Many-particle systems far from equilibrium–
from Green functions to stochastic dynamics

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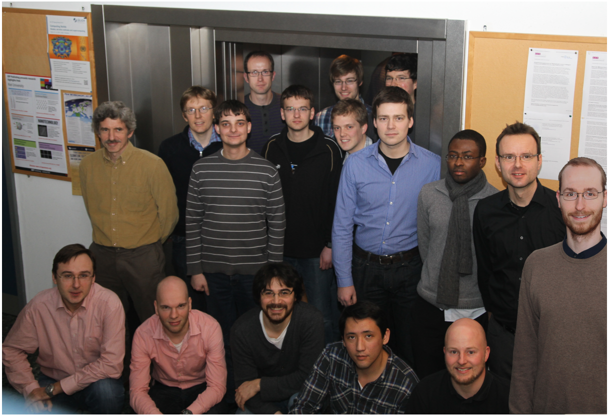
Acknowledgements[1]



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DFG

[1]thanks also to: D. Hochstuhl (MCTDHF, CI) and K. Balzer (NEGF)

Research interests: Classical and quantum many-body systems in nonequilibrium

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I. First principle simulation of strongly correlated plasmas (MC, MD), analytical concepts: kinetic theory, fluid theory [A]

II. QMC of correlated bosons and fermions (A. Filinov, [B])

III. Wave function based methods for atoms and molecules
   - Solution of Schrödinger equation, Full CI
   - Multiconfiguration time-dependent Hartree-Fock and time-dependent Restricted active space CI [1] (S. Bauch)

[*A*] *Introduction to Complex plasmas*, M. Bonitz, N. Horing, and P. Ludwig (eds.), Springer 2010 and 2014
[*B*] A. Filinov, M. Bonitz, and Yu.E. Lozovik, Phys. Rev. Lett. **86**, 3851 (2001);
A. Filinov, N. Prokof'ev, and M. Bonitz, Phys. Rev. Lett. **105**, 070401 (2010)
[1] D. Hochstuhl, C. Hinz, and M. Bonitz, EPJ-ST **223**, 177-336 (2014), review

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- Solution of Schrödinger equation, Full CI
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IV. Statistical approaches (plasmas, atoms, condensed matter)
- Nonequilibrium Green functions (NEGF, 2-time fcts [2])
- NEGF with generalized KB ansatz (GKBA, 1-time fcts [3])
- Stochastic mean field approach [4]

[1] D. Hochstuhl, C. Hinz, and M. Bonitz, EPJ-ST **223**, 177-336 (2014), review
[2] K. Balzer, and M. Bonitz, Springer Lecture Notes in Physics **867** (2013)
[3] M. Bonitz, S. Hermanns, and K. Balzer, Contrib. Plasma Phys. **53**, 778 (2013), arXiv:1309.4574
S. Hermanns, and M. Bonitz, Phys. Rev. B, sumbitted (2014), arXiv: 1402.7300
[4] D. Lacroix, S. Hermanns, C. Hinz, and M. Bonitz, Phys. Rev. Lett., submitted (2014), arXiv:1403.5098

- **High-intensity lasers, free electron lasers**
  - strong nonlinear excitation of matter
  - high photon energy: core level excitation
  - localized excitation: spatial inhomogeneity
- **Ultra-short pulses**
  - (sub-)fs dynamics of atoms, molecules, solids
  - sub-fs dynamics of electronic correlations
- **Need: Nonequilibrium many-body theory**
  - conservation laws on all time scales
  - linear and nonlinear response
  - macroscopic to finite (inhomogeneous) systems

Outline

1. Introduction
2. Quantum dynamics in second quantization
   - 1. Dynamics of the field operators
   - 2. Non-equilibrium Green functions (NEGF)
   - 3. Generalized Kadanoff-Baym ansatz (GKBA)
3. Excitation dynamics in Hubbard nanoclusters
   - 1. Testing the GKBA
   - 2. Relaxation Dynamics
   - 3. Beyond weak coupling: T-matrix selfenergy with GKBA
4. Stochastic Mean Field Approach
   - SMF–Numerical results
5. Conclusions

Quantum dynamics in second quantization (2)

Dynamics of the field operators

- use Heisenberg representation of quantum mechanics:
  $\hat{c}_{iH}(t) = U^\dagger(t, t_0)\hat{c}_i U(t, t_0)$

  with N-particle time evolution operator:
  $i\partial_t U(t, t') = \hat{H}(t) U(t, t')$, and $U(t, t) = \hat{1}$
- Heisenberg equation of motion:
  $i\partial_t \hat{c}_{iH}(t) + [\hat{H}_H(t), \hat{c}_{iH}(t)] = 0, \qquad \hat{c}_{iH}(t_0) = \hat{c}_i$

Quantum dynamics in second quantization (2)

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- evaluate commutator:

$$\boxed{i\partial_t \hat{c}_{iH}(t) = \sum_m \left(h^0_{im} + v_{im,H}(t)\right)\hat{c}_{mH} + \sum_{mln} w_{ilmn}\hat{c}^\dagger_{lH}\hat{c}_{nH}\hat{c}_{mH}}$$

- Effective single-particle (mean field) problem, nonlinear:

$$i\partial_t \hat{c}_{iH}(t) = \sum_m \left(h^0_{im} + \hat{v}^{\rm eff}_{im,H}(t)\right)\hat{c}_{mH}(t)$$

How to proceed? Simple equation for a complicated object

$$i\partial_t \hat{c}_{iH}(t) = \sum_m \left(h^0_{im} + \hat{v}^{\text{eff}}_{im,H}(t) \right) \hat{c}_{mH}(t)$$

Ensemble average

I. coordinate representation: replace $\hat{\psi}_H(\mathbf{r}, t) \to \psi(\mathbf{r}, t)$
“quasi-classical” approximation (many particles in single state)
Gross-Pitaevskii-type equation (bosons)

II. Fermions: $n_i = 0, 1$, “quantum” treatment necessary.
Ensemble average: $\langle \hat{c}_{iH} \rangle = 0, \quad \langle \hat{c}^\dagger_{iH} \hat{c}_{jH} \rangle = \rho_{ij}(t) = \langle i|\hat{\rho}_1(t)|j\rangle$
Reduced density operators: $\langle \hat{c}^\dagger_{i_1} \dots \hat{c}^\dagger_{i_s} \hat{c}_{js} \dots \hat{c}_{j1} \rangle \to \hat{\rho}_{1\dots s}(t)$
Equations of motion: BBGKY hierarchy[a]

III. Ensemble average of two(many)-time operator products:
Nonequilibrium Green functions $\langle \hat{c}^\dagger_H(t) \hat{c}_H(t') \rangle \to G^{(1)}(t, t')$

[a] M. Bonitz, *Quantum Kinetic Theory*, Teubner 1998

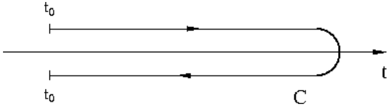
Keldysh Green functions [Keldysh, 1964]

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

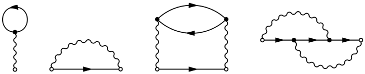
$$\boxed{G^{(1)}_{ij}(z,z') = \frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\,\hat{c}_i(z)\,\hat{c}^{\dagger}_j(z')\right\rangle}$$

Keldysh–Kadanoff–Baym equation (KBE) on $\mathcal{C}$:

$$\sum_k \left\{ \mathrm{i}\hbar \frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z) \right\} G^{(1)}_{kj}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} - \mathrm{i}\hbar \sum_{klm}\int_{\mathcal{C}} \mathrm{d}\bar{z}\, w_{iklm}(z^+,\bar{z})\, G^{(2)}_{lmjk}(z\bar{z};z'\bar{z}^+)$$



- $\int_{\mathcal{C}} wG^{(2)} \to \int_{\mathcal{C}} \Sigma G^{(1)}$, Selfenergy
- Nonequilibrium diagram technique
  Example: Hartree-Fock + Second Born selfenergy



KBE: first equation of Martin–Schwinger hierarchy for $G^{(1)}, G^{(2)} \ldots G^{(n)}$

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- Contour Green function mapped to real-time matrix Green function

$$\mathbf{G_{ij}} = \begin{pmatrix} G^{\mathsf{R}}_{ij} & G^{<}_{ij} \\ 0 & G^{\mathsf{A}}_{ij} \end{pmatrix}$$

$$G^{<}_{ij}(t_1, t_2) = \mp \mathrm{i} \left\langle \hat{c}^{\dagger}_{j}(t_2)\hat{c}_i(t_1) \right\rangle$$

$$G^{>}_{ij}(t_1, t_2) = -\mathrm{i} \left\langle \hat{c}_i(t_1)\hat{c}^{\dagger}_{j}(t_2) \right\rangle$$

- Propagators, spectral function

$$G^{\mathsf{R/A}}(t_1, t_2) = \pm\theta\left[\pm(t_1 - t_2)\right]\left\{G^{>}(t_1, t_2) - G^{<}(t_1, t_2)\right\}$$

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

$$\left[\mathrm{i}\partial_{t_1} - h_0(t_1)\right] G^{<}(t_1, t_2) = \int \mathrm{d}t_3\, \Sigma^{\mathsf{R}}(t_1, t_3)\, G^{<}(t_3, t_2) + \int \mathrm{d}t_3\, \Sigma^{<}(t_1, t_3)\, G^{\mathsf{A}}(t_3, t_2)$$

$$G^{<}(t_1, t_2)\left[-\mathrm{i}\partial_{t_2} - h_0(t_2)\right] = \int \mathrm{d}t_3\, G^{\mathsf{R}}(t_1, t_3)\Sigma^{<}(t_3, t_2) + \int \mathrm{d}t_3\, \Sigma^{\mathsf{A}}(t_1, t_3)\, G^{<}(t_3, t_2)$$

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Time-dependent single-particle operator expectation value

$$\langle \hat{O} \rangle(t) = \mp i \int dx \left[o(x' t)\, G^<(xt, x' t) \right]_{x=x'}$$

- Particle density

$$\langle \hat{n}(x,t) \rangle = n(1) = \mp i\, G^<(1,1)$$

- Density matrix

$$\rho(x_1, x_1', t) = \mp i\, G^<(1,1')\big|_{t_1=t_1'}$$

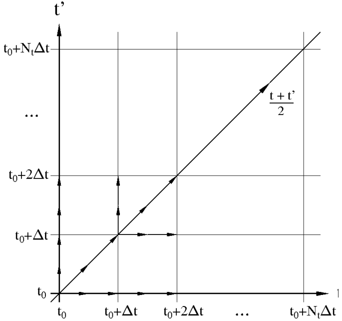
- Current density: $\langle \hat{j}(1) \rangle = \mp i \left[\left(\frac{\nabla_1}{2i} - \frac{\nabla_{1'}}{2i} + A(1) \right) G^<(1,1') \right]_{1'=1}$

Interaction energy (two-particle observable, [Baym/Kadanoff])

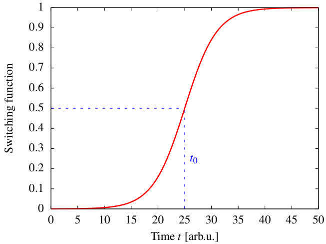
$$\langle \hat{V}_{12} \rangle(t) = \pm i \frac{\mathcal{V}}{4} \int \frac{d\vec{p}}{(2\pi\hbar)^3} \left\{ (i\,\partial_t - i\,\partial_{t'}) - \frac{p^2}{m} \right\} G^<(\vec{p}, t, t')|_{t=t'}$$

Numerical solution of the KBE

Full two-time solutions: Danielewicz, Schäfer, Köhler/Kwong, Bonitz/Semkat, Haug, Jahnke, van Leeuwen, Stefanucci, Verdozzi, Berges, Garny, Balzer ...



2. adiabatically slow switch-on of interaction for $t, t' \leq t_0$ [1, 2]

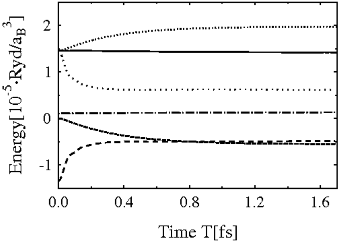


1. Uncorrelated initial state

3. solve KBE in $t - t'$ plane for $g^{\gtrless}(t, t')$

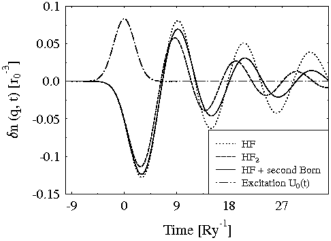
[1] A. Rios et al., Ann. Phys. **326**, 1274 (2011), [2] S. Hermanns et al., Phys. Scr. **T151**, 014036 (2012)

1. perfect conservation of total energy
2. accurate short-time dynamics:
   phase 1: correlation dynamics
   2: relaxation of orbital occupations



Example: electrons in dense hydrogen, interaction quench [1]

3. accurate long-time behavior: spectral functions and high-order correlated spectra from real-time KBE dynamics (via Fourier transform) [2]



4. extended to optical absorption, double excitations [3] etc.

[1] MB and D. Semkat, *Introduction to Computational Methods in Many-Body Physics*, Rinton Press 2006,
[2] N. Kwong and MB, PRL **84**, 1768 (2000), [3] K. Balzer, S. Hermanns, MB, EPL **98**, 67002 (2012)

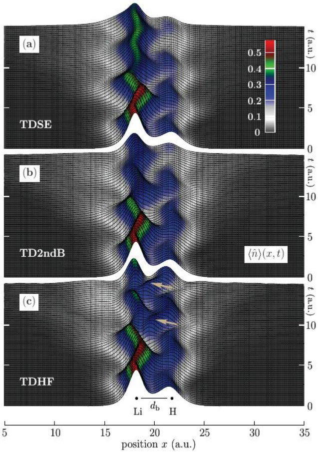
NEGF for finite inhomogeneous systems: molecules[2]

- few-electron atoms, molecules [PRA **81**, 022510 (2010), PRA **82**, 033427 (2010)]

1D He ground state

n_g (n_b)	Number of τ-grid points	E_{gs} [a.u.]
	Hartree-Fock	
	n_g (n_b)	E_{gs}^{HF} [a.u.]
	4 (43)	−2.22
	9 (98)	−2.224209
	14 (153)	−2.2242096
	Second Born	
n_g (n_b)	Number of τ-grid points	E_{gs}^{2ndB} [a.u.]
14 (153)	101	−2.23
14 (153)	301	−2.2334
14 (153)	601	−2.23341
14 (153)	1001	−2.233419
	TDSE (exact)	
		E_{gs}^{TDSE} [a.u.]
		−2.2382578

LiH, XUV-pulse excitation



[2] pioneered by N.E. Dahlen, R. van Leeuwen and K. Balzer

Challenges of inhomogeneous NEGF calculations

- Complicated structure of interaction w_{klmn} and selfenergy Σ
- Collision intergrals involve integrations over whole past
- CPU time $\sim N_t^3$, RAM $\sim N_t^2$

Typical computational parameters

- Spatial basis size: $N_b = 70$
- Time steps: $N_t = 10000$
- RAM consumption: 2 TB
- number of CPUs used: 2048
- total computation time: 2-3 days

Solutions[3]

- Finite-Element Discrete Variable Representation [PRA **81**, 022510 (2010)]
- Generalized Kadanoff–Baym ansatz [Phys. Scr. **T151**, 014036 ('12), JPCS **427**, 012006 ('13)]
- Adiabatic switch-on of interaction [Phys. Scr. **T151**, 014036 ('12)]
- Parallelization [PRA **82**, 033427 (2010)] and GPU computing

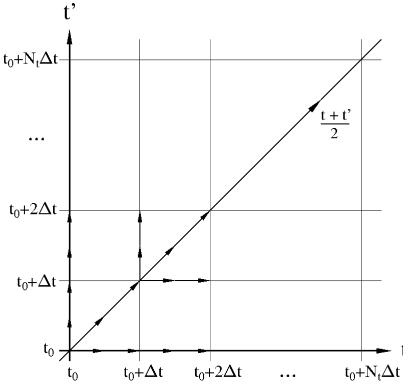
[3] K. Balzer, M. Bonitz, Lecture Notes in Phys. vol. 867 (2013)

Outline

To save CPU time and memory: Reduction to single-time propagation

- recall TD equilibrium: $G(p,\omega) = A(p,\omega)f(p)$ ("KB ansatz")
- Generalize to non-equilibrium: $\omega \to \tau = t - t'$, (Fourier trafo)

  new: dependence on $T = \frac{t+t'}{2}$
- straightforward extension of KBA: $G(p,\tau;T) = A(p,\tau;T)f(p,T)$



But: this is wrong

- violates energy conservation
- violates causality
- in contradiction to (single-time) density matrix theory[a]

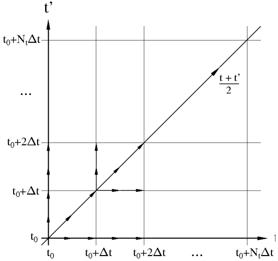
[a] M. Bonitz, *Quantum Kinetic Theory*

- Idea of the GKBA: lowest order solution [1]

$$\boxed{G^{\gtrless}_{\mathsf{GKBA}}(t_1,t_2) = -G^{\mathsf{R}}(t_1,t_2)\,\rho^{\gtrless}(t_2) + \rho^{\gtrless}(t_1)\,G^{\mathsf{A}}(t_1,t_2)}$$

$$\rho^{<}(t) = \rho(t) = \pm \mathrm{i} G^{<}(t,t), \qquad \rho^{>}(t) = 1 \pm \rho^{<}(t)$$

- correct causal structure, non-Markovian, no near-equilibrium assumption [2]



[1] P. Lipavsky, V. Spicka and B. Velicky Phys. Rev. B **34**, 6933 (1986), [2] M. Bonitz, *Quantum Kinetic Theory*

The generalized Kadanoff-Baym ansatz

- Idea of the GKBA: lowest order solution [1]

$$G^{\gtrless}_{\mathsf{GKBA}}(t_1, t_2) = -G^{\mathsf{R}}(t_1, t_2)\,\rho^{\gtrless}(t_2) + \rho^{\gtrless}(t_1)\,G^{\mathsf{A}}(t_1, t_2)$$

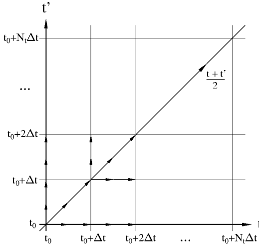
$$\rho^{<}(t) = \rho(t) = \pm \mathrm{i}\, G^{<}(t, t), \qquad \rho^{>}(t) = 1 \pm \rho^{<}(t)$$

- correct causal structure, non-Markovian, no near-equilibrium assumption [2],
- Reduction to single-time quantities by use of HF propagators

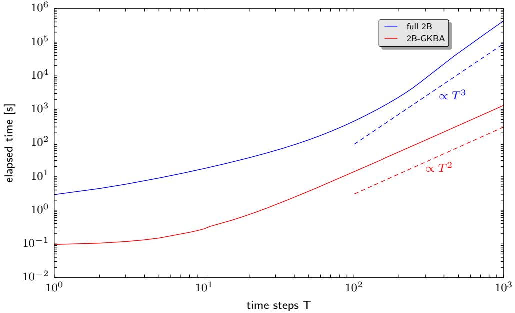
$$G^{\mathsf{R/A}}_{\mathsf{HF}}(t_1, t_2) = \mp \mathrm{i}\theta[\pm(t_1 - t_2)] \exp\left(-\mathrm{i} \int_{t_2}^{t_1} \mathrm{d}t_3\, h_{\mathsf{HF}}(t_3)\right)$$

- HF-GKBA: same conservation properties as two-time approximation
- damped propagators, local approximation violate E-conservation [3]

[1] P. Lipavsky, V. Spicka and B. Velicky Phys. Rev. B **34**, 6933 (1986), [2] M. Bonitz, *Quantum Kinetic Theory*
[3] M. Bonitz, D. Semkat, H. Haug, Eur. Phys. J. B **9**, 309 (1999)



time stepping along diagonal only. Full memory retained.



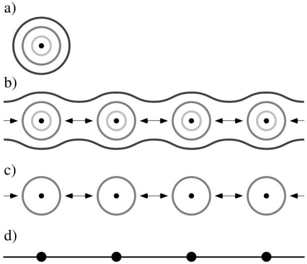
S. Hermanns, K. Balzer, and M. Bonitz, *Phys. Scripta* **T151**, 014036 (2012)

we use about 10^3 time steps for the adiabatic switching and $10^3 \dots 10^6$ for the excitation and relaxation.

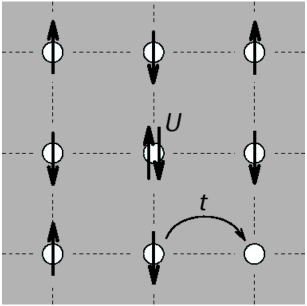
Outline

The Hubbard model

- Simple, but versatile model for solid state systems
- optical lattices, macromolecules...
- single band, small bandwidth, parameters from ab initio simulations



$\Rightarrow$

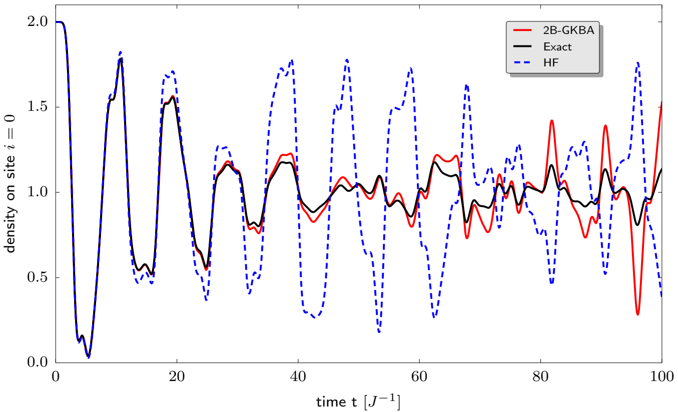


$$\hat{H}(t) = -J \sum_{ij,\,\alpha} h_{ij}\, \hat{c}^{\dagger}_{i\alpha} \hat{c}_{j\alpha} + U \sum_i \hat{c}^{\dagger}_{i\uparrow} \hat{c}_{i\uparrow} \hat{c}^{\dagger}_{i\downarrow} \hat{c}_{i\downarrow} + \sum_{ij,\alpha\beta} f_{ij,\alpha\beta}(t)\, \hat{c}^{\dagger}_{i\alpha} \hat{c}_{j\beta}$$

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

Noneq. initial state $N = 8$, half filling, $U = 0.1$

Sites $0 - 3$ doubly occupied, $4 - 7$ empty

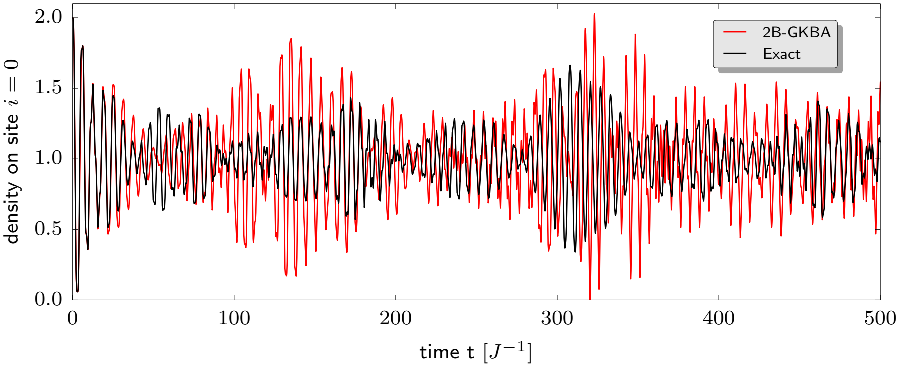


Rapid failure of HF (!), good performance of GKBA up to longer times ($t \sim 50$)

GKBA improves with particle number

Long relaxation
exact result vs. GKBA, $N = 4,\ n = 1/2,\ U = 0.1$

Sites $0-1$ doubly occupied, $2-3$ empty

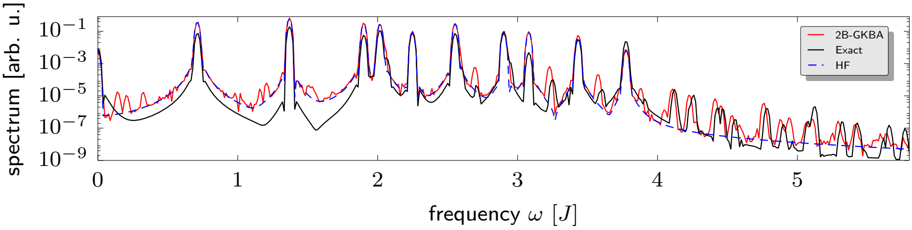


HF-GKBA: long-time stability, no divergencies. Qualitatively correct up to $t \sim 180$

- Response to weak short pulse[4] $\sim \delta(t)$
- $10 \ldots 1000$ times longer propagation compared to two-time KBE
- Increased resolution of spectra. Capture double excitations

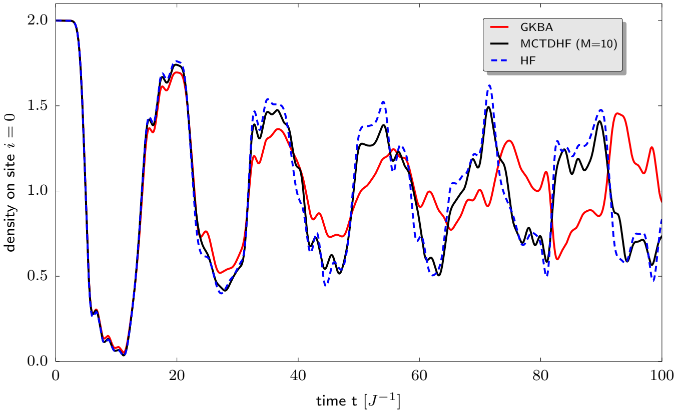
Real-time propagation following weak excitation and Fourier transform

Example: $N = 8, n = 1/2, U = 0.1$



[4] Idea: Kwong, Bonitz, PRL **84**, 1768 (2000)

$N = 16$, half filling, $U = 0.1$. Sites $0 - 7$ doubly occupied, $8 - 15$ empty



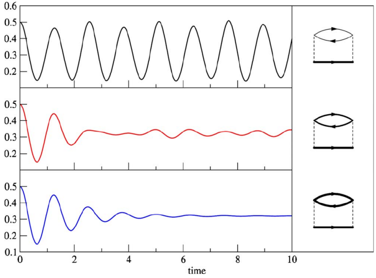
no FCI data, failure of HF (and MCTDHF), expect predictive capability of GKBA

Fix problems of two-time calculations

Problems of NEGF in second Born[5], $N = 2, n = 1/2, U = 1$

Strong excitation: $f_{ij,\alpha\beta}(t) = w_0 \delta_{i,1} \delta_{j,1} \delta_{\alpha,\beta} \Theta(t)\,, \quad w_0 = 5.0 J^{-1}$

- time-dependent density, KBE for various degrees of selfconsistency
  artif. damping, mult. steady states

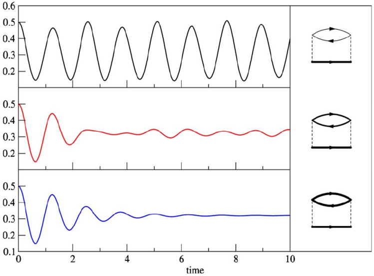


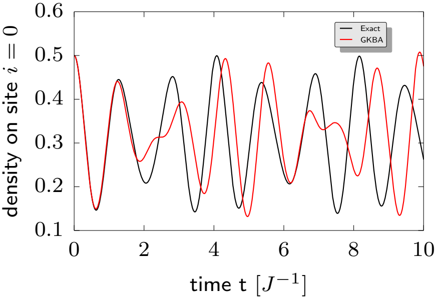
[5] P. von Friesen, C. Verdozzi, and C.O. Almbladh, Phys. Rev. B (2010)

Problems of NEGF in second Born[6], $N = 2, n = 1/2, U = 1$

Strong excitation: $f_{ij,\alpha\beta}(t) = w_0 \delta_{i,1} \delta_{j,1} \delta_{\alpha,\beta} \Theta(t)\,, \quad w_0 = 5.0 J^{-1}$

- time-dependent density, KBE for various degrees of selfconsistency artif. damping, mult. steady states
- GKBA: no damping selfconsistency problem cured

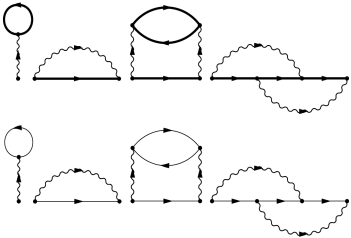




[6] P. von Friesen, C. Verdozzi, and C.O. Almbladh, Phys. Rev. B (2010), S. Hermanns, and M. Bonitz, Phys. Rev. B (2014), arXiv: 1402.7300

Hartree-Fock-GKBA vs. 2-time NEGF

$$
\begin{aligned}
G &= G_{\mathsf{id}} + G_{\mathsf{id}} \left(\bar{\Sigma}_{\mathrm{HF}} + \Sigma_{\mathsf{GKBA}} + \Delta\Sigma \right) G, \\
G_{\mathrm{HF}} &= G_{\mathsf{id}} + G_{\mathsf{id}} \bar{\Sigma}_{\mathrm{HF}} G_{\mathrm{HF}}, \\
G_{\mathrm{GKBA}} &= G_{\mathrm{HF}} + G_{\mathrm{HF}} \Sigma_{\mathrm{GKBA}} G_{\mathrm{GKBA}}, \\
G &= G_{\mathrm{GKBA}} + G_{\mathrm{GKBA}} \Delta\Sigma \, G.
\end{aligned}
$$



$\Sigma_{\mathrm{GKBA}} \equiv \Sigma_{\mathsf{cor}}[f^{\gtrless}, G^{\mathsf{R/A}}_{\mathrm{HF}}]$

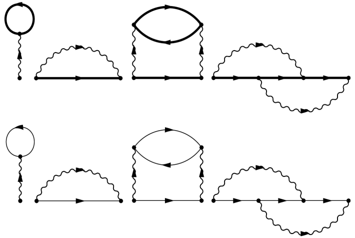
$\mathbf{G}$: 2-time NEGF, contain in addition:

$\Delta\Sigma$: terms with 1...3 full propagators

S. Hermanns, and M. Bonitz, *Phys. Rev. B* (2014), arXiv: 1402.7300

Hartree-Fock-GKBA vs. 2-time NEGF

$$\begin{aligned} G &= G_{\mathsf{id}} + G_{\mathsf{id}} \left(\bar{\Sigma}_{\rm HF} + \Sigma_{\mathsf{GKBA}} + \Delta\Sigma \right) G, \\ G_{\rm HF} &= G_{\mathsf{id}} + G_{\mathsf{id}} \bar{\Sigma}_{\rm HF}\, G_{\rm HF}, \\ G_{\rm GKBA} &= G_{\rm HF} + G_{\rm HF} \Sigma_{\rm GKBA}\, G_{\rm GKBA}, \\ G &= G_{\rm GKBA} + G_{\rm GKBA} \Delta\Sigma\; G. \end{aligned}$$



$\Sigma_{\rm GKBA} \equiv \Sigma_{\mathsf{cor}}[f^{\gtrless}, G_{\rm HF}^{\mathsf{R/A}}]$

G: 2-time NEGF, contain in addition:

$\Delta\Sigma$: terms with 1...3 full propagators

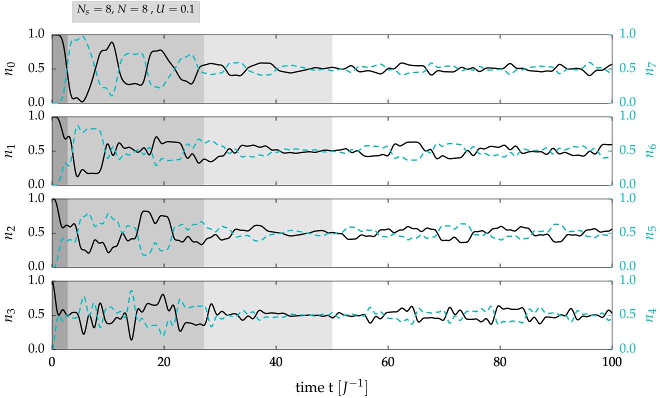
S. Hermanns, and M. Bonitz, *Phys. Rev. B* (2014), arXiv: 1402.7300

HF-GKBA reduces selfconsistency. Crucial for finite systems

Not a weak coupling approximation. Applicable to arbitrary approximation for Σ

Outline

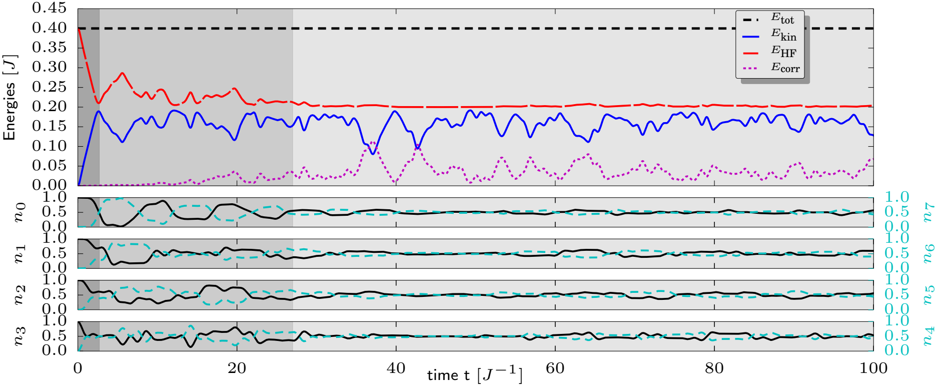
Short-time dynamics – exact calculation, $t = 0$: sites $0 - 3$ doubly occupied, $4 - 7$ empty



- Density wave to the right (diffusion)[7]
- first: depopulation of $n_3 \to n_4(t) = 1 - n_3(t)$
- delayed depopulation of n_2, n_1 (Pauli blocking)
- decay of n_0 when wave reflected at right boundary, $n_7(t) = 1 - n_0(t)$
- interferences, relaxation, revivals. Systematics? time scales? pre-thermalization?

Short-time dynamics: four stages
exact calculation, $N = 8,\ n = 1/2,\ U = 0.1$

Sites $0 - 3$ doubly occupied, $4 - 7$ empty



I: $t \leq 3$, ballistic expansion (feature of inhomogeneity)

II: $t \leq \tau_{cor} \sim 40$, correlation build-up/saturation of HF energy

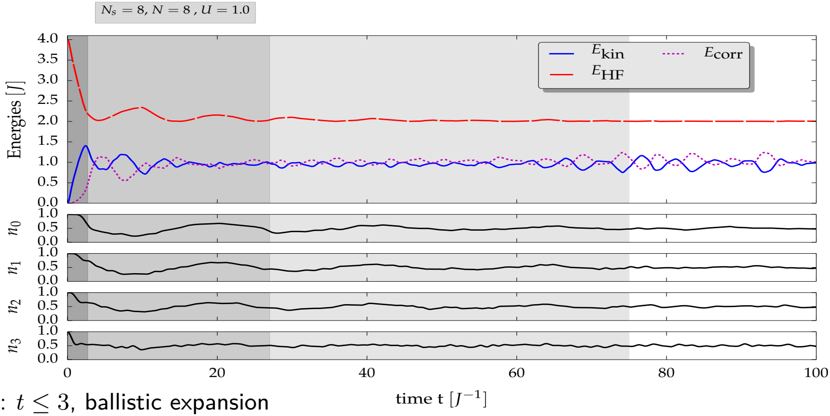
III: $t \leq 50$, one-particle equilibration (occupations)

IV: $t \geq 50$, weak revivals of occupations,

PRB (2014), arXiv: 1402.7300

Short-time dynamics ($U = 1.0$): four stages
exact calculation: $N = 8$, $n = 1/2$

Sites $0 - 3$ doubly occupied, $4 - 7$ empty



I: $t \leq 3$, ballistic expansion

II: $t \leq \tau_{cor} \sim 10$, with $\tau_{cor} \sim 1/U$

[MB, and D. Kremp, Phys. Lett. A **212**, 83 (1996)]

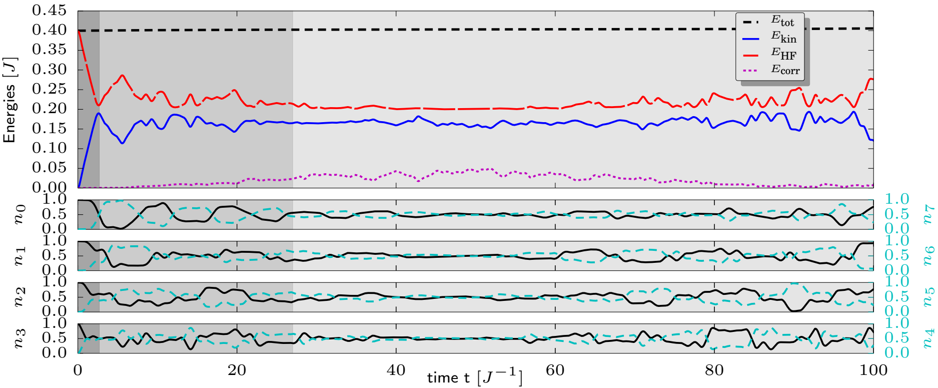
III: $t \leq 50$, one-particle equilibration (occupations)

IV: $t \geq 50$, weak revivals of occupations,

PRB (2014), arXiv: 1402.7300

GKBA calculation: Nonequilibrium initial state $N = 16,\ n = 1/2,\ U = 0.25$

Sites $0 - 7$ doubly occupied, $8 - 15$ empty



GKBA: correctly describes time-scales of stages I-III

shows incorrect return to non-equilibrated state

PRB (2014), arXiv: 1402.7300

Outline

T-Matrix selfenergy

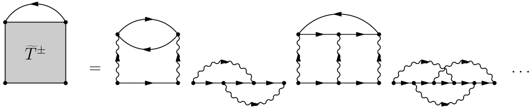
$$\boxed{\Sigma^T_{ik}(t\bar{t}) = i\hbar \int_{\mathcal{C}} d\bar{t}_1\, d\bar{t}_2\; \widetilde{T}^{\pm}_{ij'kl}(t\bar{t}_1, \bar{\bar{t}}\bar{t}_2)\, G_{lj'}(\bar{t}_2\bar{t}_1)}$$

modified T-matrix $\widetilde{T}^{\pm}$ is connected to original T-matrix T via:

$$\begin{aligned}
\widetilde{T}_{ijkl}(t_1 t_2, t_1' t_2') &:= T_{ijkl}(t_1 t_2, t_1' t_2') \mp w_{ijkl}(t_1 t_2)\delta_{\mathcal{C}}(t_1 - t_1')\delta_{\mathcal{C}}(t_2 - t_2') \\
\widetilde{T}^{\pm}_{ijkl}(t_1 t_2, t_1' t_2') &:= \widetilde{T}_{ijkl}(t_1 t_2, t_1' t_2') \pm \widetilde{T}_{ijlk}(t_1 t_2, t_2' t_1')
\end{aligned}$$

Lippmann-Schwinger equation for $\widetilde{T}^{\pm}$ on Keldysh-Contour $\mathcal{C}$:

$$\begin{aligned}
\widetilde{T}^{\pm}_{ijkl}(t_1 t_2, t_1' t_2') &= \pm i\hbar\, w_{ij\bar{k}\bar{l}}(t_1 t_2)\, G_{\bar{k}m}(t_1 t_1')\, G_{\bar{l}n}(t_2 t_2')\, w_{mnkl}(t_1' t_2') \\
&+ i\hbar\, w_{ij\bar{k}\bar{l}}(t_1 t_2)\, G_{\bar{k}m}(t_1 t_2')\, G_{\bar{l}n}(t_2 t_1')\, w_{mnlk}(t_2' t_1') \\
&+ i\hbar \int_{\mathcal{C}} d\bar{t}_1\, d\bar{t}_2\; w_{ij\bar{k}\bar{l}}(t_1 t_2)\, G_{\bar{k}m}(t_1 \bar{t}_1)\, G_{\bar{l}n}(t_2 \bar{t}_2)\, \widetilde{T}^{\pm}_{mnkl}(\bar{t}_1 \bar{t}_2, t_1' t_2')
\end{aligned}$$



Keldysh Matrix elements of GKBA-collision integral

$$I_{ij}^{(1)\gtrless}(tt) = \int_0^t d\bar{t}\,\Sigma_{ik}^{TR}(t\bar{t})G_{kj}^{\gtrless}(\bar{t}t) + \int_0^t d\bar{t}\,\Sigma_{ik}^{T\gtrless}(t\bar{t})G_{kj}^{A}(\bar{t}t)$$

$\rightarrow$ Keldysh components of $\widetilde{T}^{\pm}$ are required
in case of fermionic Hubbard clusters these components become:

$$\begin{aligned}\widetilde{T}_{ij}^{-A}(tt') = &\quad i\hbar\, U(t)\Big[G_{ij}^{>}(tt')G_{ij}^{>}(tt') - G_{ij}^{<}(tt')G_{ij}^{<}(tt')\Big]U(t') \\ + &\quad i\hbar\, U(t)\int_t^{t'} d\bar{t}\,\Big[G_{ik}^{<}(t\bar{t})G_{ik}^{<}(t\bar{t}) - G_{ik}^{>}(t\bar{t})G_{ik}^{>}(t\bar{t})\Big]\widetilde{T}_{kj}^{-A}(\bar{t}t')\end{aligned}$$

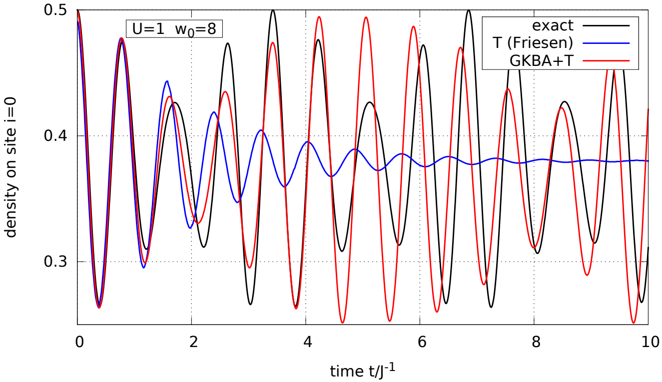
$$\begin{aligned}\widetilde{T}_{ij}^{-\gtrless}(tt') = &\quad -i\hbar\, U(t)G_{ij}^{\gtrless}(tt')G_{ij}^{\gtrless}(tt')U(t') \\ + &\quad i\hbar\, U(t)\Bigg\{\int_0^{t} d\bar{t}\,\Big[G_{ik}^{>}(t\bar{t})G_{ik}^{>}(t\bar{t}) - G_{ik}^{<}(t\bar{t})G_{ik}^{<}(t\bar{t})\Big]\widetilde{T}_{kj}^{-\gtrless}(\bar{t}t') \\ &\quad + \int_0^{t'} d\bar{t}\,G_{ik}^{\gtrless}(t\bar{t})G_{ik}^{\gtrless}(t\bar{t})\widetilde{T}_{kj}^{-A}(\bar{t}t')\Bigg\}\end{aligned}$$

$G^{\gtrless}$ reconstructed via HF-GKBA, recover density operator result

Kremp, Bonitz, Kraeft, Schlanges, Ann. Phys. **258**, 320 (1997)

Nonequilibrium initial state $N = 2,\ U = 1$

T-matrix with HF-GKBA compared to two-time T-matrix result (Friesen et al.)



HF-GKBA removes artificial damping. Good agreement of main frequency
Agreement improves for larger $N \Rightarrow$ can access strong coupling (low n)!

Outline

$$i\partial_t \hat{c}_{iH}(t) = \sum_m \left(h^0_{im} + \hat{v}^{\text{eff}}_{im,H}(t) \right) \hat{c}_{mH}(t)$$

Ensemble average $\Rightarrow$ simple(r) objects with complicated equations

I. Fermions: $n_i = 0, 1$, "quantum" treatment necessary.
Ensemble average: $\langle \hat{c}_{iH} \rangle = 0, \quad \langle \hat{c}^\dagger_{iH} \hat{c}_{jH} \rangle = \rho_{ij}(t) = \langle i|\hat{\rho}_1(t)|j\rangle$
Reduced density operators: $\langle \hat{c}^\dagger_{i_1} \ldots \hat{c}^\dagger_{i_s} \hat{c}_{js} \ldots \hat{c}_{j1} \rangle \rightarrow \hat{\rho}_{1\ldots s}(t)$
Equations of motion: BBGKY hierarchy

II. Ensemble average of two(many)-time operator products:
Nonequilibrium Green functions $\langle \hat{c}^\dagger_H(t) \hat{c}_H(t') \rangle \rangle \rightarrow G_1(t, t')$
Equations of motion: Martin-Schwinger hierarchy

$$\boxed{i\partial_t \hat{c}_{iH}(t) = \sum_m \left(h^0_{im} + \hat{v}^{\text{eff}}_{im,H}(t)\right) \hat{c}_{mH}(t)}$$

Ensemble average ⇒ simple(r) objects with complicated equations

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Equations of motion: Martin-Schwinger hierarchy

Simple equations for simple objects? Avoid the ensemble average!

Statistical approaches versus Stochastic Mean Field

Dynamics of a correlated
N-particle system with N-particle state $|\Psi(t)\rangle$

$\swarrow \qquad \searrow$

① Ensemble average	① Specify Gaussian ensemble $\left\{\bar{\rho},\ \overline{\delta\rho_{ij}\delta\rho_{kl}}\right\}$
② Many-body approximation beyond mean-field (MF): $V_{\text{xc}}[\rho],\ \rho_{12}[\rho],\ \Sigma[G]$ etc.	
③ $\rho(t_0)$	③ Sample initial state (M realizations): $\hat{n}^{(1)}(t_0)\ \ldots\ \hat{n}^{(M)}(t_0)$
④ $\mathrm{i}\,\dot{\rho} = I^{\text{MF}}[\rho] + I^{\text{cor}}[\rho]$	④ $\mathrm{i}\,\dot{\hat{n}}^{(n)} = I^{\text{MF}}[\hat{n}^{(n)}]\,;\ n = 1\ldots M$
	⑤ Ensemble average $\forall\, t$: $\frac{1}{M}\sum_{n=1}^{M}\hat{n}^{(n)}(t)$

$\searrow \qquad \swarrow$

density matrix $\rho(t)$, observables $A(t)$

- Schwinger 1951: operator correlation function in QED
- Klimontovich 1957: microscopic phase space density
- Kadomtsev, Dubois: correlation functions of EM field fluctuations
- Gurevich, Kogan...: occupation number fluctuations
- Balian, Veneroni: variational principles
- Stochastic Schrödinger equation
- Diagrammatic/real-time quantum Monte Carlo
- ...

Goal here: stochastic approach to many correlated fermions in nonequilibrium that is, both, *accurate and practically feasible*

Stochastic approach to correlated N-body dynamics[8]

Density matrix operator (not averaged): $\hat{n}_{ij} \equiv \hat{a}_i^\dagger \hat{a}_j \to \hat{\mathbf{n}}$
Heisenberg dynamics:

$$\boxed{i\partial_t \hat{n}_{ij}(t) = U^\dagger(t, t_0)[\hat{n}_{ij}, \hat{H}(t)]\, U(t, t_0), \qquad \hat{n}_{ij}(t_0) = \hat{n}_{ij}}$$

U: time evolution operator, $\hat{H}(t)$ system hamiltonian in second quantization:

$$\hat{H} = \hat{T} + \hat{V} + \hat{W}, \quad \hat{T} + \hat{U} = \sum_{i,j=1}^{\infty} \hat{a}_i^\dagger \left(t_{ij} + v_{ij}(t)\right) \hat{a}_j$$

$$\hat{W} = \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} \hat{a}_i^\dagger \hat{a}_j^\dagger \, w_{ijkl} \, \hat{a}_l \hat{a}_k .$$

Exact equation for density matrix operator:

$$\boxed{i\partial_t \widehat{\mathbf{n}}(t) = \left[\widehat{\mathbf{n}}(t), \left\{\mathbf{t}^* + \mathbf{v}_{\mathrm{H}}^*(t) + \widehat{\mathbf{U}}_{\mathrm{H}}^{\pm}(t)\right\}\right], \quad \hat{U}_{kj}^{\pm} = \sum_{ln} \frac{w_{jnkl} \pm w_{jnlk}}{2} \left\{\hat{n}_{nl} \mp \delta_{ln}\right\}}$$

[8] Single-time version. Two-time version analogous

Ensemble average. Correlations vs. fluctuations

Average, fluctuations and correlation functions:

$$\langle \hat{A} \rangle \equiv A, \quad \delta A = \hat{A} - A$$
$$\langle \hat{A}\hat{B} \rangle = AB + \langle \delta\hat{A}\delta\hat{B} \rangle$$

Ensemble average of equation of motion for $\hat{\mathbf{n}}(t)$:

$$\boxed{i\partial_t \mathbf{n}(t) - \left[\mathbf{n}(t), \mathbf{t}^* + \mathbf{v}^*_{\mathrm{H}}(t) + \mathbf{U}^{\pm}_{\mathrm{H}}(t)\right] = \left\langle \left[\delta\widehat{\mathbf{n}}(t), \delta\hat{\mathbf{U}}^{\pm}_{\mathrm{H}}(t)\right] \right\rangle \equiv \mathbf{I}(t)}$$

r.h.s.: collision integral (interactions beyond mean field, correlations)
$\Rightarrow$ determined by fluctuations of DM operator. Formal solution:

$$\begin{aligned}
\mathbf{n}(t) &= \mathcal{U}^{\mathrm{HF}\dagger}(t,t_0)\,\mathbf{n}_0\,\mathcal{U}^{\mathrm{HF}}(t,t_0) + \mathbf{n}_I(t),\\
\mathbf{n}_I(t) &= \frac{1}{i}\int_{t_0}^{t} d\bar{t}\,\mathcal{U}^{\mathrm{HF}\dagger}(t,\bar{t})\,\mathbf{I}(\bar{t})\,\mathcal{U}^{\mathrm{HF}}(t,\bar{t}),\\
i\partial_t \mathcal{U}^{\mathrm{HF}}(t,t_0) &= \mathbf{h}^{\pm}_{\mathrm{H}}(t)\mathcal{U}^{\mathrm{HF}}(t,t_0), \qquad \mathcal{U}^{\mathrm{HF}}(t,t) = \mathbf{1}.
\end{aligned}$$

Stochastic solution: $\hat{\mathbf{n}}(t) = \lim_{M\to\infty} \sum_{n=1}^{M} \hat{\mathbf{n}}^{(n)}(t), \quad \hat{\mathbf{n}}^{(n)}(t_0) = \hat{\mathbf{n}}_0^{(n)}$

Stochastic Mean Field[9]

Replace I by initial state fluctuations: $\mathbf{I}(t) \rightarrow \tilde{\mathbf{I}}(t_0)\delta(t-t_0)$

$$\mathbf{n}(t) \quad = \quad \langle\hat{\mathbf{n}}(t)\rangle = \mathcal{U}^{\mathrm{HF}\dagger}(t,t_0)\left\{\langle\hat{\mathbf{n}}_0\rangle + \langle\hat{\tilde{\mathbf{I}}}(t_0)\rangle\right\}\mathcal{U}^{\mathrm{HF}}(t,t_0)$$

pure Hartree-Fock dynamics from modified initial state.
M random TDHF-trajectories:

$$\hat{\mathbf{n}}^{(n)}(t) = \mathcal{U}^{\mathrm{HF}\dagger}_{(n)}(t,t_0)\,\hat{\mathbf{n}}_0^{(n)}\,\mathcal{U}^{\mathrm{HF}}_{(n)}(t,t_0), \quad n = 1\ldots M$$

"Classical" average: $\overline{\hat{\mathbf{n}}(t)} = \lim_{M\to\infty}\sum_{n=1}^{M}\hat{\mathbf{n}}^{(n)}(t), \quad \hat{\mathbf{n}}^{(n)}(t_0) = \hat{\mathbf{n}}_0^{(n)}$

Select $\hat{\mathbf{n}}_0^{(n)}$ from Gaussian ensemble:

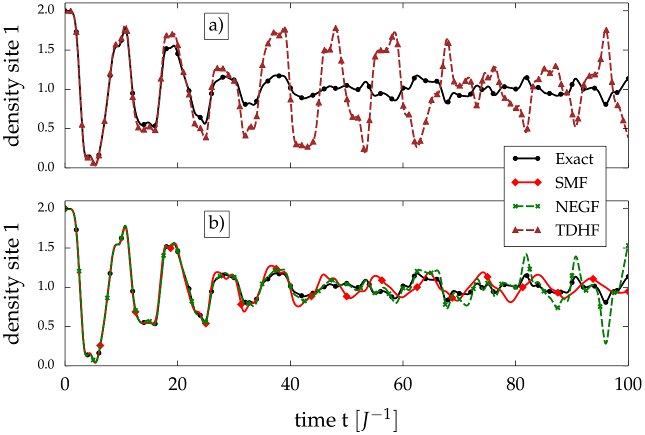
$$\overline{n_{ij}^{(n)}} = n_i\delta_{ij}$$

$$\overline{\delta n_{ij}^{(n)}\delta n_{kl}^{(n)}} = \frac{1}{2}n_i(1-n_j)\delta_{il}\delta_{jk}$$

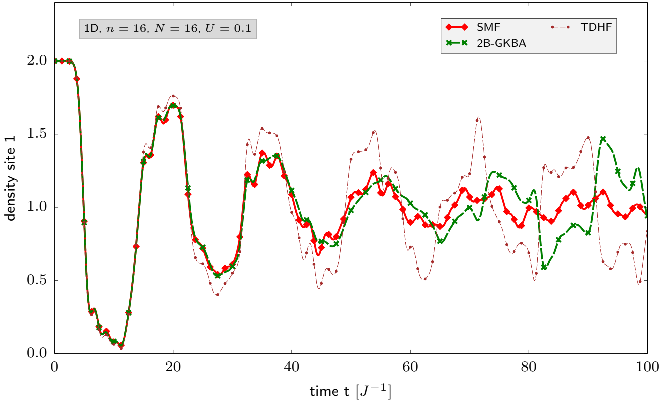
Simple TDHF-dynamics, correlations via efficient Monte Carlo sampling of trajectories

[9] Ayik 2008; Lacroix, Hermanns, Hinz and Bonitz, arXiv: 1403.5098

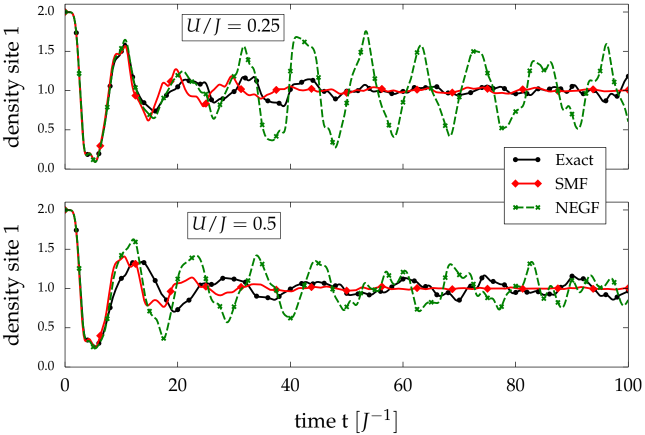
Short-time dynamics: $N = 8,\ n = 1/2,\ U = 0.1$



Short-time dynamics: $N = 16,\ n = 1/2,\ U = 0.1$



Short-time dynamics: $N = 8$, $n = 1/2$, $U \leq 0.5$

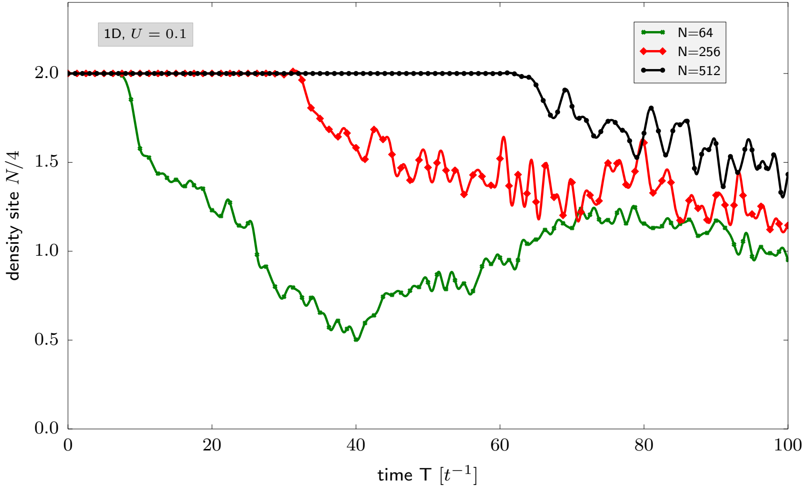


Present SMF becomes worse for increasing U

accurate for initial relaxation phase, $t \lesssim \tau_{cor} \sim 1/U$, captures correlation buildup

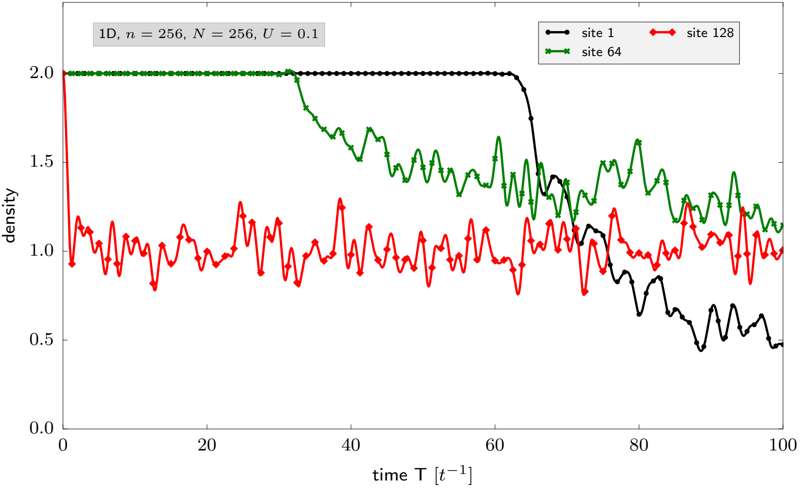
Short-time dynamics of long Hubbard chains

$n = 1/2, N = 64, 256, 512$, occupation of site $N/4$, $U = 0.1$



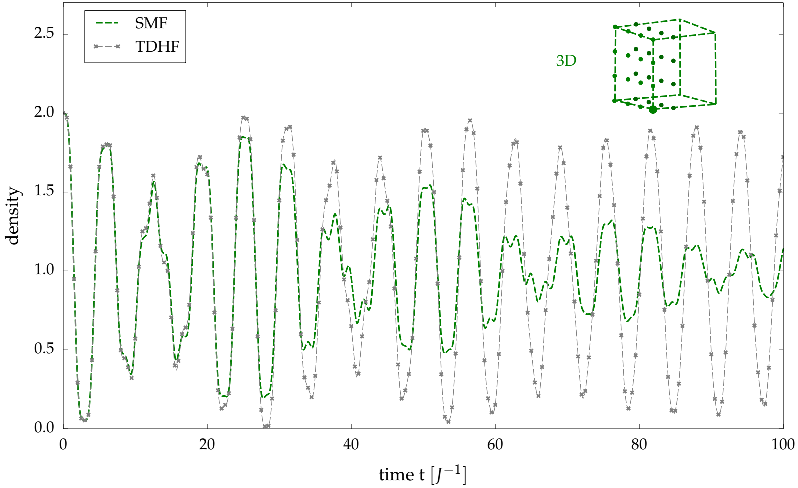
Space resolved dynamics of long Hubbard chains

$n = 1/2, N = 256, \ U = 0.1$



Dynamics of 3D Hubbard cluster, $4 \times 4 \times 4$

Influence of dimensionality: 3D vs. 2D and 1D, $U = 0.1$



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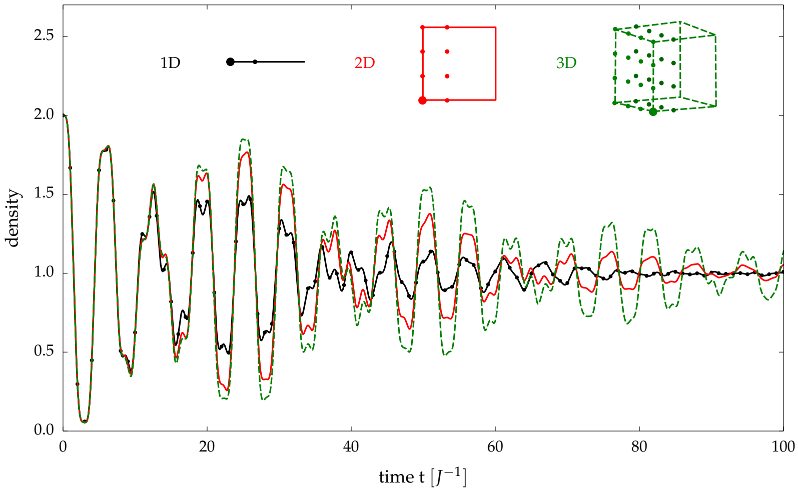

Conclusions and Outlook

Correlated quantum systems in non-equilibrium – Goals:

- self-consistent description of correlation, exchange and nonlinear response to fields; short-time to long-time dynamics

NEGF: can treat mixed and pure states, conserving

1. advantageous scaling with N (limitation: basis size)
2. GKBA $\Rightarrow$ efficiency gain, no artificial damping
3. T-matrix selfenergy with GKBA: access to strong coupling

Stochastic Mean Field: Monte Carlo sampling of TDHF trajectories

1. highly efficient, large systems, arbitrary geometry

Response of finite Hubbard clusters to strong excitation

1. non-trivial dynamics of occupations, correlations, coherences
2. extension to materials via DMFT-type schemes

Thank you for your attention!

References

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- D. Hochstuhl, C. Hinz, and M. Bonitz, EPJ-ST **223**, 177-336 (2014)
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