The G1–G2 Scheme
—Nonequilibrium Green Functions in Linear Time—

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with:

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Ab initio simulations of correlated fermions
Kiel University, July 8–9, 2020

Nonequilibrium Green Functions (NEGF)

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2nd quantization

- Fock space $\mathcal{F} \ni |n_1, n_2 \ldots\rangle$, $\quad \mathcal{F} = \bigoplus_{N_0 \in \mathbb{N}} \mathcal{F}^{N_0}$, $\quad \mathcal{F}^{N_0} \subset \mathcal{H}^{N_0}$
- $\hat{c}_i, \hat{c}_i^\dagger$ creates/annihilates a particle in single-particle orbital ϕ_i
- spin accounted for by canonical (anti-)commutator relations
  $\left[\hat{c}_i^{(\dagger)}, \hat{c}_j^{(\dagger)}\right]_\mp = 0, \quad \left[\hat{c}_i, \hat{c}_j^\dagger\right]_\mp = \delta_{i,j}$
- Hamiltonian: $\hat{H}(t) = \underbrace{\sum_{k,m} h^0_{km} \hat{c}_k^\dagger \hat{c}_m}_{\hat{H}_0} + \underbrace{\frac{1}{2} \sum_{k,l,m,n} w_{klmn} \hat{c}_k^\dagger \hat{c}_l^\dagger \hat{c}_n \hat{c}_m}_{\hat{W}} + \hat{F}(t)$

Particle interaction w_{klmn}

- Coulomb interaction
- electronic correlations

Time-dependent excitation $\hat{F}(t)$

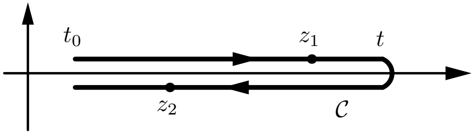
- single-particle type
- em field, quench, particles

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

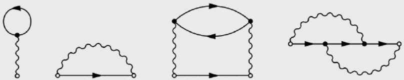
Keldysh–Kadanoff–Baym equations (KBE) on $\mathcal{C}$ (2×2 matrix):

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



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



Selfenergy Approximations[1]

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

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

GW: ∞ bubble summation,
dynamical screening effects

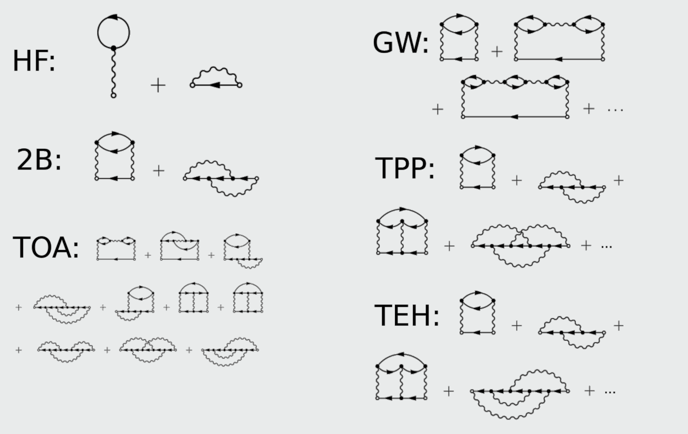
particle-particle T-matrix (TPP):
∞ ladder sum in pp channel

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

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

dynamically screened ladder (DSL):
$\sim \mathrm{2B} + GW + \mathrm{TPP} + \mathrm{TPH}$

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

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

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

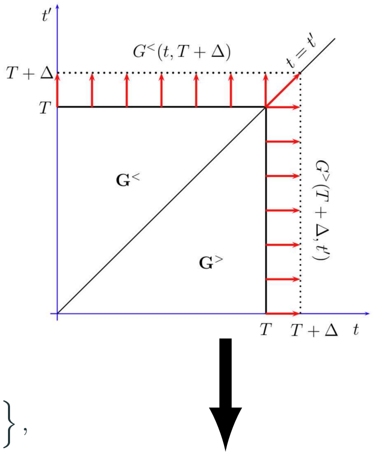
with the effective single-particle **Hartree–Fock Hamiltonian**

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

and the collision integrals

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

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



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

- numerically demanding due to N_{t}^3 scaling (most competing methods time linear)

Generalized Kadanoff–Baym Ansatz[2] (GKBA)

- full propagation on the time diagonal ($I := I^{(1),<}$):

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

- reconstruct off-diagonal NEGF from time diagonal:

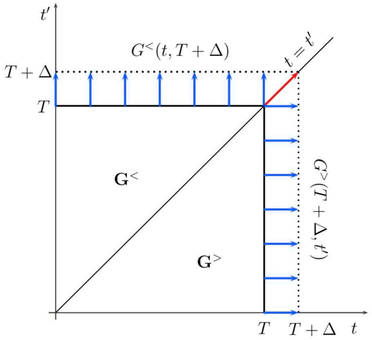
$$G^{\gtrless}_{ij}(t,t') = \pm\left[G^{\mathrm{R}}_{ik}(t,t')\rho^{\gtrless}_{kj}(t') - \rho^{\gtrless}_{ik}(t)G^{\mathrm{A}}_{kj}(t,t')\right]$$

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

- 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 total energy and reduces artificial damping problems



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

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

The fast GKBA allows for studying:[3]

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

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

Organic compounds
G. Pal *et al.*, EPJB 79, 327 (2011)
E. V. Boström *et al.*, Nano Lett. 18, 785 (2018)

Extended systems
D. Sangalli *et al.*, PRB 93, 195205 (2016)

Two-dimensional layered materials
E. A. Pogna *et al.*, ACS Nano 10, 1182 (2016)
A. Molina-Sánchez *et al.*, Nano Lett. 17, 4549 (2017)

Doublon formation by ion impact
K. Balzer *et al.*, PRL 121, 267602 (2018)

← improved scaling led to new applications

but

- improvement to N_t^2 scaling only possible for 2B selfenergy
- typical systems with small $N_\mathrm{b} \sim 10$–100 but large $N_\mathrm{t} \sim 1000$–10000
- still huge numerical disadvantage compared to other linearly scaling methods (TD-DMRG, TDDFT, TDSE)

Is $\mathcal{O}(N_\mathrm{t}^1)$ scaling possible?

[3] D. Karlsson, *Speeding up GKBA calculations using initial correlations*, KBEt^2 workshop, Kiel (2019)

Reformulating the GKBA

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

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

time integral — off-diagonal functions

Reformulating the GKBA

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

$$I_{ij}(t) = \sum_k \int_{t_0}^{t} d\bar{t} \left[\Sigma^>_{ik}(t,\bar{t}) G^<_{kj}(\bar{t},t) - \Sigma^<_{ik}(t,\bar{t}) G^>_{kj}(\bar{t},t)\right] =: \pm i\hbar \sum_{klp} w_{iklp}(t)\mathcal{G}_{lpjk}(t)$$

time integral — off-diagonal functions

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

Reformulating the GKBA

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time integral — off-diagonal functions — **Idea:** solve differential equation for $\mathcal{G}$ instead of time integral for I

- example for 2B selfenergy[4]

$$\Sigma^{\gtrless}_{ij}\left(t,t'\right) = \pm\left(\mathrm{i}\hbar\right)^2 \sum_{klpqrs} w_{iklp}\left(t\right) w^{\pm}_{qrjs}\left(t'\right) G^{\gtrless}_{lq}\left(t,t'\right) G^{\gtrless}_{pr}\left(t,t'\right) G^{\lessgtr}_{sk}\left(t',t\right)$$

- respective $\mathcal{G}$ can be identified as

$$\mathcal{G}_{ijkl}(t) = \mathrm{i}\hbar \sum_{pqrs} \int_{t_0}^{t} \mathrm{d}\bar{t}\, w^{\pm}_{pqrs}\left(\bar{t}\right) \left[\mathcal{G}^{\mathrm{H},>}_{ijpq}(t,\bar{t}) \mathcal{G}^{\mathrm{H},<}_{rskl}(\bar{t},t) - \mathcal{G}^{\mathrm{H},<}_{ijpq}(t,\bar{t}) \mathcal{G}^{\mathrm{H},>}_{rskl}(\bar{t},t)\right]$$

with the two-particle Hartree Green function

$$\mathcal{G}^{\mathrm{H},\gtrless}_{ijkl}(t,t') := G^{\gtrless}_{ik}(t,t') G^{\gtrless}_{jl}(t,t')$$

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

Hartree–Fock Time-Evolution Operators

- it is convenient to introduce the single- and two-particle propagators

$$\mathcal{U}_{ij}(t,t') = G^{\mathrm{R}}_{ij}(t,t') - G^{\mathrm{A}}_{ij}(t,t')$$
$$\mathcal{U}^{(2)}_{ijkl}(t,t') = \mathcal{U}_{ik}(t,t')\mathcal{U}_{jl}(t,t')$$

- they obey Schrödinger-type EOMs

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathcal{U}^{(2)}_{ijkl}(t,\bar{t})\right] = \frac{1}{\mathrm{i}\hbar}\sum_{pq} h^{(2),\mathsf{HF}}_{ijpq}(t)\mathcal{U}^{(2)}_{pqkl}(t,\bar{t})$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\mathcal{U}^{(2)}_{ijkl}(\bar{t},t)\right] = -\frac{1}{\mathrm{i}\hbar}\sum_{pq} \mathcal{U}^{(2)}_{ijpq}(\bar{t},t)h^{(2),\mathsf{HF}}_{pqkl}(t)$$

with the effective two-particle Hamiltonian

$$h^{(2),\mathsf{HF}}_{ijkl}(t) = \delta_{jl}h^{\mathsf{HF}}_{ik}(t) + \delta_{ik}h^{\mathsf{HF}}_{jl}(t)$$

Properties

- Symmetries

$$\mathcal{U}^{(2)}_{jilk}(t,t') = \mathcal{U}^{(2)}_{ijkl}(t,t')$$
$$\left[\mathcal{U}^{(2)}_{klij}(t,t')\right]^* = \mathcal{U}^{(2)}_{ijkl}(t',t)$$

- Group property

$$\mathcal{U}^{(2)}_{ijkl}(t,t') = (\mathrm{i}\hbar)^2\sum_{pq}\mathcal{U}^{(2)}_{ijpq}(t,\bar{t})\mathcal{U}^{(2)}_{pqkl}(\bar{t},t')$$

- Initial values

$$\mathcal{U}_{ij}(t,t) = \frac{1}{\mathrm{i}\hbar}\delta_{ij}$$
$$\mathcal{U}^{(2)}_{ijkl}(t,t) = \frac{1}{(\mathrm{i}\hbar)^2}\delta_{ik}\delta_{jl}$$

Reformulating the GKBA

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- original expression for $\mathcal{G}$ in 2B approximation

$$\mathcal{G}_{ijkl}(t) = \mathrm{i}\hbar \sum_{pqrs} \int_{t_0}^{t} \mathrm{d}\bar{t}\, w^{\pm}_{pqrs}\left(\bar{t}\right) \left[\mathcal{G}^{\mathsf{H},>}_{ijpq}(t,\bar{t})\mathcal{G}^{\mathsf{H},<}_{rskl}(\bar{t},t) - \mathcal{G}^{\mathsf{H},<}_{ijpq}(t,\bar{t})\mathcal{G}^{\mathsf{H},>}_{rskl}(\bar{t},t)\right]$$

- reconstruction of off-diagonal Hartree Green functions using $\mathcal{U}^{(2)}$ in the HF-GKBA

$$\mathcal{G}^{\mathsf{H},\gtrless}_{ijpq}(t' \leq t) = (\mathrm{i}\hbar)^2 \sum_{pq} \mathcal{G}^{\mathsf{H},\gtrless}_{ijpq}(t',t')\mathcal{U}^{(2)}_{pqkl}(t',t)$$

$$\mathcal{G}^{\mathsf{H},\gtrless}_{ijpq}(t \geq t') = (\mathrm{i}\hbar)^2 \sum_{pq} \mathcal{U}^{(2)}_{ijpq}(t,t')\mathcal{G}^{\mathsf{H},\gtrless}_{pqkl}(t',t')$$

Reformulating the GKBA

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$$\mathcal{G}^{\mathrm{H},\gtrless}_{ijpq}(t \geq t') = (\mathrm{i}\hbar)^2 \sum_{pq} \mathcal{U}^{(2)}_{ijpq}(t,t')\mathcal{G}^{\mathrm{H},\gtrless}_{pqkl}(t',t')$$

- resulting in more convenient expression for $\mathcal{G}$

$$\mathcal{G}_{ijkl}(t) = (\mathrm{i}\hbar)^3 \sum_{pqrs} \int_{t_0}^{t} \mathrm{d}\bar{t}\, \mathcal{U}^{(2)}_{ijpq}(t,\bar{t})\Psi^{\pm}_{pqrs}(\bar{t})\mathcal{U}^{(2)}_{rskl}(\bar{t},t)$$

with the single-time source term (which no longer depends on the outer time)

$$\Psi^{\pm}_{ijkl}(t) = (\mathrm{i}\hbar)^2 \sum_{pqrs} w^{\pm}_{pqrs}(t)\left[\mathcal{G}^{\mathrm{H},>}_{ijpq}(t,t)\mathcal{G}^{\mathrm{H},<}_{rskl}(t,t) - \mathcal{G}^{\mathrm{H},<}_{ijpq}(t,t)\mathcal{G}^{\mathrm{H},>}_{rskl}(t,t)\right]$$

Reformulating the GKBA

- **Goal:** find equation of motion for

$$\mathcal{G}_{ijkl}(t) = (\mathrm{i}\hbar)^3 \sum_{pqrs} \int_{t_0}^{t} \mathrm{d}\bar{t}\, \underbrace{\mathcal{U}^{(2)}_{ijpq}(t,\bar{t})\Psi^{\pm}_{pqrs}(\bar{t})\mathcal{U}^{(2)}_{rskl}(\bar{t},t)}_{f(t,\bar{t})}$$

- Leibniz integral rule:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_{t_0}^{t} f(t,\bar{t})\mathrm{d}\bar{t}\right] = f\left(t,t\right) + \int_{t_0}^{t} \frac{\partial}{\partial t} f(t,\bar{t})\mathrm{d}\bar{t}$$

- thus, the time derivative has two contributions

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}_{ijkl}(t) = \left[\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}_{ijkl}(t)\right]_{\int} + \left[\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}_{ijkl}(t)\right]_{\mathcal{U}^{(2)}}$$

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- the first from the integral boundary

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}_{ijkl}(t)\right]_{\int} = (\mathrm{i}\hbar)^3 \sum_{pqrs} \mathcal{U}^{(2)}_{ijpq}(t,t)\Psi^{\pm}_{pqrs}(t)\mathcal{U}^{(2)}_{rskl}(t,t) = \frac{1}{\mathrm{i}\hbar}\Psi^{\pm}_{ijkl}(t)$$

- the second using the EOMs of $\mathcal{U}^{(2)}$

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}_{ijkl}(t)\right]_{\mathcal{U}^{(2)}} = \frac{1}{\mathrm{i}\hbar}\sum_{pq} h^{(2),\mathrm{HF}}_{ijpq}(t)\,\mathcal{G}_{pqkl}(t) - \frac{1}{\mathrm{i}\hbar}\sum_{pq}\mathcal{G}_{ijpq}(t)\,h^{(2),\mathrm{HF}}_{pqkl}(t)$$

The G1–G2 Scheme

- full propagation on the time diagonal as for ordinary HF-GKBA:

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

- but collision integral defined by correlated two-particle Green function

$$I_{ij}(t) = \pm\mathrm{i}\hbar\sum_{klp} w_{iklp}(t)\mathcal{G}_{lpjk}(t)$$

- which obeys an ordinary differential equation[5]

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}_{ijkl}(t) = \left[h^{(2),\mathrm{HF}}, \mathcal{G}\right]_{ijkl}(t) + \Psi^{\pm}_{ijkl}(t)$$

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

[5] two-particle commutator: $[A, B]_{ijkl}(t) = \sum_{pq}\left[A_{ijpq}(t)B_{pqkl}(t) - B_{ijpq}(t)A_{pqkl}(t)\right]$

The G1–G2 Scheme

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$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{G}_{ijkl}(t) = \left[h^{(2),\mathrm{HF}}, \mathcal{G}\right]_{ijkl}(t) + \Psi^{\pm}_{ijkl}(t)$$

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

- the initial values

$$G^{0,<}_{ij} = \pm \frac{1}{\mathrm{i}\hbar} n_{ij}(t_0) =: \pm \frac{1}{\mathrm{i}\hbar} n^0_{ij} ,$$

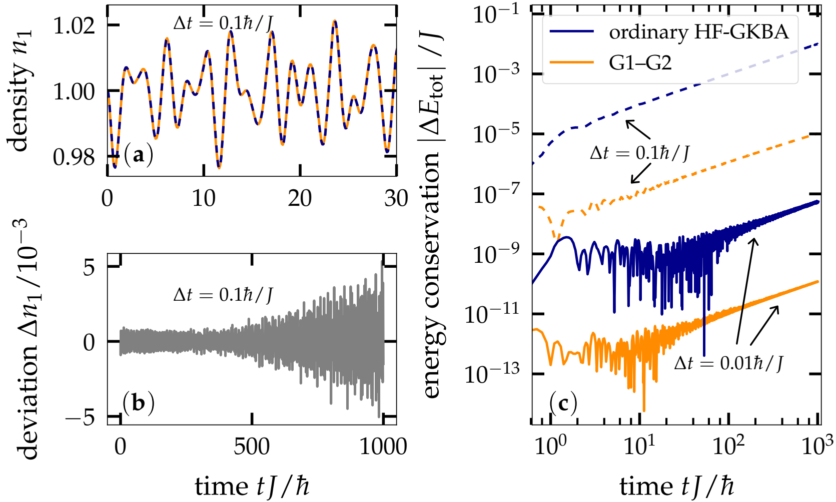
$$\mathcal{G}^0_{ijkl} = \frac{1}{(\mathrm{i}\hbar)^2} \left\{ n^0_{ijkl} - n^0_{ik} n^0_{jl} \mp n^0_{il} n^0_{jk} \right\} ,$$

  determine the density and the pair correlations existing in the system at the initial time $t = t_0$

[5] two-particle commutator: $[A, B]_{ijkl}(t) = \sum_{pq} [A_{ijpq}(t) B_{pqkl}(t) - B_{ijpq}(t) A_{pqkl}(t)]$

Comparing G1–G2 to Standard HF-GKBA (four-site Hubbard chain)

- G1–G2 scheme introduces no further approximation, results (here: 2B) exactly coincide with the standard HF-GKBA implementation



- other selfenergy approximations can be reformulated in the G1–G2 scheme in similar fashion:[6]

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}_{ijkl}(t) = \left[h^{(2),\mathsf{HF}}(t), \mathcal{G}(t)\right]_{ijkl} + \Psi^{\pm}_{ijkl}(t) + \underbrace{L_{ijkl}(t)}_{\mathsf{TPP}} + \underbrace{P_{ijkl}(t)}_{GW} \pm \underbrace{P_{jikl}(t)}_{\mathsf{TPH}}$$

with (times dropped)

$$L_{ijkl} := \sum_{pq}\left\{\mathfrak{h}^{L}_{ijpq}\mathcal{G}_{pqkl} - \mathcal{G}_{ijpq}\left[\mathfrak{h}^{L}_{klpq}\right]^*\right\}, \qquad \mathfrak{h}^{L}_{ijkl} := (\mathrm{i}\hbar)^2\sum_{pq}\left[\mathcal{G}^{\mathsf{H},>}_{ijpq} - \mathcal{G}^{\mathsf{H},<}_{ijpq}\right]w_{pqkl}\,,$$

$$P_{ijkl} := \sum_{pq}\left\{\mathfrak{h}^{\Pi}_{qjpl}\mathcal{G}_{piqk} - \mathcal{G}_{qjpl}\left[\mathfrak{h}^{\Pi}_{qkpi}\right]^*\right\}, \qquad \mathfrak{h}^{\Pi}_{ijkl} := \pm(\mathrm{i}\hbar)^2\sum_{pq}w^{\pm}_{qipk}\left[\mathcal{G}^{\mathsf{F},>}_{jplq} - \mathcal{G}^{\mathsf{F},<}_{jplq}\right]$$

and the Hartree/Fock (H/F) two-particle Green functions

$$\mathcal{G}^{\mathsf{H},\gtrless}_{ijkl}(t) := G^{\gtrless}_{ik}(t,t)G^{\gtrless}_{jl}(t,t)\,, \qquad \mathcal{G}^{\mathsf{F},\gtrless}_{ijkl}(t) := G^{\gtrless}_{il}(t,t)G^{\lessgtr}_{jk}(t,t)$$

- including all terms results in the dynamically-screened-ladder (DSL) approximation

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

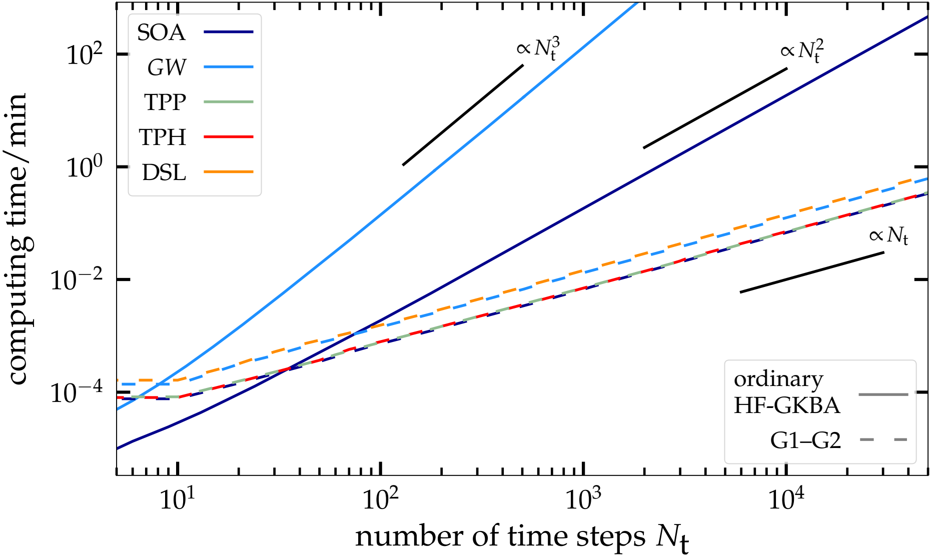
Numerical Scaling of G1–G2 vs. Standard HF-GKBA

- linear time scaling outweights introduction of 4-dimensional two-particle Green function
  $\rightarrow$ new scheme an improvement in most cases of practical relevance

Basis	HF-GKBA	2B (Σ)	GW (Σ)	TPP (Σ)	TPH (Σ)	DSL (Σ)
general	standard	$\mathcal{O}\left(N_b^5 N_t^2\right)$	$\mathcal{O}\left(N_b^6 N_t^3\right)$	$\mathcal{O}\left(N_b^6 N_t^3\right)$	$\mathcal{O}\left(N_b^6 N_t^3\right)$	–
	G1–G2	$\mathcal{O}\left(N_b^5 N_t^1\right)$	$\mathcal{O}\left(N_b^6 N_t^1\right)$	$\mathcal{O}\left(N_b^6 N_t^1\right)$	$\mathcal{O}\left(N_b^6 N_t^1\right)$	$\mathcal{O}\left(N_b^6 N_t^1\right)$
	speedup ratio	$\mathcal{O}\left(N_t\right)$	$\mathcal{O}\left(N_t^2\right)$	$\mathcal{O}\left(N_t^2\right)$	$\mathcal{O}\left(N_t^2\right)$	–
Hubbard	standard	$\mathcal{O}\left(N_b^3 N_t^2\right)$	$\mathcal{O}\left(N_b^3 N_t^3\right)$	$\mathcal{O}\left(N_b^3 N_t^3\right)$	$\mathcal{O}\left(N_b^3 N_t^3\right)$	–
	G1–G2	$\mathcal{O}\left(N_b^4 N_t^1\right)$	$\mathcal{O}\left(N_b^4 N_t^1\right)$	$\mathcal{O}\left(N_b^4 N_t^1\right)$	$\mathcal{O}\left(N_b^4 N_t^1\right)$	$\mathcal{O}\left(N_b^4 N_t^1\right)$
	speedup ratio	$\mathcal{O}\left(N_t/N_b\right)$	$\mathcal{O}\left(N_t^2/N_b\right)$	$\mathcal{O}\left(N_t^2/N_b\right)$	$\mathcal{O}\left(N_t^2/N_b\right)$	–
Jellium	standard	$\mathcal{O}\left(N_b^3 N_t^2\right)$	$\mathcal{O}\left(N_b^3 N_t^3\right)$	$\mathcal{O}\left(N_b^3 N_t^3\right)$	$\mathcal{O}\left(N_b^3 N_t^3\right)$	–
	G1–G2	$\mathcal{O}\left(N_b^3 N_t^1\right)$	$\mathcal{O}\left(N_b^3 N_t^1\right)$	$\mathcal{O}\left(N_b^4 N_t^1\right)$	$\mathcal{O}\left(N_b^4 N_t^1\right)$	$\mathcal{O}\left(N_b^4 N_t^1\right)$
	speedup ratio	$\mathcal{O}\left(N_t\right)$	$\mathcal{O}\left(N_t^2\right)$	$\mathcal{O}\left(N_t^2/N_b\right)$	$\mathcal{O}\left(N_t^2/N_b\right)$	–

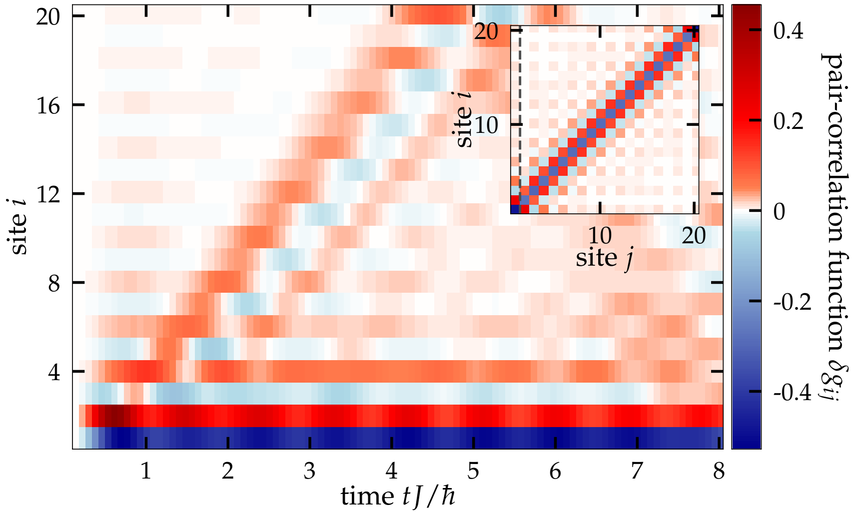
Numerical Scaling of G1–G2 vs. Standard HF-GKBA

- time-linear scaling illustrated for the 10-site Hubbard chain

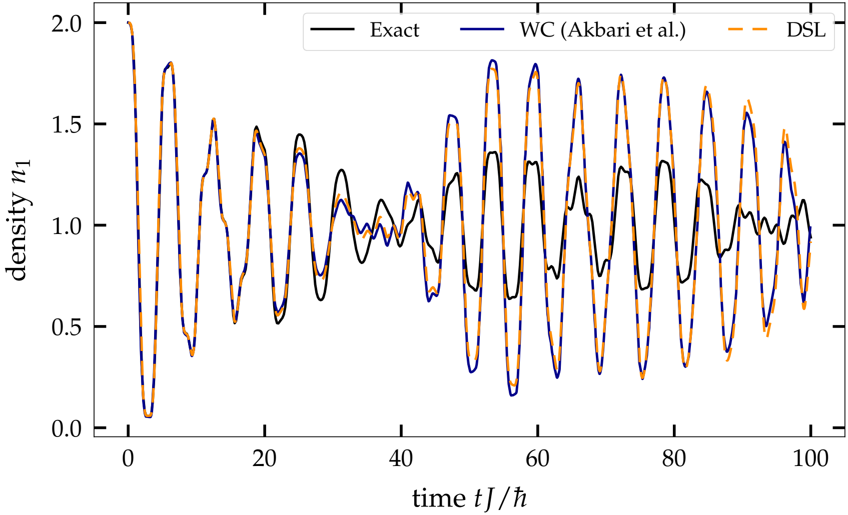


Two-Particle Observables ($N_s = 20$, $U = 2J$ quench)

- access to two-particle observables such as the pair-distribution function (PDF) $g(\boldsymbol{r}_1, \sigma_1; \boldsymbol{r}_2, \sigma_2; t)$ and its Fourier transform—the static structure factor
- here: pair-correlation function (PCF) relative to site 1, $\delta g_{i\uparrow,1\downarrow} = g_{i\uparrow,1\downarrow} - n_{i\uparrow} n_{1\downarrow}$



- DSL: neglecting three-particle correlations in BBGKY hierarchy (Wang–Cassing approximation)[7]



[7] A. Akbari *et al.*, Phys. Rev. B **85**, 235121 (2012)

Jellium

Summary

	approximation		**no approximation!**	
Full NEGF	⟶	HF-GKBA	⟶	G1–G2
$\mathcal{O}(N_\mathrm{t}^3)$		$\mathcal{O}(N_\mathrm{t}^2)$		$\mathcal{O}(N_\mathrm{t}^1)$

Summary

approximation | **no approximation!**

Full NEGF → HF-GKBA → G1–G2

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

- HF-GKBA calculations can be done in linear time (G1–G2 scheme[8]) for various selfenergy approximations: 2B, GW, particle–particle and particle–hole T matrix, DSL
- general idea: solve differential equation for $\mathcal{G}$ instead of time integral for I
- in most cases this results in significant speed-ups ($\times 10^2$–10^4, despite rank-4 $\mathcal{G}$)
- should greatly increase the realm of applicability of the HF-GKBA especially for more advanced selfenergy approximations

[8] 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 NEGF —approximation→ HF-GKBA —no approximation!→ G1–G2

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

Thank you!