

Accelerating Nonequilibrium Green functions simulations: the G1-G2 scheme

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FQMT'24

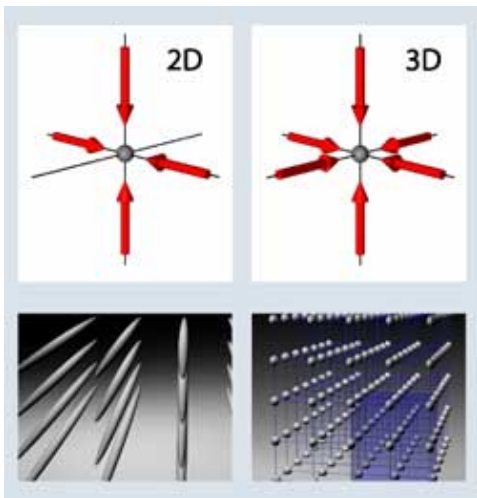
Prague, July 2024

pdf of talk: <https://www.itap.uni-kiel.de//theophysik/bonitz/talks.html>

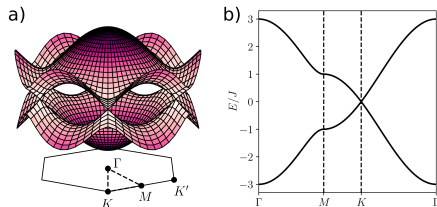
Recent review: Bonitz et al., *phys. stat. sol. (b)*
2024, DOI: 10.1002/pssb.202300578



Fermionic atoms in optical lattices
tunable lattice depth and interaction



Graphene: high mobility, no bandgap



Graphene nanoribbons (GNR):
finite tunable bandgap, topological states

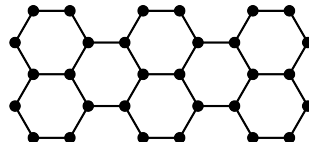
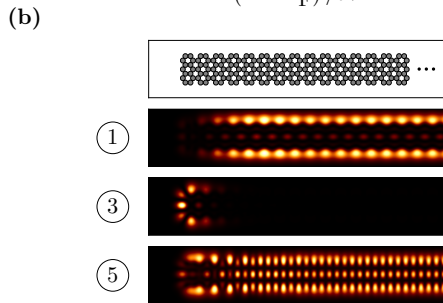
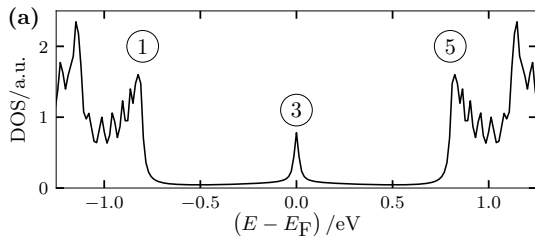


Fig.: M. Greiner (Harvard)



- top: total density of states (DOS)
- DOS size and shape dependent
- many degrees of freedom:
combination of two GNRs:
heterostructures, combination of
materials (TMDs), multiple layers,
twist angle
- bottom-up synthesis with atomic
precision

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

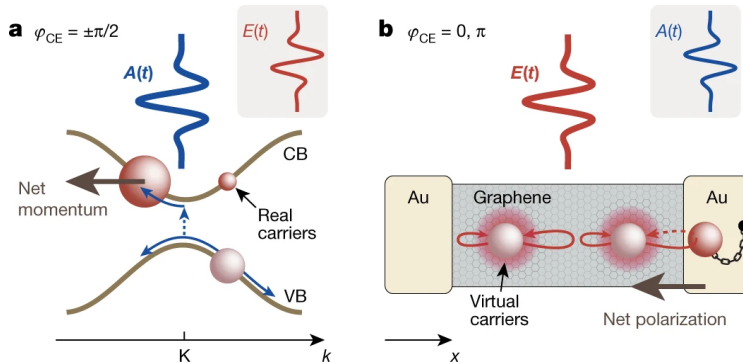
¹7 armchair GNR of 504 atoms, GW-NEGF ground state simulation,

J.-P. Joost, A.-P. Jauho, and M. Bonitz, Nano Letters **19**, 9045 (2019)

Experiments by P. Hommelhoff *et al.*: logic gate for lightwave electronics, variation of carrier envelope phase ϕ_{CE} of few cycle fs-laser pulse

a: momentum asymmetry ($A(t)$) creates $f_c(-k) \neq f_c(k)$ and net current

b: real space asymmetry ($E(t)$) of density creates net polarization



²Boolakee et al., Nature **605**, 251 (2022)

- time-dependent many-electron Hamiltonian

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

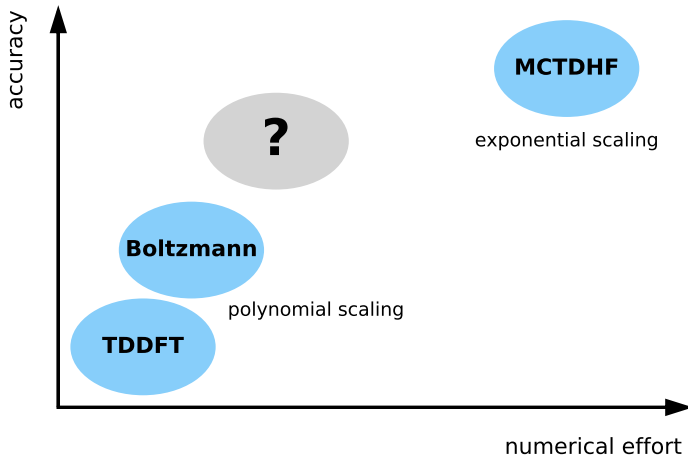
- time-dependent Schrödinger equation (TDSE)

$$i\partial_t \Psi(\mathbf{r}_1, \dots, \mathbf{r}_N; t) = H(t) \Psi(\mathbf{r}_1, \dots, \mathbf{r}_N; t)$$

direct solution
~~↯~~
exponential scaling of numerical effort

- solutions to overcome exponential scaling:**

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



*MCTDHF and other wavefunction-based methods

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

2nd quantization

- Fock space $\mathcal{F} \ni |n_1, n_2 \dots\rangle$, $\mathcal{F} = \bigoplus_{N_0 \in \mathbb{N}} \mathcal{F}^{N_0}$, $\mathcal{F}^{N_0} \subset \mathcal{H}^{N_0}$
- $\hat{c}_i, \hat{c}_i^\dagger$ 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:
$$\hat{H}(t) = \underbrace{\sum_{k,m} h_{km}^0 \hat{c}_k^\dagger \hat{c}_m}_{\hat{H}_0} + \frac{1}{2} \underbrace{\sum_{k,l,m,n} w_{klmn} \hat{c}_k^\dagger \hat{c}_l^\dagger \hat{c}_n \hat{c}_m}_{\hat{W}} + \hat{F}(t)$$

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)

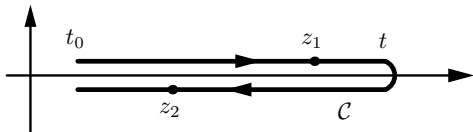
two times $z, z' \in \mathcal{C}$ ("Keldysh contour"), arbitrary one-particle basis $|\phi_i\rangle$

$$G_{ij}(z, z') = \frac{i}{\hbar} \langle \hat{T}_{\mathcal{C}} \hat{c}_i(z) \hat{c}_j^\dagger(z') \rangle \quad \text{average with } \hat{\rho}_N$$

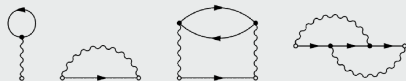
pure or mixed state

Keldysh–Kadanoff–Baym equations (KBE) on \mathcal{C} (2×2 matrix)³:

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



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



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

³L.V. Keldysh ZhETF (1964),

obituary: Bonitz, Jauho, Sadovskii, and Tikhodeev, phys. stat. sol. (b)(2019)

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

$$\sum_l \left[i\hbar \frac{d}{dt} \delta_{i,l} - h_{il}^{\text{eff}}(t) \right] G_{lj}^>(t, t') = I_{ij}^{(1),>}(t, t'),$$

$$\sum_l G_{il}^<(t, t') \left[-i\hbar \frac{d}{dt'} \delta_{l,j} - h_{lj}^{\text{eff}}(t') \right] = I_{ij}^{(2),<}(t, t'),$$

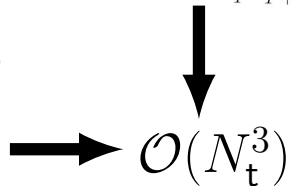
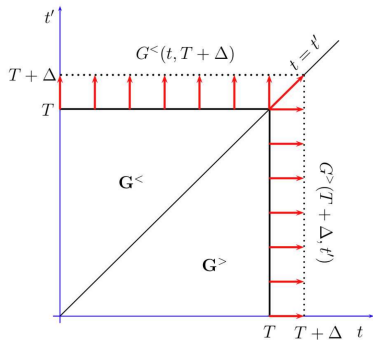
with the effective single-particle **Hartree–Fock Hamiltonian**

$$h_{ij}^{\text{eff}}(t) = h_{ij}^0 \pm i\hbar \sum_{kl} w_{ikjl}^{\pm} G_{lk}^<(t)$$

and the collision integrals

$$I_{ij}^{(1),>}(t, t') := \sum_l \int_{t_s}^{\infty} d\bar{t} \left\{ \Sigma_{il}^R(t, \bar{t}) G_{lj}^>(\bar{t}, t') + \Sigma_{il}^>(t, \bar{t}) G_{lj}^A(\bar{t}, t') \right\},$$

$$I_{ij}^{(2),<}(t, t') := \sum_l \int_{t_s}^{\infty} d\bar{t} \left\{ G_{il}^R(t, \bar{t}) \Sigma_{lj}^<(\bar{t}, t') + G_{il}^<(t, \bar{t}) \Sigma_{lj}^A(\bar{t}, t') \right\}.$$



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

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):

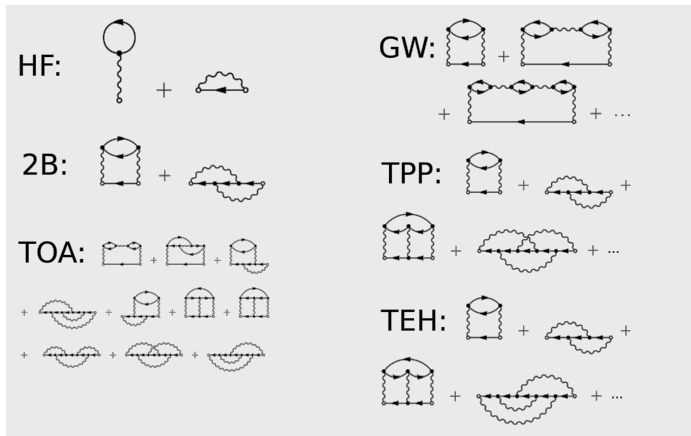
∞ ladder sum in ph channel

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

dynamically screened ladder (DSL)*:

$\sim 2B + GW + TPP + TPH$

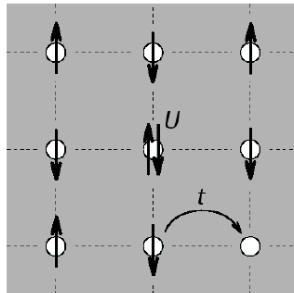
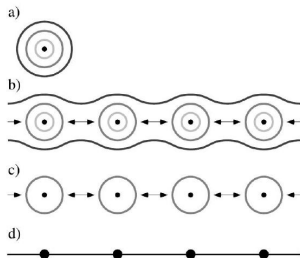
Choice depends on coupling strength, density (filling)



⁴Conserving 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)

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



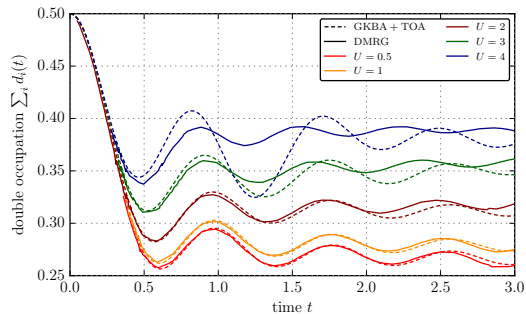
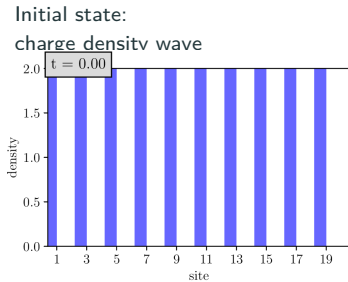
$$\hat{H}(t) = J \sum_{ij, \alpha} h_{ij} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\alpha} + U \sum_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} + \sum_{ij, \alpha\beta} f_{ij, \alpha\beta}(t) \hat{c}_{i\alpha}^\dagger \hat{c}_{j\beta}$$

$h_{ij} = -\delta_{\langle i, j \rangle}$ 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

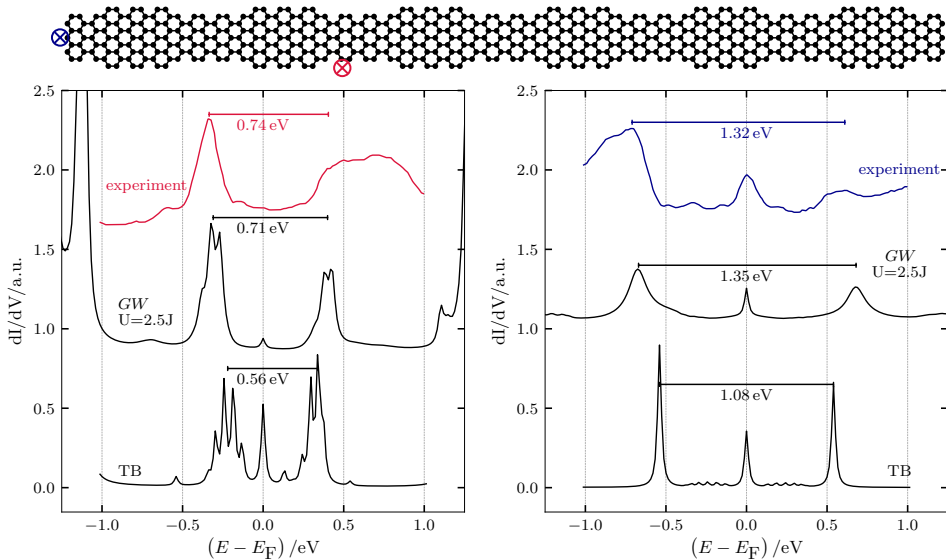
- systematic improvements: extended Hubbard and PPP model [Joost *et al.*, *phys. stat. sol. (b)* 2019]



- 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 filling⁵

⁵N. Schlünzen, S. Hermanns, M. Scharnke, and M. Bonitz, J. Phys.: Cond. Matt. 32 (10), 103001 (2020)

⁶N. Schlünzen, J.-P. Joost, F. Heidrich-Meisner, and M. Bonitz, Phys. Rev. B 95, 165139 (2017)



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)⁷

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

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

- **reconstruct off-diagonal NEGF** from time diagonal:

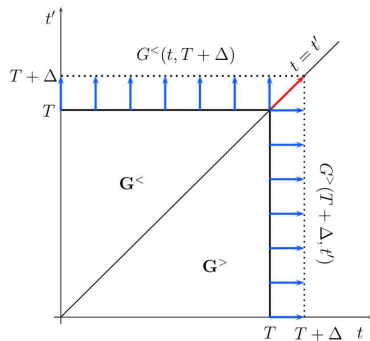
$$G_{ij}^{\geq}(t, t') = \pm \left[G_{ik}^{\text{R}}(t, t') \rho_{kj}^{\geq}(t') - \rho_{ik}^{\geq}(t) G_{kj}^{\text{A}}(t, t') \right]$$

with $\rho_{ij}^{\geq}(t) = \pm i\hbar G_{ij}^{\geq}(t, t)$

- HF-GKBA: use Hartree–Fock propagators for $G_{ij}^{\text{R/A}}$

$$G_{ij}^{\text{R/A}}(t, t') = \mp i \Theta_C(\pm[t - t']) \exp\left(-\frac{i}{\hbar} \int_{t'}^t d\bar{t} h_{\text{HF}}(\bar{t})\right) \Big|_{ij}$$

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



$$\mathcal{O}(N_t^2)$$

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)

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

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

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 selfenergy⁸

$$\Sigma_{ij}^{\gtrless}(t, t') = \pm (i\hbar)^2 \sum_{klpqrs} w_{iklp}(t) w_{qrjs}^{\pm}(t') G_{lq}^{\gtrless}(t, t') G_{pr}^{\gtrless}(t, t') G_{sk}^{\lesseqgtr}(t', t)$$

- respective \mathcal{G} can be identified as

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

with the two-particle Hartree Green function

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

⁸ N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. Lett. **124**, 076601 (2020)

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

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⁸ N. Schlünzen, J.-P. Joost and M. Bonitz, Phys. Rev. Lett. **124**, 076601 (2020)

- two-particle \mathcal{G} in GKBA

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

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

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

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

$$\begin{aligned} \frac{d}{dt} \left[\mathcal{U}_{ijkl}^{(2)}(t, \bar{t}) \right] &= \frac{1}{i\hbar} \sum_{pq} h_{ijpq}^{(2),\text{HF}}(t) \mathcal{U}_{pqkl}^{(2)}(t, \bar{t}) \\ \frac{d}{dt} \left[\mathcal{U}_{ijkl}^{(2)}(\bar{t}, t) \right] &= -\frac{1}{i\hbar} \sum_{pq} \mathcal{U}_{ijpq}^{(2)}(\bar{t}, t) h_{pqkl}^{(2),\text{HF}}(t) \end{aligned}$$

with the effective two-particle Hamiltonian

$$h_{ijkl}^{(2),\text{HF}}(t) = \delta_{jl} h_{ik}^{\text{HF}}(t) + \delta_{ik} h_{jl}^{\text{HF}}(t)$$

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

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

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

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

- which obeys an ordinary differential equation

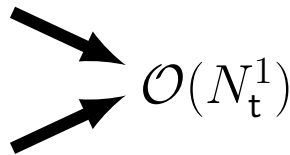
$$i\hbar \frac{d}{dt} \mathcal{G}_{ijkl}(t) = [h^{(2),\text{HF}}, \mathcal{G}]_{ijkl}(t) + \Psi_{ijkl}^\pm(t)$$

- the initial values

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

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

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



⁹N. Schlünzen, J.-P. Joost, and M. Bonitz, Phys. Rev. Lett. **124**, 076601 (2020)

- other selfenergy approximations can be reformulated in the G1–G2 scheme in similar fashion:¹⁰

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

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

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

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

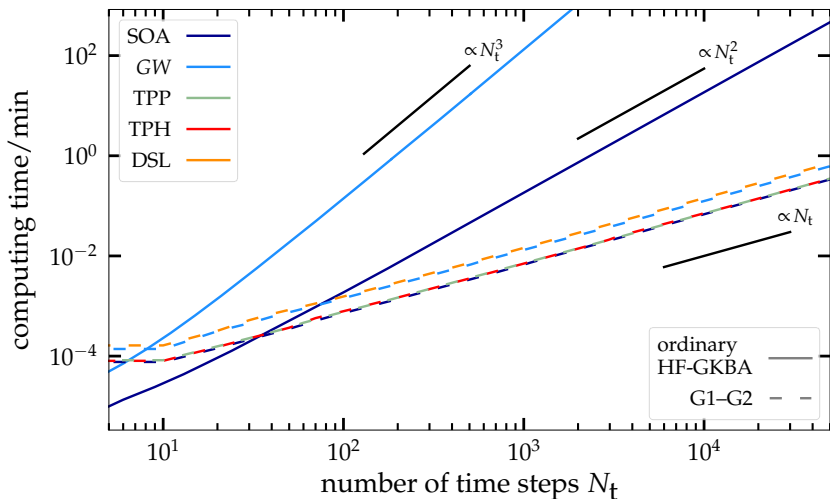
$$\mathcal{G}_{ijkl}^{\text{H},\gtrless}(t) := G_{ik}^{\gtrless}(t,t) G_{jl}^{\gtrless}(t,t), \quad \mathcal{G}_{ijkl}^{\text{F},\gtrless}(t) := G_{il}^{\gtrless}(t,t) G_{jk}^{\gtrless}(t,t)$$

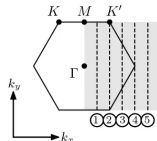
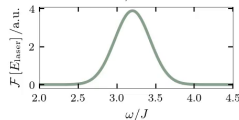
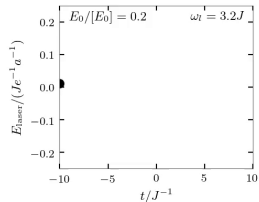
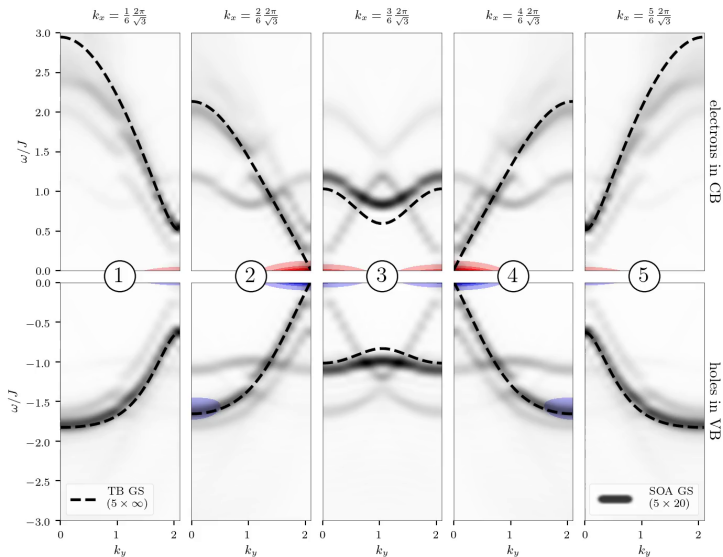
- include TPP, GW and TPH terms simultaneously: dynamically-screened-ladder (DSL) approximation. Conserving, applicable to short times. No explicit selfenergy known.¹¹
- nonequilibrium generalization of ground state result (Bethe-Salpeter equation)

¹⁰ J.-P. Joost, N. Schlünzen, and M. Bonitz, PRB **101**, 245101 (2020), Joost et al., PRB **105**, 165155 (2022);

¹¹ J.-P. Joost, PhD thesis, Kiel University 2023

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

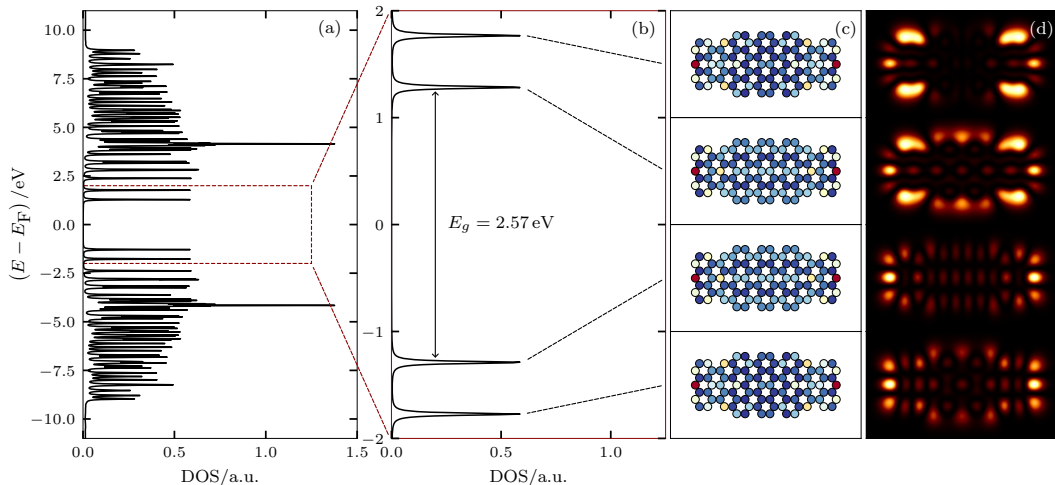




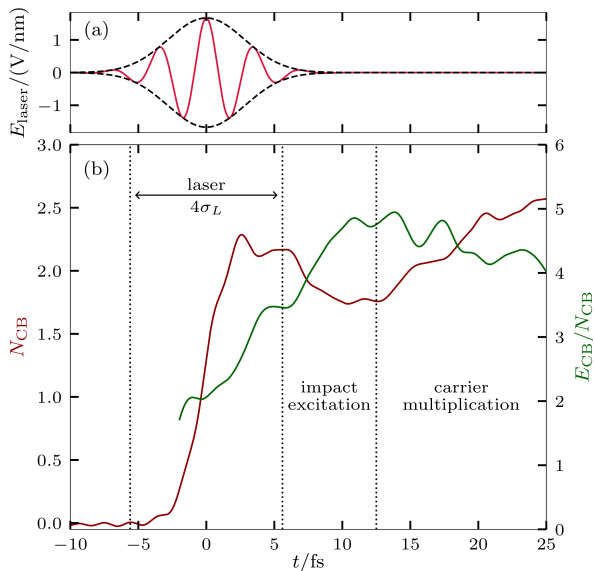
(5 × 4)-AGNR at $U = 3.5J$
 second order selfenergy (SOA)

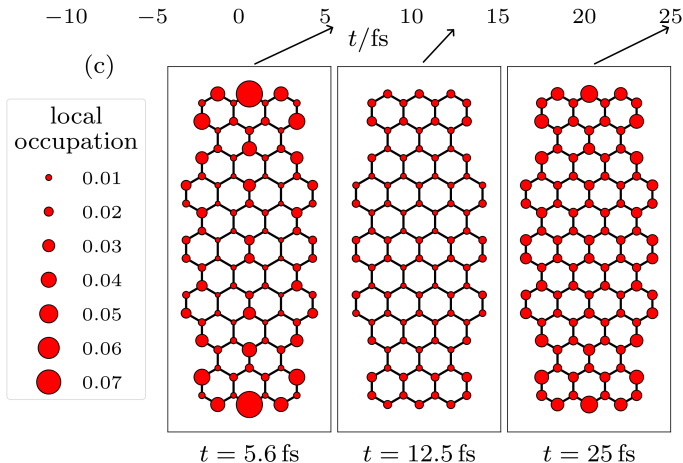
¹²Nonequilibrium GW simulations: J.-P. Joost, PhD thesis, Kiel University 2022

DOS and Edge States of the Unit Cell using Equilibrium *GW*



¹³J.-P. Joost, PhD thesis, Kiel University 2022

¹⁴Nonequilibrium GW simulations: J.-P. Joost, PhD thesis, Kiel University 2022



- Site-selective excitation on fs time scale. **Promising for PHz nanoelectronics**
- But: G1-G2 simulations currently **limited to small systems due to large memory** for \mathcal{G}

¹⁵J.-P. Joost, PhD thesis, Kiel University 2022

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

$$G_{ij}^>(t) = \langle \hat{G}_{ij}^>(t) \rangle, \quad \hat{G}_{ij}^>(t) = \frac{1}{i\hbar} \hat{a}_i(t) \hat{a}_j^\dagger(t)$$

$$G_{ij}^<(t) = \langle \hat{G}_{ij}^<(t) \rangle, \quad \hat{G}_{ij}^<(t) = \pm \frac{1}{i\hbar} \hat{a}_j^\dagger(t) \hat{a}_i(t)$$

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

- Extension to N -particle fluctuations:

$$L_{i_1 i_2 \dots i_N; j_1 j_2 \dots j_N}^{(N)}(t) := \langle \delta\hat{G}_{i_1 j_1}(t) \delta\hat{G}_{i_2 j_2}(t) \dots \delta\hat{G}_{i_N j_N}(t) \rangle$$

- Short notations: $L_{ijkl}(t) := L_{ij;kl}^{(2)}(t) = G_{ijkl}^{(2)}(t) - G_{ik}(t)G_{jl}(t)$, XC function
- I.) Replace two-particle NEGF \mathcal{G}_2 via $L_{ijkl}(t) = \pm G_{il}^>(t)G_{jk}^<(t) + \mathcal{G}_{ijkl}(t)$

¹⁶E. Schroedter, J.-P. Joost, and M. Bonitz, *Cond. Matt. Phys.* **25**, 23401 (2022);
 classical theory. Yu.L. Klimontovich, cf. E. Schroedter *et al.*, *Contrib. Plasma Phys.* **64**, e202400015 (2024)

In G_1 equation: reformulate collision integral in terms of fluctuations

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

$$h_{ij}^H(t) = h_{ij}(t) + U_{ij}^H(t); \quad U_{ij}^H(t) = \pm i\hbar \sum_{kl} w_{ikjl}(t) G_{lk}^<(t)$$

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

II.) Eliminate dynamics of $L_{ijkl}(t) = \langle \delta\hat{G}_{ik}(t) \cdot \delta\hat{G}_{jl}(t) \rangle$ by propagating $\delta\hat{G}(t)$:

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

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

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

¹⁷E. Schroedter, J.-P. Joost, and M. Bonitz, Cond. Matt. Phys. **25**, 23401 (2022);
E. Schroedter et al., PRB **108**, 205109 (2023)

Stochastic Mean field idea:¹⁸

- III.) Replace quantum expectation value by semiclassical mean over realizations A^λ , $\langle \hat{A} \rangle \rightarrow \overline{A^\lambda}$, exactly preserve first two moments
- Random sampling of initial conditions of non-interacting system:

$$\overline{\Delta G_{ij}^\lambda(t_0)} = 0,$$
$$\overline{\Delta G_{ik}^\lambda(t_0) \Delta G_{jl}^\lambda(t_0)} = -\frac{1}{2\hbar^2} \delta_{il} \delta_{jk} \{n_i(1 \pm n_j) + n_j(1 \pm n_i)\}.$$

- interactions turned on via adiabatic switching
- Careful test of probability distribution and sampling methods¹⁹
- IV.) find approximations that have product form: $\mathcal{G}^{\text{app}} \rightarrow L^{\text{app}}(t) = \langle \delta \hat{G}(t) \cdot \delta \hat{G}(t) \rangle$

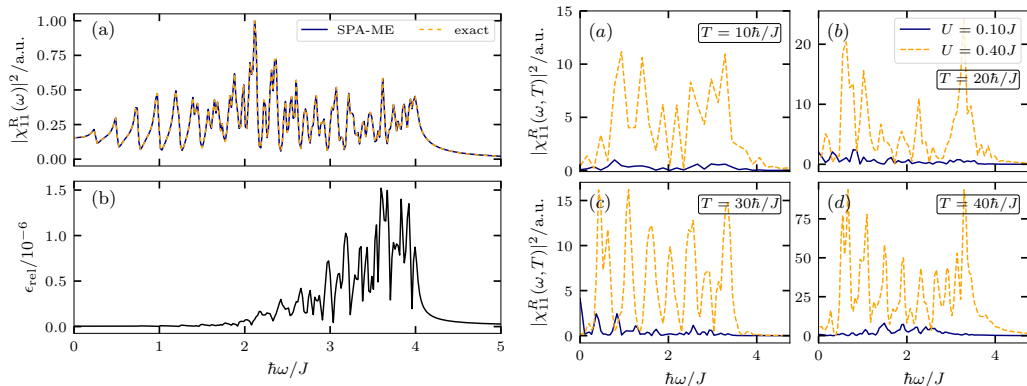
¹⁸S. Ayik, Phys. Lett. B **658**, 174 (2008);

D. Lacroix, S. Hermanns, C. M. Hinz, and M. Bonitz, PRB **90**, 125112 (2014)

¹⁹E. Schroedter, J.-P. Joost, and M. Bonitz, Cond. Matt. Phys. **25**, 23401 (2022);

E. Schroedter *et al.*, PRB **108**, 205109 (2023)

Two-time density response function: $\chi_{ij}^R(t, t') = 2\hbar\Theta(t - t')\text{Im}\left[\overline{\Delta G_{ii}^\lambda(t)(\Delta G_{jj}^\lambda(t'))^*}\right]$

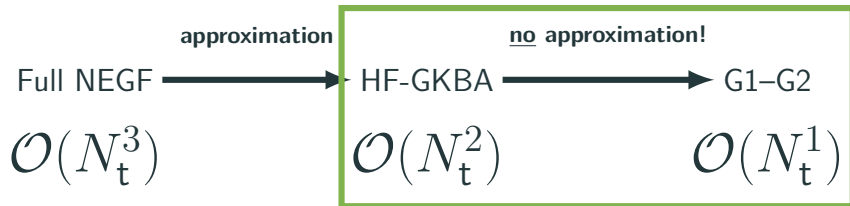


Left: Ground state of a half-filled 50 site ring for $U = 0$. **Right:** Nonequilibrium density response, for different times T , after a confinement quench, for a half-filled 30 site ring.

²⁰E. Schroedter, B.J. Wurst, J.-P. Joost, and M. Bonitz, Phys. Rev. B **108**, 205109 (2023);
equivalent to BSE in GW with HF-GKBA: E. Schroedter and M. Bonitz, phys. stat. sol. (b), 2300564 (2024)



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



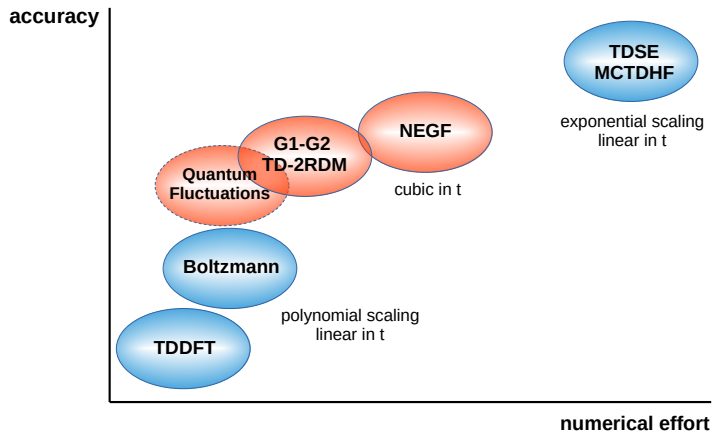
- HF-GKBA recovers Boltzmann-type kinetic equations and overcomes their problems: total energy conservation, correct short-time dynamics, correlated equilibrium state
- G1-G2 calculations can be done in **linear time**²¹, typical speed-ups: $\times 10^3$ – 10^6
- **Full nonequilibrium DSL** (combining dyn. screening and strong coupling) simulations possible
- **Memory bottleneck** for $\mathcal{G}_{ijkl}(t) \rightarrow$ mitigated via quantum fluctuations approach²²

²¹N. 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 *et al.*, Phys. Rev. B **105**, 165155 (2022);

Review: M. Bonitz *et al.*, phys. stat. sol. (b), 2300578 (2024)

²²**Review:** E. Schroedter and M. Bonitz, Contrib. Plasma Phys. **64**:5, e202400015 (2024)

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

Applications

- highly charged ion impact on 2D quantum materials, fs-neutralization dynamics and secondary electron emission²³
- Laser excitation of macroscopic graphene, TMDCs
- optimized graphene clusters for PHz electronics

Method development

- Quantum fluctuations approach for strong coupling²⁴
- Spectra and density of states beyond HF and beyond (extended) Koopmans theorem
- extension to open/large systems via embedding selfenergies²⁵
- improved selfenergies (3-particle correlations), G1–G2 scheme beyond HF-GKBA

²³Niggas *et al.*, Phys. Rev. Lett. **129**, 086802 (2022)

²⁴E. Schroedter, J.-P. Joost, and M. Bonitz, to be published

²⁵Balzer *et al.*, PRB **107**, 155141 (2023)

²⁶pdf file of talk at <https://www.itap.uni-kiel.de//theo-physik/bonitz/talks.html>