Correlated Electron Dynamics in Finite Hubbard Clusters: Benchmarking the G1—G2 Scheme

Jan-Philip Joost

with:

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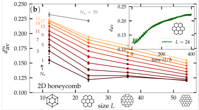
slides at: www.theo-physik.uni-kiel.de/bonitz/talks.html

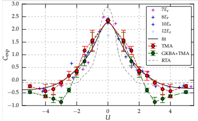
Motivation: Dynamics of Correlated Electron Systems

Ion Stopping in Hexagonal Lattices



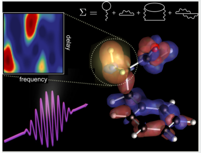
K. Balzer *et al.*, PRL **121**, 267602 (2018)

Cold Atoms in Optical Lattices



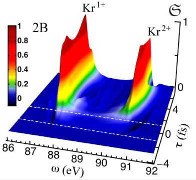
N. Schlünzen and M. Bonitz, CPP **56**, 5 (2016)

Biologically Relevant Molecules



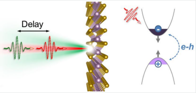
E. Perfetto *et al.*, JCPL **9**, 1353 (2018)

Atoms

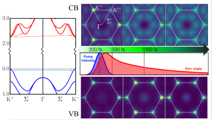


E. Perfetto *et al.*, PRA **92**, 033419 (2015)

2D Layered Materials



E. A. Pogna *et al.*, ACS Nano **10**, 1182 (2016)



A. Molina-Sánchez *et al.*, Nano Lett. **17**, 4549 (2017)

- nonequilibrium theory often more demanding than equilibrium counterpart:
  - (TD)DFT
  - (TD)DMRG
  - (TD)DMFT

- nonequilibrium Green function theory (NEGF) **versatile** (see left) but **slow** approach [$\mathcal{O}(N_t^3)$ scaling]

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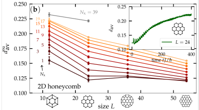

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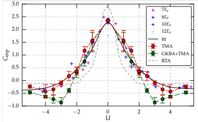

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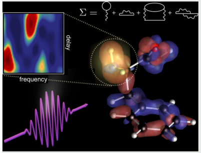

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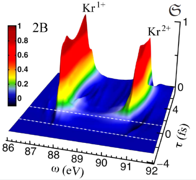
Atoms



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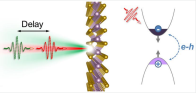

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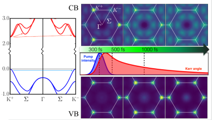

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  - (TD)DFT
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- nonequilibrium Green function theory (NEGF) **versatile** (see left) but **slow** approach [$\mathcal{O}(N_t^3)$ scaling]

This talk:

(I) present **G1–G2 scheme**: time-linear [$\mathcal{O}(N_t^1)$] formulation of NEGF theory, greatly increasing its applicability

(II) improve approximation and stability using two-electron reduced density matrix (**2RDM**) theory

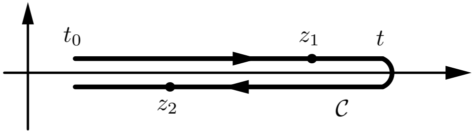
Nonequilibrium Green Functions (NEGF)

two times $z, z' \in \mathcal{C}$ (“Keldysh contour”), arbitrary one-particle basis $|\phi_i\rangle$

$$\boxed{G_{ij}(z,z') = \frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\hat{c}_i(z)\hat{c}_j^\dagger(z')\right\rangle}$$ average with ρ^N

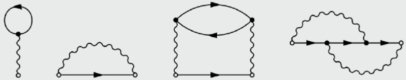
Keldysh–Kadanoff–Baym equations (KBE) on $\mathcal{C}$ (2×2 matrix):

$$\sum_k \left\{\mathrm{i}\hbar\frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z)\right\} G_{kj}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} - \mathrm{i}\hbar\sum_{klm}\int_{\mathcal{C}} \mathrm{d}\bar{z}\, w_{iklm}(z^+,\bar{z})G^{(2)}_{lmjk}(z,\bar{z};z',\bar{z}^+)$$



KBE: first equation of Martin–Schwinger hierarchy for $G, G^{(2)}\dots G^{(n)}$

- $\int_{\mathcal{C}} wG^{(2)} \to \int_{\mathcal{C}} \Sigma G$, Selfenergy
- Nonequilibrium Diagram technique
  Example: Hartree–Fock + Second Born selfenergy



Talk by M. Bonitz in this session: D48.00015 Electronic excitations in correlated finite 2D materials generated by ion impact

Selfenergy Approximations[1]

Hartree–Fock (HF, mean field): $\sim w^1$

Second Born (2B): $\sim w^2$

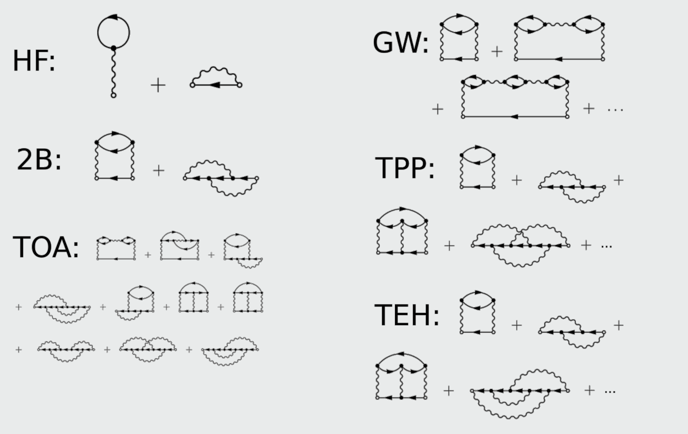
3rd order approx. (TOA): $\sim w^3$

GW: ∞ bubble summation, dynamical screening effects

particle-particle T-matrix (TPP): ∞ ladder sum in pp channel

particle-hole T-matrix (TPH/TEH): ∞ ladder sum in ph channel

Choice depends on coupling strength, density (filling)



[1] Conserving, nonequilibrium $\Sigma(t, t')$, applies for ultra-short to long times

Real-Time Keldysh–Kadanoff–Baym Equations (KBE)

- Correlation functions $G^{\gtrless}$ obey real-time KBE

$$\sum_l \left[\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\delta_{i,l} - h^{\mathrm{eff}}_{il}(t)\right] G^{>}_{lj}(t,t') = I^{(1),>}_{ij}(t,t')\,,$$

$$\sum_l G^{<}_{il}(t,t')\left[-\mathrm{i}\hbar \frac{\overleftarrow{\mathrm{d}}}{\mathrm{d}t'}\delta_{l,j} - h^{\mathrm{eff}}_{lj}(t')\right] = I^{(2),<}_{ij}(t,t')\,,$$

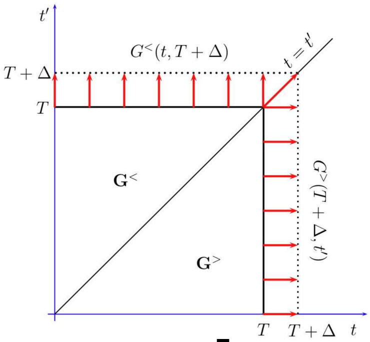
with the effective single-particle **Hartree–Fock Hamiltonian**

$$h^{\mathrm{eff}}_{ij}(t) = h^0_{ij} \pm \mathrm{i}\hbar \sum_{kl} w^{\pm}_{ikjl} G^{<}_{lk}(t)$$

and the collision integrals

$$I^{(1),>}_{ij}(t,t') := \sum_l \int_{t_\mathrm{s}}^{\infty} \mathrm{d}\bar{t} \left\{\Sigma^{\mathrm{R}}_{il}(t,\bar{t})G^{>}_{lj}(\bar{t},t') + \Sigma^{>}_{il}(t,\bar{t})G^{\mathrm{A}}_{lj}(\bar{t},t')\right\},$$

$$I^{(2),<}_{ij}(t,t') := \sum_l \int_{t_\mathrm{s}}^{\infty} \mathrm{d}\bar{t} \left\{G^{\mathrm{R}}_{il}(t,\bar{t})\Sigma^{<}_{lj}(\bar{t},t') + G^{<}_{il}(t,\bar{t})\Sigma^{\mathrm{A}}_{lj}(\bar{t},t')\right\}.$$



$$\mathcal{O}(N_\mathrm{t}^3)$$

- numerically demanding due to N_t^3 scaling (most competing methods time linear)

Generalized Kadanoff–Baym Ansatz (GKBA)

- full propagation on the time diagonal ($I := I^<$):

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} G^<_{ij}(t) = \left[h^{\mathrm{HF}}, G^<\right]_{ij}(t) + \left[I + I^\dagger\right]_{ij}(t)$$

- reconstruct off-diagonal NEGF from time diagonal:

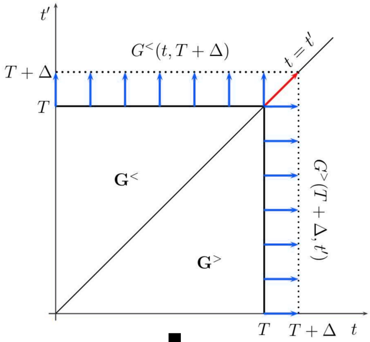
$$G^{\gtrless}_{ij}(t,t') = \pm \left[G^{\mathrm{R}}_{ik}(t,t')\rho^{\gtrless}_{kj}(t') - \rho^{\gtrless}_{ik}(t) G^{\mathrm{A}}_{kj}(t,t') \right]$$

with $\rho^{\gtrless}_{ij}(t) = \pm \mathrm{i}\hbar G^{\gtrless}_{ij}(t,t)$

- HF-GKBA: use Hartree–Fock propagators for $G^{\mathrm{R/A}}_{ij}$

$$G^{\mathrm{R/A}}_{ij}(t,t') = \mp \mathrm{i}\Theta_{\mathcal{C}}\left(\pm[t-t']\right) \exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} \mathrm{d}\bar{t}\, h_{\mathrm{HF}}(\bar{t})\right)\Bigg|_{ij}$$

- conserves particle number and total energy



$\mathcal{O}(N_{\mathrm{t}}^2)$

(for 2B)

P. Lipavský, V. Špička, and B. Velický, Phys. Rev. B **34**, 6933 (1986)

Reformulating the GKBA

- quadratic/cubic scaling is caused by the structure of the collision integral

$$I_{ij}(t) = \sum_k \int_{t_0}^{t} \mathrm{d}\bar{t} \left[\Sigma^>_{ik}(t,\bar{t}) G^<_{kj}(\bar{t},t) - \Sigma^<_{ik}(t,\bar{t}) G^>_{kj}(\bar{t},t) \right]$$

time integral   two-time quantities

N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. Lett. **124**, 076601 (2020)

J.-P. Joost, N. Schlünzen, and M. Bonitz, Phys. Rev. B **101**, 245101 (2020)

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time integral

two-time quantities

Idea: solve differential equation for $\mathcal{G}$ instead of time integral for I

N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. Lett. **124**, 076601 (2020)

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time integral — two-time quantities

Idea: solve differential equation for $\mathcal{G}$ instead of time integral for I

- **Solution:** G1–G2 scheme:

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{G}_{ijkl}(t) = \left[h^{(2),\mathrm{HF}}, \mathcal{G}\right]_{ijkl}(t) + \underbrace{\Psi_{ijkl}(t)}_{\text{2B}} + \underbrace{\Lambda_{ijkl}(t)}_{\text{TPP}} + \underbrace{\Pi_{ijkl}(t)}_{GW} \pm \underbrace{\Pi_{ijlk}(t)}_{\text{TPH}},$$

with $h^{(2),\mathrm{HF}}_{ijkl}(t) := \delta_{ik} h^{\mathrm{HF}}_{jl}(t) + \delta_{jl} h^{\mathrm{HF}}_{ik}(t)$ and the selfenergy contributions

$$\Psi \sim w^{\pm} G^< G^< G^< , \qquad \Lambda \sim w G^< \mathcal{G} , \qquad \Pi \sim w^{\pm} G^< \mathcal{G}$$

N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. Lett. **124**, 076601 (2020)

J.-P. Joost, N. Schlünzen, and M. Bonitz, Phys. Rev. B **101**, 245101 (2020)

- full propagation on time diagonal with collision integral coupling to correlated $\mathcal{G}$

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} G^<_{ij}(t) = \left[h^{\mathrm{HF}}, G^<\right]_{ij}(t) + \left[I + I^\dagger\right]_{ij}(t)\,, \qquad I_{ij}(t) = \pm \mathrm{i}\hbar \sum_{klp} w_{iklp}(t)\mathcal{G}_{lpjk}(t)\,,$$

- which obeys an ordinary differential equation

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$$\boxed{\mathcal{O}(N_\mathrm{t}^1)}$$

[1] R. Zimmermann et al., Phys. Status Solidi B **90**, 175 (1978); H. Haug et al., Phys. Status Solidi B **85**, 561 (1978)

[2] F. Colmenero, et al., Phys. Rev. A **47**, 971 (1993)

The G1–G2 Scheme: DSL

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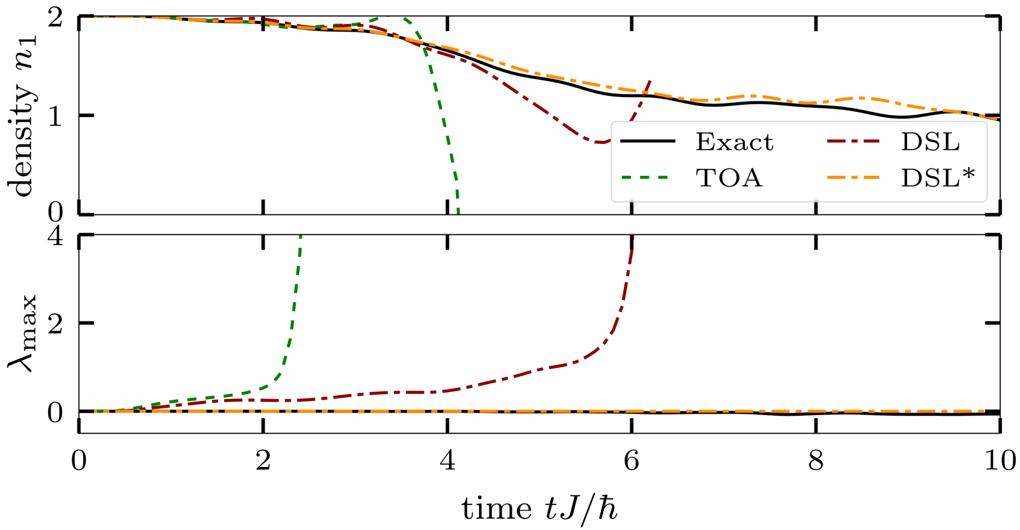
$$\boxed{\mathcal{O}(N_\mathrm{t}^1)}$$

- DSL combines **strong electronic correlations** and **dynamical screening** out of equilibrium
- in the context of Green functions previously discussed for equilibrium systems[1]

[1] R. Zimmermann et al., Phys. Status Solidi B **90**, 175 (1978); H. Haug et al., Phys. Status Solidi B **85**, 561 (1978)

[2] F. Colmenero, et al., Phys. Rev. A **47**, 971 (1993)

6-Site Hubbard Chain: Sites 1–3 Full, Sites 4–6 Empty, $U/J = 4$



- λ_{max}: largest eigenvalue of the two-particle Green function

The G1–G2 Scheme: Relations to 2RDM Theory

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- full propagation on time diagonal with collision integral coupling to correlated $\mathcal{G}$

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$$\boxed{\mathcal{O}(N_{\mathrm{t}}^{1})}$$

- DSL combines **strong electronic correlations** and **dynamical screening** out of equilibrium
- in the context of Green functions previously discussed for equilibrium systems[1]

- fully equivalent to the well-known **Valdemoro approximation** emerging from the BBGKY hierarchy in 2RDM theory[2]
  $\longrightarrow$ apply knowledge from 2RDM theory to further improve G1–G2 scheme

[1] R. Zimmermann et al., Phys. Status Solidi B **90**, 175 (1978); H. Haug et al., Phys. Status Solidi B **85**, 561 (1978)

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Contraction Consistency and Purification (DSL*)

- trace relations of (full) single-time Green functions: $(G^{(2)}_{ijkl} = G^{<}_{ik}G^{<}_{jl} \pm G^{<}_{il}G^{<}_{jk} + \mathcal{G}_{ijkl})$

$$N = \pm \mathrm{i}\hbar\, \mathrm{Tr}_1 G^{(1)}_1 \,, \qquad (N-1)G^{(1)}_1 = \pm \mathrm{i}\hbar\, \mathrm{Tr}_2 G^{(2)}_{12} \,, \qquad (N-2)G^{(2)}_{12} = \pm \mathrm{i}\hbar\, \mathrm{Tr}_3 G^{(3)}_{123} \,, \qquad \ldots$$

J.-P. Joost, N. Schlünzen, H. Ohldag, M. Bonitz, F. Lackner, and I. Březinová, submitted for publication, arXiv:2202.10061

F. Lackner, et al., Phys. Rev. A **91**, 023412 (2015); F. Lackner, et al., Phys. Rev. A **95**, 033414 (2017)

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(a) enforcing **contraction consistency** results in additional correction term

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}_{ijkl}(t) = \left[h^{(2),\mathsf{HF}}, \mathcal{G}\right]_{ijkl}(t) + \Psi_{ijkl}(t) + \Lambda_{ijkl}(t) + \Pi^{\pm}_{ijkl}(t) + \underbrace{C^{\mathsf{CC}}_{ijkl}(t)}_{\text{contraction consistency}}$$

where

$$C^{\mathsf{CC}}_{ijkl}(t) = \pm i\hbar \sum_{pqr} w_{ipqr} G^{(3),\mathsf{CC}}_{qrjkpl}(t) + \text{symmetries}$$

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where

$$C^{\mathsf{CC}}_{ijkl}(t) = \pm \mathrm{i}\hbar \sum_{pqr} w_{ipqr} G^{(3),\mathsf{CC}}_{qrjkpl}(t) + \text{symmetries}$$

(b) **purification:** enforcing partial **N-representability** by keeping $(\mathrm{i}\hbar)^2\, G^{(2)}$ positive semidefinite

$$(\mathrm{i}\hbar)^2\, G^{(2)}_{ijkl} = \langle \Psi | \, \hat{c}^{\dagger}_i \hat{c}^{\dagger}_j \hat{c}_l \hat{c}_k \, | \Psi \rangle \succeq 0$$

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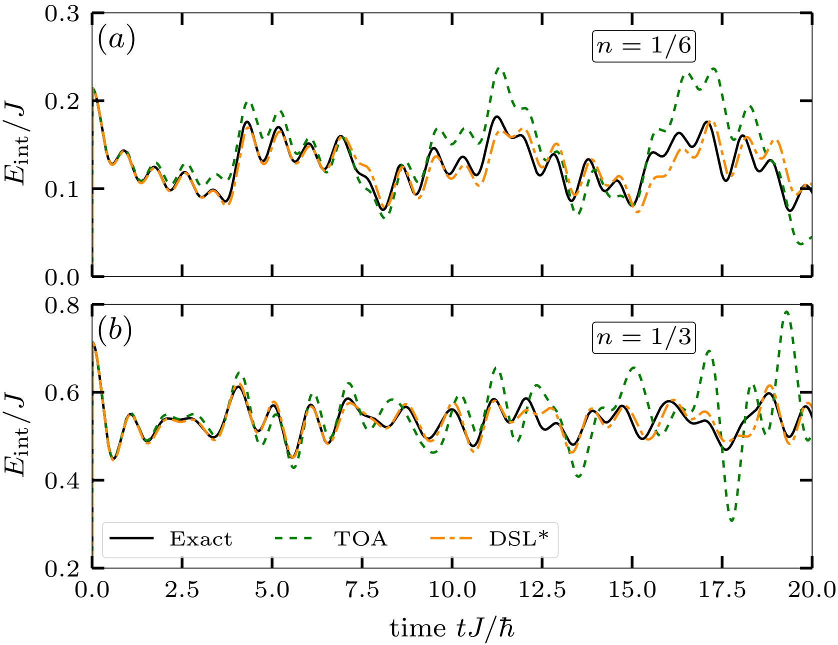
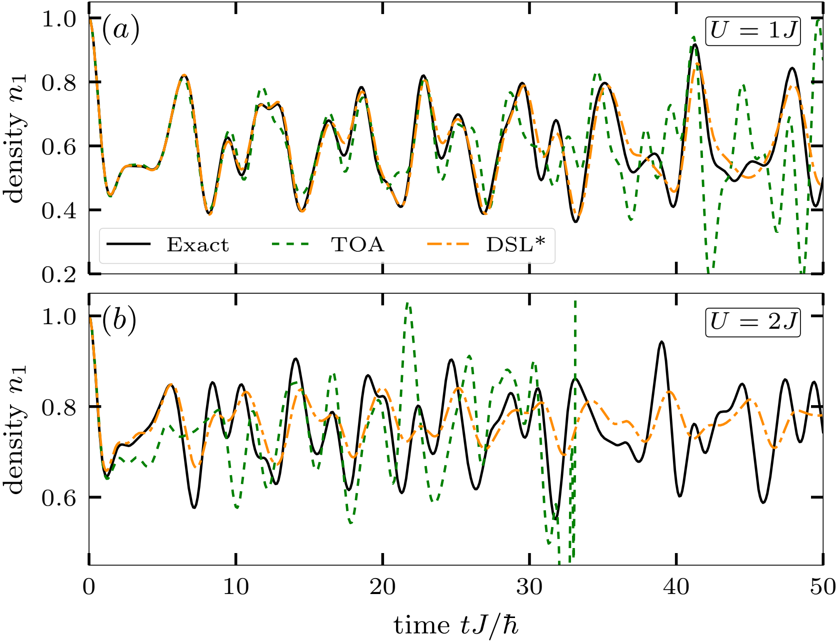
F. Lackner, et al., Phys. Rev. A **91**, 023412 (2015); F. Lackner, et al., Phys. Rev. A **95**, 033414 (2017)

6-Site Hubbard Chain: Interaction Quench $U = 0 \rightarrow J$



6-Site Hubbard Chain: External Potential on First Site $w_0 = J$



Summary and Outlook [contact: joost@theo-physik.uni-kiel.de]

approximation — **no approximation!**

Full NEGF → HF-GKBA → G1–G2

$\mathcal{O}(N_\mathrm{t}^3)$ → $\mathcal{O}(N_\mathrm{t}^2)$ → $\mathcal{O}(N_\mathrm{t}^1)$

(I) G1–G2 scheme[1]:

- NEGF (HF-GKBA) calculations can be done in **linear time** for various selfenergy approximations: 2B, GW, particle–particle and particle–hole T matrix
- DSL combines **strong electronic correlations** and **dynamical screening** out of equilibrium[2]
- greatly increases the realm of applicability of the NEGF approach (HF-GKBA):

  Y. Pavlyukh et al., PRB **104**, 035124 (2021); D. Karlsson et al., PRL **127**, 036402 (2021); E. Perfetto et al., PRL **128**, 016801 (2022)

[1] N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. Lett. **124**, 076601 (2020)

[2] J.-P. Joost, N. Schlünzen, and M. Bonitz, Phys. Rev. B **101**, 245101 (2020)

[3] J.-P. Joost, N. Schlünzen, H. Ohldag, M. Bonitz, F. Lackner, and I. Březinová, submitted for publication, arXiv:2202.10061

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approximation — **no** approximation!

Full NEGF → HF-GKBA → G1–G2

$\mathcal{O}(N_\mathrm{t}^3)$ → $\mathcal{O}(N_\mathrm{t}^2)$ → $\mathcal{O}(N_\mathrm{t}^1)$

(I) G1–G2 scheme[1]:

- NEGF (HF-GKBA) calculations can be done in **linear time** for various selfenergy approximations: 2B, GW, particle–particle and particle–hole T matrix
- DSL combines **strong electronic correlations** and **dynamical screening** out of equilibrium[2]
- greatly increases the realm of applicability of the NEGF approach (HF-GKBA):

  Y. Pavlyukh et al., PRB **104**, 035124 (2021); D. Karlsson et al., PRL **127**, 036402 (2021); E. Perfetto et al., PRL **128**, 016801 (2022)

(II) 2RDM theory: enforce contraction consistency, and N-representability by purification (DSL*)[3]

[1] N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. Lett. **124**, 076601 (2020)

[2] J.-P. Joost, N. Schlünzen, and M. Bonitz, Phys. Rev. B **101**, 245101 (2020)

[3] J.-P. Joost, N. Schlünzen, H. Ohldag, M. Bonitz, F. Lackner, and I. Březinová, submitted for publication, arXiv:2202.10061