Calculations of spectral quantities in quantum systems using kernel polynomial method

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Outline

Outline for section 1

Introduction

Behavior of particles depending on eigenvalues of Hamiltonian.

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Dimensions $\sim D$,

- memory requirement $\sim D^2$,
- computation time requirement $\sim D^3$.

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KPM scales:

- for sparse matrices: $\sim D$,
- for dense matrices: $\sim D^2$.

Outline for section 2

Mathematical formalism

Define scalar product:

$$\langle f|g\rangle = \int_a^b w(x)f(x)g(x)dx, \tag{1}$$

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Function can be expanded:

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty} \alpha_n p_n(x) \\ \alpha_n &= \langle p_n|f\rangle h_n \end{aligned} \tag{3}$$

Interval of definition for Chebyshev polynomials $[-1, 1]$

Definition

$$
\begin{aligned}
w_1(x) &= \left(\pi\sqrt{1-x^2}\right)^{-1}, \quad w_2(x) = \pi\sqrt{1-x^2}, \\
\langle T_n | T_m \rangle_1 &= \frac{1+\delta_{n,0}}{2}\delta_{n,m}, \quad \langle U_n | U_m \rangle_2 = \frac{\pi^2}{2}\delta_{n,m}.
\end{aligned}
\tag{4}
$$

Chebyshev polynomials can be expressed as:

$$T_n(x) = \cos\left[n \arccos\left(x\right)\right], \tag{5}$$

and

$$U_n(x) = \frac{\sin\left[(n+1)\arccos\left(x\right)\right]}{\sin\left[\arccos(x)\right]}. \tag{6}$$

Polynomials are obeying recursive relations:

$$P_{m+1}(x) = 2xP_m(x) - P_{m-1}(x), \quad P \equiv T \vee U \tag{7}$$

Mathematical formalism
Modified moments

$$
\begin{aligned}
f(x) &= \sum_{n=0}^{\infty} \frac{\langle f | T_n \rangle_1}{\langle T_n | T_n \rangle_1} T_n(x) = \alpha_0 + 2 \sum_{n=1}^{\infty} \alpha_n T_n(x), \\
\alpha_n &= \langle f | T_n \rangle_1 = \int_{-1}^{1} \frac{f(x) T_n(x)}{\pi \sqrt{1 - x^2}} dx.
\end{aligned}
\tag{8}
$$

we can modify the moments:

$$
\begin{aligned}
f(x) &= \frac{1}{\pi \sqrt{1 - x^2}} \left[\mu_0 + 2 \sum_{n=1}^{\infty} \mu_n T_n(x) \right], \\
\mu_n &= \int_{-1}^{1} f(x) T_n(x) dx.
\end{aligned}
\tag{9}
$$

Problems may arise after the simple truncation of series:

$$f(x) \approx \frac{1}{\pi\sqrt{1-x^2}}\left(\mu_0 + 2\sum_{n=1}^{N-1}\mu_n T_n(x)\right), \tag{10}$$

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$$f(x) \approx \frac{1}{\pi\sqrt{1-x^2}}\left(g_0\mu_0 + 2\sum_{n=1}^{N-1}g_n\mu_n T_n(x)\right). \tag{11}$$

Mathematical formalism
Kernel polynomials

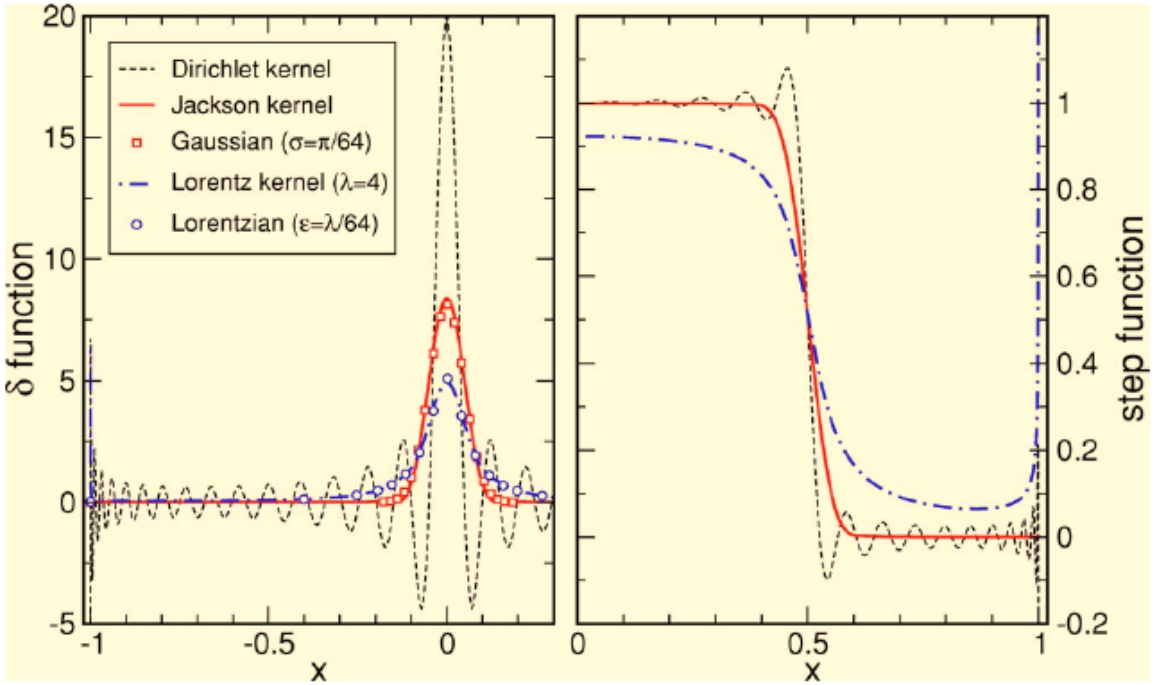

Figure 1 : *N=64 expansion moments of $\delta(x)$ (left) and step function (right).*[Weiße et al., 2006]

Mathematical formalism
Kernel polynomials

Name	g_n
Dirichlet	1
Fejér	$1 - \frac{n}{N}$
Jackson	$\left[(N-n+1)\cos(\frac{\pi n}{N+1}) + \sin(\frac{\pi n}{N+1})\cot(\frac{\pi n}{N+1})\right] / (N+1)$
Lorentz	$\sinh\left[\lambda(1-\frac{n}{N})\right] / \sinh(\lambda), \lambda \in \mathbb{R}$
Lanzos	$\left(\sin(\pi\frac{n}{N})/(\pi\frac{n}{N})\right)^M, M \in \mathbb{N}$

Table 1 : *Kernels.*

Chebyshev polynomials are defined on the real interval $[-1, 1]$.

Mathematical formalism
Requirements of the expansion

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Modify our matrix (Hamiltonian):

$$\begin{aligned} \tilde{H} &= \frac{(H - bI)}{a}, \\ \tilde{E} &= \frac{(E - b)}{a}. \end{aligned} \tag{12}$$

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Where a and b are:

$$\begin{aligned} a &= \frac{(E_{max} - E_{min})}{2 - \varepsilon}, \\ b &= \frac{(E_{max} + E_{min})}{2}, \quad \varepsilon = 0.01. \end{aligned} \tag{13}$$

Depending on the function two types of moments can arise:

Expectation values (case 1):

$$\mu_n = \langle \beta | T_n(H) | \alpha \rangle, \tag{14}$$

and

Mathematical formalism
Calculating the moments

Depending on the function two types of moments can arise:

Expectation values (case 1):

$$\mu_n = \langle \beta | T_n(H) | \alpha \rangle, \tag{14}$$

and

trace of operator and polynomial (case 2):

$$\mu_n = \mathrm{Tr}\left[A T_n(\tilde{H}) \right]. \tag{15}$$

Handling case 1

$$\mu_n = \langle\beta| T_n(\tilde{H})|\alpha\rangle,$$
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$$|\alpha_{n+1}\rangle = 2\tilde{H}|\alpha_n\rangle - |\alpha_{n-1}\rangle. \tag{16}$$

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Stochastic evaluation of trace.

Comparing with previous example numerical effort should be D^2 (D states of a given basis)

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$$\mu_n = \mathrm{Tr}\left[AT_n(\tilde{H})\right],$$

$$\mathrm{Tr}\left[AT_n(\tilde{H})\right] \approx \frac{1}{R}\sum_{r=0}^{R-1}\langle r|T_n(\tilde{H})|r\rangle, \quad R << D$$

where $r(i) \in \{\mathrm{rand}(\xi_{ri})\}, \quad \xi_{ri} \in \mathbb{C}.$

Handling case 2

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$$|r\rangle = \sum_{i=0}^{D-1} \xi_{ri}|i\rangle.$$

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Absorbing boundary conditions

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Apply boundary conditions:

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Modify the eq. 16:

$$|\alpha_{n+1}\rangle = \exp^{-\gamma}\left(2\tilde{H}|\alpha_n\rangle - \exp^{-\gamma}|\alpha_{n-1}\rangle\right). \tag{17}$$

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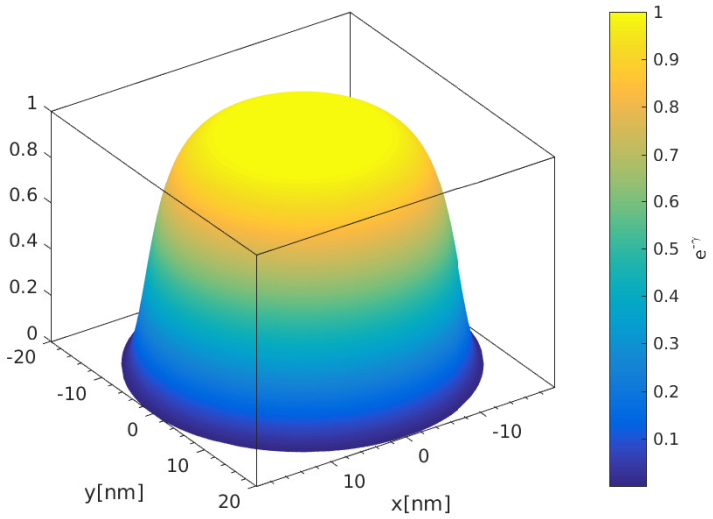

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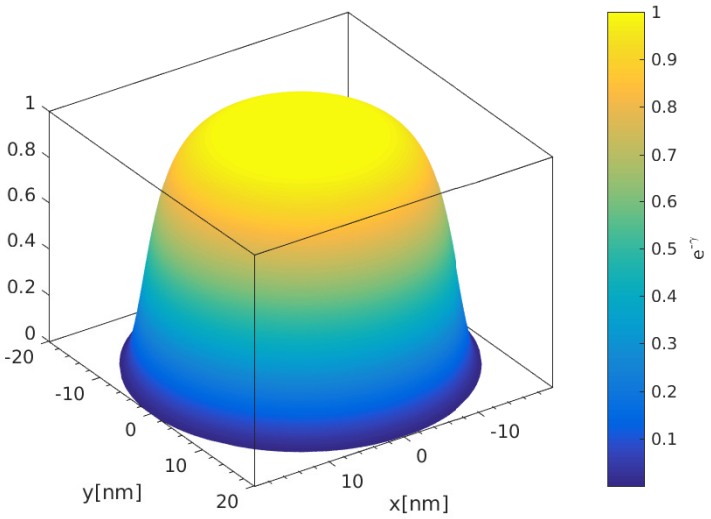

Bad back reflections!

Outline for section 3

Application of kpm

Matrix H of size D, with eigenvalues E_k:

Density of states

$$\rho(E) = \frac{1}{D}\sum_{k=0}^{D-1}\delta(E - E_k) \rightarrow \tilde{\rho}(\tilde{E}) = \frac{1}{D}\sum_{k=0}^{D-1}\delta(\tilde{E} - \tilde{E}_k) \tag{18}$$

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$$\begin{aligned}\mu_n &= \int_{-1}^{1}\tilde{\rho}(\tilde{E})T_n(\tilde{E})d\tilde{E} = \frac{1}{D}\sum_{k=0}^{D-1}T_n(\tilde{E}_k) \\ &= \frac{1}{D}\sum_{k=0}^{D-1}\langle k|T_n(\tilde{H})|k\rangle = \frac{1}{D}Tr\left[T_n(\tilde{H})\right]\end{aligned} \tag{19}$$

Application of kpm

Similar, we can start from expression for local density of states:

$$\tilde{\rho}_i(\tilde{E}) = \frac{1}{D}\sum_{k=0}^{D-1} |\langle i|k\rangle|^2 \delta(\tilde{E} - \tilde{E}_k). \tag{20}$$

and get:

$$\begin{aligned} \mu_n &= \int_{-1}^{1} \tilde{\rho}_i(\tilde{E}) T_n(\tilde{E}) d\tilde{E} \\ &= \frac{1}{D}\sum_{k=0}^{D-1} |\langle i|k\rangle|^2 T_n(\tilde{E}_k) \\ &= \frac{1}{D}\sum_{k=0}^{D-1} \langle i| T_n(\tilde{H})|k\rangle\langle k|i\rangle = \frac{1}{D}\langle i| T_n(\tilde{H})|i\rangle. \end{aligned} \tag{21}$$

Application of kpm
Conductivity calculation

Start with $\delta(\tilde{\varepsilon} - \tilde{H})$ and Green's function $G^{\pm}(\tilde{\varepsilon}, \tilde{H})$.

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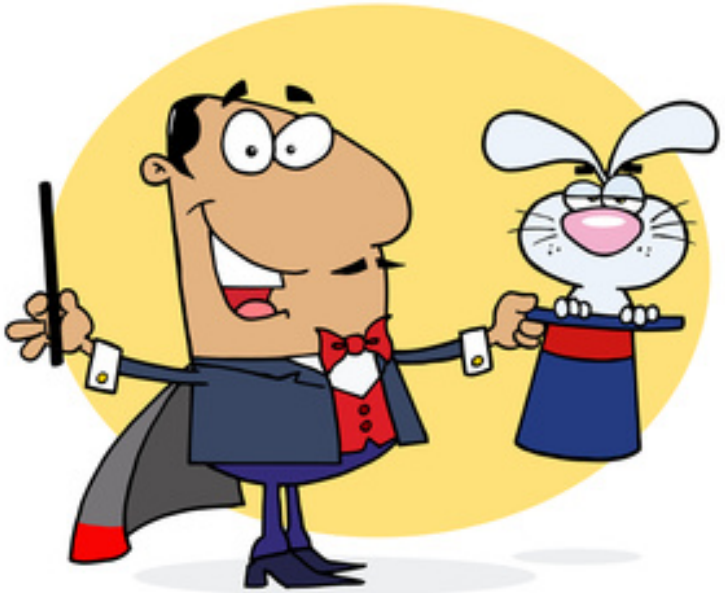

Expanded Kubo-Bastin formula in the linear response

$$\sigma_{\alpha,\beta}(\mu, T) = \frac{4e^2\hbar}{\pi\sigma}\frac{4}{\Delta E^2}\int_{-1}^{1} d\tilde{E}\frac{f(\tilde{\varepsilon}, \mu, T)}{(1-\varepsilon^2)^2}\sum_{m,n}\Gamma_{nm}(\tilde{\varepsilon})\mu_{nm}^{\alpha\beta}. \tag{22}$$

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$$\mu_{nm}^{\alpha\beta} \equiv [g_m g_n/(1+\delta_{n0})(1+\delta_{m0})\,\mathrm{Tr}\left[\upsilon_\alpha T_m(\tilde{H}) \times \upsilon_\beta T_n(\tilde{H})\right],$$

$$\Gamma_{nm} \equiv \left[\left(\tilde{\varepsilon} - im\sqrt{1-\tilde{\varepsilon}^2}\right)\exp^{im\arccos(\tilde{\varepsilon})}\, T_n(\tilde{\varepsilon}) + \left(\tilde{\varepsilon} + in\sqrt{1-\tilde{\varepsilon}^2}\right)\exp^{in\arccos(\tilde{\varepsilon})}\, T_m(\tilde{\varepsilon})\right],$$

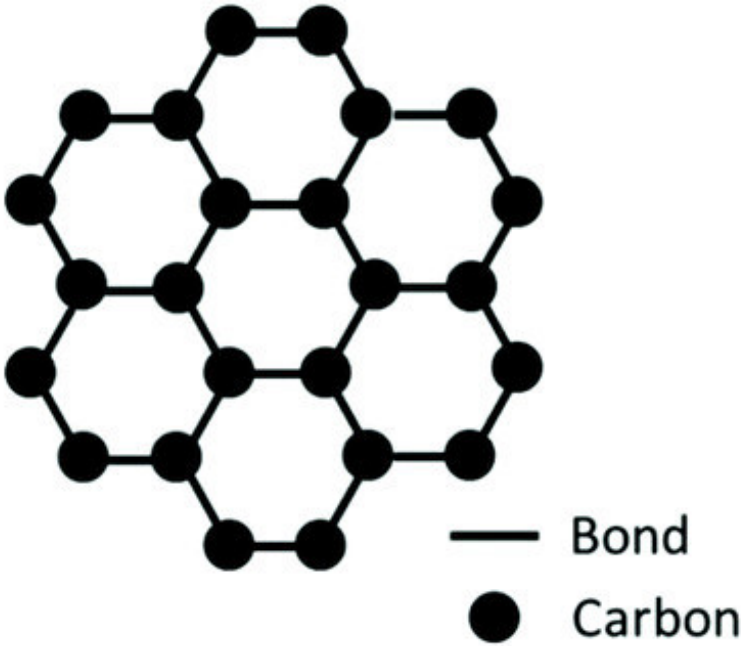
$\alpha, \beta \in \{x, y\}$.

[García et al., 2015]

Outline for section 4

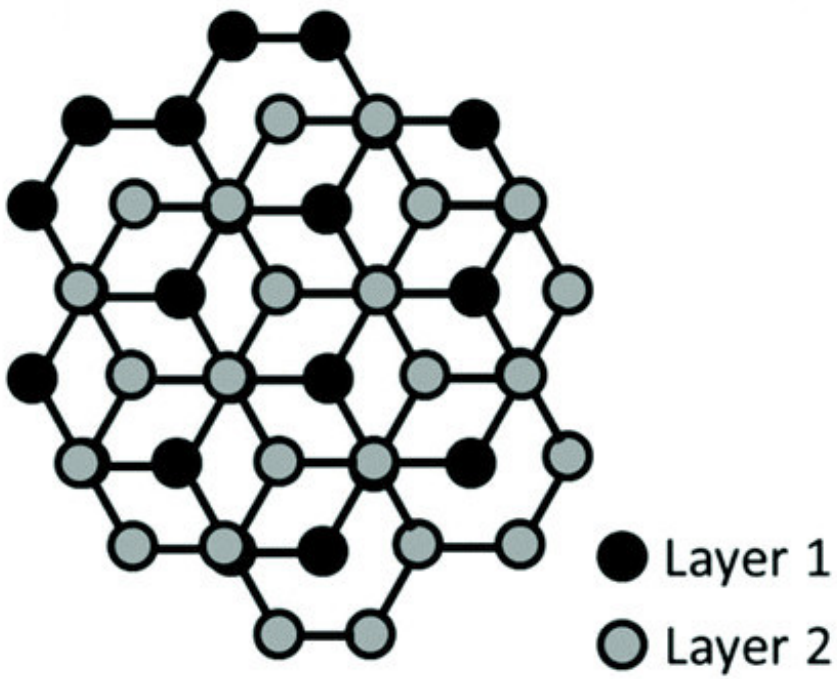
Examples

Material: Graphene - monolayer.



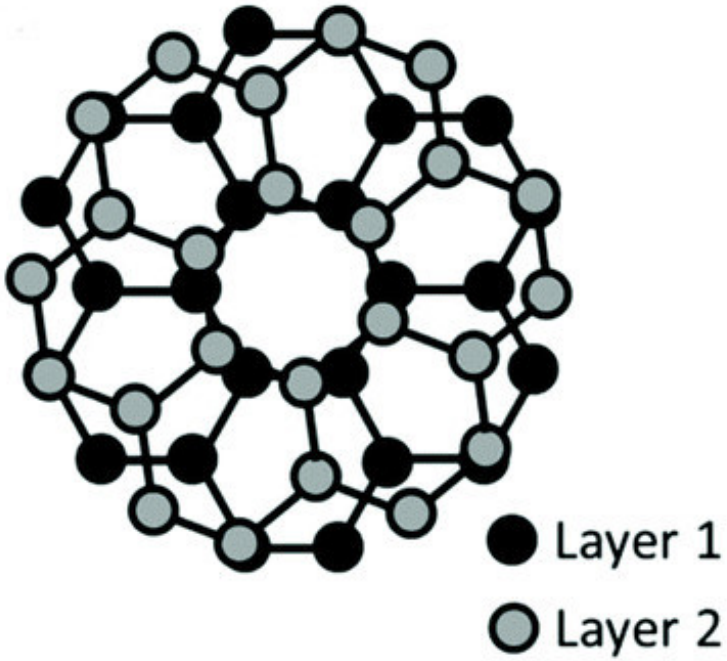
Examples

Material: Graphene - bilayer Bernal stacking.



Examples

Material: Graphene - twisted bilayer.



Examples

Graphene with nearest neighbours

$$H = -t \sum_{\langle i,j \rangle} \exp^{i\cancelto{0}{\phi_{ij}}} c_i^\dagger c_j + \sum_i \cancelto{0}{\varepsilon_i} c_i^\dagger c_j$$

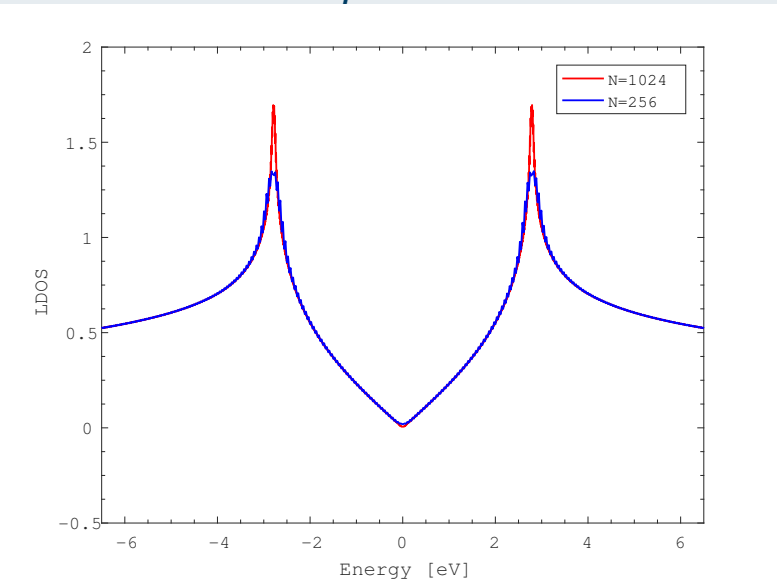


Figure 2 : *LDOS - comparing $N = 256$ and $N = 1024$ moments.*

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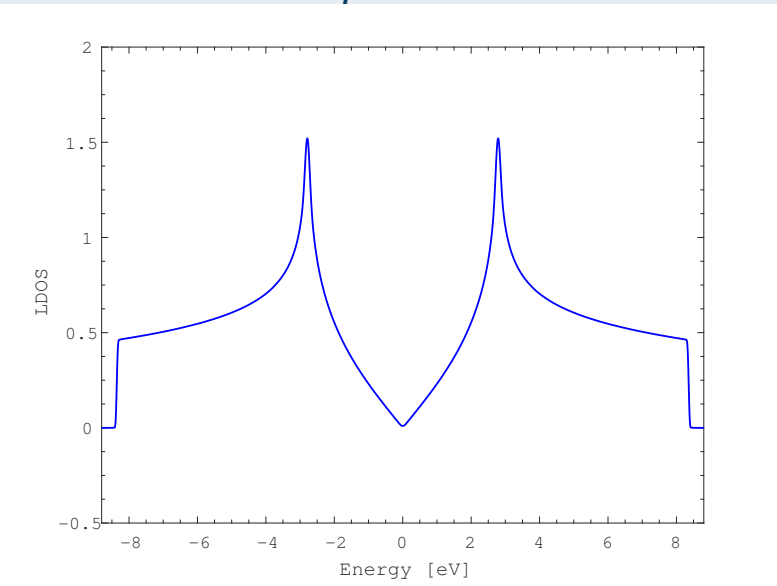

Figure 2 : *LDOS* $N = 512$ *moments.*

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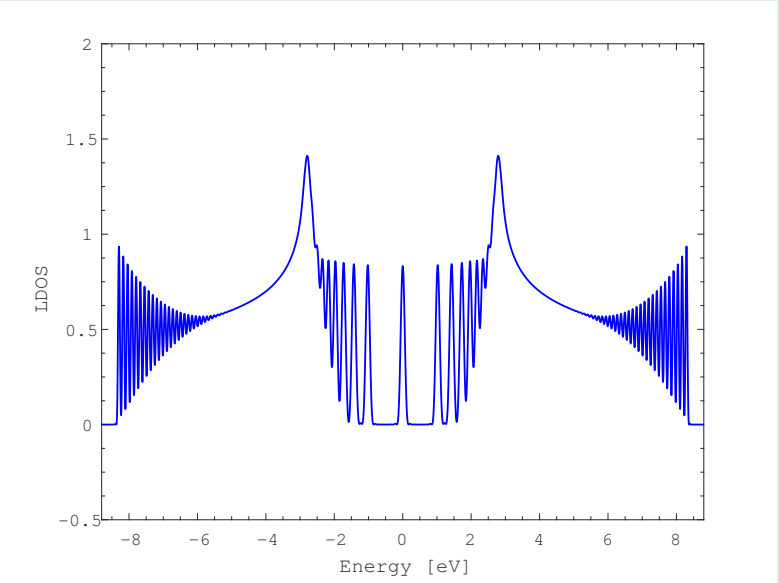

Figure 2 : *LDOS $N = 512$ moments with magnetic field.*

Examples

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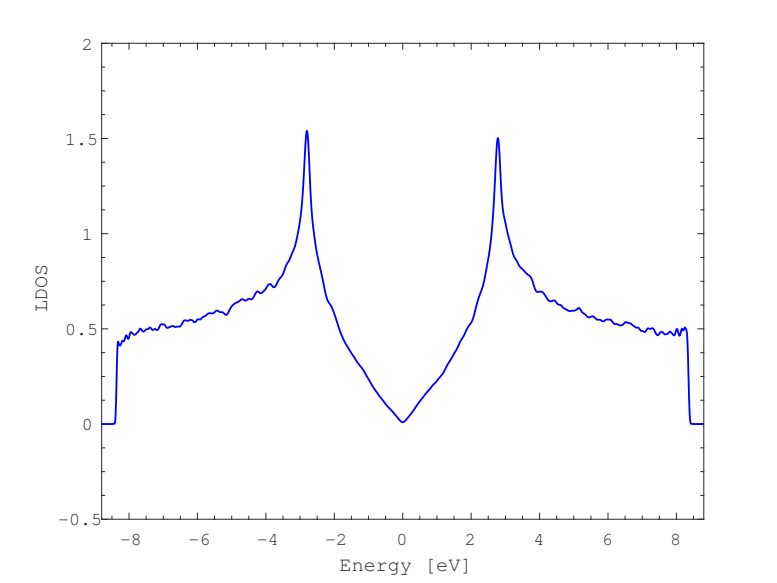

Figure 2 : *LDOS $N = 512$ moments with disorder.*

Examples

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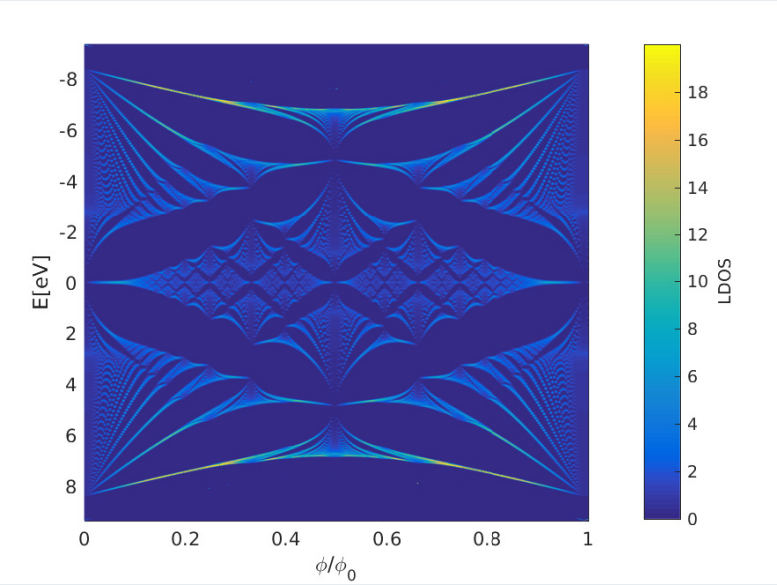

Figure 3 : *Hofstadter butterfly*

Examples

Bilayer graphene, Bernal stacking

$$H = -\sum_{\langle i,j \rangle} t(\vec{R}_i, \vec{R}_j) \exp^{i\cancelto{0}{\phi_{ij}}} c_i^\dagger c_j + \sum_i \cancelto{0}{\varepsilon_i} c_i^\dagger c_j \pm \frac{\cancelto{0}{\Delta_{AB}}}{2} \sum_{i \in A/B} c_i^\dagger c_j$$

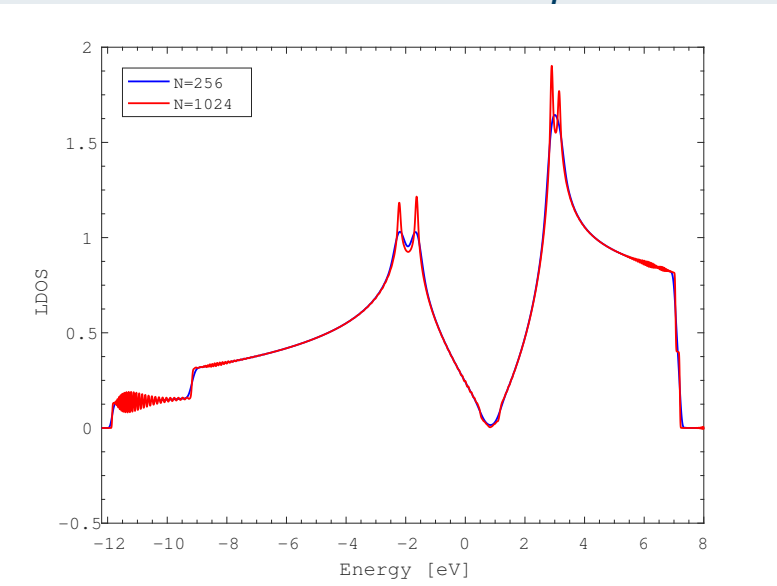

Figure 4 : *LDOS - comparing $N = 256$ and $N = 1024$ moments.*

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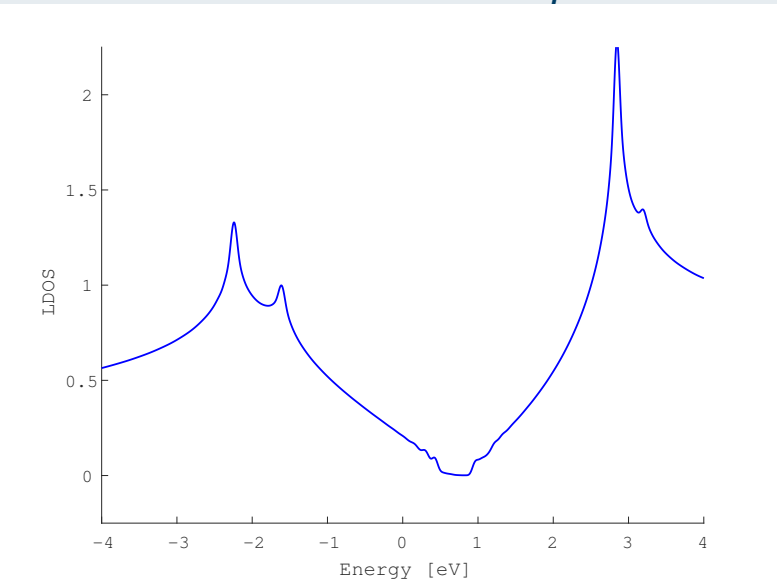

Figure 4 : *LDOS $N = 1024$ moments with applied voltage.*

Examples

Twisted bilayer graphene

Start from Bernal stacking and rotate for 4.14°.

$$H = -\sum_{\langle i,j \rangle} t(\vec{R}_i, \vec{R}_j) \exp^{i\phi_{ij}} c_i^\dagger c_j + \sum_i \cancelto{0}{\varepsilon_i} c_i^\dagger c_j \pm \frac{\cancelto{0}{\Delta_{AB}}}{2} \sum_{i \in A/B} c_i^\dagger c_j$$

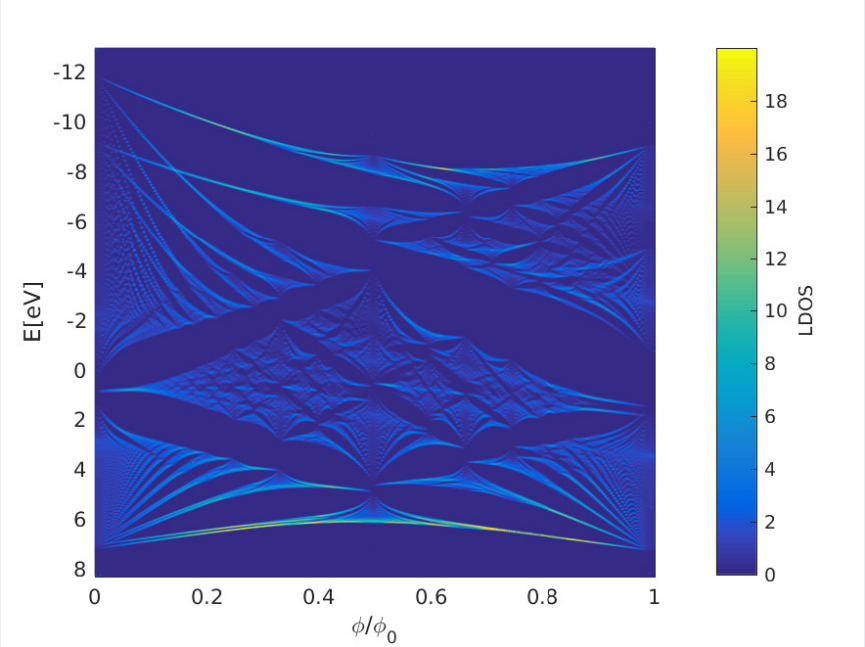

Figure 5 : *Hofstadter butterfly in twisted bilayer graphene.*

Conductivity of graphene from Kubo-Bastin formula

$$H = -t \sum_{\langle i,j \rangle} \exp^{i\phi_{ij}} c_i^\dagger c_j + \sum_i \varepsilon_i c_i^\dagger c_j$$

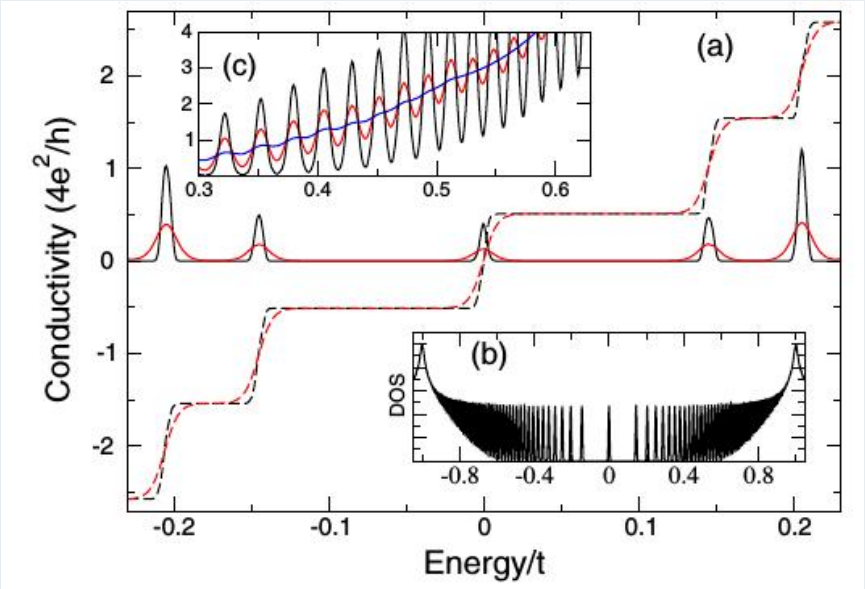

Figure 6 : *(a) Conductivity σ_{xx} and σ_{xy}, (b) DOS, (c) Shubnikovde Haas oscillations.*[García et al., 2015]

Outline for section 5

Conclusion

Kernel polynomial method and Chebyshev expansion.

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Linearly scalable.

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- Cons:
  - Energy resolution $\sim \frac{1}{N}$.

Conclusion

Kernel polynomial method and Chebyshev expansion.

- Pros:
  - Linearly scalable.
  - Paralelization (CPU + GPU).
  - Applying of boundary conditions.
- Cons:
  - Energy resolution $\sim \frac{1}{N}$.
- Future work:
  - Conductivity of twisted bilayer graphene.
  - Different types of materials, transition metal dichalcogenides.

References

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Thank you for your attention!