Ultrafast dynamics of quantum many-body systems including dynamical screening and strong coupling

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Michael Bonitz, Jan-Philip Joost, Hannes Ohldag, and Erik Schroedter

Institute for Theoretical Physics and Astrophysics, Kiel University
in collaboration with Iva Brezinova, TU Vienna

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

Finite correlated quantum systems

Fermionic atoms in optical lattices

tunable lattice depth and interaction

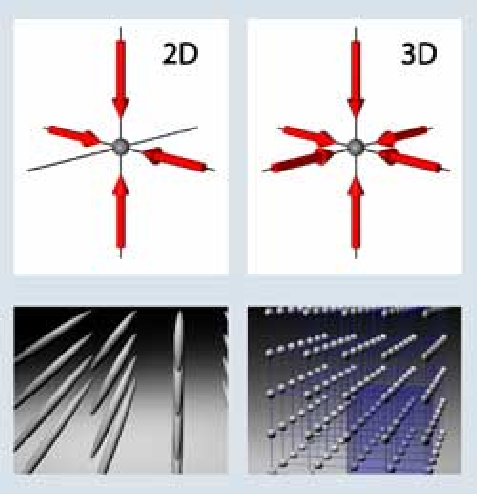
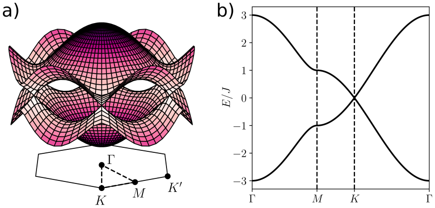


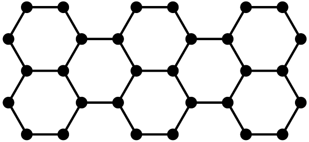
Fig.: M. Greiner (Harvard)

Graphene: high mobility, no bandgap

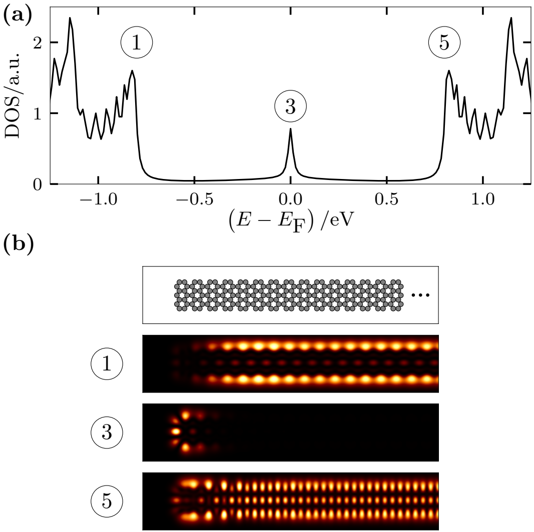


Graphene nanoribbons:

finite tunable bandgap



GNR: spatially localized spectral contributions[1]



- top: total density of states (DOS)

- DOS size and shape dependent
- many degrees of freedom: combination of materials, multiple layers

- importance of e-e interactions
- what will happen in nonequilibrium, upon external excitation (e.g. by lasers)?

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[1] 7 armchair GNR of 504 atoms, GW-NEGF ground state simulation,
J.-P. Joost, A.-P. Jauho, and M. Bonitz, Nano Letters **19**, 9045 (2019)

Time-dependent Schrödinger equation. Scaling bottleneck

- time-dependent many-electron Hamiltonian

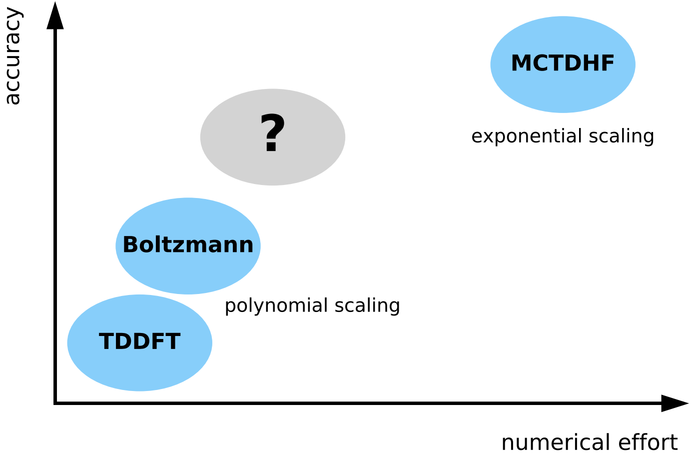
$$H(t) = \underbrace{\sum_{i=1}^{N} h(\boldsymbol{r}_i, t)}_{\text{one-body operators}} + \underbrace{\frac{1}{2}\sum_{i\neq j}^{N} W(\boldsymbol{r}_i, \boldsymbol{r}_j)}_{\textbf{pair-wise}\text{ interactions}}$$

- time-dependent Schrödinger equation (TDSE)

$$i\partial_t \Psi(\boldsymbol{r}_i, \ldots, \boldsymbol{r}_N; t) = H(t)\Psi(\boldsymbol{r}_i, \ldots, \boldsymbol{r}_N; t) \qquad \underset{\text{exponential scaling of numerical effort}}{\overset{\text{direct solution}}{\not\longrightarrow}} \qquad \Psi(\boldsymbol{r}_i, \ldots, \boldsymbol{r}_N; t)$$

- **solutions to overcome exponential scaling:**
  1. approximations to TDSE: TD-RASCI, TD-CASSCF, truncated CC, TD-R-matrix etc.
     D. Hochstuhl and M. Bonitz, PRA (2012) and EJP-ST (2014)
  2. propagation of simpler observables: density (TDDFT), distribution function (Kinetic theory), correlation functions etc.

Scaling of quantum many-body methods



*MCTDHF and other wavefunction-based methods

? Can one achieve sufficient accuracy (including e-e correlations) at non-exponential cost?

Nonequilibrium Green Functions (NEGF)

2nd quantization

- Fock space $\mathcal{F} \ni |n_1, n_2 \ldots\rangle$, $\mathcal{F} = \bigoplus_{N_0 \in \mathbb{N}} \mathcal{F}^{N_0}$, $\mathcal{F}^{N_0} \subset \mathcal{H}^{N_0}$
- $\hat{c}_i$,$\hat{c}_i^\dagger$ 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

Nonequilibrium Green Functions (NEGF)

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

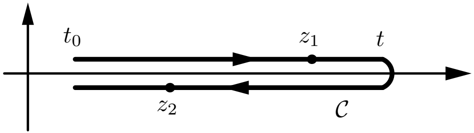
$$\boxed{G_{ij}(z,z') = \tfrac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\hat{c}_i(z)\hat{c}_j^\dagger(z')\right\rangle}$$

average with $\hat{\rho}_N$

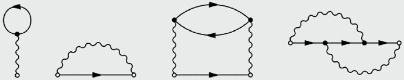
pure or mixed state

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

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



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



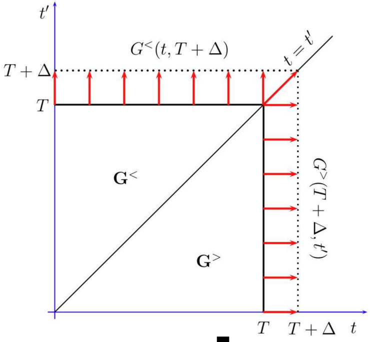
KBE: first equation of Martin–Schwinger hierarchy for $G, G^{(2)} \dots G^{(n)}$

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

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

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

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



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

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

$$I^{(2),<}_{ij}(t,t') := \sum_l \int_{t_{\mathsf{s}}}^{\infty} \mathrm{d}\bar{t}\left\{G^{\mathsf{R}}_{il}(t,\bar{t})\Sigma^{<}_{lj}(\bar{t},t') + G^{<}_{il}(t,\bar{t})\Sigma^{\mathsf{A}}_{lj}(\bar{t},t')\right\}. \longrightarrow \mathcal{O}(N_{\mathsf{t}}^3)$$

- two-time structure contains spectral information
- numerically demanding due to cubic scaling with number of time steps N_t

Selfenergy Approximations[2]

Choice depends on coupling strength, density (filling)

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

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

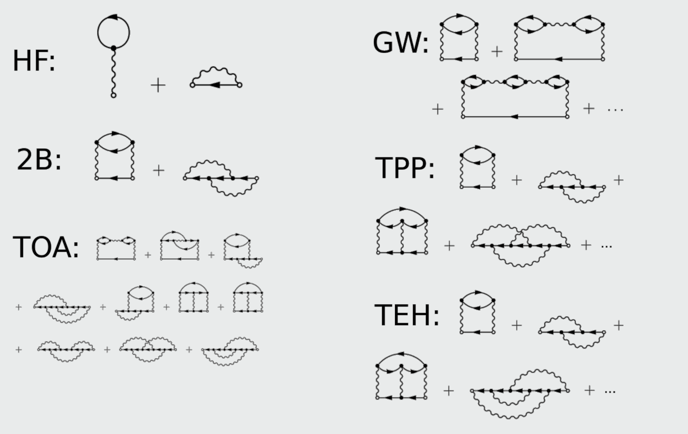
GW: ∞ bubble summation,
dynamical screening effects

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)*:
$\sim \mathrm{2B} + GW + \mathrm{TPP} + \mathrm{TPH}$



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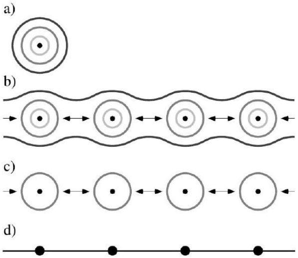
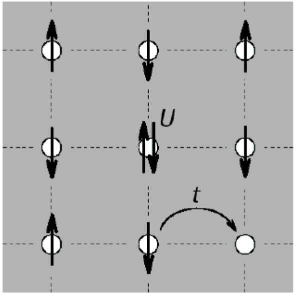
[2] Conserving approximations, nonequilibrium $\Sigma(t, t')$, applies for ultra-short to long times
Review: Schlünzen *et al.*, J. Phys. Cond. Matt. **32**, 103001 (2020); *Joost *et al.*, PRB (2022)

Testing various selfenergies: the Hubbard model

- Simple, but versatile model for strongly correlated solid state systems, 2D materials
- Suitable for single band, small bandwidth; atoms in optical lattices



$\Rightarrow$



$$\boxed{\hat{H}(t) = J \sum_{ij,\,\alpha} h_{ij}\, \hat{c}^\dagger_{i\alpha}\hat{c}_{j\alpha} + U \sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow} + \sum_{ij,\alpha\beta} f_{ij,\alpha\beta}(t)\, \hat{c}^\dagger_{i\alpha}\hat{c}_{j\beta}}$$

$h_{ij} = -\delta_{\langle i,\,j\rangle}$ and $\delta_{\langle i,\,j\rangle} = 1$, if (i, j) is nearest neighbor, $\delta_{\langle i,\,j\rangle} = 0$ otherwise

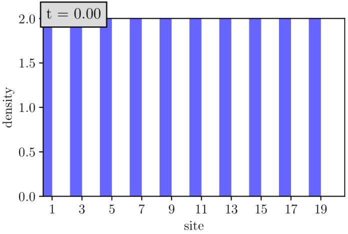
use $J = 1$, on-site repulsion $(U > 0)$ or attraction $(U < 0)$, tunable interaction strength

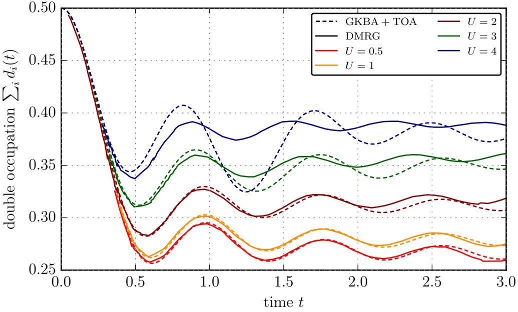
- parameters from electronic structure calculations or experiment
- systematic improvements: extended Hubbard and PPP model

Benchmarks of NEGF against DMRG (1D)[4]

Initial state:

charge density wave





- sensitive observable: total double occupation
- good quality transients NEGF up to $U \simeq$ bandwidth
- accurate long-time behavior of GKBA+T-matrix (not shown)
- performance of different selfenergies vs. coupling and filling[3]

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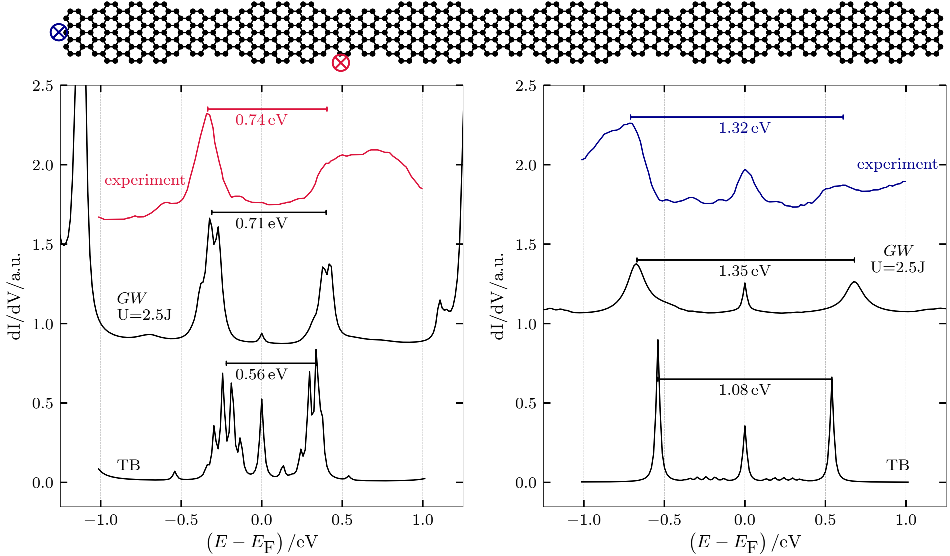
[3] N. Schlünzen, S. Hermanns, M. Scharnke, and M. Bonitz, J. Phys.: Cond. Matt. 32 (10), 103001 (2020)

[4] N. Schlünzen, J.-P. Joost, F. Heidrich-Meisner, and M. Bonitz, Phys. Rev. B **95**, 165139 (2017)

Local density of states of graphene nanoribbons: Bulk vs. End



Failure of tight binding and Hartree-Fock results. Electronic correlations crucial

Experiments: Rizzo et al. Nature, **560**, 204 (2018), NEGF simulations: Joost et al. Nano Lett. **19**, 9045 (2019)

Acceleration: Generalized Kadanoff–Baym Ansatz (GKBA)[5]

- 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:

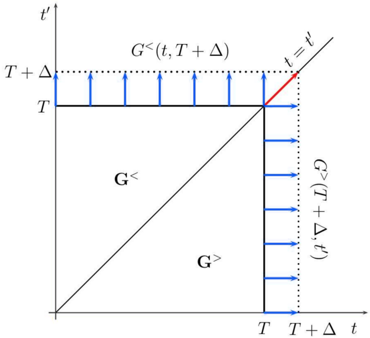
$$G^{\gtrless}_{ij}(t,t') = \pm\left[G^{\mathrm{R}}_{ik}(t,t')\rho^{\gtrless}_{kj}(t') - \rho^{\gtrless}_{ik}(t)G^{\mathrm{A}}_{kj}(t,t')\right]$$

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

- 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
- Large number of applications to atoms, molecules, condensed matter systems, plasmas



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

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[6] P. Lipavský, V. Špička, and B. Velický, Phys. Rev. B **34**, 6933 (1986); K. Balzer and M. Bonitz, Lecture Notes in Physics **867** (2013)

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

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time integral

off-diagonal functions

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

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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[6]

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

- 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

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

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

Reformulating the GKBA

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

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- example for 2B selfenergy[6]

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

Reformulating the GKBA

- two-particle $\mathcal{G}$ in GKBA

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

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

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

and the two-particle Hartree–Fock time-evolution operators obeying Schrödinger-type EOMs

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

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

with the effective two-particle Hamiltonian

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

Time-linear NEGF simulations: the G1–G2 Scheme[7]

- 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

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

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

- 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 $t = t_0$

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

The G1–G2 Scheme: beyond 2nd Born selfenergy

- other selfenergy approximations can be reformulated in the G1–G2 scheme in similar fashion:[8]

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

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

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

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

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

- include TPP, GW and TPH terms simultaneously: dynamically-screened-ladder (DSL) approximation. Conserving, applicable to short times. No explicit selfenergy known.[9]
- nonequilibrium generalization of ground state result (Bethe-Salpeter equation)

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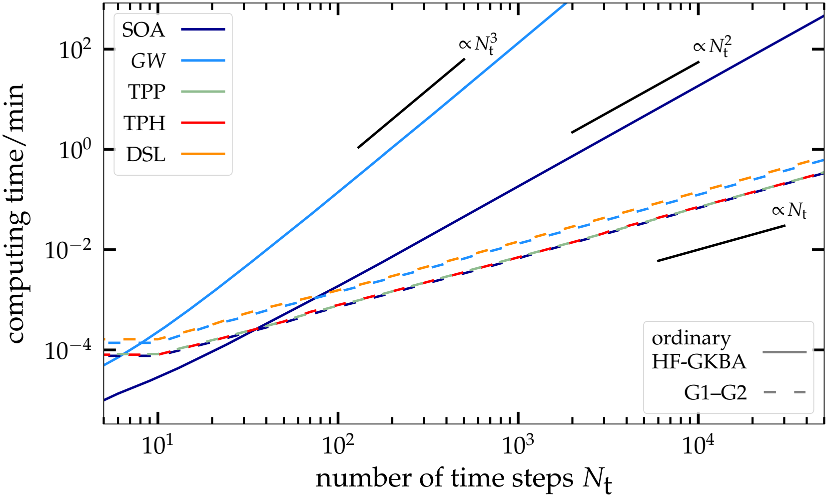
[8] J.-P. Joost, N. Schlünzen, and M. Bonitz, PRB **101**, 245101 (2020), Joost et al., PRB **105**, 165155 (2022);

[9] J.-P. Joost, PhD thesis, Kiel University 2023

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

- time-linear scaling achieved quickly for all approximations. Example: 10-site Hubbard chain



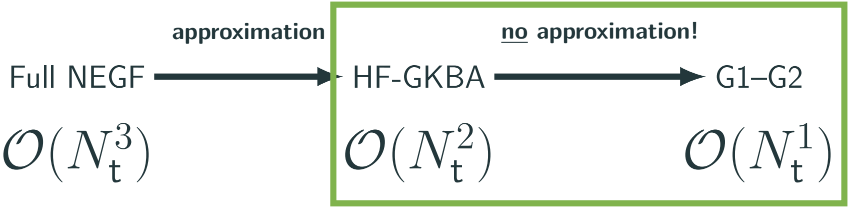
Summary and Outlook

$$\text{Full NEGF} \xrightarrow{\textbf{approximation}} \text{HF-GKBA}$$

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

- HF-GKBA recovers Boltzmann-type kinetic equations and overcomes their problems: total energy conservation, correct short-time dynamics, correlated equilibrium state

Summary and Outlook



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 recovers Boltzmann-type kinetic equations and overcomes their problems: total energy conservation, correct short-time dynamics, correlated equilibrium state
- G1–G2 calculations can be done in linear time[10], typical speed-ups: $\times 10^3$–10^6
- Full nonequilibrium DSL (combining dyn. screening and strong coupling) simulations possible
- **Price to pay:** expensive storage of $\mathcal{G}_{ijkl}(t) \rightarrow$ alternative representations of interest, e.g. quantum fluctuations approach

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[10] 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)

J.-P. Joost, N. Schlünzen, H. Ohldag, M. Bonitz, F. Lackner, and I. Brezinova, Phys. Rev. B **105**, 165155 (2022)

First principles approach to Quantum Fluctuations: Definitions[11]

- One goal: eliminate memory-costly four-point quantities ($\mathcal{G}_2$)
- Expectation values and fluctuations of Green functions: $\hat{G} = G + \delta\hat{G}$

$$G^{>}_{ij}(t) = \frac{1}{\mathrm{i}\hbar}\langle \hat{a}_i(t)\hat{a}^\dagger_j(t)\rangle, \qquad \hat{G}^{>}_{ij}(t) = \frac{1}{\mathrm{i}\hbar}\,\hat{a}_i(t)\hat{a}^\dagger_j(t)$$

$$G^{<}_{ij}(t) = \pm\frac{1}{\mathrm{i}\hbar}\,\langle \hat{a}^\dagger_j(t)\hat{a}_i(t)\rangle, \qquad \hat{G}^{<}_{ij}(t) = \pm\frac{1}{\mathrm{i}\hbar}\,\hat{a}^\dagger_j(t)\hat{a}_i(t)$$

$$\delta\hat{G}_{ij}(t) := \delta\hat{G}^{<}_{ij}(t) = \delta\hat{G}^{>}_{ij}(t)$$

- Extension to N-particle fluctuations:

$$\Gamma^{(N)}_{i_1i_2\ldots i_N;j_1j_2\ldots j_N}(t) := \langle \delta\hat{G}_{i_1j_1}(t)\delta\hat{G}_{i_2j_2}(t)\ldots\delta\hat{G}_{i_Nj_N}(t)\rangle$$

- Short notations:

$$\gamma_{ij;kl}(t) := \Gamma^{(2)}_{ij;kl}(t)\,, \qquad \Gamma_{ijk;lmn}(t) := \Gamma^{(3)}_{ijk;lmn}(t)$$

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[11] E. Schroedter, J.-P. Joost, and M. Bonitz, Cond. Matt. Phys. **25**, 23401 (2022); arXiv:2204.08250

Quantum Fluctuations: Single-particle dynamics[12]

Exact single-particle dynamics:

Collision integral in terms of fluctuations (instead of $\mathcal{G}$)

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

$$h^{\mathrm{H}}_{ij}(t) = h_{ij}(t) + U^{\mathrm{H}}_{ij}(t)\,; \quad U^{\mathrm{H}}_{ij}(t) = \pm\mathrm{i}\hbar\sum_{kl} w_{ikjl}(t) G^<_{lk}(t)$$

$$\left[\tilde{I} + \tilde{I}^\dagger\right]_{ij}(t) = \pm\mathrm{i}\hbar\sum_{klp}\left\{w_{iklp}(t)\gamma_{plkj}(t) - w_{kljp}(t)\gamma_{ipkl}(t)\right\}$$

Eliminate dynamics of $\gamma_{ij;kl}(t) = \langle\delta\hat{G}_{ik}(t)\delta\hat{G}_{jl}(t)\rangle$ by propagating $\delta\hat{G}(t)$:

Exact equation for single-particle fluctuation (two-point function)

$$\mathrm{i}\hbar\partial_t\delta\hat{G}_{ij}(t) = \left[h^{\mathrm{H}}, \delta\hat{G}\right]_{ij}(t) + \left[\delta\hat{U}^{\mathrm{H}}, G^<\right]_{ij}(t) + \left[\delta\hat{U}^{\mathrm{H}}, \delta\hat{G}\right]_{ij}(t) - \left[\tilde{I} + \tilde{I}^\dagger\right]_{ij}(t)$$

$$\delta\hat{U}^{\mathrm{H}}_{ij}(t) = \pm\mathrm{i}\hbar\sum_{kl} w_{ikjl}(t)\delta\hat{G}^<_{lk}(t)$$

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[12] E. Schroedter, J.-P. Joost, and M. Bonitz, Cond. Matt. Phys. **25**, 23401 (2022); arXiv:2204.08250

Quantum Fluctuations: Semiclassical averaging

Stochastic Mean field idea:[13]

- replace quantum-mechanical expectation value by semiclassical mean over realizations A^λ,

$$\langle \hat{A} \rangle \longrightarrow \overline{A^\lambda}$$

- Random sampling of initial conditions of non-interacting system:

$$\begin{aligned} \overline{\Delta G^\lambda_{ij}(t_0)} &= 0, \\ \overline{\Delta G^\lambda_{ik}(t_0) \Delta G^\lambda_{jl}(t_0)} &= -\frac{1}{2\hbar^2} \delta_{il}\delta_{jk}\{n_i(1 \pm n_j) + n_j(1 \pm n_i)\}. \end{aligned}$$

- Careful test of probability distribution and sampling methods[14]
- interactions turned on via adiabatic switching
- Stochastic polarization approximation reproduces time-dependent GW–G1–G2 results[22]

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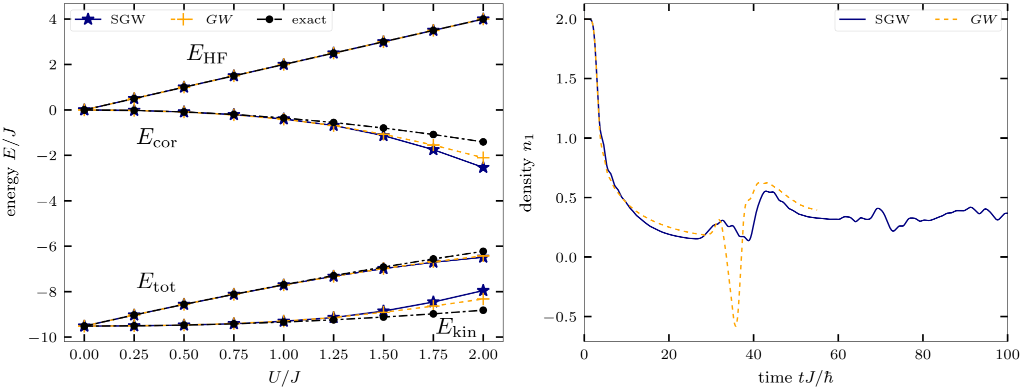
[13] S. Ayik, Phys. Lett. B **658**, 174 (2008), D. Lacroix, S. Hermanns, C. M. Hinz, and M. Bonitz, PRB **90**, 125112 (2014)

[14] E. Schroedter, J.-P. Joost, and M. Bonitz, Cond. Matt. Phys. **25**, 23401 (2022); arXiv:2204.08250

Quantum Fluctuations: Testing the stochastic GW-approximation[15]



Left: Ground state for $N_s = N = 8$. **Right:** Density dynamics following confinement quench for $N_s = 30$, $N = 10$, $\nu = 1/6$, $U = 1$. Initially leftmost 5 sites doubly occupied, rest empty.

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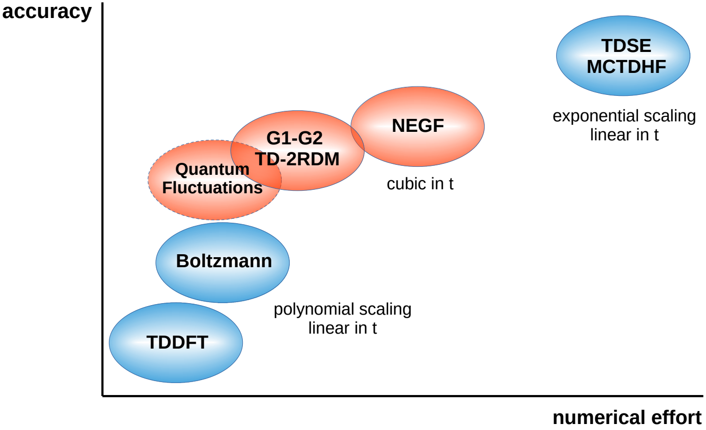
[15] E. Schroedter, J.-P. Joost, and M. Bonitz, Cond. Matt. Phys. **25**, 23401 (2022); arXiv:2204.08250

Scaling of selected quantum many-body methods revisited

G1–G2 scheme: highly efficient accurate, long and stable correlated quantum dynamics, for systems of any geometry and time scale



External input: parameters of lattice models, efficient atomic basis sets

Other results. Outlook[18]

- highly charged ion impact on 2D quantum materials, fs-neutralization dynamics[16]
- improved selfenergies (3-particle correlations), G1–G2 scheme beyond HF-GKBA
- extension to open systems via embedding selfenergies[17]
- More quantum many-body physics: Conference *Progress in Nonequilibrium Green Functions 8*

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[16] Niggas et al., Phys. Rev. Lett. **129**, 086802 (2022)

[17] Schlünzen et al., submitted to PRB, arXiv: 2211.09615

[18] pdf file of talk at http://www.theo-physik.uni-kiel.de/bonitz/talks.html