Ultrafast dynamics of strongly correlated fermions – a Nonequilibrium Green functions approach

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Acknowledgements

M. Bonitz (Kiel University)
Chair Statistical Physics - Research Directions

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
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}
Measured “Core expansion velocity”

- Measured HWHM of density distribution\(^1\)
- Strongly correlated fermions. Core shrinks for \( |U| \lesssim 3 \)

\[ C_{\text{exp}} = \begin{cases} 7E_r & \text{fit} \\ 8E_r & \text{} \\ 10E_r & \text{} \end{cases} \]

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\(^1\) U. Schneider et al., Nature Physics 8, 213-218 (2012)
Model used by Schneider et al.\(^2\)

Semiclassical Boltzmann equation in relaxation time approximation:

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

General problems of Boltzmann-type (Markovian) equations:
- incorrect asymptotic state, conservation laws
- isolated dynamics: expect reversibility

Additional limitations of RTA:
- local TD equilibrium assumption questionable (Heisenberg)
- no quantum dynamics effects
- linear response assumption questionable

⇒ cannot describe ultrafast quantum dynamics of correlated fermions

\(^2\) U. Schneider et al., Nature Physics 8, 213-218 (2012)
A challenge for theory...

Quote from Schneider et al., (p. 216):

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\(^3\).

Not exactly true...\(^4\).

- NEGF can treat Hubbard clusters in any dimension
- we know how to access strong correlations
- some limitations apply

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\(^3\) common theme in experimental papers, justification (?) of experiments

\(^4\) Nonequilibrium Green Functions (NEGF) exist for 50 years..., other approaches: DFT (Verdozzi et al.)
Can we simulate this with NEGF in 2D, 3D?\textsuperscript{5}

**Goal: Modeling of transport of strongly correlated fermions**

- retain full spatial resolution (single-site)
- retain full temporal resolution
- explore particle number dependence, finite-size effects
- explore effects of inhomogeneity, geometry, dimensionality

\textsuperscript{5}Yes we can: arXiv:1508.02957
Measured core expansion velocity

![Graph showing measured core expansion velocity with markers at $7E_r$, $8E_r$, $10E_r$, and $12E_r$. The graph includes a fitted curve.](image)

- $C_{exp}$ vs. $U$

- Markers at $7E_r$, $8E_r$, $10E_r$, and $12E_r$.

- Fitted curve.

- M. Bonitz (Kiel University)

Nonequilibrium Green functions

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NEG F result\textsuperscript{6} vs. experiment\textsuperscript{7}

- 2D T-matrix data symmetric w.r. to $U \to -U$. Zero crossing close to $|U = 3|$
- excellent agreement with experiment within error bars without free parameters

\textsuperscript{6}N. Schlünzen, S. Hermanns, M. Bonitz, and C. Verdozzi, arXiv:1508.02957
\textsuperscript{7}U. Schneider et al., Nature Physics 8, 213-218 (2012)
- agreement with measurements for the final stage of the dynamics
- in addition: NEGF predict early stages, correlation dynamics etc.

\[^8\]U. Schneider et al., Nature Physics 8, 213-218 (2012)
1 Introduction: why generalized quantum kinetic equations?

2 Nonequilibrium Green Functions
   - I. Two-time (Keldysh) Green functions
   - II. Inhomogeneous Systems

3 Excitation dynamics in Hubbard nanoclusters
   - I. NEGF on a lattice
   - II. NEGF Results for the expansion dynamics

4 Conclusions
Outline

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4 Conclusions
(too) Fast carrier relaxation in semiconductors

Consecutive times: (0, 21, 75, 147, 796) fs.

\[ W \text{ arbitrarily large due to nonequilibrium plasmons} \]
Failure of Boltzmann-type equations\textsuperscript{9}

\[
\left\{ \frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial r_1} + \frac{1}{m} F_1 \frac{\partial}{\partial v_1} \right\} f(r_1, p_1, t) = I(r_1, p_1, t),
\]

\[
I(r_1, p_1, t) = \int d^3 p_2 \int d^3 \bar{p}_1 \int d^3 \bar{p}_2 \ P(p_1, p_2; \bar{p}_1, \bar{p}_2; t)
\]

\[
\times \left\{ f(r_1, \bar{p}_1, t)f(r_1, \bar{p}_2, t) - f(r_1, p_1, t)f(r_1, p_2, t) \right\},
\]

\[
P(p_1, p_2; \bar{p}_1, \bar{p}_2; t) = \left\lfloor \frac{V(q)}{\epsilon(q, \omega; t)} \right\rfloor^2 \delta(p_{12} - \bar{p}_{12})\delta(E_{12} - \bar{E}_{12})
\]

\[
q = |p_1 - \bar{p}_1|, \quad p_{12} = p_1 + p_2, \quad \hbar \omega = E_1 - \bar{E}_1, \quad \text{Pauli blocking factors}(1 \pm \tilde{f})\text{omitted}
\]

- Eq. (1) conserves quasi-particle energy,
- Eq. (1) relaxes towards Fermi (Bose) function, \(f_{F,B}(p)\)
- Eq. (1) fails at short times, misses buildup of correlations, screening
  \(\Rightarrow\) unphysical fast relaxation dynamics \(\Rightarrow\) generalized quantum kinetic theory needed

\textsuperscript{9}M. Bonitz, Quantum Kinetic theory, Teubner 1998, 2nd ed.: Springer 2015
Build up of dynamical screening\textsuperscript{10}

- finite time for build up of binary correlations: MB and D. Kremp, Phys. Lett. A 1996
- first results for build up of screening, plasmon spectrum: MB, 1996

Build up of dynamical screening in semiconductors:

Experiment

- Drude: \( \tau = 84 \, \text{fs} \)
  \( \omega_{\text{pl}} = 14.4 \, \text{THz} \)

Huber et al., Nature 414, 216 (2001)

Numerical solution of non-Markovian Balescu equation:
Generalized quantum kinetic equations

1. Non-Markovian kinetic equations, starting from BBGKY-hierarchy
   - “top-down”, starting from $N$-particle density operator $\hat{\rho}_{1\ldots N}$:
   - construct hierarchy for reduced operators $\hat{F}_1, \hat{F}_{12}, \ldots$
   Bogolyubov, Klimontovich, Silin, Cassing, ...

2. Second quantization, Nonequilibrium Green functions
   - “bottom-up”, from field operators $\hat{c}, \hat{c}^\dagger$
   - construct expectation values of field operator products
   Bonch-Bruevich, Abrikosov, Keldysh, ...
   Schwinger, Martin, Kadanoff, Baym, Danielewicz, ...

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11 M. Bonitz, *Quantum Kinetic Theory, Teubner 1998*
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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
  $[\hat{c}_i^{(\dagger)}, \hat{c}_j^{(\dagger)}] = 0$, $[\hat{c}_i, \hat{c}_j^\dagger] = \delta_{i,j}$
- Hamiltonian: $\hat{H}(t) = \sum_{k,m} h_{km}^0 \hat{c}_k^\dagger \hat{c}_m + \frac{1}{2} \sum_{k,l,m,n} w_{klmn} \hat{c}_k^\dagger \hat{c}_m^\dagger \hat{c}_n \hat{c}_l + \hat{F}(t)$

Particle interaction $w_{klmn}$

- Only electron dynamics
- Coulomb interaction

Time-dependent excitation $\hat{F}(t)$

- 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 $|\phi_i\rangle$

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

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

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

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

\[
G_{ij} = \begin{pmatrix} G_{ij}^R & G_{ij}^< \\ 0 & G_{ij}^A \end{pmatrix}
\]

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

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

- Propagators, nonequilibrium spectral function

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

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

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

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

Time-dependent single-particle operator expectation value

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

- Particle density \((1 = r_1, s_1, t_1)\)

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

- Density matrix

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

- 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, 1962])

\[ \langle \hat{V}_{12} \rangle(t) = \pm i \, \frac{V}{4} \int \frac{d\vec{p}}{(2\pi\hbar)^3} \left\{ (i \partial_t - i \partial_{t'}) - \frac{p^2}{m} \right\} \, G^< (\vec{p}, t, t') \bigg|_{t=t'} \]
**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 $t, t' \leq t_0$ [1-3]

\[ f_{AS}^{\tau,t_H}(t) = \exp \left( - \frac{A_{t_H}^{\tau}}{t / (2t_H)} \right) \exp \left( \frac{B_{t_H}^{\tau}}{t / (2t_H) - 1} \right) \]

\[
B_{t_H}^{\tau} := \frac{t_H}{\tau \ln(2)} - \frac{1}{2}, \quad A_{t_H}^{\tau} := \frac{\ln(2)}{2} e^{2B_{t_H}^{\tau}}
\]

3. Solve KBE in $t - t'$ plane for $g(t, t')$

Two-time simulations (homogeneous): Summary

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

Inhomogeneous systems: atoms and molecules

1D He ground state energy (left)  
e-density in small molecules (right)

<table>
<thead>
<tr>
<th></th>
<th>Hartree-Fock</th>
<th>Second Born</th>
<th>TDSE (exact)</th>
</tr>
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<tbody>
<tr>
<td>$n_g$ ($n_h$)</td>
<td>$E^{HF}_{gs}$ [a.u.]</td>
<td>$E^{2nd,Born}_{gs}$ [a.u.]</td>
<td>$E^{TDSE}_{gs}$ [a.u.]</td>
</tr>
<tr>
<td>4 (43)</td>
<td>-2.22</td>
<td>-2.33</td>
<td>-2.2382578</td>
</tr>
<tr>
<td>9 (98)</td>
<td>-2.224209</td>
<td>-2.2334</td>
<td></td>
</tr>
<tr>
<td>14 (153)</td>
<td>-2.2242096</td>
<td>-2.23341</td>
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</tbody>
</table>

Laser excitation dynamics of small molecules

- strong excitation of molecules: Balzer et al., PRA 82, 033427 (2010)

- XUV-pulse excitation of LiH (1d-model)

- goal: correlated (sub-)fs-electron dynamics beyond Hartree-Fock

- difficulty: spatial resolution of density matrix expensive
strong excitation and ionization of atoms and molecules: need to resolve nucleus and large distances

FEDVR combines grid and basis expansion approaches

Selfenergy in FEDVR largely diagonal

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13 Balzer et al., PRA 81, 022510 (2010)
**NEGF**: Full memory plus time stepping in 2-time plain. Expensive!

**Independent Alternative**: 1-time non-Markovian equations

1. Density operator theory (BBGKY-hierarchy)\(^{14}\)
2. NEGF: special case of KBE via generalized Kadanoff-Baym ansatz (GKBA)

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\(^{14}\)M. Bonitz, *Quantum Kinetic Theory*
The Generalized Kadanoff-Baym Ansatz

Equivalent form of the KBE\textsuperscript{15}: 

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 $t_0 < t_1 < t_2$:

$$G^<(t_1, t_2) = \rho(t_1)\, G^A(t_1, t_2)$$

$$- \int_{t_0}^{t_1} dt_3 \int_{t_1}^{t_2} dt_4 \, G^R(t_1, t_3)\Sigma^<(t_3, t_4)\, G^A(t_4, t_2)$$

$$- \int_{t_0}^{t_1} dt_3 \int_{t_1}^{t_2} dt_4 \, G^<(t_1, t_3)\Sigma^A(t_3, t_4)\, G^A(t_4, t_2).$$

\textsuperscript{15}P. Lipavsky, V. Spicka and B. Velicky Phys. Rev. B 34, 6933 (1986)
The generalized Kadanoff-Baym ansatz (GKBA)

- Idea of the GKBA: lowest order solution\textsuperscript{16}

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

\[
f^\leq(t) = f(t) = \pm i G^<(t, t), \quad f^>(t) = 1 \pm f^<(t)
\]

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

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

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

- applicable to any selfenergy (2nd Born, T-matrix etc.)

- same conserving properties as 2-time KBE\textsuperscript{17}

- Direct derivation from density operator theory possible\textsuperscript{18}

- via GKBA controlled derivation of Boltzmann-type equations possible

\textsuperscript{16} P. Lipavsky, V. Spicka and B. Velicky, Phys. Rev. B 34, 6933 (1986)

\textsuperscript{17} S. Hermanns, N. Schlünzen, and M. Bonitz, Phys. Rev. B 90, 125111 (2014)

\textsuperscript{18} M. Bonitz, Quantum Kinetic Theory
Strong excitation: T-matrix vs. GKBA+T

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

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

$\Rightarrow$ worst case: minimum $N$, half filling, strong excitation

rapid improvement of NEGF with $N$, lower density

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Reducing selfconsistency with the HF-GKBA

Selfenergy diagrams in Hartree-Fock plus second Born approximation

- full 2-time version (full G-lines)

- 1-time version with HF-GKBA (non-interacting G-lines)

- case of Hubbard model (exchange missing)

For small particle numbers: improved performance of HF-GKBA \(^{20}\)

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.
- Less significant gain for T-matrix selfenergies (GKBA+T remains order $T^3$)

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4. Conclusions
The Hubbard model

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

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

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

use \( J = 1 \), on-site repulsion \((U > 0)\) or attraction \((U < 0)\)
Test 1: “Diffusion” in 1D cluster with $N = 8$

$t = 0$: Sites $0 - 3$ doubly occupied, $4 - 7$ empty, $U = 0.1$

Occupation dynamics on site “0”, 2nd Born vs. TDHF and CI

- failure of HF, good performance of 2nd Born (GKBA) up to long times ($t \sim 50$)
Test 2: Excitation spectrum

Real-time propagation following weak excitation and Fourier transform

Example: \( N = 8, n = 1/2, U = 0.1 \), 2nd Born approximation vs. CI and TDHF

- GKBA: increased resolution of spectra. Capture double excitations\(^{21}\) improve on earlier results\(^{22}\) \(^{23}\)

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\(^{21}\) S. Hermanns, N. Schlünzen, and M. Bonitz, PRB 90, 125111 (2014)


Strong coupling: T-matrix selfenergy

- to access strong coupling: use T-matrix selfenergy (sum entire Born series)
- for Hubbard model simplification\textsuperscript{24}

\[
\Sigma_{ss',\uparrow(\downarrow)}^{\text{cor}}(z, z') = i\hbar T_{ss'}(z, z') \, G_{s's}^{\downarrow(\uparrow)}(z', z), \\
T_{ss'}(z, z') = -i\hbar U^2 \, G_{ss'}^{\uparrow}(z, z') \, G_{ss'}^{\downarrow}(z, z') \\
+ i\hbar U \int_C \text{d}\bar{z} \, G_{ss}^{\uparrow}(z, \bar{z}) \, G_{ss}^{\downarrow}(z, \bar{z}) \, T_{ss'}(\bar{z}, z').
\]

- T-matrix: well defined and conserving strong coupling approximation
- limitation: low density (binary collision approximations)
- numerical optimization: large systems, long propagation feasible\textsuperscript{25}
- no free parameters

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4. Conclusions
- $t = 0$: circular array of doubly occupied sites.
- Confinement quench initiates diffusion.
- Arising expansion depends on
  - dimension $D$
  - interaction strength $U$
  - particle number $N$

Experimental results ($U = 0$)

Evolution of the expansion velocity

Diffusion quantities

- mean squared displacement
  \[ R^2(t) = \frac{1}{N} \sum_s n_s(t)(s - s_0)^2 \]
  \( s_0 \): center of the system

- rescaled cloud diameter
  \[ d(t) = \sqrt{R^2(t) - R^2(0)} \]

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

- asymptotic expansion velocity
  \[ v_{\text{exp}}^\infty = \lim_{t \to \infty} v_{\text{exp}}(t) \]

- \( N = 58 \) fermions in 2D
Evolution of the expansion velocity

- single-particle part $E_{sp}$ and correlation part $E_{corr}$ of the energy
Evolution of the expansion velocity

\[ v_{\text{exp}}(t) \]

\[ U = 0.1 \]
\[ U = 1 \]
\[ U = 1.5 \]
\[ U = 2.5 \]
\[ U = 3 \]
\[ U = 4 \]
\[ U = 5 \]

-entanglement entropy

\[ S = S_{\text{sp}} + S_{\text{corr}} \]

\[ S = \sum_{s} -2 \left( \frac{n_{s}^{\downarrow\downarrow}}{2} - n_{s}^{\uparrow\downarrow} \right) \log_{2} \left( \frac{n_{s}^{\downarrow\downarrow}}{2} - n_{s}^{\uparrow\downarrow} \right) - n_{s}^{\uparrow\downarrow} \log_{2} n_{s}^{\uparrow\downarrow} - \left( 1 - n_{s} + n_{s}^{\uparrow\downarrow} \right) \log_{2} \left( 1 - n_{s} + n_{s}^{\uparrow\downarrow} \right) \]

Identification of three expansion phases:

(i) build-up of **single-particle** entanglement

(ii) build-up of **correlations** and entanglement entropy

(iii) **saturated** expansion
times decrease with interaction strength $U$

• times increase with particle number $N$

• shell effects due to finite system size
Density in quasi-momentum space

\[ p(k) = N_s^{-1} + a \cos(k), \quad \text{amplitude } a(U, N) \text{ in inset} \]

- momentum distribution \( p(k) = N_s^{-1} + a \cos(k) \), amplitude \( a(U, N) \) in inset
- amplitude shows common scaling in momentum space
- parameters: \( t = 9.5 \), 1D system, \( N_s = 65 \) sites, \( U = 3 \) and \( N = 2 \ldots 42 \)
Expansion for different particle numbers

- time evolution for different cloud sizes in 2D
- $U = 4$

\[ N = 74 \]
\[ \sqrt{n_s} \]

\[ N = 26 \]
\[ \sqrt{n_s} \]

\[ N = 2 \]
\[ \sqrt{n_s} \]

\[ t=0 \] \hspace{1cm} \[ t=1 \] \hspace{1cm} \[ t=2 \] \hspace{1cm} \[ t=3 \]
Asymptotic expansion velocity approaches macroscopic limit as

\[ v^\infty_{\exp}(U; N) - V_{\exp}(U) = \chi(U)N^{-1/2} \]
Asymptotic expansion velocity approaches macroscopic limit as

\[ \nu^\infty_{\exp}(U; N; D) - V_{\exp}(U; D) = \chi(U; D)N^{-1/2} \]

extrapolation to macroscopic system is possible
Asymptotic expansion velocity approaches macroscopic limit as

$$v_{\text{exp}}(U; N; D) - V_{\text{exp}}(U; D) = \chi(U; D)N^{-1/2}$$

similar shape of $\chi(U; D)$ for all dimensions $D$

bandwidth $b = 4JD$
Extrapolated expansion velocity: 1D–3D

- similar shape of the macroscopic \( V_{\text{exp}} \) in all dimensions
- noninteracting limit, \( V_{\text{exp}} = \sqrt{2D} = \sqrt{2}, 2, \sqrt{6} \) in 1D-3D reproduced
- the proper treatment of correlations is crucial
Site-resolved evolution of correlations

Simulations give access to correlated quantities ($U = 4$):

- double occupation $n_s^{\uparrow\downarrow}$
- local entanglement entropy $S_s$
- pair correlation function $\delta n_s^{\uparrow\downarrow} = n_s^{\uparrow\downarrow} - n_s^{\uparrow} n_s^{\downarrow}$

Insights into the early expansion phases measurable in recently developed atomic quantum microscopes
Capabilities of NEGF for fermion transport

- quantum dynamics for finite systems, size dependence
- single-site resolution, any geometry/dimension
- access arbitrary time scales, arbitrary initial state
- captures correlation (and screening) buildup, doublon formation etc.
- predictive capability for novel nonequilibrium scenarios, quenches
Numerical capabilities (approximate)

- dramatic progress compared to earlier NEGF results with full two-time T-matrix
- up to $N_s = 1000$, up to $T = 1000J^{-1}$, due to optimization, GPU hardware etc.
- ideas/wishes welcome
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, time-reversible
   - Advantageous scaling with $N$ (limitation: basis size)
   - **GKBA**: independent alternative
     - Efficiency gain (for weak coupling), no artificial damping (small $N$)

3. **Ab initio Dynamics of finite Hubbard clusters**
   - Long simulations, strong excitation possible
   - Can treat 2D, 3D systems
   - Strong correlations accessible via T-matrix selfenergy (low density)
   - Excellent agreement with measurements for the final expansion phase
   - Predict interesting correlation dynamics at short times

4. **High-quality spectra via time-propagation of KBE**
Thank you for your attention!

References

- [www.itap.uni-kiel.de/theo-physik/bonitz](http://www.itap.uni-kiel.de/theo-physik/bonitz)