TU^{2}FRG - a scalable approach for TUFRG in generic fermionic models

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Goal of a unified real and momentum space TU-FRG

- Why merging the two?
  - Source of superconductivity in quasicrystals [1]
  - Many body-localization in two and more dimensions [2]
  - Majorana/topological edge modes [3]
  - Large unit cells (twisted materials etc.)
  - Quasi-1D geometries
  - Wannierized multi-band DFT models to FRG
- Need for efficient approximations

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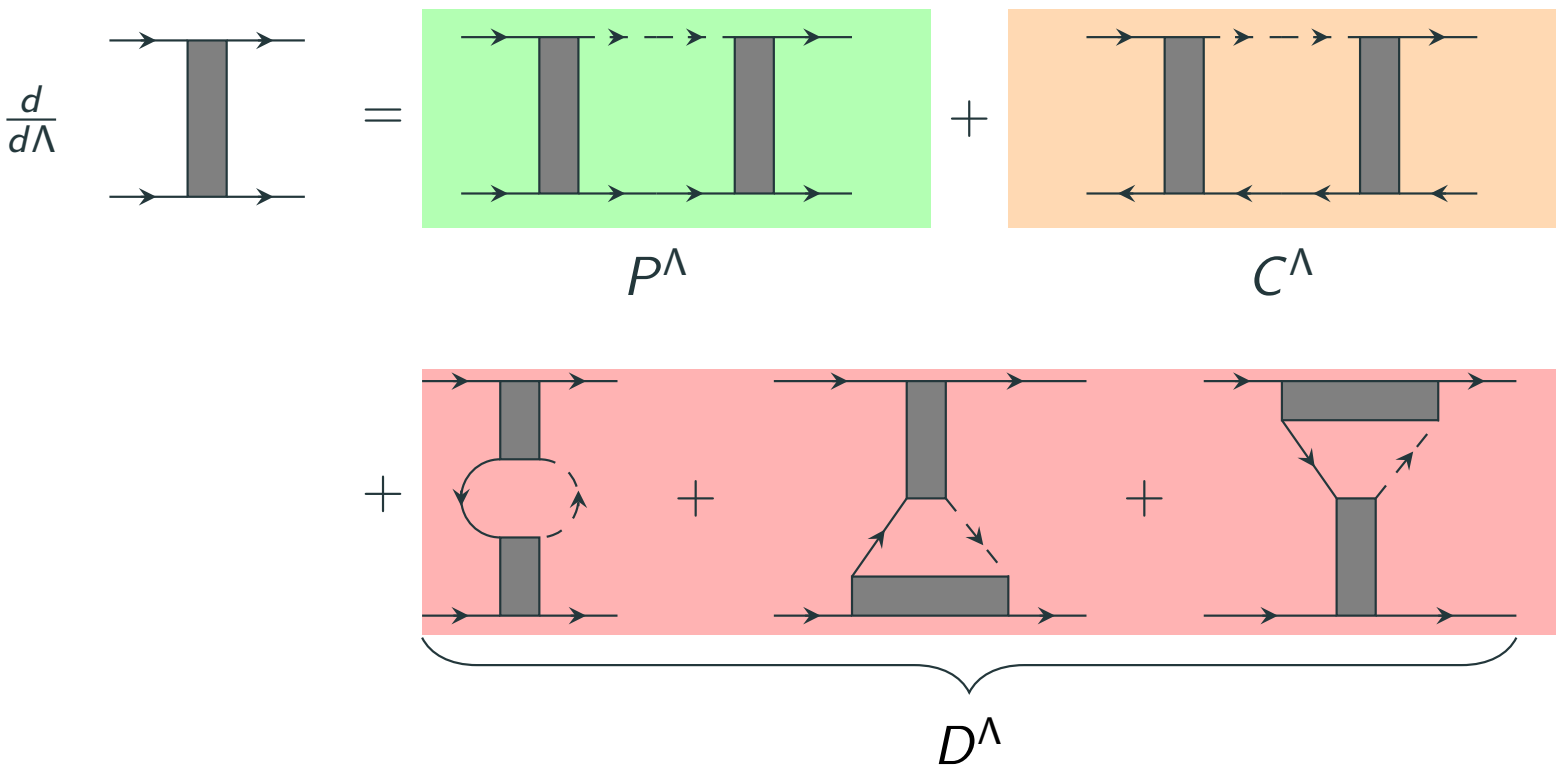
[1] K. Kamiya et al. "Discovery of superconductivity in quasicrystal". en. In: *Nature Communications* 9.1 (Dec. 2018), p. 154.

[2] Eli Chertkov, Benjamin Villalonga, and Bryan K. Clark. "Numerical Evidence for Many-Body Localization in Two and Three Dimensions". In: *Phys. Rev. Lett.* 126 (18 May 2021), p. 180602.

[3] Rahul Nandkishore, LS Levitov, and AV Chubukov. "Chiral superconductivity from repulsive interactions in doped graphene". In: *Nature Physics* 8.2 (2012). Publisher: Nature Publishing Group, p. 158.

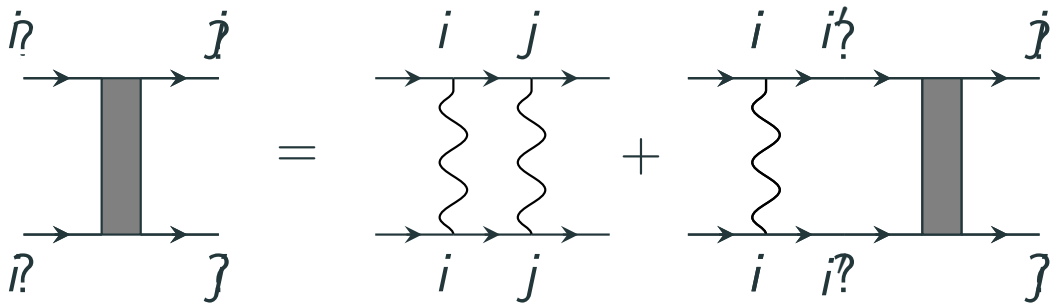
Issue

- Flow for the effective interaction
- scales $\mathcal{O}(N_o^6 N_k^3 N_\omega^3)$ and memory $\mathcal{O}(N_o^4 N_k^3 N_\omega^3)$
- impossible for more than 4 orbitals $\rightarrow$ need to find more efficient basis
- Focus on momentum and orbitals



Solution?

- momentum space - exploit diagrammatic structure[4]
- Analog in realspace - pertubative argument[5,6]
- Model interaction is short ranged - assume on-site interaction
  $U(i,k,j,l) = U\delta_{i,k}\delta_{j,l},\delta_{i,j}$
- What index structure follows from single channel FRG?



- Each channel 2 main indices
- Expand in bonds and truncate expansion

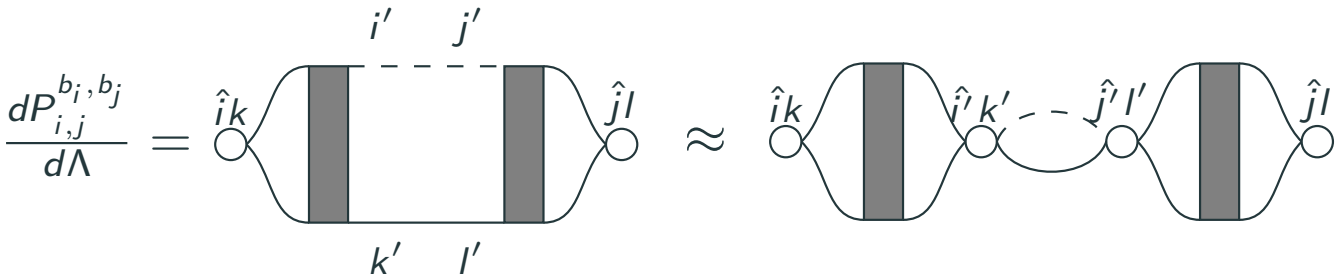
[4] J. Lichtenstein et al. "High-performance functional Renormalization Group calculations for interacting fermions". In: *Computer Physics Communications* 213 (Apr. 2017), pp. 100–110.

[5] Lukas Weidinger, Florian Bauer, and Jan von Delft. "Functional renormalization group approach for inhomogeneous one-dimensional Fermi systems with finite-ranged interactions". In: *Physical Review B* 95.3 (Jan. 2017).

[6] Lisa Markhof et al. "Detecting phases in one-dimensional many-fermion systems with the functional renormalization group". In: *Physical Review B* 97.23 (June 2018). arXiv: 1803.00272, p. 235126.

Real-Space TUFRG

- Project on main dependence $\delta_{i+b_i,k} =$ - bond b_i connecting site i and k
- Projected channels $I = \hat{I}\phi^I$



- Restrict the set of bonds
- Scaling $\mathcal{O}(N_o^3 N_{bo}^3)$ (compared to $\mathcal{O}(N_o^6)$)
- Issues:
  - Near phase boundary - multiple-channels diverge, cross feedback cut away!
  - biased towards short ranged fluctuations
  - projections from one channel to another are approximate

Add in momentum

- formally: separate unities, ff shells and real-space bonds
- site dependent momentum form-factors $g_{b_i}(o_j, \boldsymbol{k})$
- Use sharp cutoff $R(\Lambda) = \Theta(\Lambda - \omega)$ (numerically convenient)

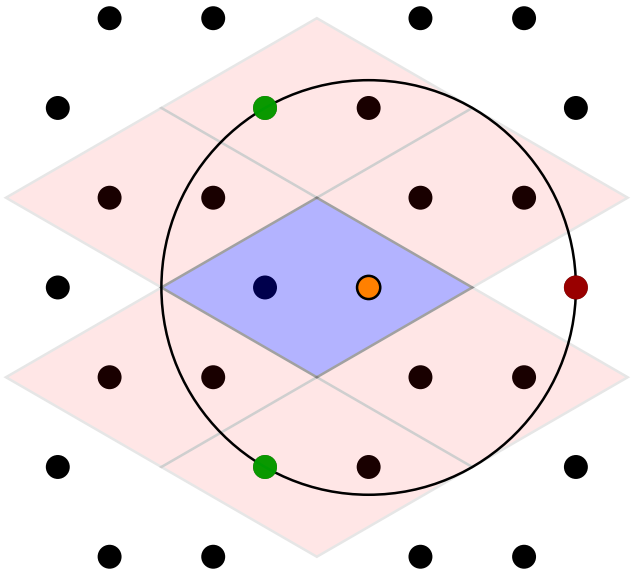
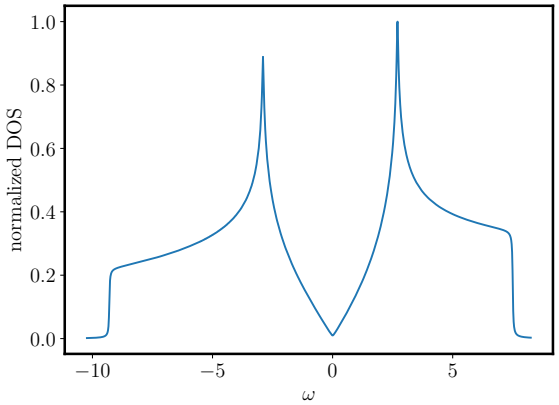
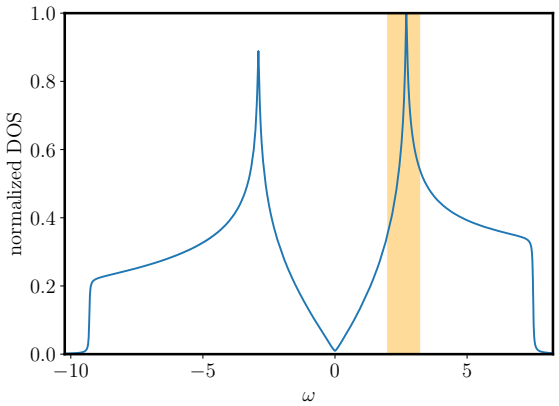


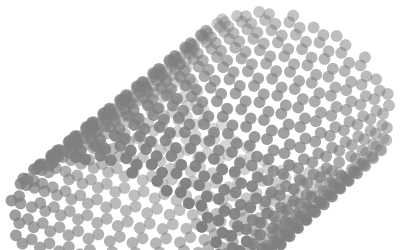
Figure 1: Taken from Jonas B. Hauck and Dante M. Kennes. "TU^{2}FRG: a scalable approach for truncated unity functional renormalization group in generic fermionic models". In: *The European Physical Journal B* 95.3 (Mar. 2022) with permission of the authors

Application: Graphene topological superconductivity





- Graphene near van-Hove $\rightarrow$ TSC [7]
- Topological edge modes [8]
- Van-Hove doping achieved [9]
- Large diameter Nanotube (C^2 symmetry)
- Hubbard-type Model
- TU^{2}FRG



Compare slab and periodic

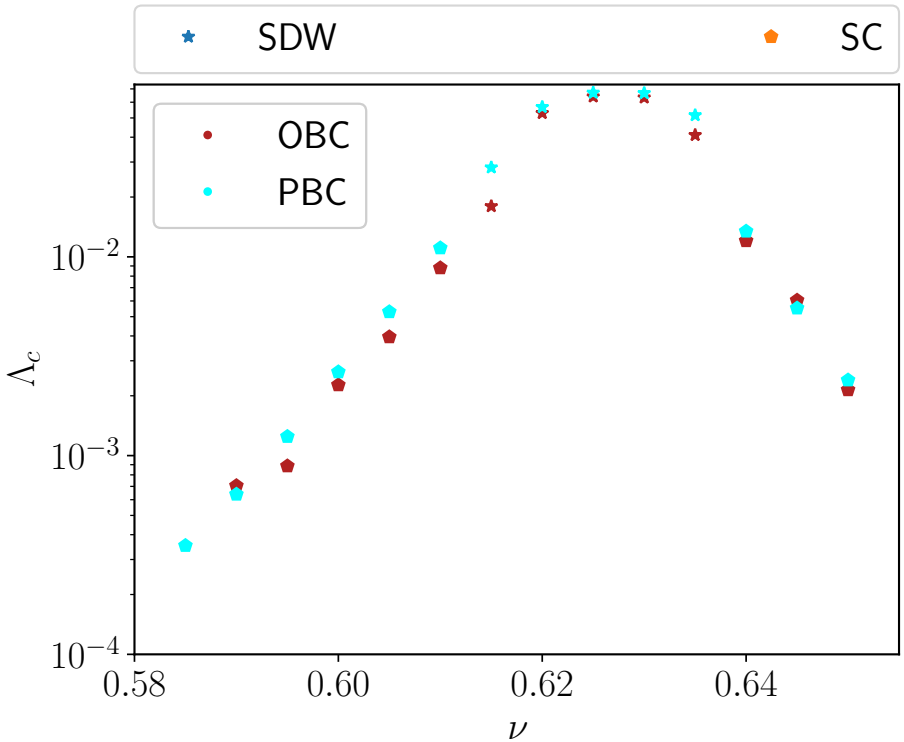


Figure 2: Slab and periodic system without self-energy feedback

- qualitative agreement
- periodic: d_{xy} and $d_{x^2-y^2}$ exactly degenerate (2D E_2 irrep)
- open: C_{6v} broken into C_2
- d_{xy} and $d_{x^2-y^2}$ in trivial irrep $\Longrightarrow$ mixing s

Behavior of the attraction at the boundary

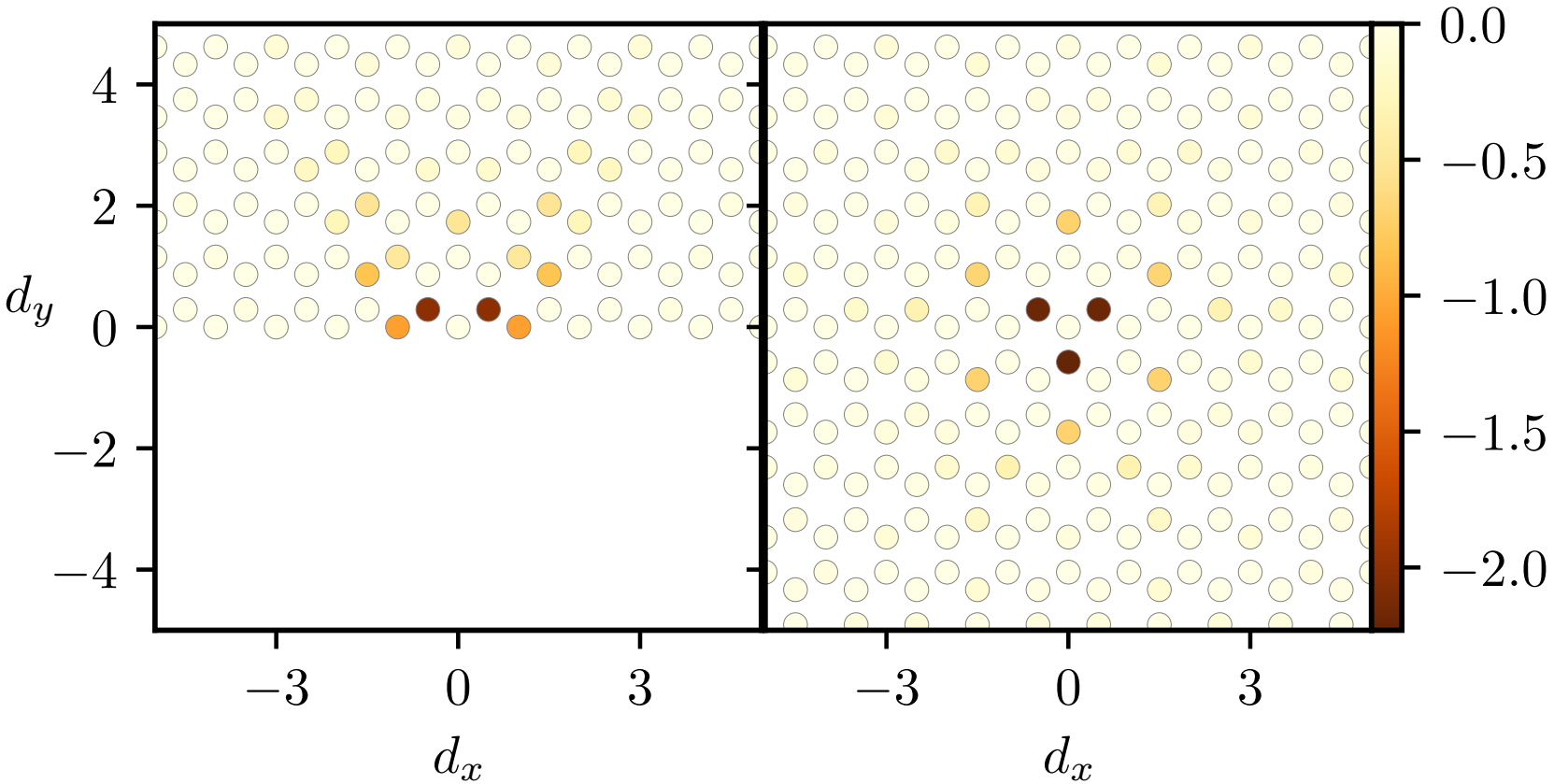


Figure 3: Attractive pairing interaction at a site at the boundary compared to a site in the bulk as a function of the real space positions

Including the static self-energy

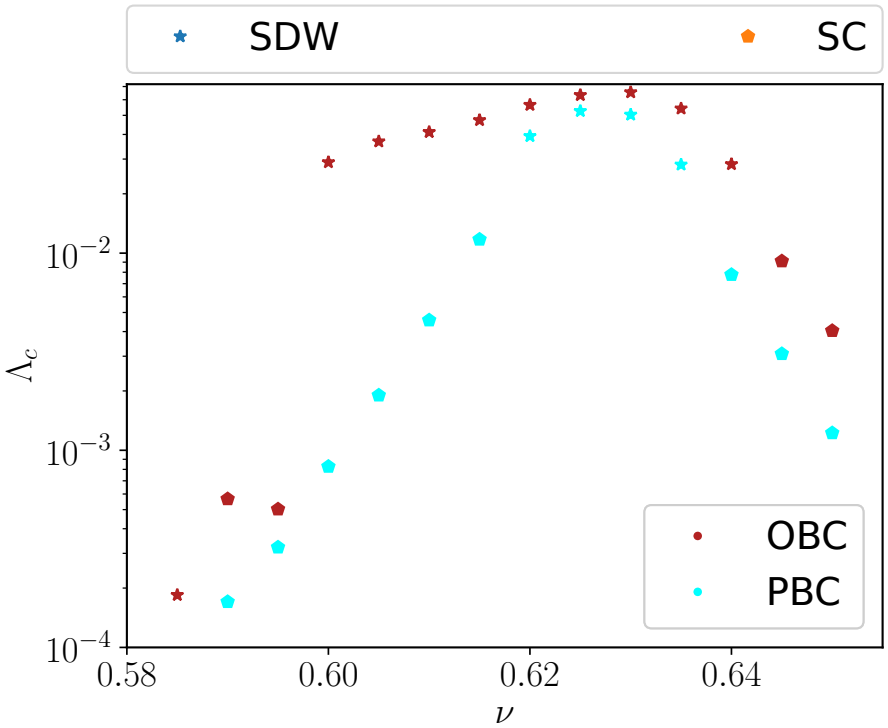


Figure 4: Slab and periodic system with self-energy feedback

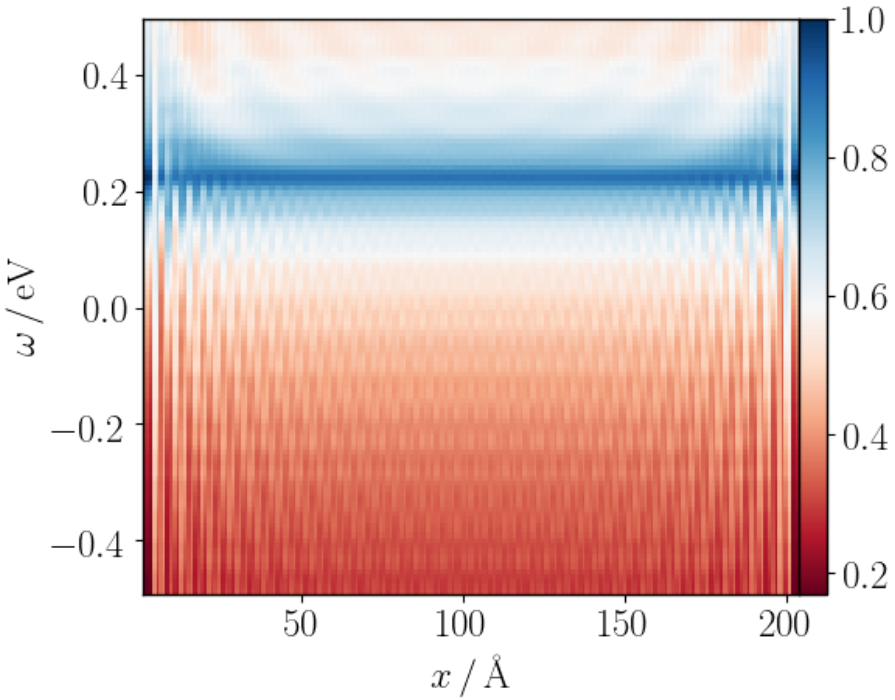
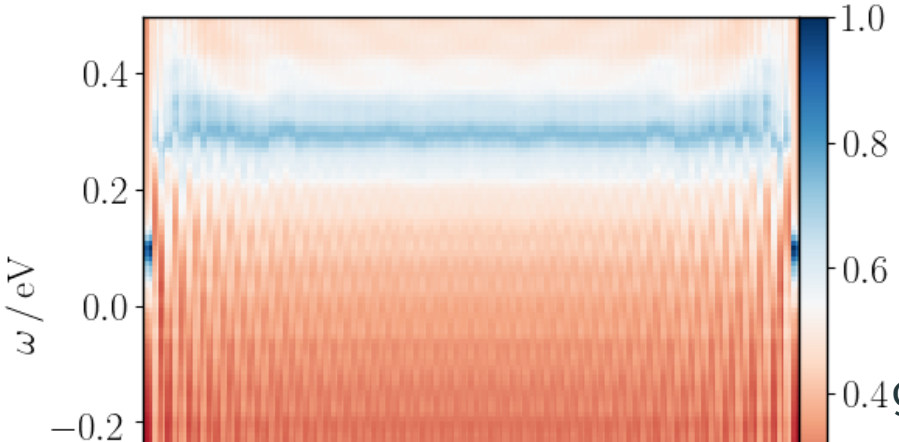


Figure 5: non interacting local density of states



Outlook/Conclusion

- New unified TU approach
- Higher harmonics at boundaries
- Charge reordering $\Longrightarrow$ splitted van-Hove
- Next steps
  - Make code open access with python interface
  - Apply to SBE-FRG
- Special Thanks to D. Kennes, L. Klebl and J. Beyer. The authors gratefully acknowledge the computing time granted through JARA on the supercomputer JURECA [10] at Forschungszentrum Jülich.

[9] Jülich Supercomputing Centre. "JURECA: Data Centric and Booster Modules implementing the Modular Supercomputing Architecture at Jülich Supercomputing Centre". In: *Journal of large-scale research facilities* 7.A182 (2021).

Implementation

Scaling

- Flow equations $\mathcal{O}(N_q N_o^3 N_{bf}^3)$
- Projections $\mathcal{O}(N_q^2 N_o^2 N_{bf}^3)$
- Loop $\mathcal{O}(N_q^2 N_{fine} N_o^2 N_{bf}^2)$
- Self energy $\mathcal{O}(N_q^2 N_o^2 N_{bf}^2)$

Run-time example: $N_o = 3$, $N_{bf} = 47$, $N_q = 1296$ and $N_{fine} = 400 \implies \approx 1h$ (rwth gpu cluster, w. o. self-energy)

Requirement for simulations:

- real-space basis of unit cell (UC)
- positions of orbitals in UC (optional: type of orbitals)
- Hamiltonian

Many optional inputs (Interaction, Distance measure etc.)

FF-generation issue