
  - Insulators differ from conductors in their dc conductivity;
  - But also: insulators and metals polarize in a different way.
- Kohn's (1964) vision:
  - Even before any probe is applied to the system, the **ground-state organization** of the electrons is different in insulators and metals (localized vs. delocalized)
- Quantitative sampling of Kohn's localization:
  - Resta-Sorella within PBCs
  - Relationship to Drude weight & conductivity
  - Quantum metric within OBCs