Bridging disorder & topology via large-scale simulation of condensed matter:
The open-source quantum KITE initiative

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KITE
quantum transport software

Topology & Disorder Beyond Perfect Crystals: NORDITA, 26 May - 13 June, 2025

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THE ROYAL SOCIETY

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Pioneering research and skills

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KITE co-founders (left to right → Ferreira, Rappoport, Lopes, João, Anđelković & Covaci)

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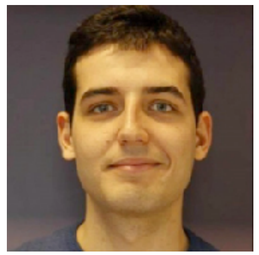

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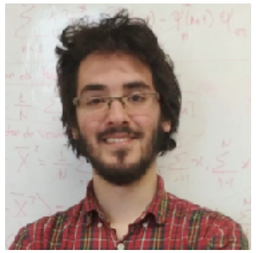

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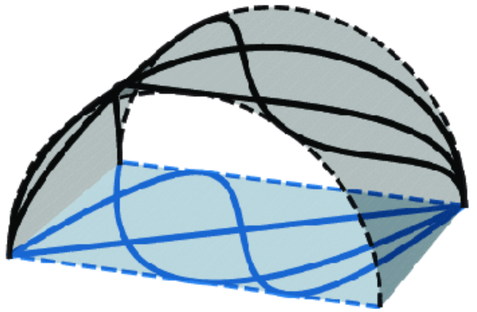
Outline

Part 1: Methodology

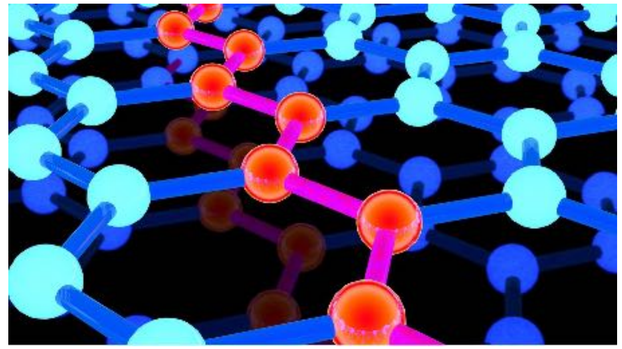


- ➡ Approximation theory (Chebyshev spectral expansions)
- ➡ Chebyshev methods in condensed matter physics

Part 2: Applications

- ➡ Disorder & Topology: from millions to billions of sites
- ➡ Open-source **KITE** initiative

KITE
quantum transport software



Motivation

$$H = H_{\mathrm{e}} + H_{\mathrm{I}} + H_{\mathrm{e\text{-}I}}$$

credit: isgs.illinois.edu

Full many-body problem is far too complex

Solution:

Break the problem into smaller parts,
construct effective theories, think differently!

Motivation

- Exact diagonalisation, many-body (diagrammatic) perturbation theory, $1/N$ expansions, etc.

- Specialised numerical / simulation tools: *DFT, DMRG, QMC, …*

- General-purpose spectral methods

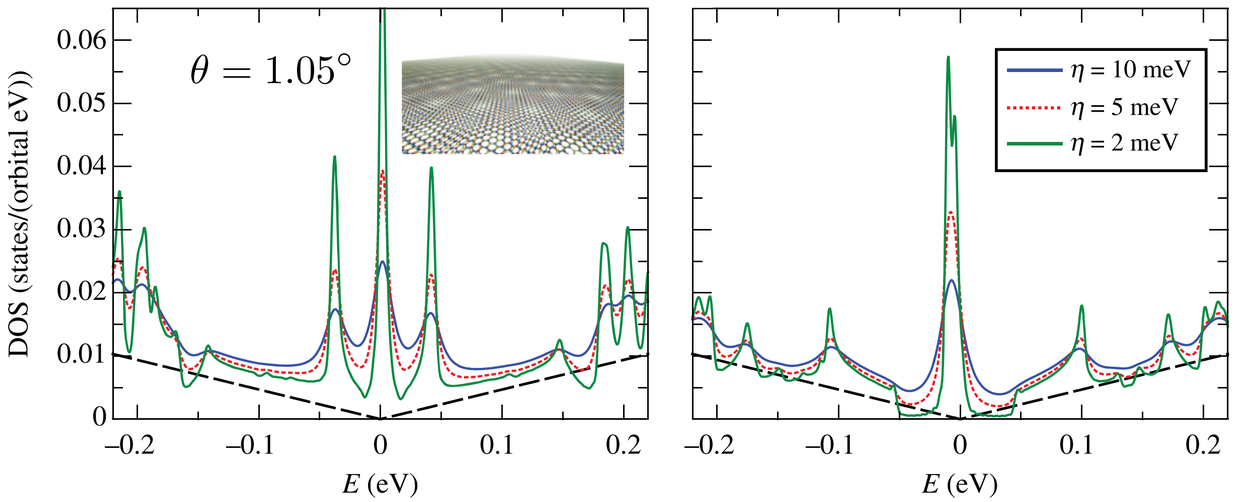
Motivation

João *et al.*, R. Soc. open sci. 7, 191809 (2020)

➡ Large-scale electronic structure in real space

DoS of twisted bilayer graphene

[(a) rigid non-relaxed lattice and (b) lattice relaxed by molecular dynamics]



- unit cell with 11908 orbitals (Z~60)
- 640 x 512 u.c. **~ 4 billion orbitals**

Approximation theory

Part 1a

“All science is dominated by the idea of approximation” (Bertrand Russel)

Approximation theory

John P. Boyd, Chebyshev & Fourier Spectral Methods (2001)

➡ Finding a suitable spectral approximation

$$f(\varepsilon) = \sum_n \langle \phi_n | f \rangle \phi_n(\varepsilon)$$

function of real variable (e.g., energy) defined on a finite interval, $\varepsilon \in [\varepsilon_{min}, \varepsilon_{max}]$

➡ Old problem in approximation theory (Chebyshev, 1854)

➡ There is an ideal polynomial interpolant, *so-called 'minimax polynomial'* $\min_{p \in P_M} \max_{\varepsilon} |f(\varepsilon) - p(\varepsilon)|$

➡ Pragmatically, near-minimax approximations based on orthogonal polynomials are best

Approximation theory

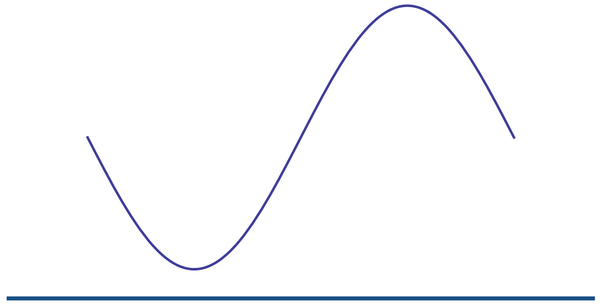
John P. Boyd, Chebyshev & Fourier Spectral Methods (2001)

➡ Choice of basis set

Boyd's moral principle:

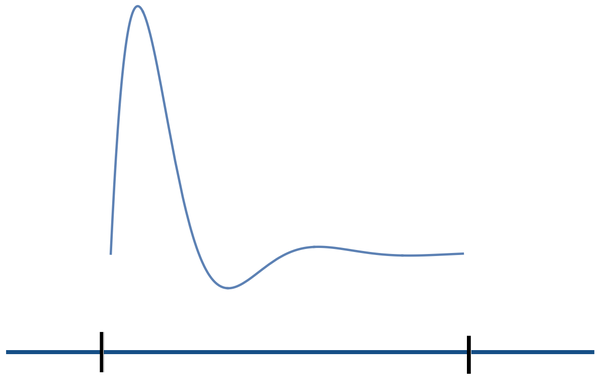
"Unless you are <u>really, really sure</u> another set of basis functions is better, use Chebyshev polynomials"

PERIODIC



Fourier

NON-PERIODIC



Chebyshev

Approximation theory

➡ Chebyshev polynomials of the first kind

A Fourier series *in disguise*, yet non-periodic and defined on a finite interval

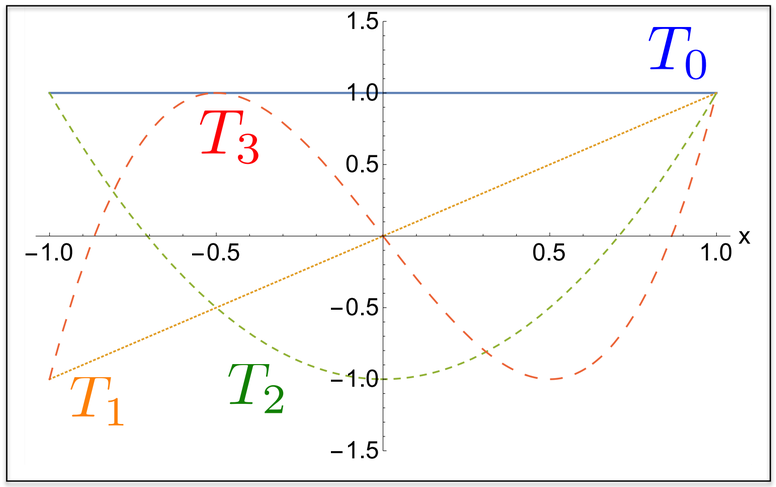
$$T_n(\cos\theta) = \cos(n\theta) \qquad n \in \mathbb{Z}_0^+$$

$$T_0(x) = 1$$

$$T_1(x) = x \qquad \ldots$$

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

Chebyshev recursion rule



Approximation theory

➡ Finding a suitable spectral approximation

1st step:

$$\{\phi_n(x)\}$$

Chebyshev polynomials: $T_n(x)$

2nd step:

$$\mu_n = \langle \phi_n | f \rangle$$

efficient determination of expansion moments

weight function associated to $\{\phi_n(x)\}$

$$f_N(x) = \omega(x) \sum_{n=0}^{N-1} \mu_n T_n(x)$$

N-order approximation

Part 1b

Large-scale real-space Chebyshev expansions: ***key ideas & milestones***

The idea

First, rescale $\hat{H}$ so that (dimensionless) eigenvalues E fall into the canonical interval $\varepsilon \in [-1:1]$

$$\hat{H} \to \hat{h} = \frac{\hat{H} - \delta E\_ \mathbf{1}}{\delta E_+}$$

$$\delta E_\pm + = \frac{E_{max} \pm E_{min}}{2}$$

$E_{max/min}$ *are some reasonable upper/lower energy bounds*

Lattice Hamiltonian

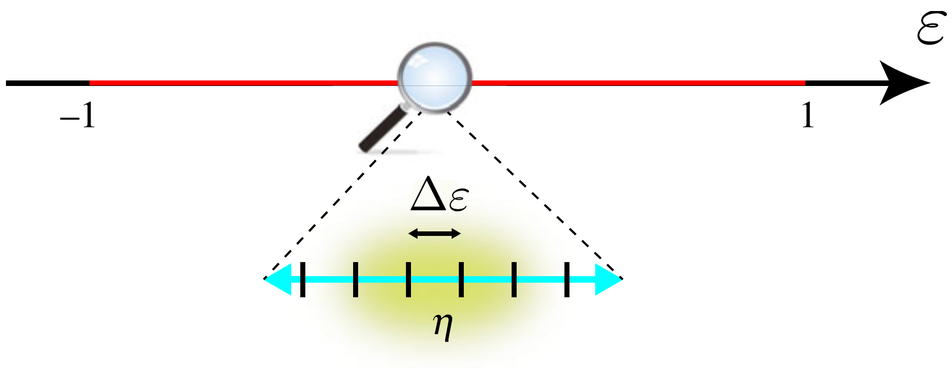
$dim\, \hat{H} = D$

Spectral expansions in condensed matter

The idea

Reconstruct target function (e.g. LDoS) with spectral resolution:

$$\Phi(\mathbf{x},\varepsilon) \simeq \omega(\varepsilon) \sum_{n<N} \mu_n(\mathbf{x}) T_n(\varepsilon)$$



resolution $\eta \approx \Lambda/N$

"Bandwidth"

$$\Lambda = 2\delta E_+$$

Mean level spacing

$$\Delta\varepsilon = \Delta\varepsilon(L)$$

Spectral expansions in condensed matter

➡ Types of Chebyshev moments

Single expansion

$$\mu_n = \mathrm{Tr}[T_n(\hat{h})]$$

For 1-particle Green's functions
and related quantities (e.g. DoS)

Double expansion

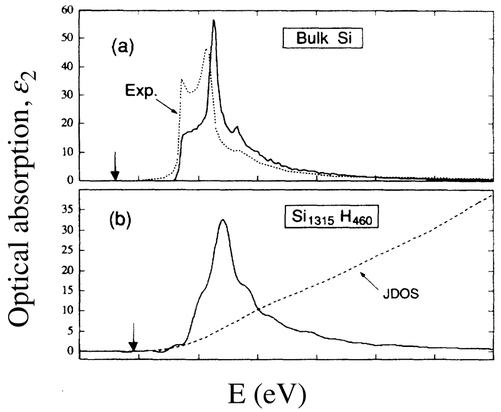
$$\mu_{nm} = \mathrm{Tr}[\hat{A}\, T_n(\hat{h})\, \hat{B}\, T_m(\hat{h})]$$

For 2-particle Green's functions
(e.g. optical conductivity)

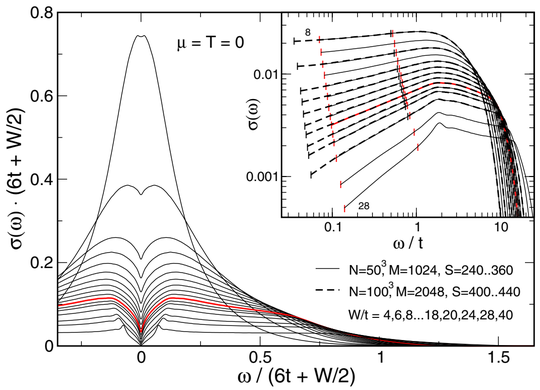
Spatially resolved quantities (e.g., local Chern marker):

$$\mu_{nm}^{i,\alpha} = \langle i,\alpha|T_n(\hat{h})\, \hat{X}\, T_m(\hat{h})\, \hat{Y}|i,\alpha\rangle$$

First large-scale calculations



Wang & Zunger, PRL 73 1039 (1994)



Weisse, EPJB 40 125 (2004)

D	*Si quantum dots with 1,000 atoms*	*Anderson model with million sites*
N	*500 x 500 moments*	*1000 x 1000 moments*
R	*tens of realisations*	*hundreds of realisations*

$$O = D \times N \times R$$

$O = 10^{10}$ → $O = 10^{14}$

However … ***"Understanding grows only logarithmically with the number of floating point operations" (J.P. Boyd)***

Bridging disorder and topology on the large scale

Part 2a

From millions ($D = 10^6$) to billions ($D = 10^9$) atomic orbitals

Bridging disorder and topology on the large scale

Ferreira & Mucciolo, Phys. Rev. Lett. 114, 116602 (2015)

➡ Chebyshev polynomial Green's function (CPGF) method

Exact decomposition of lattice Green's functions

$$\hat{\mathcal{G}}(z) = \sum_n g_n(z)\, T_n(\hat{h})$$

$z = \varepsilon + i\eta$

➡ CPGF coefficients have a simple closed-form solution

➡ Control over energy resolution

Bridging disorder and topology on the large scale

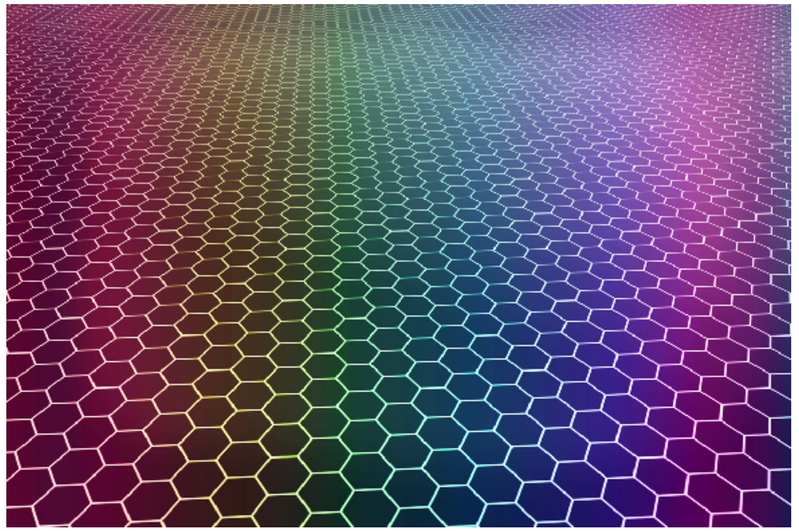
Ferreira & Mucciolo, Phys. Rev. Lett. 114, 116602 (2015)

➡ **Chiral disordered graphene (BDI class):** super-metallic zero-energy modes

Graphene with dilute random vacancies

$$\sigma_{xx}(\varepsilon = 0) = \frac{4e^2}{\pi h} + \text{weak correc.}$$

Ostrovsky, Gornyi & Mirlin, PRB 74, 235443 (2006)



A numerically-exact real-space approach would be ideal!

$$l_{\text{mfp}} \sim n_v^{-1} \qquad L \gg l_{\text{loc}}, l_{\text{mfp}}$$

Challenge: Mean free paths can easily reach hundreds *nm*!

Bridging disorder and topology on the large scale

Ferreira & Mucciolo, Phys. Rev. Lett. 114, 116602 (2015)

➡ **Chiral disordered graphene (BDI class):** super-metallic zero-energy modes

‘single-shot’ algorithm

$$\sigma_{xx}(z) \simeq \langle R|\Im\hat{\mathcal{G}}(z)\,\hat{v}_x\;\Im\hat{\mathcal{G}}(z)\,\hat{v}_x|R\rangle$$

$\langle\psi_L(z)|$ $\quad$ $|\psi_R(z)\rangle$

disorder average

$$\sigma_{xx}(z) \simeq \overline{\langle\psi_L(z)|\psi_R(z)\rangle}$$

$$O \simeq 2\,D\,N \propto D^{3/2}$$

Bridging disorder and topology on the large scale

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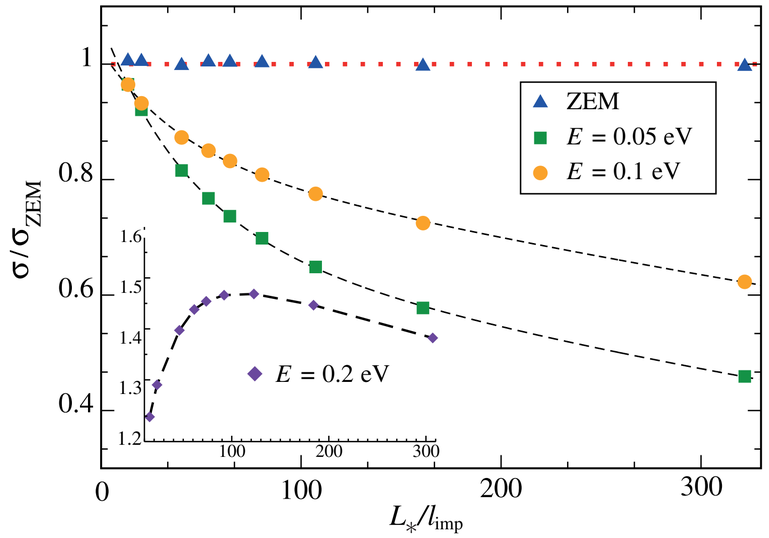
➡ **Chiral disordered graphene (BDI class):** super-metallic zero-energy modes

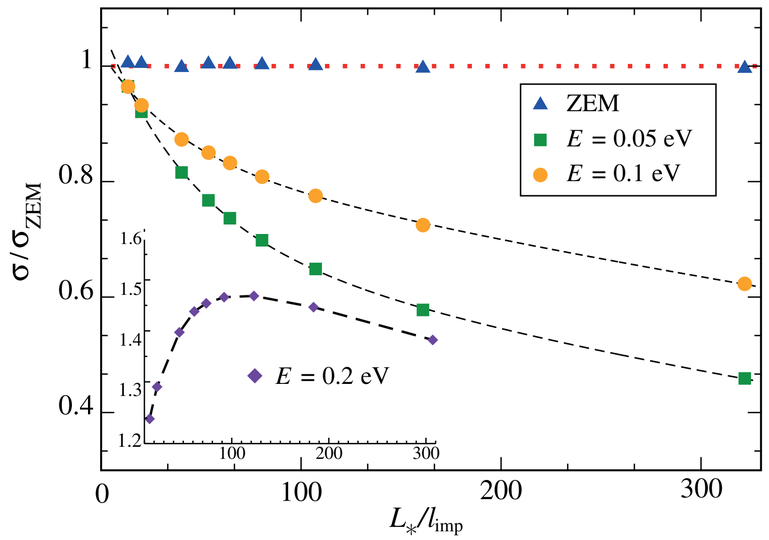


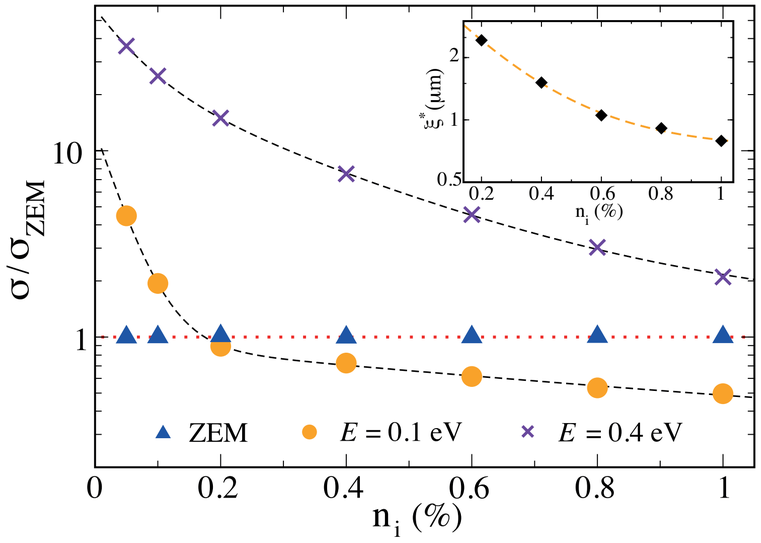
- **3.6 billion sites**
- **0.4% vacancy concentration**
- **N = 12000** (for each Green's function in the 2-particle response function)

Bridging disorder and topology on the large scale

Ferreira & Mucciolo, Phys. Rev. Lett. 114, 116602 (2015)

➡ **Chiral disordered graphene (BDI class):** super-metallic zero-energy modes





$$\sigma_{xx} = \frac{4e^2}{\pi h}\,(1 \pm 0.01)$$

Universal value within accuracy

- **3.6 billion sites**
- **N = 12000** (for each Green's function in the 2-particle response function)

Bridging disorder and topology on the large scale

Offidani & Ferreira, Phys. Rev. Lett. 121, 126802 (2018); **João *et al.***, R. Soc. open sci. 7, 191809 (2020)

➡ **Chern insulators:** quantum anomalous Hall effect & magneto-optical response

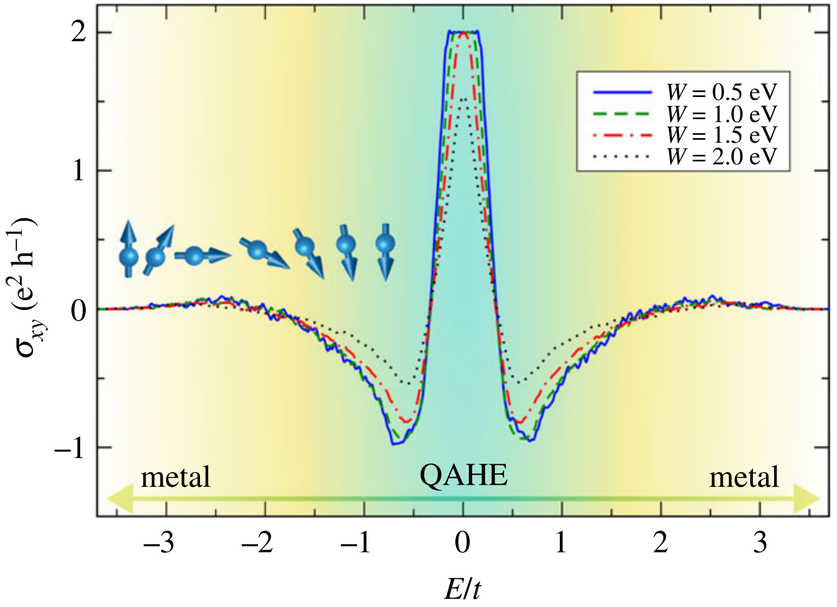
‘full-spectral’ algorithm

$$\sigma_{xy}(z) \propto \int_{-1}^{\varepsilon_F} d\varepsilon \, \mathrm{Re}\,\mathrm{Tr}\left[i\hat{v}_x \, \partial_z \hat{\mathcal{G}}(z) \, \hat{v}_y \, \Im\hat{\mathcal{G}}(z) \right]$$

➡ Double Chebyshev expansion

➡ Minimum RAM: 8 GB (double complex precision)

ferromagnetic graphene



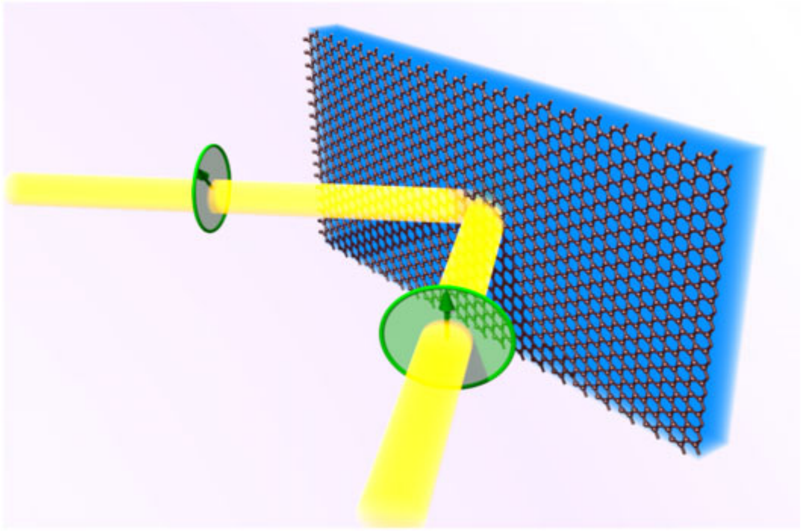
- 8192×8192 lattice
- $M_t = 4.2 \times 10^6$

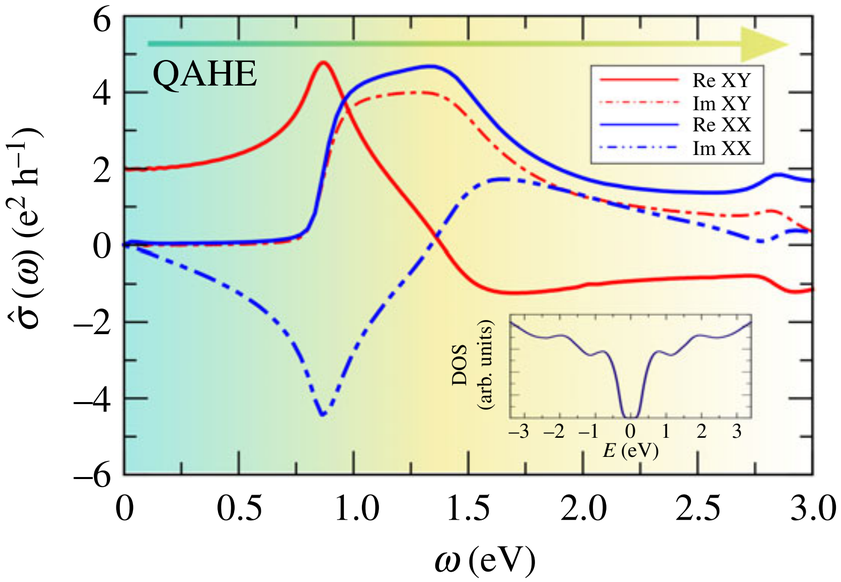
Bridging disorder and topology on the large scale

Offidani & Ferreira, Phys. Rev. Lett. 121, 126802 (2018); **João *et al.***, R. Soc. open sci. 7, 191809 (2020)

➡ **Chern insulators:** quantum anomalous Hall effect & magneto-optical response

‘full-spectral’ algorithm: optical conductivity tensor





Bridging disorder and topology on the large scale

Veiga *et al.*, to appear (2025)

➡ **Topology and geometry in disordered condensed matter**

Space-resolved quantum geometric tensor

$$\langle \mathbf{x}| \, \mathcal{P} \, x \, (1 - \mathcal{P}) \, y \, \mathcal{P} |\mathbf{x}\rangle = \Omega_{xy}(\mathbf{x}) + i \, (2\pi)^{1-d} \, \mathcal{C}(\mathbf{x})$$

Metric (geometry)

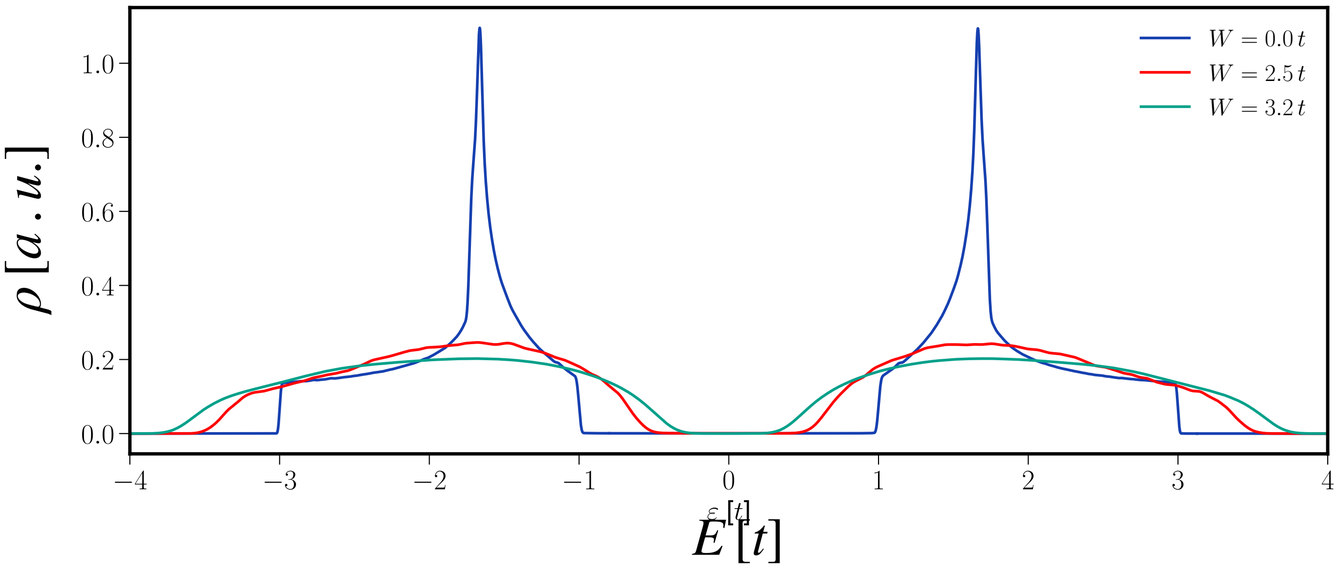
Local marker (topology)

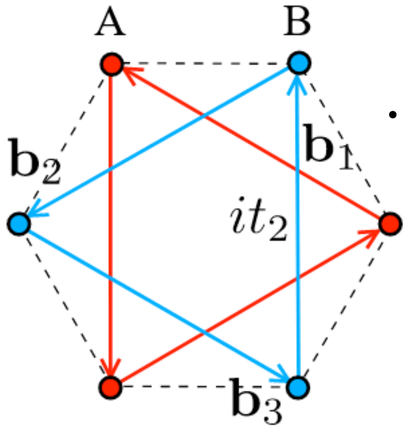
Bridging disorder and topology on the large scale

Veiga *et al.*, to appear (2025)

➡ **Local Chern marker statistics**

Average DoS overview





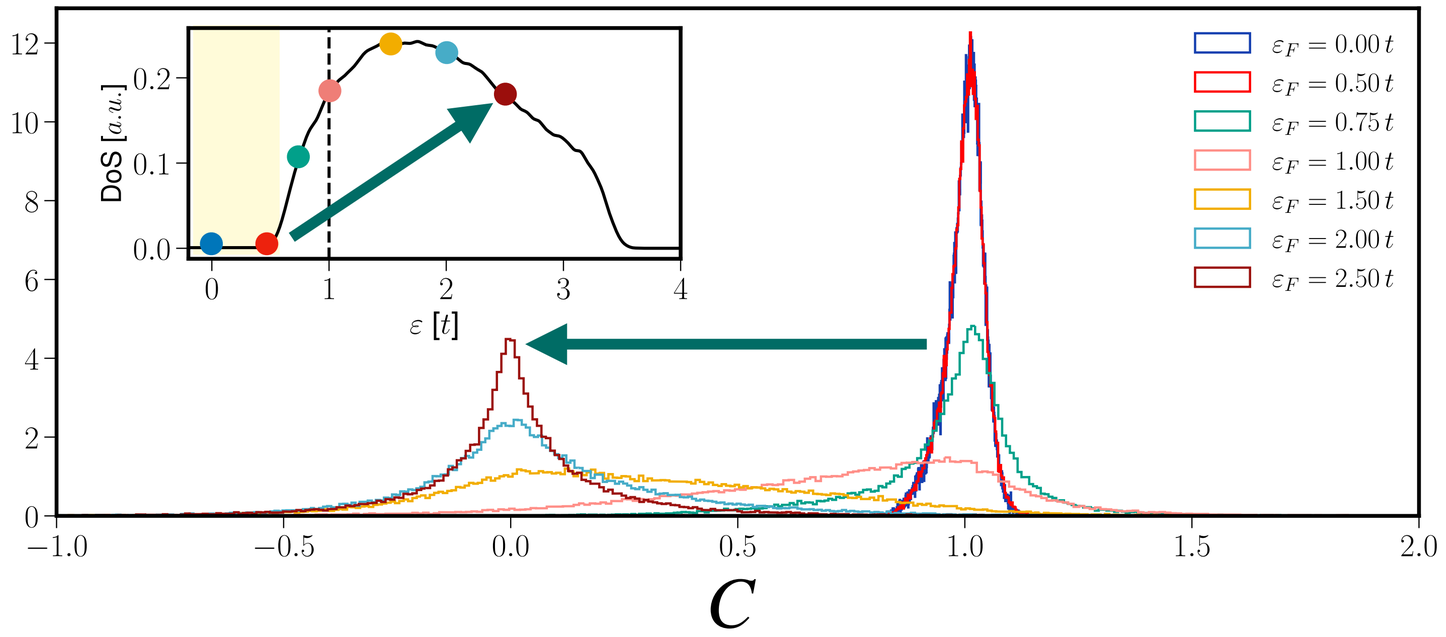
Haldane model

- $t_2 = t/3$
- 512×512 lattice
- $\eta \approx 0.01t$

Bridging disorder and topology on the large scale

Veiga *et al.*, to appear (2025)

➡ Local Chern marker statistics



$W = 2.5t$

65000 samples

512 samples take 1.5 hours to run on 4 cores.

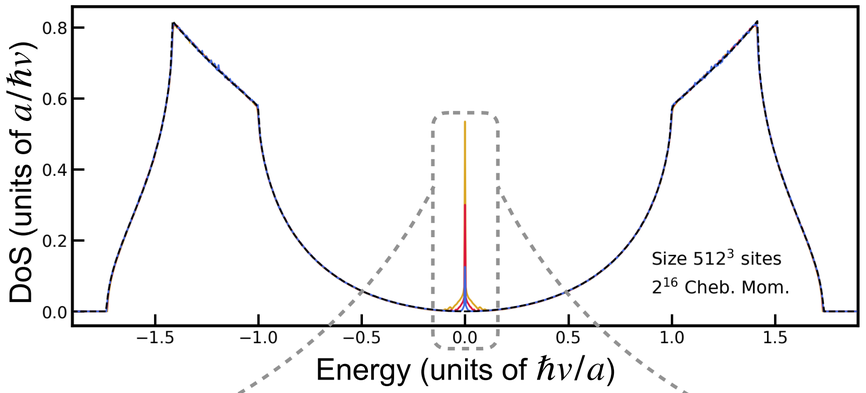
➡ Chern PDFs are stable within and near the single-particle gap

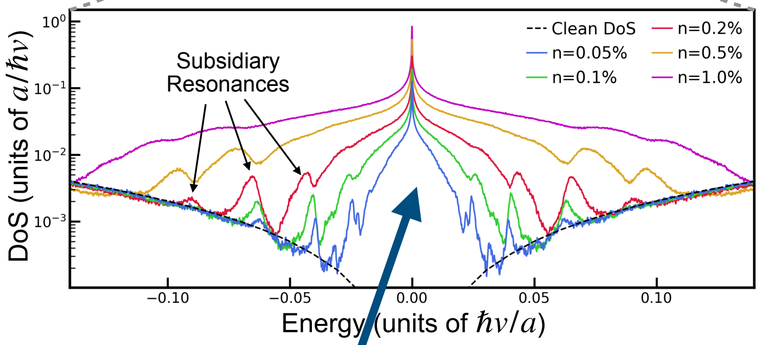
➡ Topological phase transitions are observed changing W and/or ε

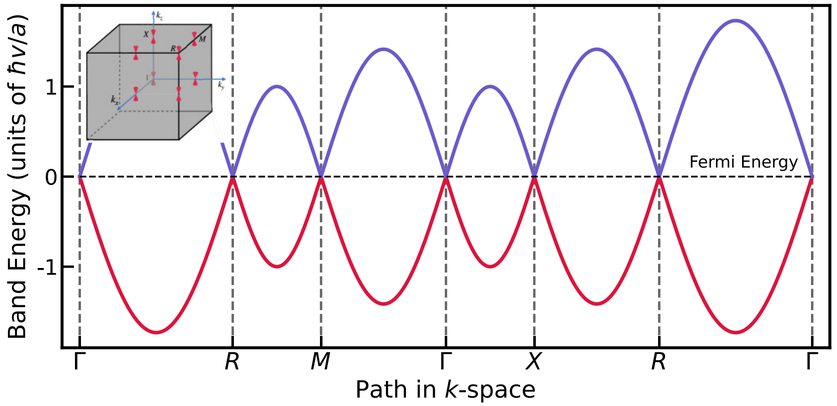
Bridging disorder and topology on the large scale

J. Pires *et al.*, Phys. Rev. Res. 3, 013183 (2021) J. Pires *et al.*, PRB 106, 184201 (2022) J. Pires *et al.*, PRL 129, 196601 (2022)

➡ **Weyl semi-metal:** diffusive metallic phase and anomalous transport due to point defects







- 256 million orbitals
- 65536 moments

Lifting of nodal DoS at arbitrary small n: no topological protection

Bridging disorder and topology on the large scale

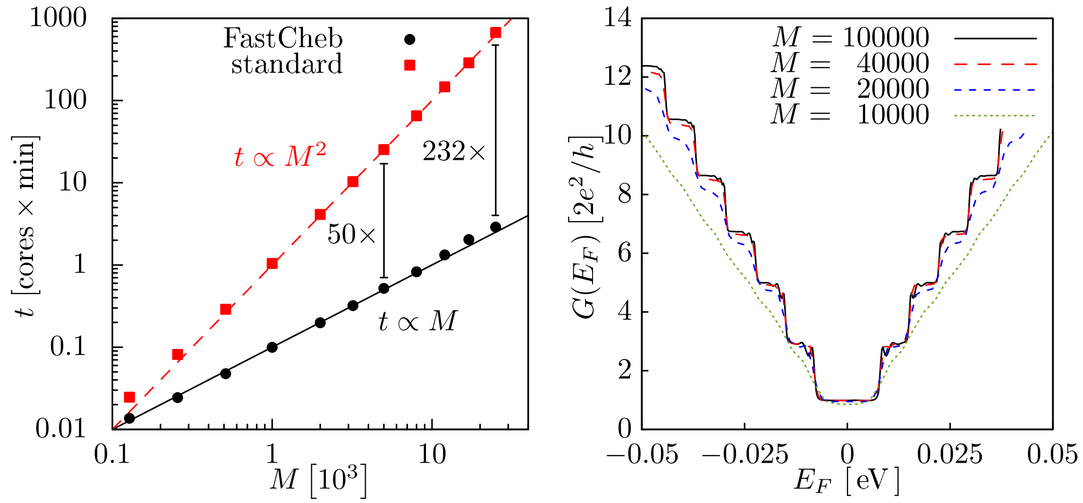
Castro *et al.*, PRB 107, 045418 (2023); Castro *et al.*, PRL 132, 076302 (2024)

➡ **FastCheb: Fast Fourier-Chebyshev algorithm for ultra-high resolution simulations**

➡ $O(DN \ln N)$ *[all energies at once]*

➡ **tens of billions** of moments - *fast & accurate*

Benchmark on a ballistic 2-terminal graphene device



- $N_t = M^2 = 10^{10}$

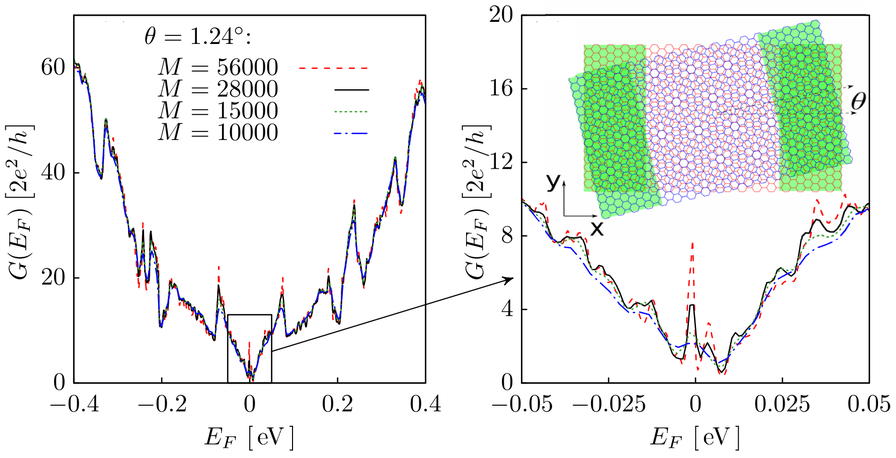
Bridging disorder and topology on the large scale

Castro *et al.*, PRB 107, 045418 (2023); Castro *et al.*, PRL 132, 076302 (2024)

➡ Ultra-high resolution quantum transport

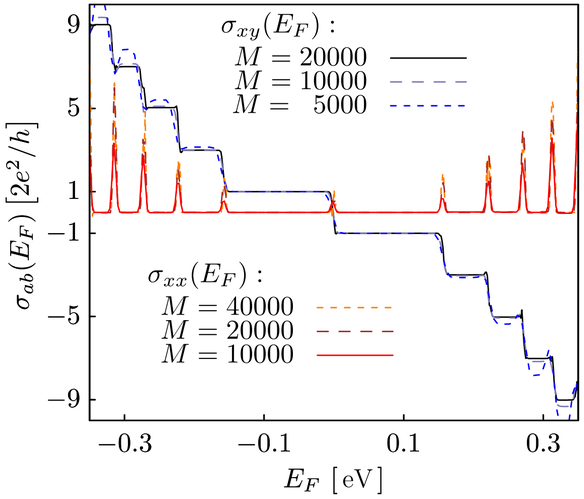
Fast Fourier-Chebyshev algorithm

Twisted bilayer graphene ($\theta = 1.1°$)



- 10^7 lattice sites
- $N_t = M^2 \simeq 3.1 \times 10^9$

Quantum Hall effect



- 10^7 lattice sites
- $W = 0.1t$
- $\Phi = 3 \times 10^{-4} h/e$

Part 2b: KITE open-source initiative

https://quantum-kite.com

Suite of algorithms for real-space simulation of condensed matter

➡ Open-source code

➡ Extensive on-line documentation

➡ Github repository (2 approvals for new push requests)

➡ Users and developers workshops

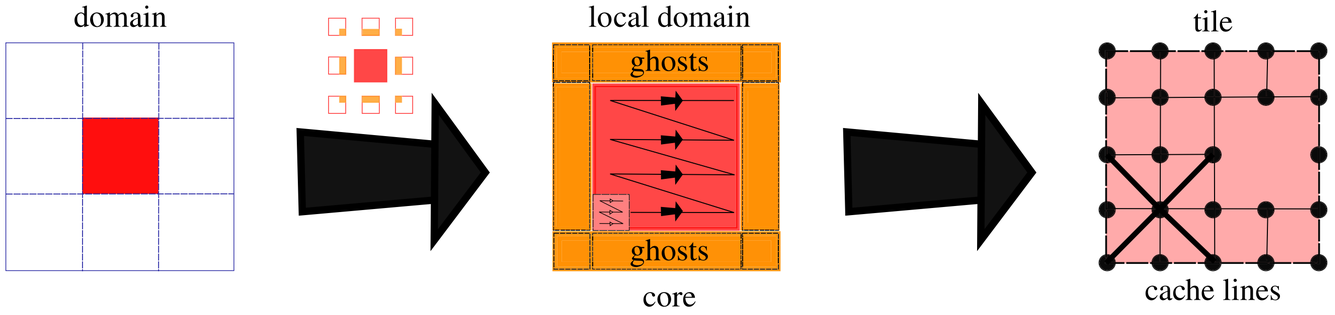
Part 2b: KITE open-source initiative

Efficiency

Design-level optimisation

- On-the-fly **matrix-free** computations
- CPU-memory “alignment” to minimise cache-to-cache transfers and cache misses
- **Optimal multi-threading scaling**

J. Lopes
(U Porto)



Inner workings

$$\mu^{m_i \ldots m_p}_{n_1 \ldots n_N} = \langle \hat{X}_{m_1} T_{n_1}(\hat{h})\, \hat{Y}_{m_1} \ldots \hat{X}_{m_p}\, T_{n_N}(\hat{h})\, \hat{Y}_{m_p} \rangle$$

$$\mathrm{LDoS}(\vec{x}, \epsilon)$$

$$\sigma_{ij}(\mu, T, \omega, \vec{q})$$

$$\Omega_{\alpha\beta}(\mathbf{x})$$

generalised Chebyshev moments (N-particle Green's functions)

- **stable**
- **accurate**
- **general-purpose**

Part 2b: KITE open-source initiative

Functionalities

	Algorithms	Type	#orbitals	Availability
Models	*N.A.*	**LCAOs 1D / 2D / 3D**	*N/A*	v1.0
Disorder	*N.A.*	**Generic multi-orbital (short-range)**	*N/A*	v1.0
B field	*N.A.*	Vector B aligned with a desired crystal axis	*N/A*	v1.0 - v1.1
LDOS/ARPES	Full Spectral	Generic, High-Resolution	$O(10^{10})$	v1.0
Linear RFs	Full Spectral	**DC, AC, XX, XY, spin, orbital, etc.**	$O(10^{8})$	v1.0 - **v1.2**
Linear RFs	Single Shot	High-Resolution (FS response)	$O(10^{10})$	v1.0
Nonlinear RFs	Full Spectral	2nd order	$O(10^{7})$	v1.0
t-Dynamics	Single Shot	Generic, High-Resolution	$O(10^{10})$	v1.0
Geometry & Topology	Single Shot	Generic, High-Resolution	$O(10^{10})$	**v1.2**

Part 2b: KITE open-source initiative

Workflow

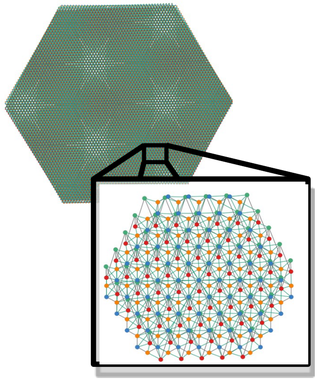
- import / build model
- ‘disorder cell‘
- target functions
- visualisation tools

KITEx (C++)

(I/O)

post-processing tools

DoS: TBLG Θ=1.05
(12k atoms, 70k hoppings p/ cell)
4 billion atoms



```
lattice = pb.load('tbl')

configuration = kite.Configuration(
        divisions=[5, 4],
        length=[640, 512],
        boundaries=[True, True],
        is_complex=False,
        precision=0,
        spectrum_range=[- 11.7, 9.3])

calculation = kite.Calculation(configuration)
calculation.dos(num_points=5000,
        num_moments=12000, num_random=1,
        num_disorder=1)

kite.config_system(lattice, configuration,
        calculation, filename='config.h5')
```

KITE + pybinding

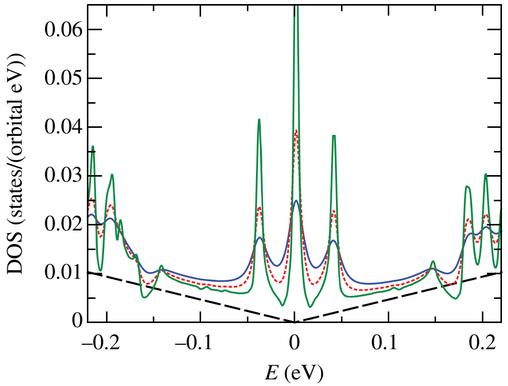
./KITEx config.h5

$$\mu_n = \mathrm{Tr}\left[T_n\left(H\right)\right]$$

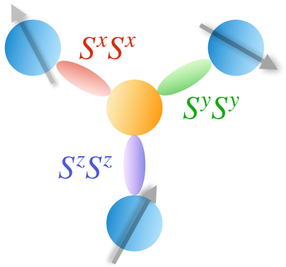
./KITE-tools config.h5

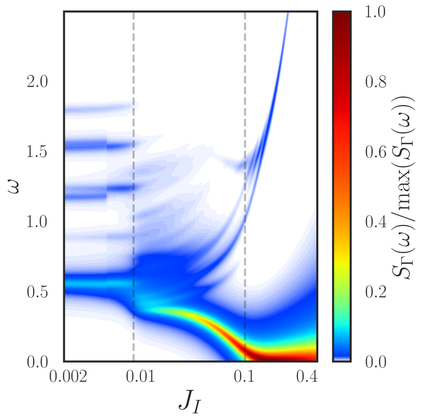
$$\rho\left(\varepsilon\right) = \sum_n \mu_n \Delta_n\left(\varepsilon\right)$$

KITE



Part 2b: KITE open-source initiative



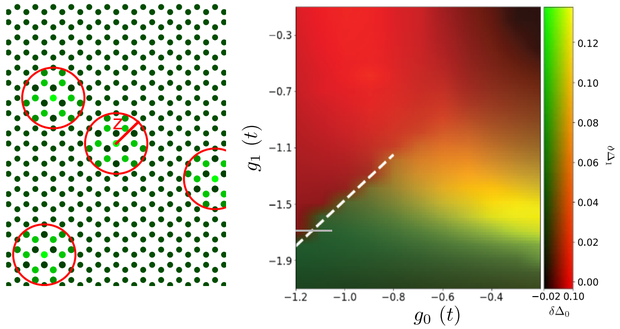


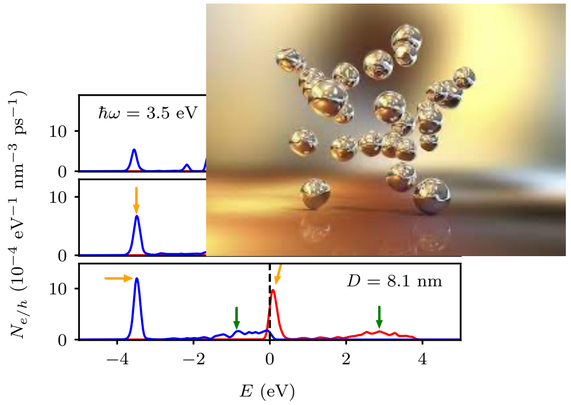
Finite-*T* Chebyshev Polynomial (FTCP) &
Hybrid Lanczos-Chebyshev (HLC) methods
(Brito & Ferreira, 2024)

strongly correlated systems

disordered superconductors

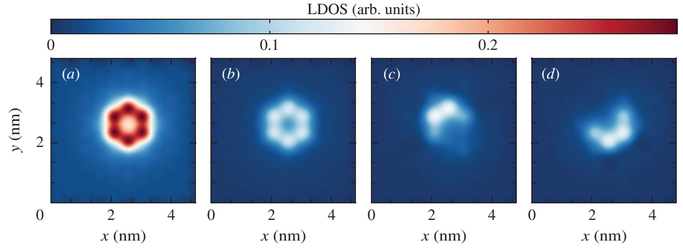
(Joao, Lopes & Ferreira, 2024)





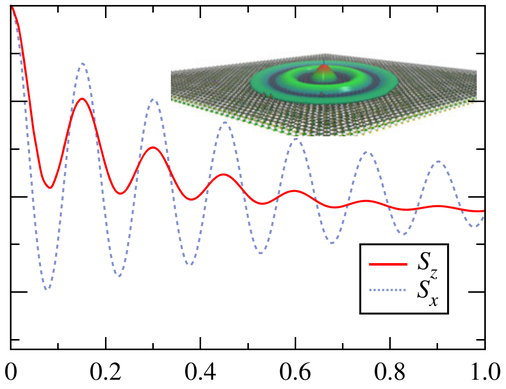
plasmonics

(Jin *et al.*, 2022)



real-space LDOS

(Joao *et al.*, 2020)



dynamics

(Joao *et al.*, 2020)

Outlook & Next steps

➡ **Chebyshev spectral methods:** real-space simulation of condensed matter on large scales

➡ **Soon, KITE v1.2 with new functionalities:** quantum geometry, topology & flavoured (orbital/spin) vertex operators

➡ **Future additions to the KITE open-source code:** superconductivity, interacting spin models, …

The community (i.e. you!) will be key to inspire and drive new developments: get in touch with us!

Thank you!