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

Michael Bonitz and Niclas Schünzen

in collaboration with: Sebastian Hermanns, and Claudio Verdozzi*

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

*Department of Mathematical Physics, Lund University, Sweden

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Kiel physics

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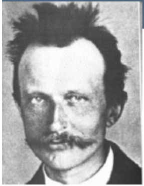
Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät



Acknowledgements

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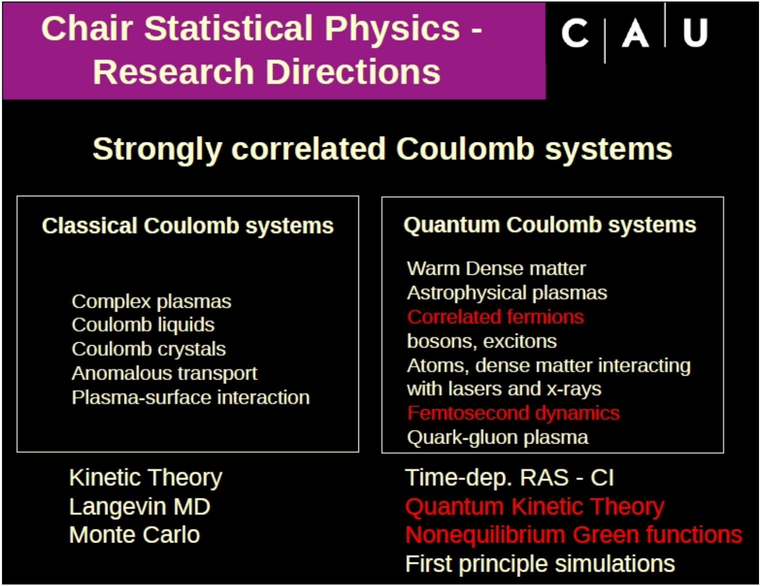
Research


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

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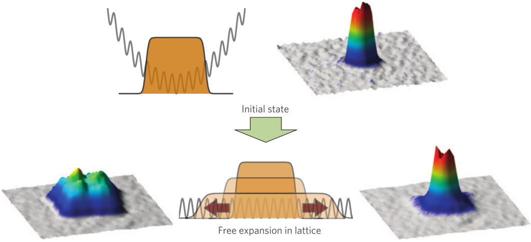
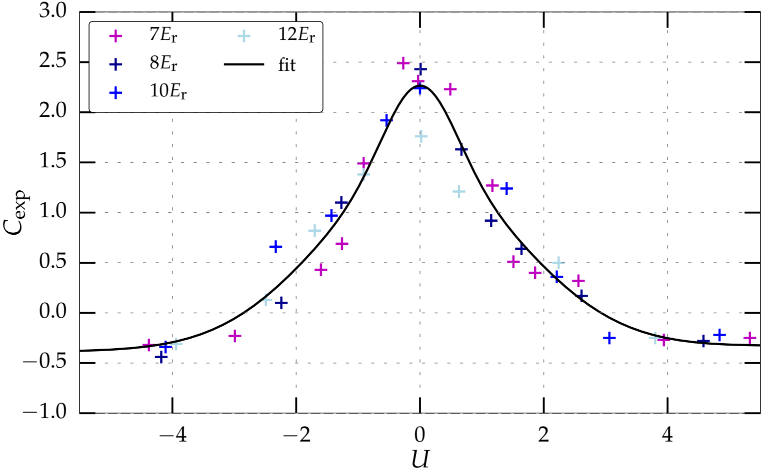
Fermionic transport and out-of-equilibrium dynamics in a homogeneous Hubbard model with ultracold atoms

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]



- Measured HWHM of density distribution[1]
- Strongly correlated fermions. Core shrinks for $|U| \lesssim 3$



[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:

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

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

$\Rightarrow$ **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

---

[3] common theme in experimental papers, justification (??) of experiments

[4] Nonequilibrium Green Functions (NEGF) exist for 50 years..., other approaches: DFT (Verdozzi et al.)

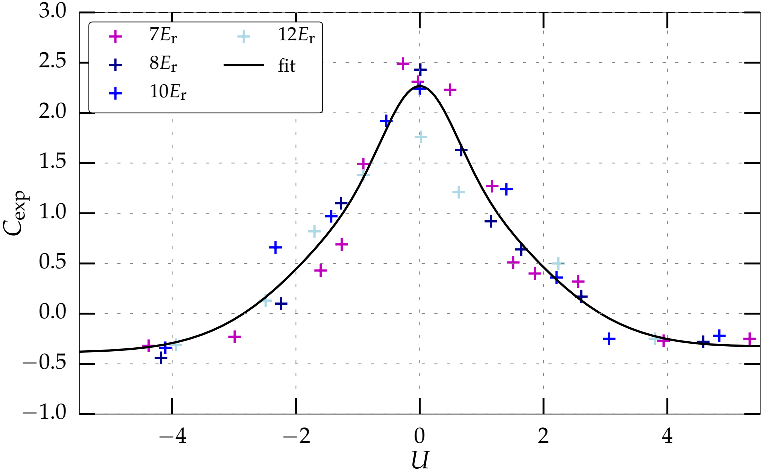
Can we simulate this with NEGF in 2D, 3D?[5]

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

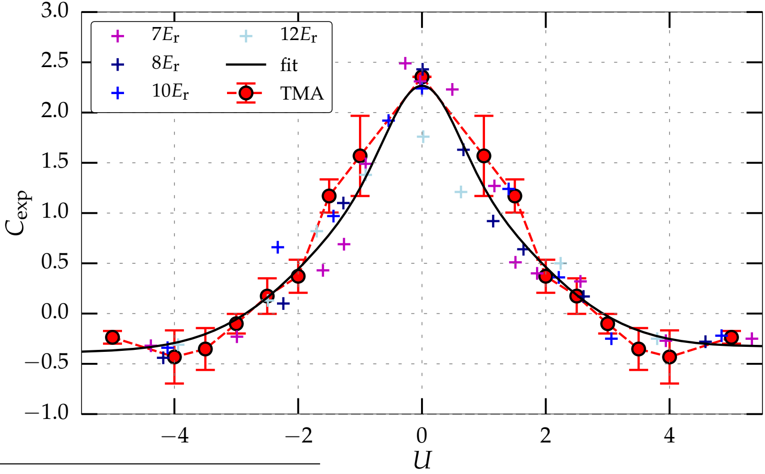
[5] Yes we can: arXiv:1508.02957

Measured core expansion velocity



NEGF result[6] vs. experiment[7]

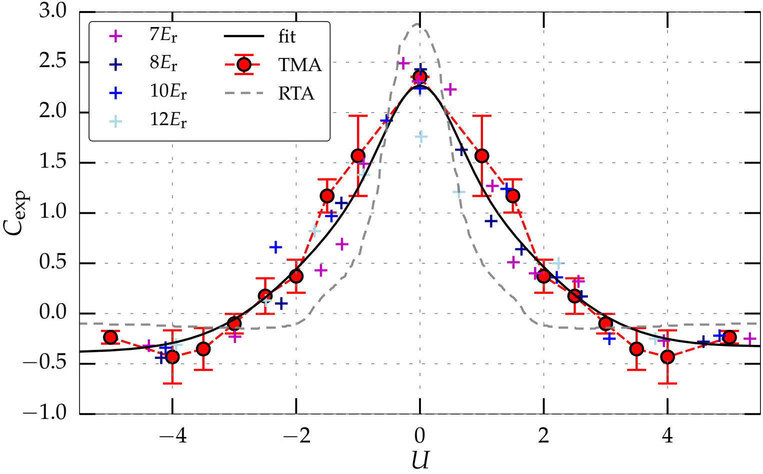
- 2D T-matrix data symmetric w.r.t. to $U \to -U$. Zero crossing close to $|U = 3|$
- excellent agreement with experiment within error bars without free parameters



[6] N. Schlünzen, S. Hermanns, M. Bonitz, and C. Verdozzi, arXiv:1508.02957

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

NEGF result vs. experiment and RTA[8]



- 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)

Outline

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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

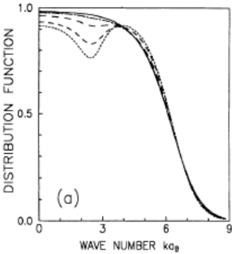
4. Conclusions

(too) Fast carrier relaxation in semiconductors

REVIEW B VOLUME 45, NUMBER 3 15 JANUARY 1992-I

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

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

Consecutive times: (0, 21, 75, 147, 796)fs, $\quad W$ arbitrarily large due to nonequilibrium plasmons

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

$$I(\mathbf{r}_1, \mathbf{p}_1, t) = \int d^3p_2 \int d^3\bar{p}_1 \int d^3\bar{p}_2 \; P(\mathbf{p}_1, \mathbf{p}_2; \bar{\mathbf{p}}_1, \bar{\mathbf{p}}_2; t)$$
$$\times \left\{ f(\mathbf{r}_1, \bar{\mathbf{p}}_1, t) f(\mathbf{r}_1, \bar{\mathbf{p}}_2, t) - f(\mathbf{r}_1, \mathbf{p}_1, t) f(\mathbf{r}_1, \mathbf{p}_2, t) \right\}, \qquad (1)$$

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

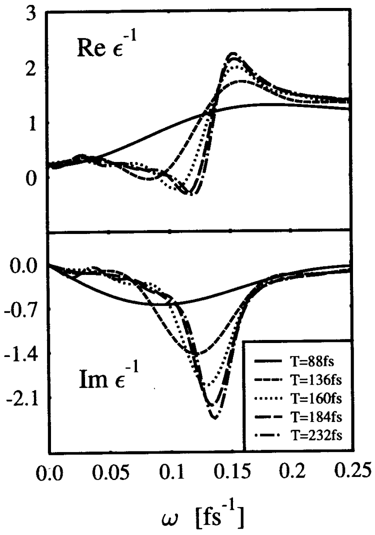
$q = |\mathbf{p}_1 - \bar{\mathbf{p}}_1|$, $\mathbf{p}_{12} = \mathbf{p}_1 + \mathbf{p}_2$, $\hbar\omega = E_1 - \bar{E}_1$, Pauli blocking factors $(1 \pm f)$ omitted

- Eq. (1) conserves quasi-particle energy,
- Eq. (1) relaxes towards Fermi (Bose) function, $f_{F,B}(\mathbf{p})$
- Eq. (1) fails at short times, misses buildup of correlations, screening

⇒ unphysical fast relaxation dynamics ⇒ generalized quantum kinetic theory needed

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

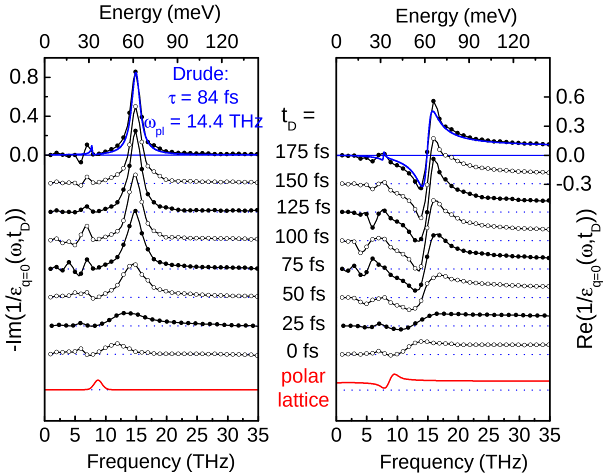
Build up of dynamical screening[10]



- 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

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

Build up of dynamical screening in semiconductors: Experiment



- Huber *et al.*, Nature **414**, 216 (2001)
- numerical solution of non-Markovian Balescu equation: Banyai, *et al.*, PRL **81**, 882 (1998)

Generalized quantum kinetic equations[11]

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, ...

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

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2nd quantization

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

Particle interaction w_{klmn}

- Only electron dynamics
- Coulomb interaction

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

- Single-particle type
- Optical/Laser-induced

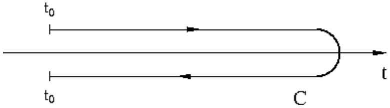
Keldysh Green functions

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

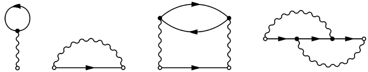
$$\boxed{G^{(1)}_{ij}(z, z') = \frac{\mathrm{i}}{\hbar} \left\langle \hat{T}_{\mathcal{C}}\, \hat{c}_i(z)\, \hat{c}^{\dagger}_j(z') \right\rangle}$$

Keldysh–Kadanoff–Baym equations (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 $G^{(1)}, G^{(2)} \dots G^{(n)}$

- 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, nonequilibrium 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

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

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

Time-dependent single-particle operator expectation value

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

- Particle density $(1 = \mathbf{r}_1, s_1, t_1)$

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

- Density matrix

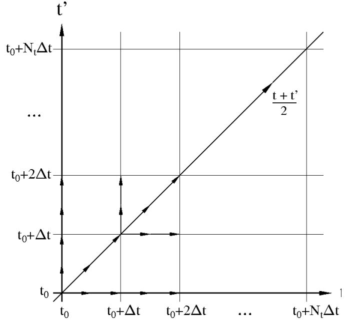
$$\rho(x_1, x_1', t) = \mp\mathrm{i}\, G^<(1,1')\big|_{t_1=t_1'}$$

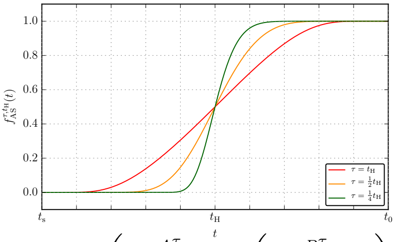
- Current density: $\langle \hat{j}(1) \rangle = \mp\mathrm{i} \left[\left(\frac{\nabla_1}{2i} - \frac{\nabla_{1'}}{2\mathrm{i}} + A(1) \right) G^<(1,1') \right]_{1'=1}$

Interaction energy (two-particle observable, [Baym/Kadanoff, 1962])

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

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





$$f_{\mathrm{AS}}^{\tau,t_\mathrm{H}}(t) = \exp\left(-\frac{A_{t_\mathrm{H}}^\tau}{t/(2t_\mathrm{H})}\exp\left(\frac{B_{t_\mathrm{H}}^\tau}{t/(2t_\mathrm{H})-1}\right)\right)$$

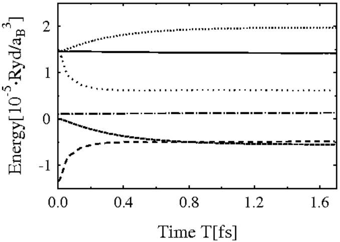
$$B_{t_\mathrm{H}}^\tau := \frac{t_\mathrm{H}}{\tau\ln(2)} - \frac{1}{2}, \quad A_{t_\mathrm{H}}^\tau := \frac{\ln(2)}{2}\mathrm{e}^{2B_{t_\mathrm{H}}^\tau}$$

1. Uncorrelated initial state
2. adiabatically slow switch-on of interaction for $t, t' \le t_0$ [1-3]
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)
[3] M. Watanabe and W. P. Reinhardt, Phys. Rev. Lett. **65**, 3301 (1990)

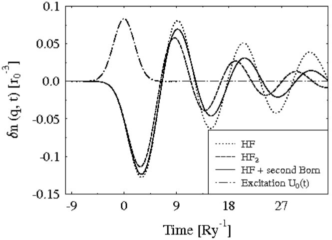
Two-time simulations (homogeneus): Summary

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]



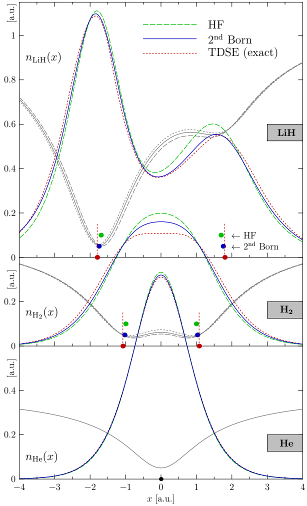
4. extended to optical absorption, double excitations [3] etc.

[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)

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

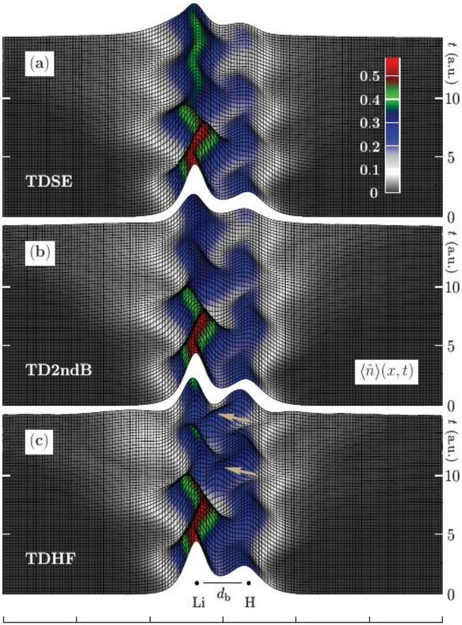
n_g (n_b)	Number of τ-grid points	E_{gs} [a.u.]
Hartree-Fock		
4 (43)		E_{gs}^{HF}: −2.22
9 (98)		E_{gs}^{HF}: −2.224209
14 (153)		E_{gs}^{HF}: −2.2242096
Second Born		
14 (153)	101	E_{gs}^{2ndB}: −2.23
14 (153)	301	E_{gs}^{2ndB}: −2.2334
14 (153)	601	E_{gs}^{2ndB}: −2.23341
14 (153)	1001	E_{gs}^{2ndB}: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



12 N. Dahlen, R. van Leeuwen, PRL **98**, 153004 (2007); K. Balzer, S. Bauch, M. Bonitz, PRA **81**, 022510 (2010)

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



FEDV-Representation[13]

- 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

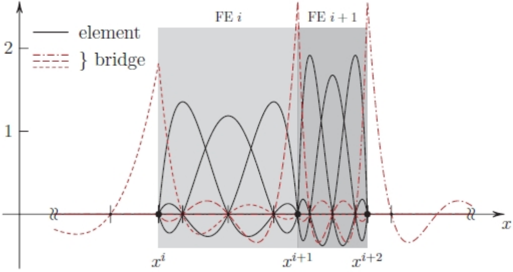
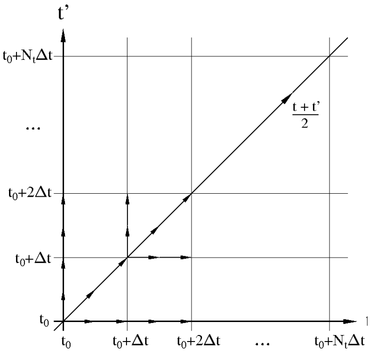


FIG. 2. (Color online) Structure of a FE-DVR basis $\{\chi_m^i(x)\}$ with $n_g = 4$ (i.e., five local DVR basis functions in each element). While the element functions (solid) are defined in a single FE, the bridge functions (dashed and dashed-dotted lines) link two adjacent FEs.

13 Balzer *et al.*, PRA **81**, 022510 (2010)

Two-time vs. one-time non-Markovian equations



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)

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

Equivalent form of the KBE[15]:

- 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 $t_0 < t_1 < t_2$:

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

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

- Idea of the GKBA: lowest order solution[16]

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

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

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

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

- applicable to any selfenergy (2nd Born, T-matrix etc.)
- same conserving properties as 2-time KBE[17]

– Direct derivation from density operator theory possible[18]

– via GKBA controlled derivation of Boltzmann-type equations possible

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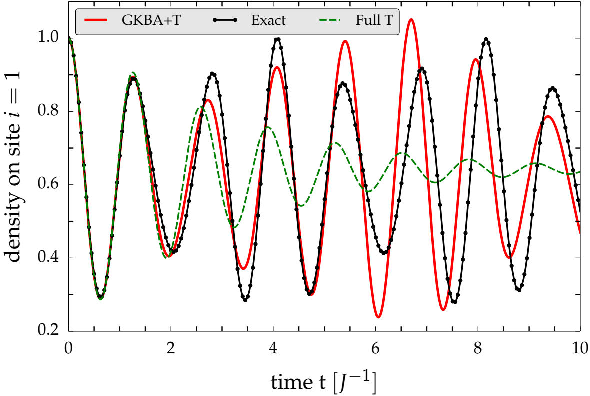
[16] P. Lipavsky, V. Spicka and B. Velicky Phys. Rev. B **34**, 6933 (1986)

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

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

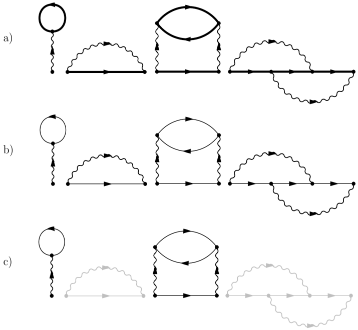
Hubbard model at medium coupling: $N = 2, n = 1/2, U = 1,$
Excitation matrix: $f_{ij,\alpha\beta}(t) = w_0 \delta_{i,1} \delta_{j,1} \delta_{\alpha,\beta} \Theta(t)\,, \quad w_0 = 5.0 J^{-1}$



$\Rightarrow$ worst case: minimum N, half filling, strong excitation
rapid improvement of NEGF with N, lower density

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

Reducing selfconsistency with the HF-GKBA



Selfenergy diagrams in Hartree-Fock plus second Born approximation

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

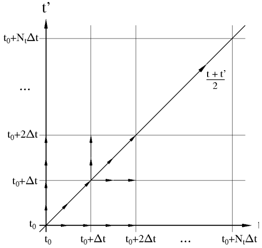
- 1-time version with HF-GKBA (non-interacting G-lines)

- case of Hubbard model (exchange missing)

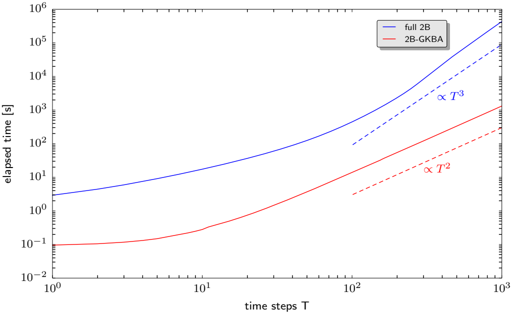
For small particle numbers: improved performance of HF-GKBA[20]

[20] 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.



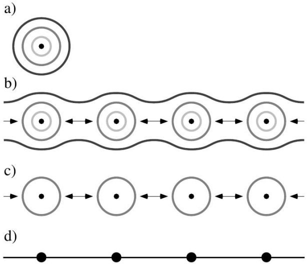
S. Hermanns, K. Balzer, and M. Bonitz, *Phys. Scripta* **T151**, 014036 (2012)

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

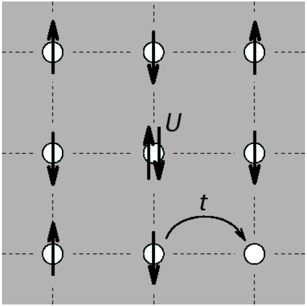
Outline

The Hubbard model

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



$\Rightarrow$



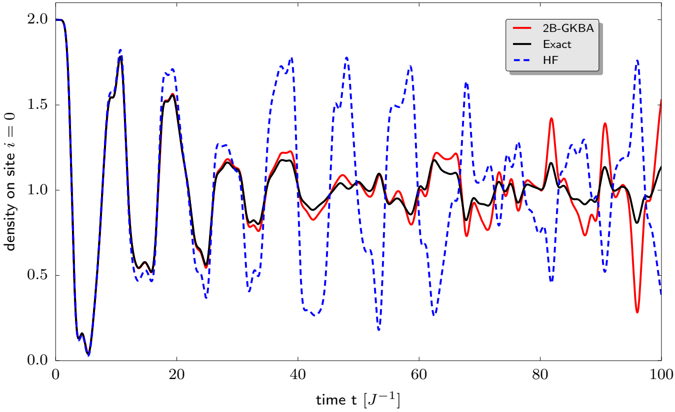
$$\hat{H}(t) = J\sum_{ij,\,\alpha} h_{ij}\,\hat{c}^\dagger_{i\alpha}\hat{c}_{j\alpha} + U\sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow} + \sum_{ij,\alpha\beta} f_{ij,\alpha\beta}(t)\,\hat{c}^\dagger_{i\alpha}\hat{c}_{j\beta}$$

$h_{ij} = -\delta_{\langle i,j\rangle}$ and $\delta_{\langle i,j\rangle} = 1$, if (i,j) is nearest neighbor, $\delta_{\langle i,j\rangle} = 0$ otherwise
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, $\quad U = 0.1$

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

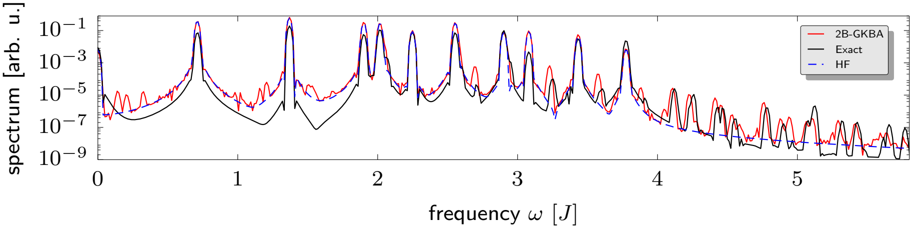


- failure of HF, good performance of 2nd Born (GKBA) up to long times ($t \sim 50$)

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]

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

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

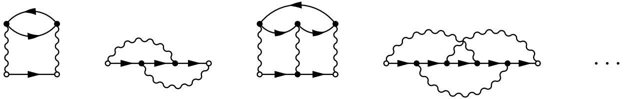
[23] K. Balzer, S. Hermanns, and M. Bonitz, Europhys. Lett. **98**, 67002 (2012).

Strong coupling: T-matrix selfenergy

- to access strong coupling: use T-matrix selfenergy (sum entire Born series)
- for Hubbard model simplification[24]

$$\Sigma^{\text{cor},\uparrow(\downarrow)}_{ss'}(z,z') = \mathrm{i}\hbar\, T_{ss'}(z,z')\, G^{\downarrow(\uparrow)}_{s's}(z',z)\,,$$

$$T_{ss'}(z,z') = -\mathrm{i}\hbar\, U^2\, G^{\uparrow}_{ss'}(z,z')\, G^{\downarrow}_{ss'}(z,z') + \mathrm{i}\hbar\, U \int_{\mathcal{C}} \mathrm{d}\bar{z}\, G^{\uparrow}_{s\bar{s}}(z,\bar{z})\, G^{\downarrow}_{s\bar{s}}(z,\bar{z})\, T_{\bar{s}s'}(\bar{z},z')\,.$$



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

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

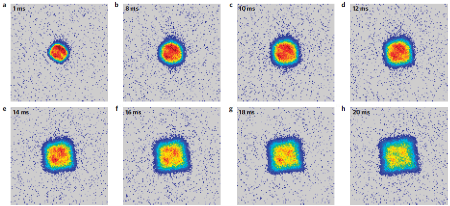
[25] M. Bonitz, N. Schlünzen, and S. Hermanns, Contrib. Plasma Phys. **55**, 152 (2015)

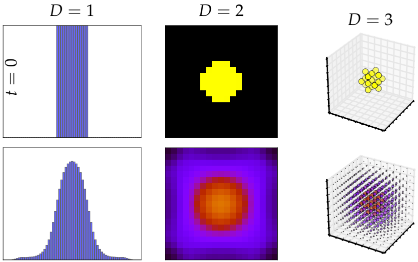
Outline

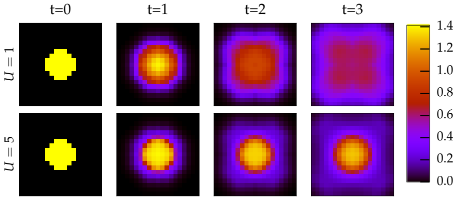
Fermion expansion and doublon decay

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

Experimental results ($U = 0$)

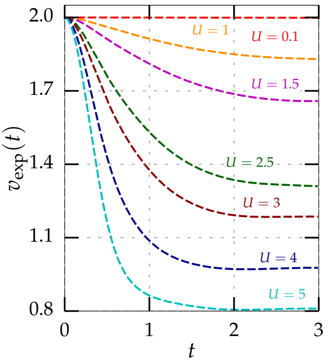






[1] U. Schneider *et al.*, Nature Physics **8**, 213-218 (2012)

Evolution of the expansion velocity



- $N = 58$ fermions in 2D

Diffusion quantities

- **mean squared displacement**

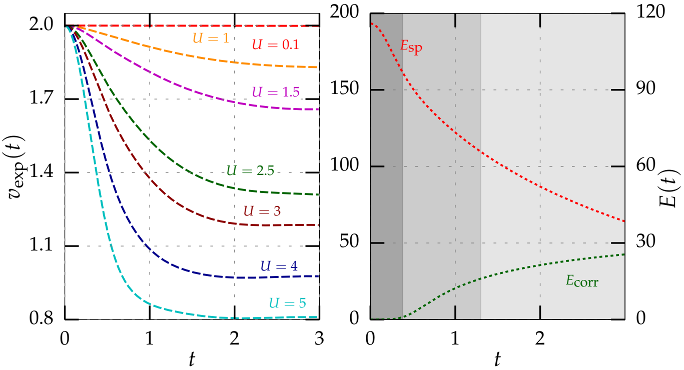
$$R^2(t) = \frac{1}{N} \sum_{\boldsymbol{s}} n_{\boldsymbol{s}}(t)[\boldsymbol{s} - \boldsymbol{s}_0]^2$$

  $\boldsymbol{s}_0$: center of the system

- rescaled cloud **diameter** $d(t) = \sqrt{R^2(t) - R^2(0)}$
- **expansion velocity** $v_{\mathrm{exp}}(t) = \frac{\mathrm{d}}{\mathrm{d}t} d(t)$
- **asymptotic expansion velocity**

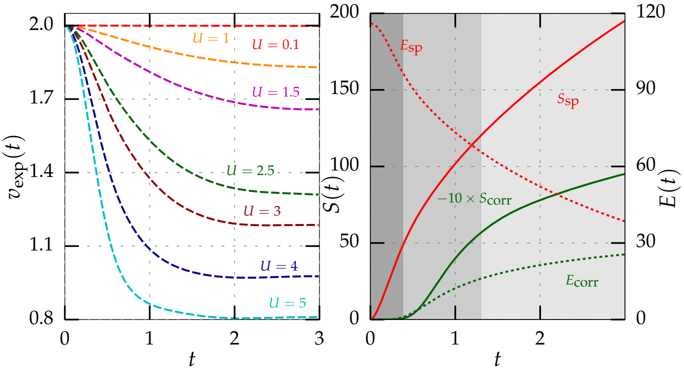
$$v_{\mathrm{exp}}^{\infty} = \lim_{t \to \infty} v_{\mathrm{exp}}(t)$$

Evolution of the expansion velocity



- single-particle part E_{sp} and correlation part E_{corr} of the energy

Evolution of the expansion velocity



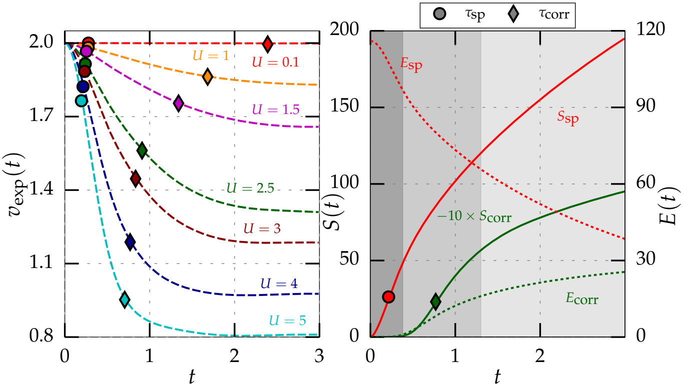
-entanglement entropy [26] [27] $S = S_{\rm sp} + S_{\rm corr}$ [in $S_{\rm sp}$: doublon density $n_s^{\uparrow\downarrow} \rightarrow n_s^{\uparrow} n_s^{\downarrow}$]

$$S = \sum_{\bar{s}} -2\left(\frac{n_{\bar{s}}}{2} - n_{\bar{s}}^{\uparrow\downarrow}\right)\log_2\left(\frac{n_{\bar{s}}}{2} - n_{\bar{s}}^{\uparrow\downarrow}\right) - n_{\bar{s}}^{\uparrow\downarrow}\log_2 n_{\bar{s}}^{\uparrow\downarrow} - \left(1 - n_{\bar{s}} + n_{\bar{s}}^{\uparrow\downarrow}\right)\log_2\left(1 - n_{\bar{s}} + n_{\bar{s}}^{\uparrow\downarrow}\right)$$

[26] D. Larsson, and H. Johannesson, Phys. Rev. Lett. **95**, 196406 (2005).

[27] M. Puig von Friesen, C. Verdozzi and C.-O. Almbladh, Europ. Phys. Lett. **95**, 27005 (2011).

3 phases of the dynamics



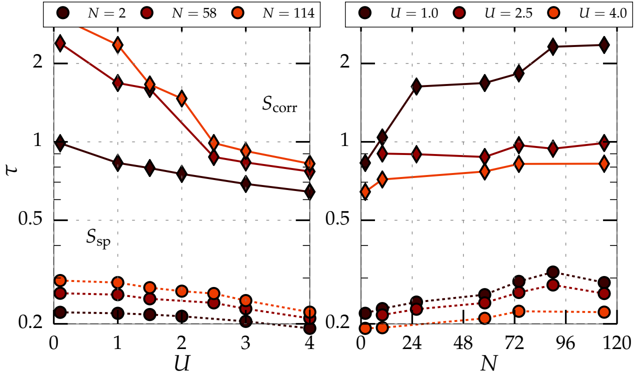
Identification of three expansion phases:

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

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

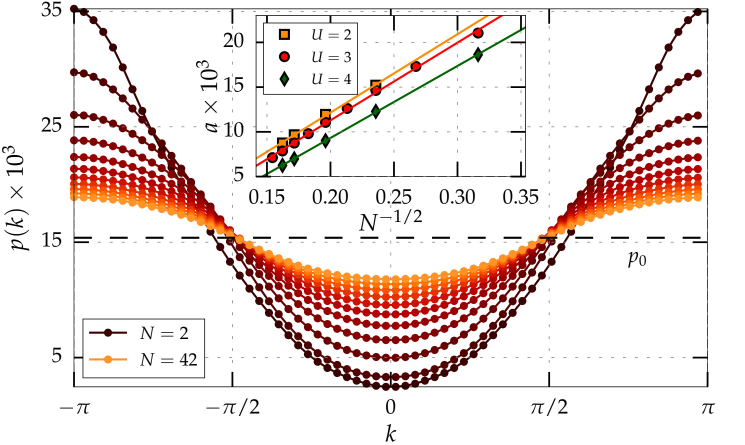
(iii) **saturated** expansion

U/N-Dependencies of the characteristic phases



- times decrease with interaction strength U
- times increase with particle number N
- shell effects due to finite system size

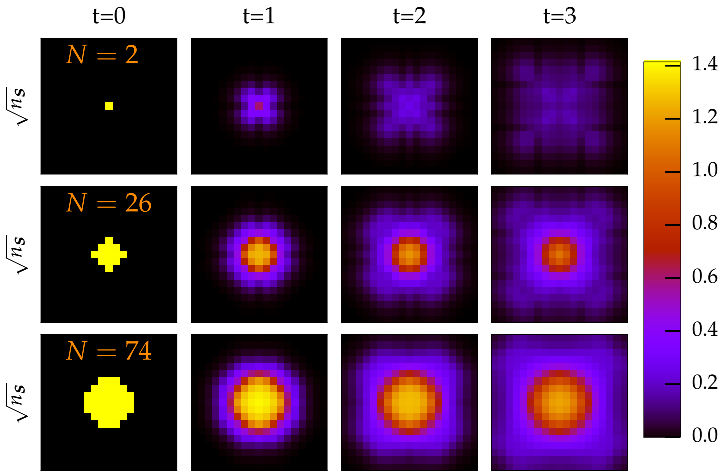
Density in quasi-momentum space

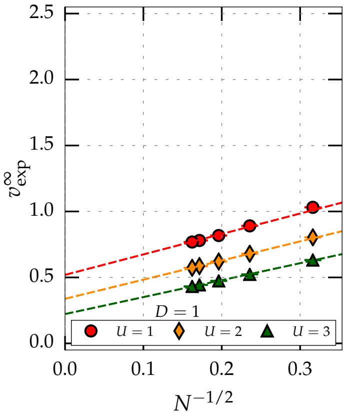


- momentum distribution $p(k) = N_s^{-1} + a\cos(k)$, amplitude $a(U, N)$ in inset
- amplitude shows common scaling in momentum space
- parameters: $t = 9.5$, 1D system, $N_s = 65$ sites, $U = 3$ and $N = 2 \ldots 42$

Expansion for different particle numbers

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

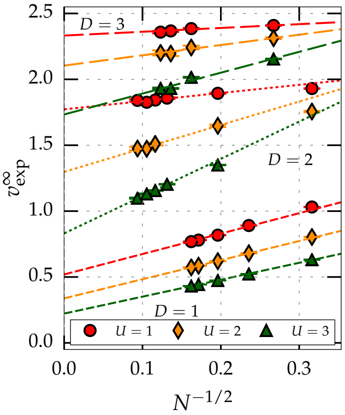




- asymptotic expansion velocity approaches macroscopic limit as

$$v^\infty_{\rm exp}(U;N) - V_{\rm exp}(U) = \chi(U)N^{-1/2}$$

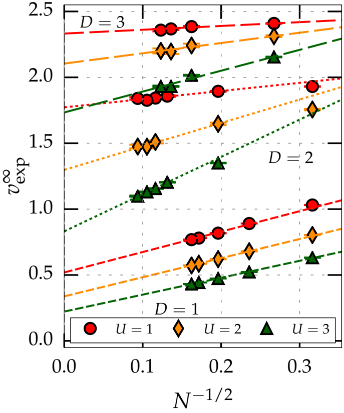
Asymptotic expansion velocity: 1D–3D

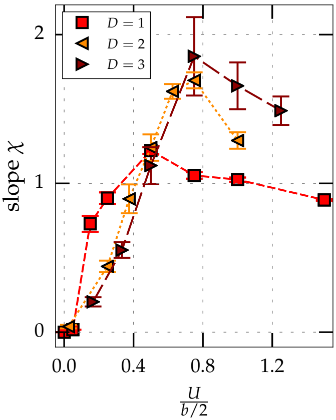


- asymptotic expansion velocity approaches macroscopic limit as

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

- **extrapolation** to macroscopic system is possible



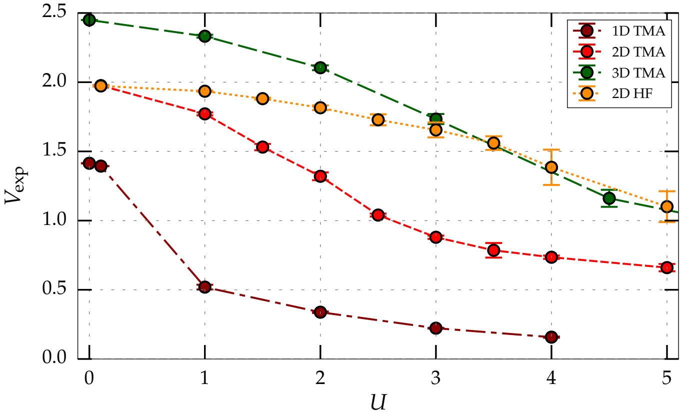


- asymptotic expansion velocity approaches macroscopic limit as

$$v^{\infty}_{\mathrm{exp}}(U;N;D) - V_{\mathrm{exp}}(U;D) = \chi(U;D)N^{-1/2}$$

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

bandwidth $b = 4JD$

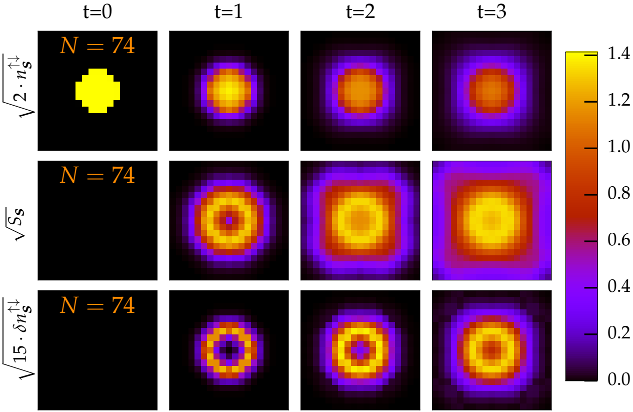


- similar shape of the macroscopic V_{exp} in all dimensions
- noninteracting limit, $V_{\mathrm{exp}} = \sqrt{2D} = \sqrt{2},\ 2,\ \sqrt{6}$ in 1D-3D reproduced
- the proper treatment of correlations is crucial

Site-resolved evolution of correlations

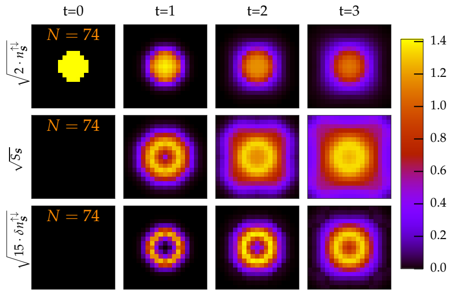
Simulations give access to correlated quantities ($U = 4$):

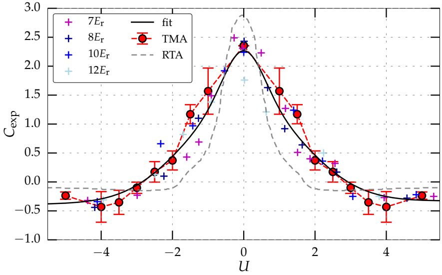
- double occupation $n_s^{\uparrow\downarrow}$
- local entanglement entropy S_s
- pair correlation function $\delta n_s^{\uparrow\downarrow} = n_s^{\uparrow\downarrow} - n_s^{\uparrow} n_s^{\downarrow}$



- insights into the early expansion phases
- measurable in recently developed atomic quantum microscopes

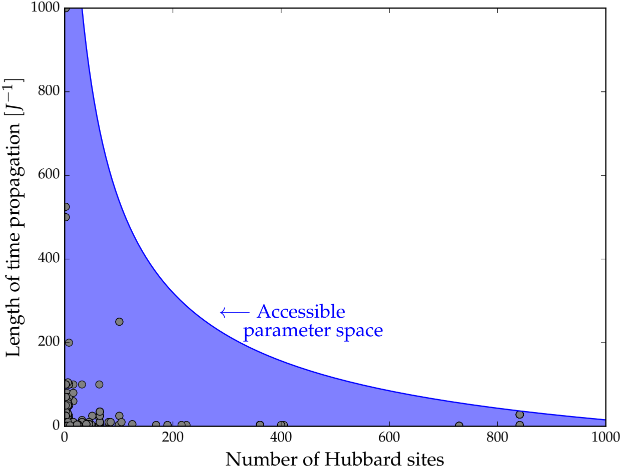
- quantum dynamics for finite systems, size dependence
- single-site resolution, any geometry/dimension
- access arbitrary time scales, arbitrary initial state
- captures correlation (and screening) buildup, doublon formation etc.
- predictive capability for novel nonequilibrium scenarios, quenches





Numerical capabilities (approximate)

- dramatic progress compared to earlier NEGF results with full two-time T-matrix
- up to $N_s = 1000$, up to $T = 1000 J^{-1}$, 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
   1. advantageous scaling with N (limitation: basis size)
   2. GKBA: independent alternative
      $\Rightarrow$ efficiency gain (for weak coupling), no artificial damping (small N)

3. ***Ab initio* Dynamics of finite Hubbard clusters**
   1. long simulations, strong excitation possible
   2. can treat 2D, 3D systems
   3. strong correlations accessible via T-matrix selfenergy (low density)
   4. excellent agreement with measurements for the final expansion phase
   5. predict interesting correlation dynamics at short times

4. **High-quality spectra via time-propagation of KBE**

Thank you for your attention!

CAU
Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

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- www.itap.uni-kiel.de/theo-physik/bonitz