Can we treat strong correlations, spatial inhomogeneity and ultrafast dynamics with Green functions?

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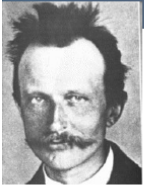
Kiel physics



Chair Statistical Physics - Research Directions

C | A | U

Strongly correlated Coulomb systems

Classical Coulomb systems

Complex plasmas
Coulomb liquids
Coulomb crystals
Anomalous transport
Plasma-surface interaction

Quantum Coulomb systems

Warm Dense matter
Astrophysical plasmas
Correlated fermions
bosons, excitons
Atoms, dense matter interacting with lasers and x-rays
Femtosecond dynamics
Quark-gluon plasma

Kinetic Theory
Langevin MD
Monte Carlo

Time-dep. RAS - CI
Quantum Kinetic Theory
Nonequilibrium Green functions
First principle simulations

Acknowledgements

DFG

Bundesministerium
für Bildung
und Forschung

Outline

1. Introduction
2. Nonequilibrium Green Functions
   - I. Two-time (Keldysh) Green functions
   - II. Inhomogeneous Systems
   - III. Generalized Kadanoff-Baym ansatz (GKBA)
3. Excitation dynamics in Hubbard nanoclusters
   - I. Testing the GKBA
   - II. Transport properties of finite Hubbard clusters
   - III. Excitation spectra
4. Conclusions

(too) Fast carrier relaxation in semiconductors

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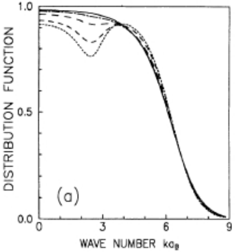
Carrier-carrier scattering and optical dephasing in highly excited semiconductors

R. Binder, D. Scott, A. E. Paul, M. Lindberg, K. Henneberger,* and S. W. Koch
Optical Sciences Center and Physics Department, University of Arizona, Tucson, Arizona 85721
(Received 3 June 1991; revised manuscript received 3 September 1991)



Lenard-Balescu collision integral, Phys. of Fluids **3**, 52 (1960)

dynamically screened Coulomb potential

$$W(q,\omega) = \frac{V(q)}{1 - V(q)\,P(q,\omega)} = V(q)\,\epsilon^{-1}(q,\omega)$$

unscreened potential $\quad V(q) = \dfrac{4\pi e^2}{Vq^2}$

$$P(\mathbf{q},\omega) = \lim_{\delta\to 0} 2\sum_{\alpha,\mathbf{k}} \frac{f_\alpha(k) - f_\alpha(|\mathbf{q}+\mathbf{k}|)}{\epsilon_\alpha(k) - \epsilon_\alpha(|\mathbf{q}+\mathbf{k}|) + \hbar\omega + i\delta}$$

Failure of the Boltzmann equation[1]

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$$\left\{\frac{\partial}{\partial t} + \mathbf{v}_1\frac{\partial}{\partial \mathbf{r}_1} - \frac{1}{m}\mathbf{F}_1\frac{\partial}{\partial \mathbf{v}_1}\right\} f(\mathbf{r}_1,\mathbf{p}_1,t) = I(\mathbf{r}_1,\mathbf{p}_1,t),$$

$$I(\mathbf{r}_1,\mathbf{p}_1,t) = \int d^3p_2 \int d^3\bar{p}_1 \int d^3\bar{p}_2 \; P(\mathbf{p}_1,\mathbf{p}_2;\bar{\mathbf{p}}_1,\bar{\mathbf{p}}_2;t)$$
$$\times \left\{ f(\mathbf{r}_1,\bar{\mathbf{p}}_1,t) f(\mathbf{r}_1,\bar{\mathbf{p}}_2,t) - f(\mathbf{r}_1,\mathbf{p}_1,t) f(\mathbf{r}_1,\mathbf{p}_2,t) \right\}, \tag{1.1}$$

$$P(\mathbf{p}_1,\mathbf{p}_2;\bar{\mathbf{p}}_1,\bar{\mathbf{p}}_2;t) = \left|\frac{V(q)}{\epsilon(q,\omega;t)}\right|^2 \delta(\mathbf{p}_{12}-\bar{\mathbf{p}}_{12})\delta(E_{12}-\bar{E}_{12})$$

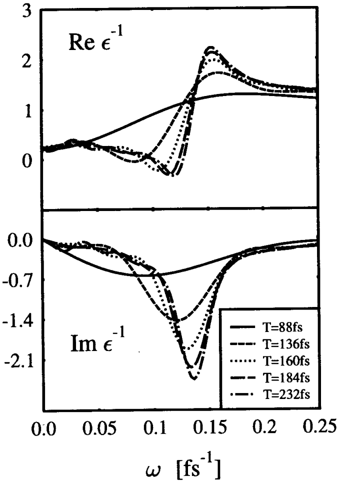
$q = |\mathbf{p}_1 - \bar{\mathbf{p}}_1|$, $\mathbf{p}_{12} = \mathbf{p}_1 + \mathbf{p}_2$, $\hbar\omega = E_1 - \bar{E}_1$, Pauli blocking factors $(1 \pm f)$ omitted

- Equation (1.1): conserves quasi-particle energy, relaxes towards Fermi (Bose) function
- Equation (1.1): fails at short times, misses buildup of correlations, screening

$\Rightarrow$ unphysical fast relaxation dynamics $\Rightarrow$ generalized quantum kinetic theory needed

[1] M. Bonitz, *Quantum Kinetic theory*, Teubner 1998, 2nd ed.: Springer 2015

Build up of dynamical screening[2]



- first results: MB, 1996
- numerical solution of non-Markovian Balescu equation: Banyai, *et al.*, PRL **81**, 882 (1998)
- Experimental verification of screening build up: Huber *et al.*, Nature **414**, 216 (2001)

[2] M. Bonitz, *Quantum Kinetic theory*, Teubner 1998, 2nd ed.: Springer 2015

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2nd quantization

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

Particle interaction w_{klmn}

- Only electron dynamics
- Coulomb interaction

Time-dependent excitation F(t)

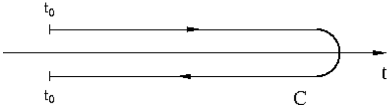
- Single-particle type
- Optical/Laser-induced

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

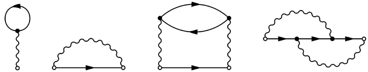
$$G^{(1)}_{ij}(z,z') = \frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\,\hat{c}_i(z)\hat{c}^\dagger_j(z')\right\rangle$$

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

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



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



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

Real-time Dyson equation/ KBE

- 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

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

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

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

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

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

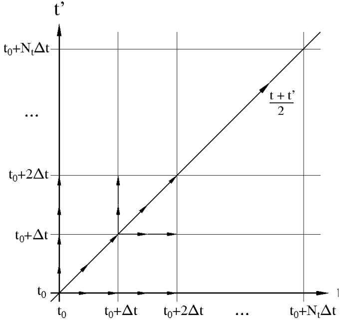
$$\rho(x_1, x_1', t) = \mp\, i\, g^{<}(1,1')\Big|_{t_1=t_1'}$$

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

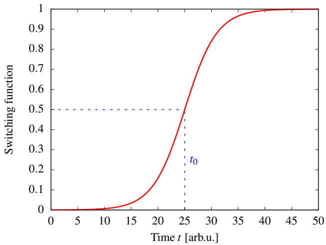
Interaction energy (two-particle observable, [Baym/Kadanoff])

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

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



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



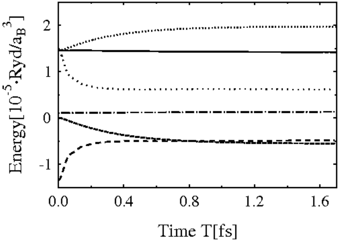
1. Uncorrelated initial state

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)

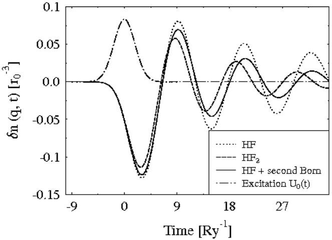
Two-time simulations: Summary

1. perfect conservation of total energy
2. accurate short-time dynamics:
   phase 1: correlation dynamics
   2: relaxation of $f(p)$, 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)

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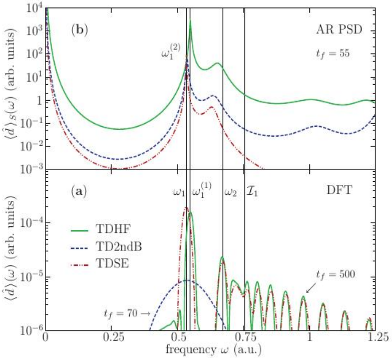
- few-electron atoms, molecules: Balzer *et al.*, PRA **81**, 022510 (2010)

1D He ground state

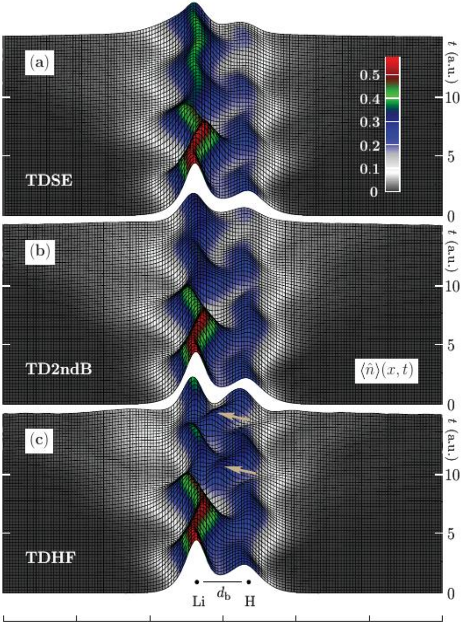
	Hartree-Fock	
	n_g (n_b)	E_{gs}^{HF} [a.u.]
	4 (43)	−2.22
	9 (98)	−2.224209
	14 (153)	−2.2242096
	Second Born	
n_g (n_b)	Number of τ-grid points	E_{gs}^{2ndB} [a.u.]
14 (153)	101	−2.23
14 (153)	301	−2.2334
14 (153)	601	−2.23341
14 (153)	1001	−2.233419
	TDSE (exact)	
		E_{gs}^{TDSE} [a.u.]
		−2.2382578

1D He dipole spectra



[3] pioneered by N. Dahlen and R. van Leeuwen, PRL **98**, 153004 (2007)

- strong excitation of molecules: Balzer *et al.*, PRA **82**, 033427 (2010)
- XUV-pulse excitation of LiH (1d-model)
- Goals: correlated electron dynamics beyond Hartree-Fock



Numerical challenges of 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[4]

- 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

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

FEDV-Representation[5]

- strong excitation and ionization of atoms and molecules: need to resolve nucleus and large distances
- Selfenergy in FEDVR largely diagonal

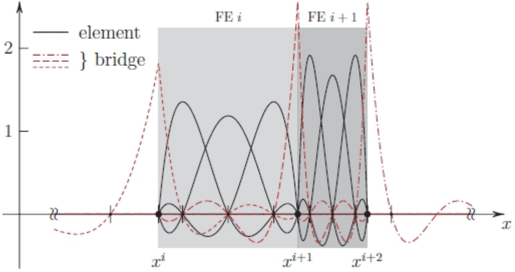


FIG. 2. (Color online) Structure of a FE-DVR basis $\{\chi_m^i(x)\}$ with $n_g = 4$ (i.e., five local DVR basis functions in each element). While the element functions (solid) are defined in a single FE, the bridge functions (dashed and dashed-dotted lines) link two adjacent FEs.

[5] Balzer *et al.*, PRA **81**, 022510 (2010)

The Generalized Kadanoff-Baym Ansatz

Equivalent form of the KBE [*Lipavskii et. al.*]:

- For times $t_1 > t_2 > t_0$:

$$G^<(t_1,t_2) = -G^{\mathrm{R}}(t_1,t_2)\rho(t_2) + \int_{t_2}^{t_1} \mathrm{d}t_3 \int_{t_0}^{t_2} \mathrm{d}t_4\, G^{\mathrm{R}}(t_1,t_3)\Sigma^<(t_3,t_4)G^{\mathrm{A}}(t_4,t_2) + \int_{t_2}^{t_1} \mathrm{d}t_3 \int_{t_0}^{t_2} \mathrm{d}t_4\, G^{\mathrm{R}}(t_1,t_3)\Sigma^{\mathrm{R}}(t_3,t_4)G^<(t_4,t_2)\,.$$

- For times $t_0 < t_1 < t_2$:

$$G^<(t_1,t_2) = \rho(t_1)G^{\mathrm{A}}(t_1,t_2) - \int_{t_0}^{t_1} \mathrm{d}t_3 \int_{t_1}^{t_2} \mathrm{d}t_4\, G^{\mathrm{R}}(t_1,t_3)\Sigma^<(t_3,t_4)G^{\mathrm{A}}(t_4,t_2) - \int_{t_0}^{t_1} \mathrm{d}t_3 \int_{t_1}^{t_2} \mathrm{d}t_4\, G^<(t_1,t_3)\Sigma^{\mathrm{A}}(t_3,t_4)G^{\mathrm{A}}(t_4,t_2)\,.$$

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- Idea of the GKBA: lowest order solution[6]

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

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

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

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

- Direct derivation from density operator theory possible[7]

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[6] P. Lipavsky, V. Spicka and B. Velicky Phys. Rev. B **34**, 6933 (1986)

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

The generalized Kadanoff-Baym ansatz: Conserving properties

- HF-GKBA: same conservation properties as two-time approximation[8]
- damped propagators, local approximation violate total energy conservation[9]
- Generalization of the energy conservation theorem of Baym and Kadanoff (relaxed conditions)[10]

Extensions: Gauge invariant generalization of the GKBA to strong electro-magnetic fields[11]

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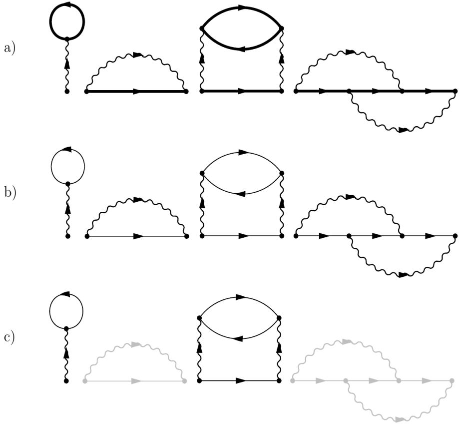
[8] G. Baym and L.P. Kadanoff, Phys. Rev. **124**, 287 (1961)

[9] M. Bonitz, D. Semkat, H. Haug, Eur. Phys. J. B **9**, 309 (1999)

[10] S. Hermanns, N. Schlünzen, and M. Bonitz, Phys. Rev. B **90**, 125111 (2014)

[11] D. Kremp, Th. Bornath, M. Bonitz, and M. Schlanges, Phys. Rev. E **60**, 4725 (1999)

HF-GKBA: reducing the selfconsistency

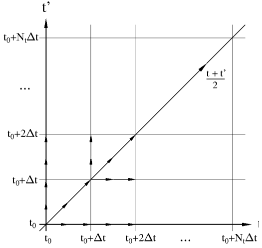


HF-GKBA: All propagators replaced by HF-propagators[12]

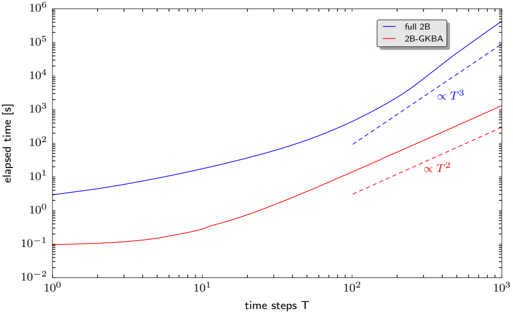
Example: 2nd Born selfenergy. a) two-time, b) HF-GKBA, c) Hubbard

[12] S. Hermanns, N. Schlünzen, and M. Bonitz, Phys. Rev. B **90**, 125111 (2014)

Performance gain with the GKBA+2B



time stepping along diagonal only. Full memory retained.



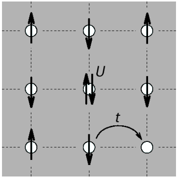
S. Hermanns, K. Balzer, and M. Bonitz, *Phys. Scripta* **T151**, 014036 (2012)

we use about $5 \cdot 10^3 \ldots 5 \cdot 10^4$ time steps for the adiabatic switching and $10^5 \ldots 10^6$ for the excitation and relaxation.

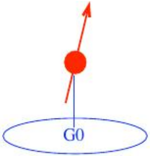
Outline

Lattice models

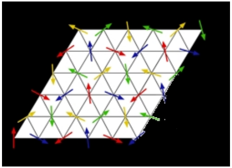
Hubbard



Anderson impurity



Heisenberg

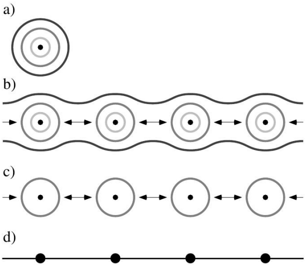


- simplification of the many-body problem
  - localized sites
  - interaction and exchange effects tractable
- macroscopic and finite systems

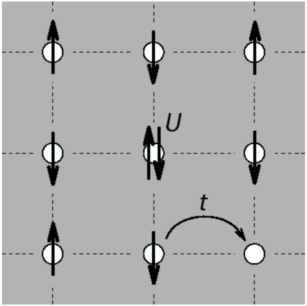
- derived from many-body theory for many systems
  - condensed matter (transition metal oxides, ...)
  - ultracold particles in optical lattices
  - molecules

The Hubbard model

- Simple, but versatile model for strongly correlated solid state systems
- Suitable for single band, small bandwidth



$$\Rightarrow$$



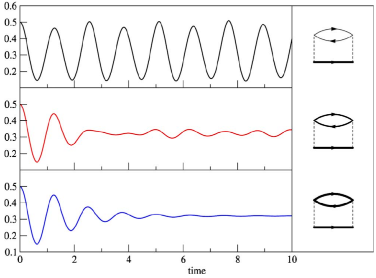
$$\hat{H}(t) = J \sum_{ij,\,\alpha} h_{ij}\, \hat{c}^\dagger_{i\alpha} \hat{c}_{j\alpha} + U \sum_i \hat{c}^\dagger_{i\uparrow} \hat{c}_{i\uparrow} \hat{c}^\dagger_{i\downarrow} \hat{c}_{i\downarrow} + \sum_{ij,\alpha\beta} f_{ij,\alpha\beta}(t)\, \hat{c}^\dagger_{i\alpha} \hat{c}_{j\beta}$$

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

Two-site Hubbard—strong excitation[13]

Problems of NEGF in second Born: $N = 2, n = 1/2, U = 1,$
Excitation matrix: $f_{ij,\alpha\beta}(t) = w_0 \delta_{i,1}\delta_{j,1}\delta_{\alpha,\beta}\Theta(t)\,, \quad w_0 = 5.0 J^{-1}$

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

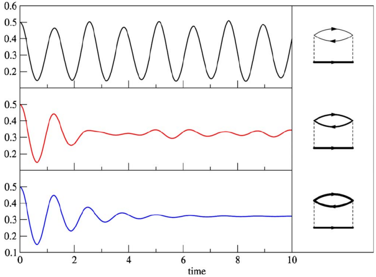


[13] P. von Friesen, C. Verdozzi, and C.O. Almbladh, Phys. Rev. B **82**, 155108 (2010)

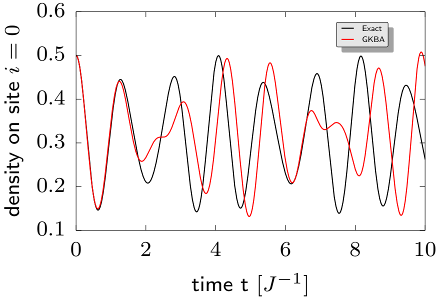
Two-site Hubbard—strong excitation[14][15]

Problems of NEGF in second Born: $N = 2, n = 1/2, U = 1$ [1],
Excitation matrix: $f_{ij,\alpha\beta}(t) = w_0 \delta_{i,1}\delta_{j,1}\delta_{\alpha,\beta}\Theta(t)\,, \quad w_0 = 5.0J^{-1}$

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



- GKBA+2B: no damping!
  selfconsistency problem "cured"

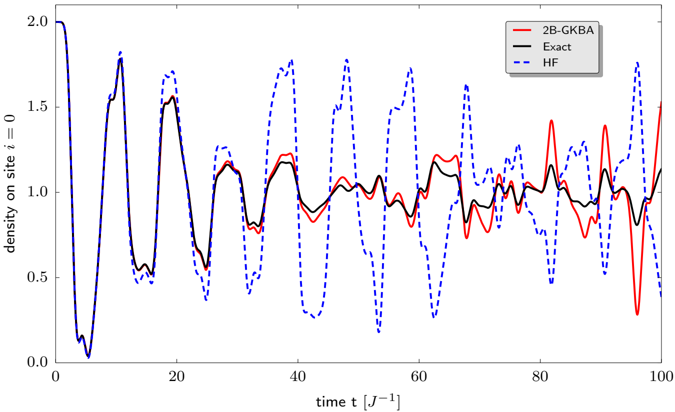


[14] P. von Friesen, C. Verdozzi, and C.O. Almbladh, Phys. Rev. B **82**, 155108 (2010)

[15] S. Hermanns, N. Schlünzen, and M. Bonitz, Phys. Rev. B **90**, 125111 (2014)

Half filling—noneq. initial state $N = 8, \; U = 0.1$

No field. Sites $0 - 3$ doubly occupied, $4 - 7$ empty



- failure of HF, good performance of GKBA up to long times ($t \sim 50$)
- GKBA improves with particle number

T-matrix selfenergy and HF-GKBA+T

- To access strong coupling: need T-matrix selfenergy
- For Hubbard model simplification[16]

$$\Sigma^{\mathrm{cor}}_{ik}(t_1,t_2) = \mathrm{i}T_{ik}(t_1,t_2)G_{ki}(t_2,t_1),$$

$$T_{ik}(t_1,t_2) = \pm\mathrm{i}U^2\, G^{\mathrm{H}}_{ik}(t_1,t_2) + \mathrm{i}U \int_{\mathcal{C}} \mathrm{d}\bar{t}\, G^{\mathrm{H}}_{il}(t_1,\bar{t})T_{lk}(\bar{t},t_2),$$

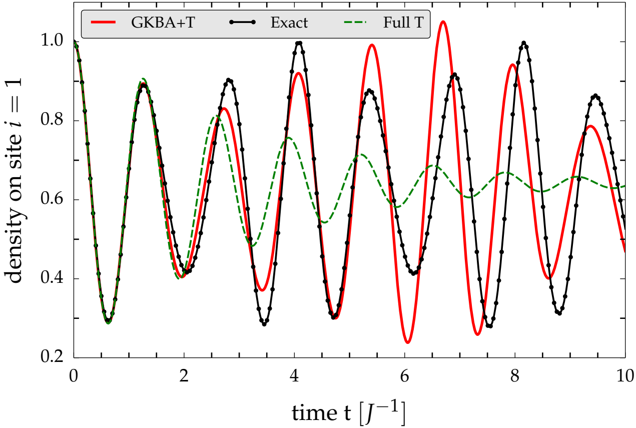
$$G^{\mathrm{H}}_{ik}(t_1,t_2) = G^{\uparrow}_{ik}(t_1,t_2)\, G^{\downarrow}_{ik}(t_1,t_2),$$

- T-matrix + HF-GKBA: well defined and conserving strong coupling approximation
- larger systems, long propagation feasible[17]

[16] P. von Friesen, C. Verdozzi, and C.O. Almbladh, Phys. Rev. B **82**, 155108 (2010)

[17] M. Bonitz, S. Hermanns, and N. Schlünzen, Contrib. Plasma Phys. **55**, 152 (2015)

Hubbard model at medium coupling: $N = 2, n = 1/2, U = 1,$
Excitation matrix: $f_{ij,\alpha\beta}(t) = w_0 \delta_{i,1}\delta_{j,1}\delta_{\alpha,\beta}\Theta(t)\,, \quad w_0 = 5.0J^{-1}$



[18] S. Hermanns, N. Schlünzen, and M. Bonitz, Phys. Rev. B **90**, 125111 (2014)

Goals :

- study transport (diffusion, heat conductivity etc.) by a nonequilibrium approach[19]
- retain full spatial resolution (single-site)
- retain full temporal resolution
- explore particle number dependence, finite-size effects
- explore effects of inhomogeneity, geometry, dimensionality

[19] in contrast to standard equilibrium approaches based on fluctuation-dissipation relations

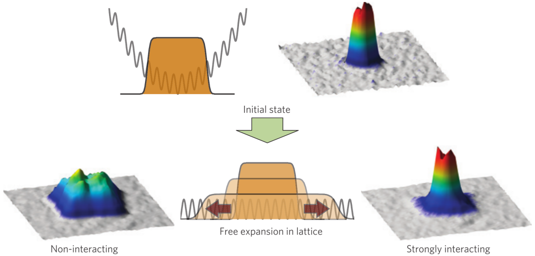
nature physics

ARTICLES

PUBLISHED ONLINE: 15 JANUARY 2012 | DOI: 10.1038/NPHYS2205

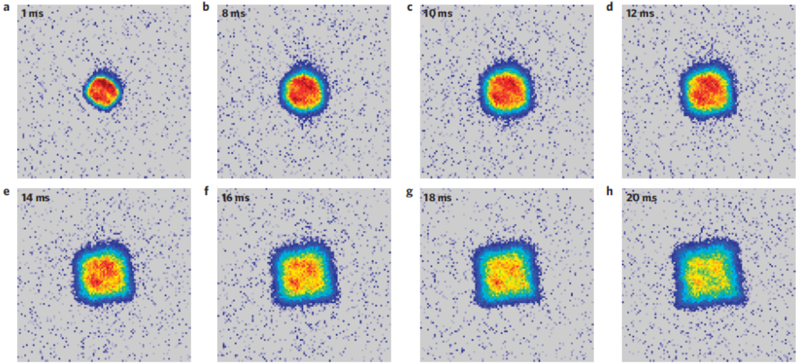
Fermionic transport and out-of-equilibrium dynamics in a homogeneous Hubbard model with ultracold atoms

Ulrich Schneider[1,2]★, Lucia Hackermüller[1,3], Jens Philipp Ronzheimer[1,2], Sebastian Will[1,2], Simon Braun[1,2], Thorsten Best[1], Immanuel Bloch[1,2,4], Eugene Demler[5], Stephan Mandt[6], David Rasch[6] and Achim Rosch[6]



Time-resolved expansion of Fermi gas[20]

- Experimental snapshots for ^{40}K-atoms in optical lattice
- Expansion initiated by turn-off ("quench") of harmonic confinement.
- Hubbard model with variable U, $T \sim 0.13\,T_F$, $N \sim 200,000$.



[20] U. Schneider *et al.*, Nature Physics **8**, 213-218 (2012)

Theory:

use semiclassical Boltzmann equation in relaxation time approximation

$$\partial_t f_{\mathbf{q}} + \mathbf{v}_{\mathbf{q}} \nabla_{\mathbf{r}} f_{\mathbf{q}} + \mathbf{F}(\mathbf{r}) \nabla_{\mathbf{q}} f_{\mathbf{q}} = -\frac{1}{\tau(\mathbf{n})} \left(f_{\mathbf{q}} - f_{\mathbf{q}}^{0}(\mathbf{n}) \right)$$

Quote:

Although the expansion can be modelled in 1D (ref. 31) using DMRG methods (ref. 32), so far no methods are available to calculate the dynamics quantum-mechanically in higher dimensions.

[21] U. Schneider *et al.*, Nature Physics **8**, 213-218 (2012)

A challenge for NEGF...

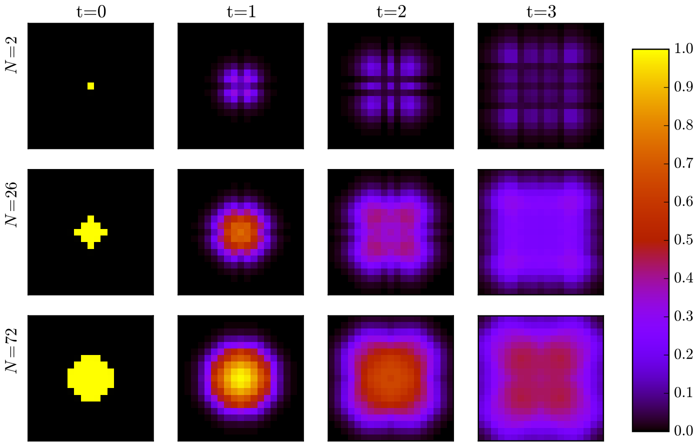
- NEGF can treat Hubbard clusters in *any* dimension
- with T-matrix selfenergy: strong correlations accessible, $U \lesssim 4$
- problem: direct inhomogeneous expansion feasible only for small N
- idea: simulations for fixed N; attempt numerical extrapolation[22]
- concept and first results[23] for $N \leq 8$

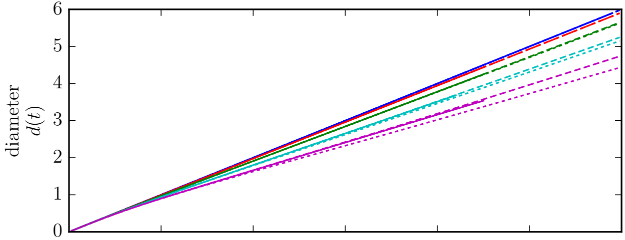
[22] S. Hermanns, N. Schlünzen, and M. Bonitz, to be published

[23] M. Bonitz, S. Hermanns, and N. Schlünzen, Contrib. Plasma Phys. **55**, 152 (2015)

Fermion expansion and doublon decay

- $t = 0$: circular array of doubly occupied sites. Confinement quench initiates diffusion.
- T-matrix selfenergy for $U = 1$ and 3 values of N.
- Plots show $\sqrt{N_\uparrow}$



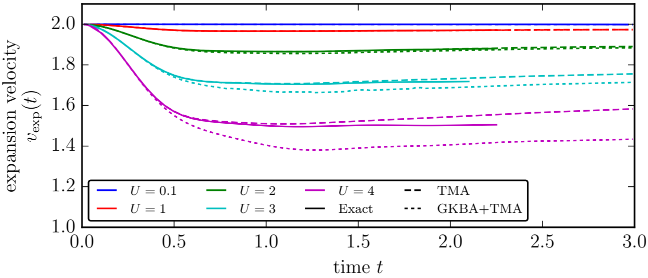


Time evolution of cloud diameter for different U:

$d(t) = \sqrt{R^2(t) - R^2(0)}$

$R^2 = \frac{1}{N} \sum_{i=1}^{N_s} (i - l_0)^2 \cdot n_i$

Full T-matrix and GKBA+T vs. exact solution ($N = 2$).



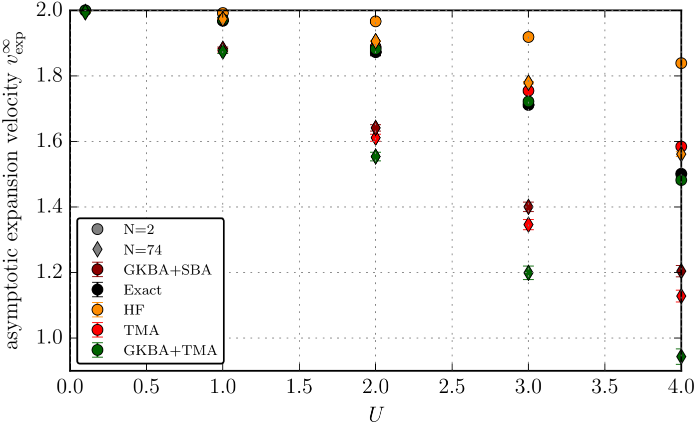
Time evolution of the cloud expansion velocity

$v_{\text{exp}}(t) = \frac{\mathrm{d}}{\mathrm{d}t} d(t)$

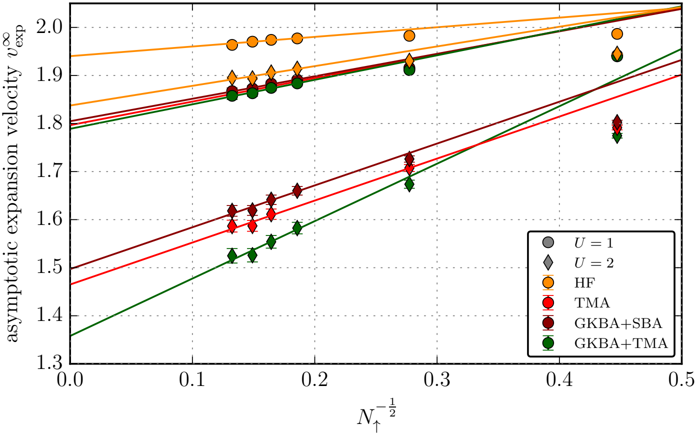
Extract asymptote $v_{\text{exp}}^{\infty}(U)$

Correlations slow down expansion. Exact result between T, GKBA+T

- Expansion of initially circular doubly occupied cloud for $U = 1$ and $N = 2, 74$
- Strong correlation effect. Error of HF grows with N



- Expansion of initially circular doubly occupied cloud for $U = 1$ and $U = 2$ at fixed N
- Extrapolation $N \to \infty$.



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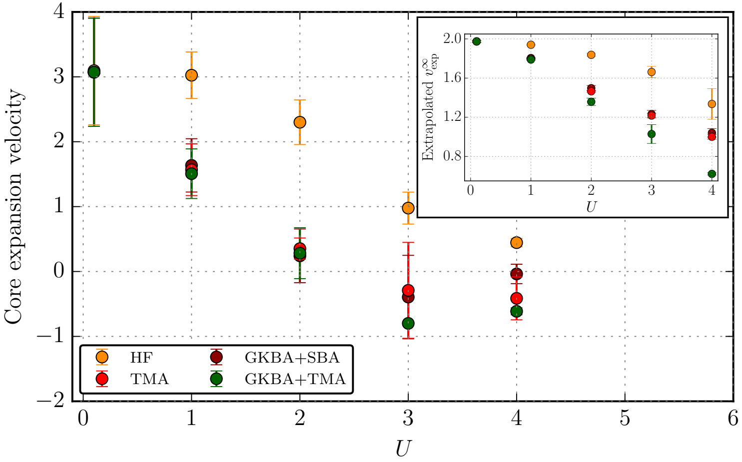
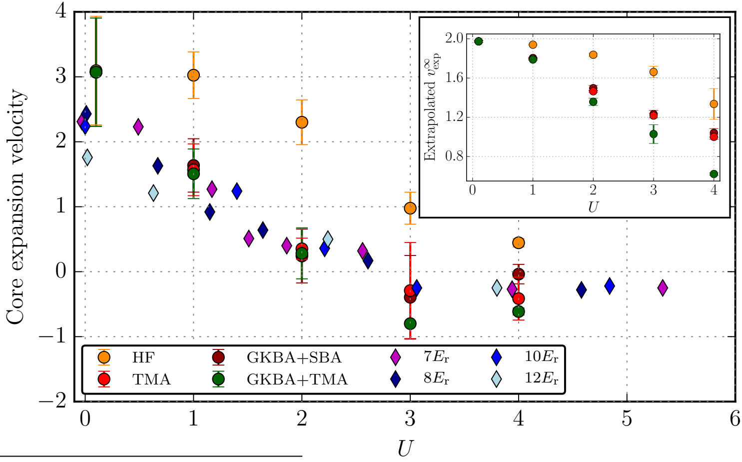
- Extrapolation results for expansion velocity for different approximations
- Comparison to extrapolated "core expansion velocity" (HWHM)
- Core shrinks for $U \lesssim 3$, as in experiment



NEGF vs. experimental results

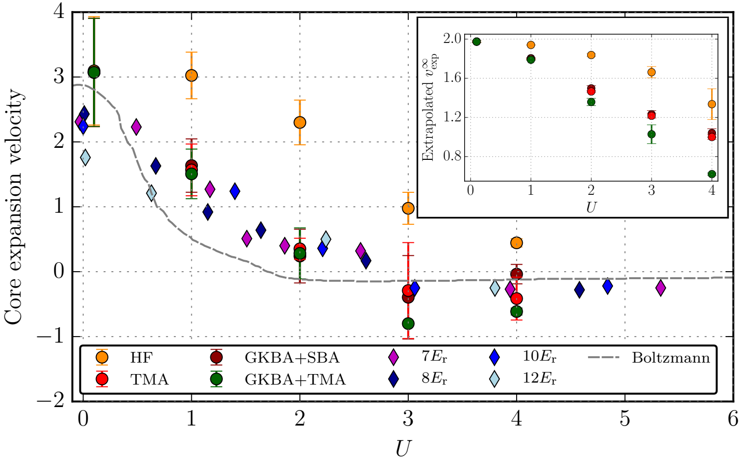
- Compare macroscopic T-matrix data to *core* expansion velocities of Schneider *et al.*[24]
- Inset: theoretical results for full expansion velocity



[24] U. Schneider *et al.*, Nature Physics **8**, 213-218 (2012)

NEGF vs. experimental results and RTA-model

- Compare macroscopic T-matrix data to *core* expansion velocities of Schneider *et al.*[25]
- grey line: relaxation time model (Rosch)



[25] U. Schneider *et al.*, Nature Physics **8**, 213-218 (2012)

Outline

- Charge-conserving spectral properties accessible via two-particle XC function

$$L(1,2,3,4) = \pm\left[G_2(1,2;3,4) - G(1;3)\,G(2;4)\right] \,,$$

or reducible polarizability/density response function χ,

$$\chi(1;2) = \pm\mathrm{i}L(1,2;1^+,2^+)\,.$$

- L fulfills Bethe–Salpeter equation (BSE)

$$\begin{aligned} L(1,2;3,4) =& \; G(1;4)\,G(2;3) \\ & \pm \int_{\mathcal{C}} \mathrm{d}1'\mathrm{d}2'\mathrm{d}3'\mathrm{d}4' \; G(1;1')\,G(3';3)\,K(1',2';3',4')\,L(4',2;2',4)\,, \end{aligned}$$

- BSE successfully used for ground state and equilibrium spectra
- examples: optical spectra in semiconductors and insulators, formation of particle–hole pairs, excitons, plasmons etc.
- Even for stationary case (in Fourier space) BSE can be solved only for simple kernels K

Alternative approach:
- obtain response functions from time-dependent solution of KB equations
- consider weak change of single-particle Hamiltonian $h \to h + \delta h$,
- linear response from correlated equilibrium state: $G \to G + \delta G$,

$$\delta G(1;3) = \int_{\mathcal{C}} L(1,2';3,4')\delta h(4';2')\,.$$

General concept 1999: N. Kwong and MB[26]
- 1998: optical absorption of semiconductors, exciton formation[27]
- 2000: application to plasmon spectrum of correlated electron gas[28]
- 2007: optical absorption of atoms[29]
- 2012: double excitations of correlated systems[30]

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[26] M. Bonitz, N.H. Kwong, D. Semkat, and D. Kremp, Contrib. Plasma Phys. **39**, 37 (1999)

[27] N.H. Kwong, M. Bonitz, R. Binder and S. Köhler, phys. stat. sol. (b) **206**, 197 (1998)

[28] N.H. Kwong, and M. Bonitz, Phys. Rev. Lett. **84**, 1768 (2000)

[29] N. Dahlen and R. van Leeuwen, PRL **98**, 153004 (2007)

[30] K. Balzer, S. Hermanns and M. Bonitz, EPL **98**, 67002 (2012);

N. Säkkinen, M. Manninen and R. van Leeuwen, New J. Phys. **14**, 013032 (2012)

Complex Spectra from simple selfenergies

Contrib. Plasma Phys. **39** (1999) 1–2, 37–40

Generalized Kadanoff–Baym Theory for Non–Equilibrium Many–Body Systems in External Fields. An Effective Multi–Band Approach

M. Bonitz, N.H. Kwong, D. Semkat, D. Kremp

correlated system in ext. field U: Dyson equation (on Keldysh contour)

$$G = G_0^{[0]} + G_0^{[0]}(\Sigma + U)G,$$ equivalent to system:

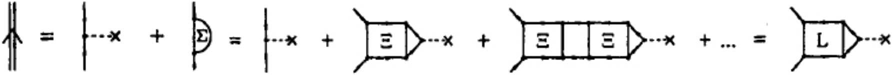
$$G^{[0]} = G_0^{[0]} + G_0^{[0]}\Sigma^{[0]}G^{[0]},$$ $^{[0]}$: field-free, but correlated

$$G = G^{[0]} + G^{[0]}(\Sigma^{[1]} + \Sigma^{[2]} + \cdots + U)G,$$ add field

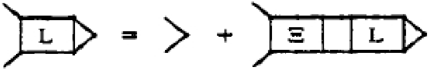
in linear response the last eq. becomes ($\Xi^{[0]}$: field-free 2-particle kernel):

$$G^{[1]} = G^{[0]} + G^{[0]}(\Sigma^{[1]} + U)G^{[0]}, \quad \Sigma^{[1]} \equiv \Xi^{[0]}G^{[1]}$$

First order (in U) Green function (particle-hole NEGF):



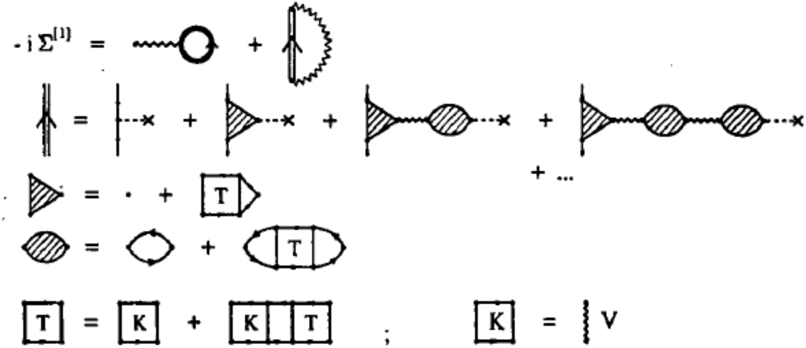
L obeys Bethe-Salpeter equation ($\Sigma^{[1]} \equiv \Xi^{[0]} G^{[1]}$):



equivalent to[31]:

$$\Xi^{[0]} \to K(1,2;3,4) = V \pm \delta\Sigma(1;3)/\delta G(4;2)\,.$$

[31] N.H. Kwong, and M. Bonitz, Phys. Rev. Lett. **84**, 1768 (2000)



K includes T-matrix and ring diagrams, i.e. exciton-like bound states

Example 2: $\Sigma = \Sigma^{\mathrm{F}} + \Sigma^{\mathrm{2Bdirect}}$

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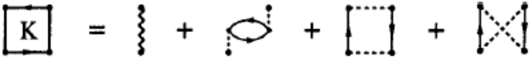


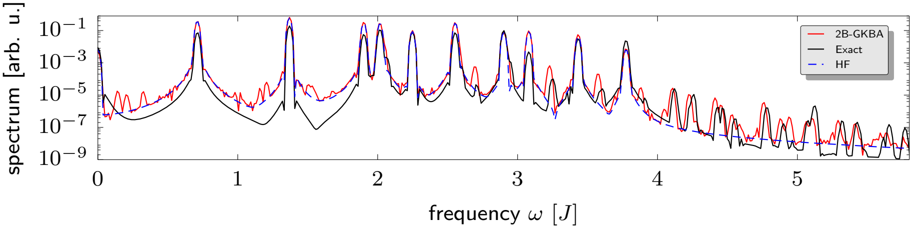
- K includes particle-hole T-matrix diagrams
- when applied to uniform electron gas:

$\rightarrow$ yields correlated plasmon spectrum with vertex corrections (f-sum rule preserving)[32]

[32] N.H. Kwong, and M. Bonitz, Phys. Rev. Lett. **84**, 1768 (2000)

Real-time propagation following weak excitation and Fourier transform

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



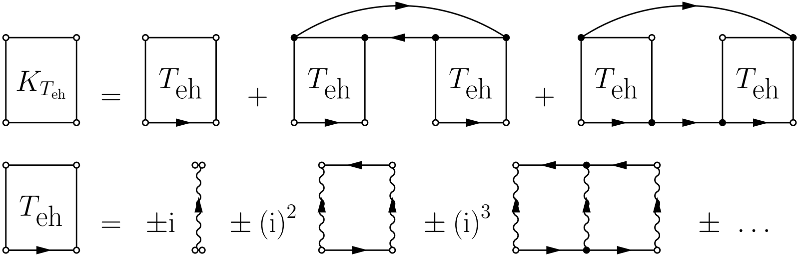
- GKBA: increased resolution of spectra. Capture double excitations[33] improve on earlier results[34] [35]

[33] S. Hermanns, N. Schlünzen, and M. Bonitz, PRB **90**, 125111 (2014)

[34] N. Säkkinen, M. Manninen, and R. van Leeuwen, New J. Phys. **14**, 013032 (2012).

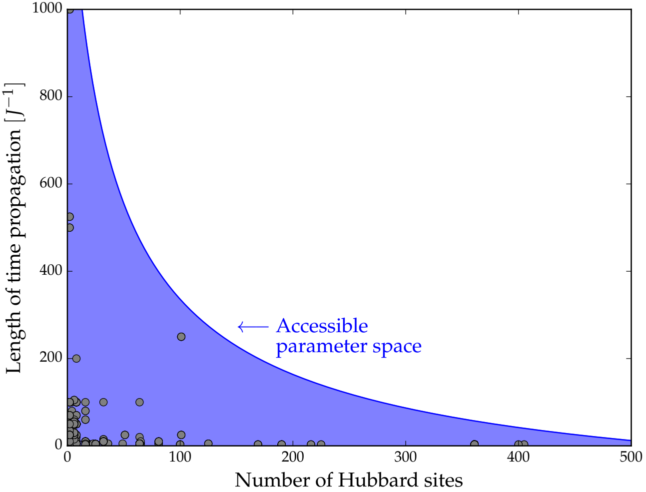
[35] K. Balzer, S. Hermanns, and M. Bonitz, Europhys. Lett. **98**, 67002 (2012).

Outlook:
time-propagation with T–Matrix selfenergy yields BSE kernel $K^{\mathsf{T}_{\mathsf{eh}}}$:



S. Hermanns, N. Schlünzen, and M. Bonitz, to be published

Up to $N_s = 500$, up to $T = 1000 J^{-1}$



Conclusions and Outlook

1. **Correlated quantum systems in non-equilibrium –** failure of Boltzmann-type kinetic equations
2. **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. **Dynamics of finite Hubbard clusters**
   1. long Hubbard simulations, strong excitation (small U)
   2. strong correlations accessible via T-matrix and GKBA+T
   3. Transport of strongly correlated fermions: good agreement with cold atom experiments
4. **High-quality spectra via time-propagation of KBE**

Thank you for your attention!

References

- MB and D. Semkat, *Introduction to Computational Methods in Many-Body Physics*, Rinton Press 2006
- K. Balzer, and M. Bonitz, Springer Lect. Not. Phys. **867** (2013)
- www.itap.uni-kiel.de/theo-physik/bonitz

Don't miss: (see web page above)
→ *Progress in Nonequilibrium Green functions VI*, Lund August 17-21

→ *Isolated many-body quantum systems out of equilibrium: from unitary time evolution to quantum kinetic equations* (Heraeus-Seminar)
30 Nov - 3 Dec, Bad Honnef, Germany