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

Sebastian Hermanns, Niclas Schlünzen, Michael Bonitz, and Claudio Verdozzi*

Institut für Theoretische Physik und Astrophysik
Christian-Albrechts-Universität zu Kiel, Germany

*Department of Mathematical Physics, Lund University, Sweden

CECAM Lausanne, May 6 2015
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

M. Bonitz (Kiel University)

Nonequilibrium Green functions

CECAM, May 6 2015
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
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

\[ V(q) = \frac{4\pi e^2}{Vq^2} \]

\[ P(q, \omega) = \lim_{\delta \to 0} 2 \sum_{\alpha, k} \frac{f_\alpha(k) - f_\alpha(|q + k|)}{\epsilon_\alpha(k) - \epsilon_\alpha(|q + k|) + i\delta + \hbar\omega} \]
Equation (1.1): conserves quasi-particle energy, relaxes towards Fermi (Bose) function

Equation (1.1): fails at short times, misses buildup of correlations, screening

⇒ unphysical fast relaxation dynamics ⇒ generalized quantum kinetic theory needed

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

\[ I(\mathbf{r}_1, \mathbf{p}_1, t) = \int d^3 p_2 \int d^3 \bar{p}_1 \int d^3 \bar{p}_2 P(\mathbf{p}_1, \mathbf{p}_2; \bar{\mathbf{p}}_1, \bar{\mathbf{p}}_2; t) \]

\[ \times \left\{ f(\mathbf{r}_1, \bar{\mathbf{p}}_1, t)f(\mathbf{r}_1, \bar{\mathbf{p}}_2, t) - f(\mathbf{r}_1, \mathbf{p}_1, t)f(\mathbf{r}_1, \mathbf{p}_2, t) \right\} \]

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

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

\[ ^1 \text{M. Bonitz, Quantum Kinetic theory, Teubner 1998, 2nd ed.: Springer 2015} \]
Build up of dynamical screening

- first results: MB, 1996
- Experimental verification of screening build up: Huber et al., Nature 414, 216 (2001)

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\[ \text{M. Bonitz, } Quantum Kinetic theory, \text{ Teubner 1998, 2nd ed.: Springer 2015} \]
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Nonequilibrium Green functions

2nd quantization

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

Particle interaction $w_{klmn}$

- Only electron dynamics
- Coulomb interaction

Time-dependent excitation $F(t)$

- Single-particle type
- Optical/Laser-induced
Keldysh Green functions

time-ordered one-particle Nonequilibrium Green function, two times \(z, z' \in C\) (“Keldysh contour”), arbitrary one-particle basis \(|\phi_i\rangle\)

\[
G^{(1)}_{ij}(z, z') = \frac{i}{\hbar} \langle \hat{T}_C \hat{c}_i(z) \hat{c}_j^\dagger(z') \rangle
\]

Keldysh–Kadanoff–Baym equation (KBE) on \(C\):

\[
\sum_k \left\{ i\hbar \frac{\partial}{\partial z} \delta_{i k} - h_{i k}(z) \right\} G^{(1)}_{kj}(z, z') = \delta_C(z, z') \delta_{ij} - i\hbar \sum_{klm} \int_C d\bar{z} \ w_{iklm}(z^+, \bar{z}) G^{(2)}_{lmjk}(z, \bar{z}; z', \bar{z}^+) \]

\(\int_C w G^{(2)} \rightarrow \int_C \Sigma G^{(1)}\), 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

\[ G_{ij} = \begin{pmatrix} G^R_{ij} & G^<_{ij} \\ 0 & G^A_{ij} \end{pmatrix} \]

\[ G^<_{ij}(t_1, t_2) = \mp i \left\langle \hat{c}_j(t_2) \hat{c}_i(t_1) \right\rangle \]

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

- Propagators

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

- Correlation functions \( G^\geq \) obey real-time KBE

\[ \left[ i\partial_{t_1} - h_0(t_1) \right] G^<(t_1, t_2) = \int dt_3 \Sigma^R(t_1, t_3) G^<(t_3, t_2) + \int dt_3 \Sigma^<(t_1, t_3) G^A(t_3, t_2) , \]

\[ G^<(t_1, t_2) \left[ -i\partial_{t_2} - h_0(t_2) \right] = \int dt_3 G^R(t_1, t_3) \Sigma^<(t_3, t_2) + \int dt_3 \Sigma^A(t_1, t_3) G^<(t_3, t_2) \]
Information in the Nonequilibrium Green functions

Time-dependent single-particle operator expectation value

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

- **Particle density**

\[ \langle \hat{n}(x, t) \rangle = n(1) = \mp i \, g^<(1, 1) \]

- **Density matrix**

\[ \rho(x_1, x'_1, t) = \mp i \, g^<|_{t_1=t'_1}^{(1, 1')} \]

- **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])

\[ \langle \hat{V}_{12}(t) \rangle = \pm i \, \frac{\nu}{4} \int \frac{d\vec{p}}{(2\pi\hbar)^3} \left\{ (i \partial_t - i \partial_{t'}) - \frac{p^2}{m} \right\} g^<|_{t=t'}^{(\vec{p}, t, t')} \]
Numerical solution of the KBE

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

1 Uncorrelated initial state

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

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

Two-time simulations: Summary

1. perfect conservation of total energy

2. accurate short-time dynamics:
   - phase 1: correlation dynamics
   - phase 2: relaxation of $f(p)$, occupations

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.

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


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

1D He ground state

<table>
<thead>
<tr>
<th>$n_g$ ($n_b$)</th>
<th>$E_{gs}^{\text{HF}}$ [a.u.]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 (43)</td>
<td>-2.22</td>
</tr>
<tr>
<td>9 (98)</td>
<td>-2.224209</td>
</tr>
<tr>
<td>14 (153)</td>
<td>-2.2242096</td>
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</table>

Second Born

<table>
<thead>
<tr>
<th>$n_g$ ($n_b$)</th>
<th>Number of $\tau$-grid points</th>
<th>$E_{gs}^{\text{2ndB}}$ [a.u.]</th>
</tr>
</thead>
<tbody>
<tr>
<td>14 (153)</td>
<td>101</td>
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</tr>
<tr>
<td>14 (153)</td>
<td>301</td>
<td>-2.2334</td>
</tr>
<tr>
<td>14 (153)</td>
<td>601</td>
<td>-2.23341</td>
</tr>
<tr>
<td>14 (153)</td>
<td>1001</td>
<td>-2.233419</td>
</tr>
</tbody>
</table>

TDSE (exact)

$E_{gs}^{\text{TDSE}}$ [a.u.]

-2.2382578

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3 pioneered by N. Dahlen and R. van Leeuwen, PRL 98, 153004 (2007)
Inhomogeneous systems: small molecules

- 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 self-energy $\Sigma$
- Collision integrals 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**

- Finite-Element Discrete Variable Representation [PRA 81, 022510 (2010)]
- Adiabatic switch-on of interaction [Phys. Scr. T151, 014036 ('12)]
- Parallelization [PRA 82, 033427 (2010)] and GPU computing

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strong excitation and ionization of atoms and molecules: need to resolve nucleus and large distances

Selfenergy in FEDVR largely diagonal

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5Balzer et al., PRA 81, 022510 (2010)
The Generalized Kadanoff-Baym Ansatz

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

- For times $t_1 > t_2 > t_0$:
  \[
  G^<(t_1, t_2) = -G^R(t_1, t_2)\rho(t_2) \\
  + \int_{t_2}^{t_1} dt_3 \int_{t_0}^{t_2} dt_4 \, G^R(t_1, t_3)\Sigma^<(t_3, t_4)G^A(t_4, t_2) \\
  + \int_{t_2}^{t_1} dt_3 \int_{t_0}^{t_2} dt_4 \, G^R(t_1, t_3)\Sigma^R(t_3, t_4)G^<(t_4, t_2).
  \]

- For times $t_0 < t_1 < t_2$:
  \[
  G^<(t_1, t_2) = \rho(t_1)G^A(t_1, t_2) \\
  - \int_{t_0}^{t_1} dt_3 \int_{t_1}^{t_2} dt_4 \, G^R(t_1, t_3)\Sigma^<(t_3, t_4)G^A(t_4, t_2) \\
  - \int_{t_0}^{t_1} dt_3 \int_{t_1}^{t_2} dt_4 \, G^<(t_1, t_3)\Sigma^A(t_3, t_4)G^A(t_4, t_2).
  \]
The generalized Kadanoff-Baym ansatz II

- Idea of the GKBA: lowest order solution

\[ G_{\text{GKBA}}^\geq(t_1, t_2) = -G_{\text{R}}^\geq(t_1, t_2)f^\geq(t_2) + f^\geq(t_1)G_{\text{A}}(t_1, t_2) \]

\[ f^\leq(t) = f(t) = \pm iG^\leq(t, t), \quad f^\geq(t) = 1 \pm f^\leq(t) \]

- correct causal structure, non-Markovian, no near-equilibrium assumption,

- Reduction to single-time quantities by use of HF propagators

\[ G_{\text{HF}}^{R/A}(t_1, t_2) = \mp i\theta[\pm(t_1 - t_2)] \exp\left(-i \int_{t_2}^{t_1} dt_3 \, h_{\text{HF}}(t_3) \right) \]

- Direct derivation from density operator theory possible

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\[ ^6 \text{P. Lipavsky, V. Spicka and B. Velicky Phys. Rev. B 34, 6933 (1986)} \]

\[ ^7 \text{M. Bonitz, Quantum Kinetic Theory} \]
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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HF-GKBA: All propagators replaced by HF-propagators\textsuperscript{12}

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

\textsuperscript{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.


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.
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Lattice models

Hubbard

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

Anderson impurity

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

Heisenberg

...
The Hubbard model

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

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

\[h_{ij} = -\delta_{\langle i, j \rangle} \text{ and } \delta_{\langle i, j \rangle} = 1, \text{ if } (i, j) \text{ is nearest neighbor, } \delta_{\langle i, j \rangle} = 0 \text{ otherwise}\]
Problems of NEGF in second Born: \( N = 2, n = 1/2, U = 1 \),

Excitation matrix: \( f_{ij,\alpha\beta}(t) = w_0 \delta_{i,1} \delta_{j,1} \delta_{\alpha,\beta} \Theta(t) \), \( w_0 = 5.0 J^{-1} \)

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

---

Two-site Hubbard—strong excitation

Problems of NEGF in second Born: \( N = 2, n = 1/2, U = 1 \) [1],

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

- time-dependent density, KBE for various degrees of selfconsistency
- artif. damping, mult. steady states
- GKBA+2B: no damping! selfconsistency problem “cured”

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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

\[
\Sigma_{ik}^{\text{cor}}(t_1, t_2) = iT_{ik}(t_1, t_2)G_{ki}(t_2, t_1),
\]
\[
T_{ik}(t_1, t_2) = \pm iU^2 G_{ik}^H(t_1, t_2) + iU \int_C d\tau G_{il}^H(t_1, \tau)T_{lk}(\tau, t_2),
\]
\[
G_{ik}^H(t_1, t_2) = G_{ik}^{\uparrow}(t_1, t_2) G_{ik}^{\uparrow}(t_1, t_2),
\]

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

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Strong excitation: T-matrix vs. GKBA+T

Hubbard model at medium coupling: $N = 2$, $n = 1/2$, $U = 1$,

Excitation matrix: $f_{ij,\alpha\beta}(t) = w_0 \delta_{i,1} \delta_{j,1} \delta_{\alpha,\beta} \Theta(t)$, \hspace{1em} $w_0 = 5.0 J^{-1}$

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II. Transport in finite Hubbard clusters

Goals:

- study transport (diffusion, heat conductivity etc.) by a nonequilibrium approach\(^\text{19}\)
- 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
Fermionic transport and out-of-equilibrium dynamics in a homogeneous Hubbard model with ultracold atoms

Ulrich Schneider\textsuperscript{1,2,*}, Lucia Hackermüller\textsuperscript{1,3}, Jens Philipp Ronzheimer\textsuperscript{1,2}, Sebastian Will\textsuperscript{1,2}, Simon Braun\textsuperscript{1,2}, Thorsten Best\textsuperscript{1}, Immanuel Bloch\textsuperscript{1,2,4}, Eugene Demler\textsuperscript{5}, Stephan Mandt\textsuperscript{6}, David Rasch\textsuperscript{6} and Achim Rosch\textsuperscript{6}
Time-resolved expansion of Fermi gas

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

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$^{20}$U. Schneider et al., Nature Physics 8, 213-218 (2012)
Theory:

use semiclassical Boltzmann equation in relaxation time approximation

\[ \partial_t f_q + v_q \nabla f_q + F(r) \nabla q f_q = -\frac{1}{\tau(n)} (f_q - f_q^0(n)) \]

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.

\[ \text{\footnotesize \cite{Schneider2012}} \]

\[ U. \ Schneider \ et \ al., \ Nature \ Physics \ 8, \ 213-218 \ (2012) \]
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\(^\text{22}\)
- concept and first results\(^\text{23}\) for $N \leq 8$

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\(^{22}\) S. Hermanns, N. Schlünzen, and M. Bonitz, to be published

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 $\sqrt{N_{\uparrow}}$
Quantifying the expansion. Correlation effects.

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 

\[ v_{\text{exp}}(t) = \frac{d}{dt} d(t) \]

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

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

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Asymptotic expansion velocity vs. $U$

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

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

![Graph showing system size dependence of expansion velocity](image) 

**Legend:**
- $U = 1$
- $U = 2$
- HF
- TMA
- GKBA+SBA
- GKBA+TMA

**Asymptotic expansion velocity $v_\infty$**

**$N_\uparrow^{-\frac{1}{2}}$**
- Extrapolation results for expansion velocity for different approximations
- Comparison to extrapolated “core expansion velocity” (HWHM)
- Core shrinks for $U \lesssim 3$, as in experiment
NEG F vs. experimental results

- Compare macroscopic T-matrix data to core expansion velocities of Schneider et al.\textsuperscript{24}
- Inset: theoretical results for full expansion velocity

\textsuperscript{24}U. Schneider \textit{et al}., \textit{Nature Physics} 8, 213-218 (2012)
NEGFR vs. experimental results and RTA-model

- Compare macroscopic T-matrix data to core expansion velocities of Schneider et al.\textsuperscript{25}
- grey line: relaxation time model (Rosch)

\textsuperscript{25}U. Schneider \textit{et al.}, Nature Physics \textbf{8}, 213-218 (2012)
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III. Spectra from nonequilibrium calculations

- Charge-conserving spectral properties accessible via two-particle XC function
  \[ L(1, 2, 3, 4) = \pm [G_2(1, 2; 3, 4) - G(1; 3) G(2; 4)] , \]
  or reducible polarizability/density response function \( \chi \),
  \[ \chi(1; 2) = \pm iL(1, 2; 1^+, 2^+) . \]

- \( L \) fulfills Bethe–Salpeter equation (BSE)
  \[ L(1, 2; 3, 4) = G(1; 4) G(2; 3) \]
  \[ \pm \int_C d1'd2'd3'd4' G(1; 1') G(3'; 3) K(1', 2'; 3', 4') L(4', 2; 2', 4) , \]

- 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 $h \rightarrow h + \delta h$,
- linear response from correlated equilibrium state: $G \rightarrow G + \delta G$,

$$\delta G(1; 3) = \int_C L(1, 2'; 3, 4') \delta h(4'; 2') .$$

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

30 K. Balzer, S. Hermanns and M. Bonitz, EPL 98, 67002 (2012);
Complex Spectra from simple selfenergies


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

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

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

$$G^{[0]} = G_0^{[0]} + G_0^{[0]} \Sigma^{[0]} G^{[0]},$$

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

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 ($\Sigma^{[1]} \equiv \Xi^{[0]} G^{[1]}$):

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

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Example 1: $\Sigma = \Sigma^{\text{HF}}$

$K$ includes T-matrix and ring diagrams, i.e. exciton-like bound states
Example 2: $\Sigma = \Sigma^F + \Sigma^{2B_{\text{direct}}}$

- $K$ includes particle-hole T-matrix diagrams
- when applied to uniform electron gas:
  $\rightarrow$ yields correlated plasmon spectrum with vertex corrections
  (f-sum rule preserving)$^{32}$

Hubbard cluster spectrum for $\Sigma = \Sigma^{\text{GKBA}} + 2\text{B}$

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\textsuperscript{33} improve on earlier results\textsuperscript{34, 35}

\textsuperscript{33} S. Hermanns, N. Schlünzen, and M. Bonitz, PRB 90, 125111 (2014)
Hubbard cluster spectrum for $\Sigma = \Sigma^T$

**Outlook:**
time-propagation with $T$–Matrix selfenergy yields BSE kernel $K_{Teh}^T$:

$$K_{Teh} = T_{eh} + T_{eh} T_{eh} + T_{eh} T_{eh} = \pm i \pm (i)^2 \pm (i)^3 \pm \ldots$$

S. Hermanns, N. Schlünzen, and M. Bonitz, to be published
Numerical possibilities (approximate)

Up to $N_s = 500$, up to $T = 1000J^{-1}$
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
   - advantageous scaling with $N$ (limitation: basis size)
   - GKBA $\Rightarrow$ efficiency gain, no artificial damping

3. Dynamics of finite Hubbard clusters
   - long Hubbard simulations, strong excitation (small $U$)
   - strong correlations accessible via T-matrix and GKBA+T
   - 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

- 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