Ultrafast Dynamics of Strongly Correlated Fermions – a Nonequilibrium Green Functions Approach

Michael Bonitz

in collaboration with: Niclas Schlünzen, Sebastian Hermanns, Jan-Philip Joost, and Karsten Balzer[†]

further collaborations: Claudio Verdozzi[*], Fabian Heidrich-Meisner[1]

Institut für Theoretische Physik und Astrophysik; [†]Rechenzentrum, Christian-Albrechts-Universität zu Kiel, Germany

[*]Department of Mathematical Physics, Lund University, Sweden
[1]Ludwig Maximilians Univrsität München

CECAM meeting Lausanne, April 2016

Acknowledgements

C A U
Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

DFG

Bundesministerium für Bildung und Forschung

Contents

1. Nonequlibrium dynamics of correlated fermions:
   experiments with fermionic atoms in optical lattices

2. Nonequilibrium Green functions (NEGF): basics and capabilities

3. NEGF simulation of the fermion expansion dynamics

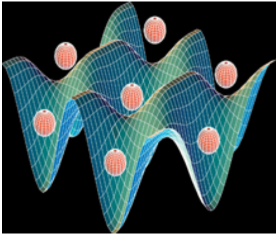
4. Outlook: quantum kinetic approach to plasma-surface interaction

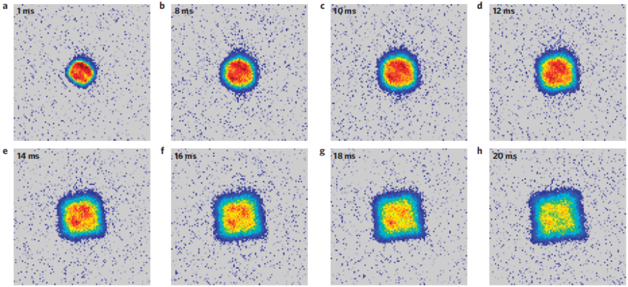
Expansion of fermionic atoms–Experiment

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]

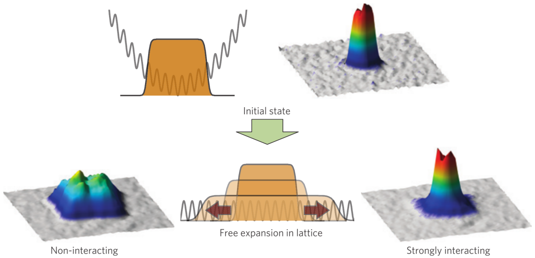




Expansion of fermionic atoms–Experiment

- 2D optical lattice, ca. 200 000 atoms
- atom-atom interaction strength tuned (via Feshbach resonance)
- t<0: confinement in trap center, doubly occupied lattice sites
- t=0: confinement rapidly removed ("quench"):

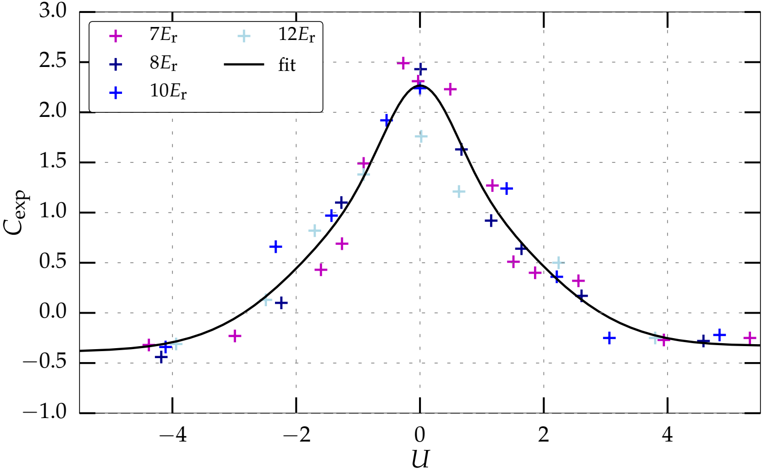
  system far from equilibrium ⇒ start of diffusion, equilibration



- at strong coupling: center ("core") does not expand

Measured “Core expansion velocity”

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



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

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:

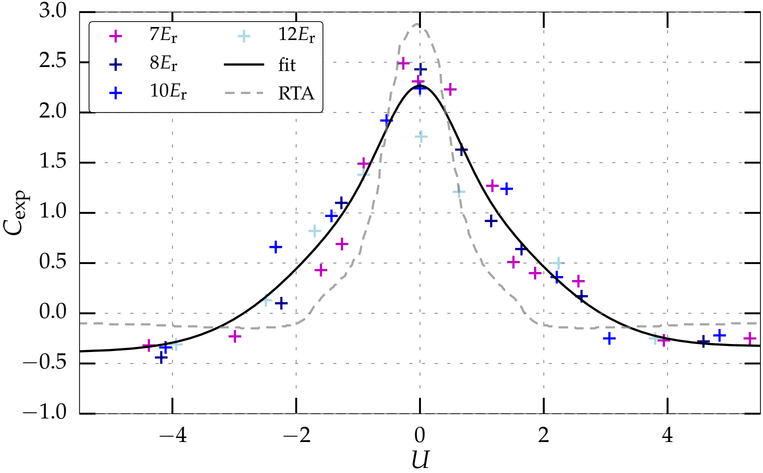
- local TD equilibrium assumption questionable (Heisenberg)
- no quantum dynamics effects
- linear response assumption questionable

⇒ **cannot describe ultrafast quantum dynamics of correlated fermions**

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

"Core expansion velocity": Expt. vs. RTA

- RTA reproduces qualitative trends
- But strong deviations for most U, even for ideal system



A challenge for quantum many-body dynamics...

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

"Although the expansion can be modelled in 1D (...) using DMRG[3] *methods (...), so far no methods are available to calculate the dynamics quantum-mechanically in higher dimensions"*

Similar claims in many experimental papers, for example:

"Quantengase unter dem Mikroskop", M. Greiner, I. Bloch, Phys. Journal Okt. 2015:

"*Ein anderes Gebiet, in dem Experimente schon heute leistungsfähiger als Computersimulationen sind, ist die Untersuchung von Nichtgleichgewichtsprozessen in Quanten-Vielteilchensystemen ... bisherige Algorithmen auf eindimensionale Systeme beschränkt sind und meistens nur die Dynamik für sehr kurze Zeiten berechnen können.*"

Not exactly true...[4].

[3] Density Matrix Renormalization Group

[4] Nonequilibrium Green Functions (NEGF) exist for 50 years...

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

Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

Requirements for theory

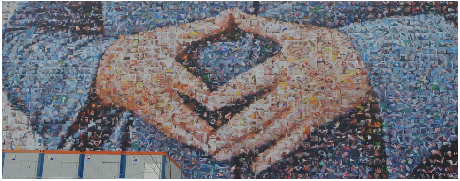
- fully include quantum and spin effects
- retain full space and time resolution
- obey conservation laws
- capture strong correlations

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

Requirements for theory

- fully include quantum and spin effects
- retain full space and time resolution
- obey conservation laws
- capture strong correlations

Yes, we can![5]



[5] Foto: Moritz Kozinsky

Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

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: $\hat{H}(t) = \underbrace{\sum_{k,m} h^0_{km}\, \hat{c}_k^\dagger \hat{c}_m}_{\hat{H}_0} + \underbrace{\frac{1}{2} \sum_{k,l,m,n} w_{klmn}\, \hat{c}_k^\dagger \hat{c}_m^\dagger \hat{c}_n \hat{c}_l}_{\hat{W}} + \hat{F}(t)$

Particle interaction w_{klmn}

- Only electron dynamics
- Coulomb interaction

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

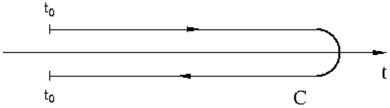
- Single-particle type
- Optical/Laser-induced

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

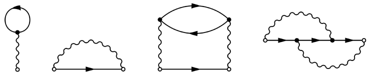
$$G^{(1)}_{ij}(z, z') = \frac{\mathrm{i}}{\hbar} \left\langle \hat{T}_{\mathcal{C}} \hat{c}_i(z) \hat{c}^\dagger_j(z') \right\rangle$$

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 $G^{(1)}, G^{(2)} \dots G^{(n)}$

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, nonequilibrium spectral function

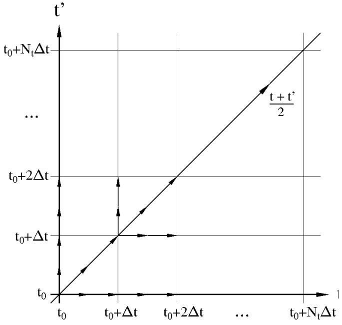
$$G^{\mathsf{R/A}}(t_1, t_2) = \pm\theta\left[\pm(t_1 - t_2)\right]\left\{G^{>}(t_1, t_2) - G^{<}(t_1, t_2)\right\}$$

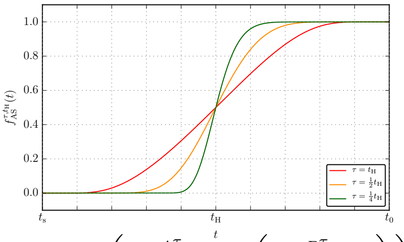
- Correlation functions $G^{\gtrless}$ obey real-time KBE

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

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

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 $t, t' \leq t_0$ [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)

The generalized Kadanoff-Baym ansatz (GKBA)

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

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

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

- 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[7]
  - Direct derivation from density operator theory possible[8]
  - via GKBA controlled derivation of Boltzmann-type equations possible

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

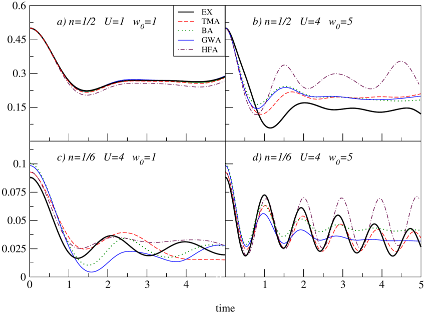
[7] S. Hermanns, N. Schlünzen, and M. Bonitz, Phys. Rev. B **90**, 125111 (2014)

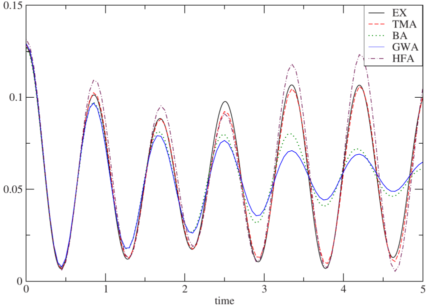
[8] M. Bonitz, *Quantum Kinetic Theory*

PHYSICAL REVIEW B **82**, 155108 (2010)

Kadanoff-Baym dynamics of Hubbard clusters: Performance of many-body schemes, correlation-induced damping and multiple steady and quasi-steady states

Marc Puig von Friesen, C. Verdozzi, and C.-O. Almbladh
Mathematical Physics and European Theoretical Spectroscopy Facility (ETSF), Lund University, 22100 Lund, Sweden



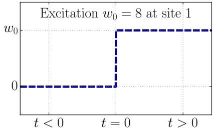


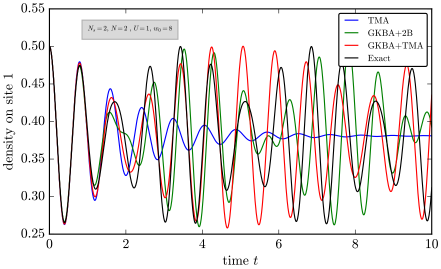
small Hubbard clusters. Strong external excitation (Right Fig.: $N_s = 6, n = 1/6, U = 2, w_0 = 5$)

$\Rightarrow$ artificial damping of *many-body* approximations. Best behavior: T-matrix

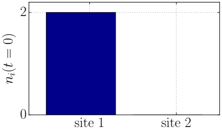
[9] see also: M. P. von Friesen, C. Verdozzi, and C.-O. Almbladh, Phys. Rev. Lett. **103**, 176404 (2009)

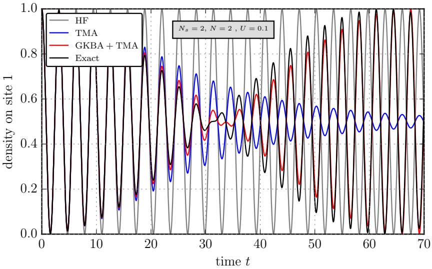
Time-dependent excitation



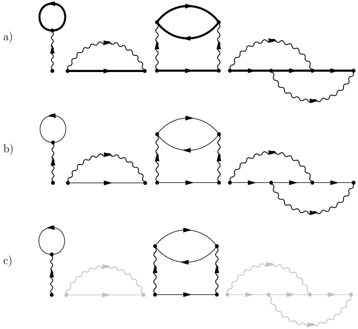


Nonequilibrium initial state





- KBE with all many-body approximations show unphysical damping effects
- HF-GKBA: reduction or even removal of damping (*small clusters*)



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[10]

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

Summary: properties of the KBE

Advantages:

- perfect conservation of total energy[11] and particle number
- time reversible (unitary) dynamics
- accurate description of dynamics far from equilibrium
- convenient and easy way to implement various many-body approximations

Problems and solutions for *strongly excited small systems*:

- full two-time KBE show unphysical damping dynamics[12]:
  ($\Rightarrow$ self-consistency leads to diagrams of infinite order that would cancel in exact case)
- get rid of damping by reducing the degree of self-consistency via HF-GKBA:
  - "reconstruction" of two-time Green functions eliminates infinite order iterations
  - Retains conserving behavior, additional class of conserving approximations[13]
- large systems: two-time and one-time approximations of comparable accuracy
  further benchmarks below

[11] "Conserving approximations" by Baym and Kadanoff

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

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

PHYSICAL REVIEW B **93**, 041103(R) (2016)

On the unphysical solutions of the Kadanoff-Baym equations in linear response: Correlation-induced homogeneous density-distribution and attractors

Adrian Stan*

Sorbonne Universités, UPMC Université Paris VI, UMR8112, LERMA, F-75005 Paris, France;
LERMA, Observatoire de Paris, PSL Research University, CNRS, UMR8112, F-75014 Paris, France;
Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France;
and European Theoretical Spectroscopy Facility (ETSF)

(Received 13 September 2015; revised manuscript received 12 December 2015; published 8 January 2016)

PHYSICAL REVIEW B **93**, 041103(R) (2016)

On the unphysical solutions of the Kadanoff-Baym equations in linear response: Correlation-induced homogeneous density-distribution and attractors

Adrian Stan*
Sorbonne Universités, UPMC Université Paris VI, UMR8112, LERMA, F-75005 Paris, France; LERMA, Observatoire de Paris, PSL Research University, CNRS, UMR8112, F-75014 Paris, France; Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France; and European Theoretical Spectroscopy Facility (ETSF)
(Received 13 September 2015; revised manuscript received 12 December 2015; published 8 January 2016)

1. The density dynamics obtained from the KBE in the case of strong excitation is damped, in agreement with previous studies of Friesen *et al.*
2. For sufficiently long propagation time a state with homogeneous density (HDD) is reached indicating the existence of an attractor.
3. In addition to previous observations, the unphysical damping occurs also for weak excitation (linear response regime).
4. Damping occurs also for an uncorrelated system (Hartree or Hartree-Fock selfenergies), although no HDD is approached.

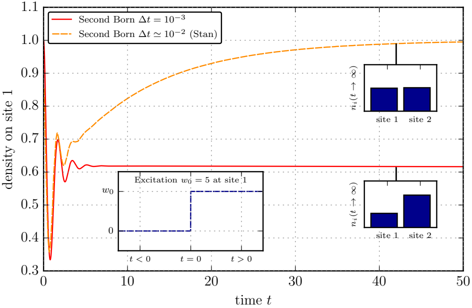
$\Rightarrow$ Previous studies were bad (overlooked the physics)

$\Rightarrow$ KBE are practically useless (negligible range of validity)

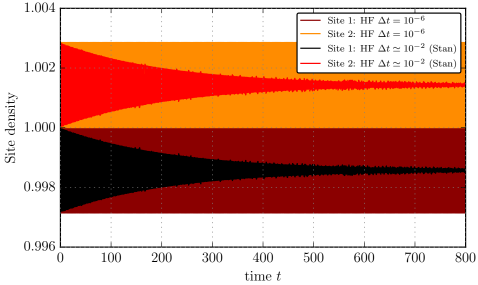
Testing Adrian's Claims

- "KBE possess a global attractor towards a homogeneous density distribution".
- "The unphysical behavior is universal, i.e., across all regimes..."

Hubbard dimer in second Born approx.



Hartree(-Fock) dynamics

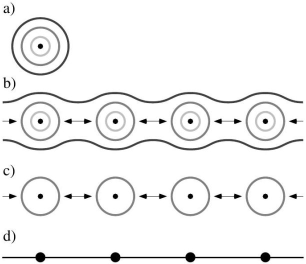


$\Rightarrow$ Unwarrented claims and generalizations (from Hubbard dimer).
$\Rightarrow$ Scientifically questionable. No reliable tests.
$\Rightarrow$ All statements are wrong and numerical artefacts[14] (too large time step).

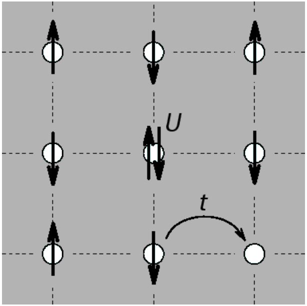
[14] N. Schlünzen and M. Bonitz, to be published

Dynamics of strongly correlated systems. The Hubbard model

- Useful model for strongly correlated solid state systems, ultracold atoms
- 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

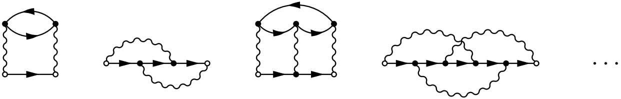
use $J = 1$, on-site repulsion ($U > 0$) or attraction ($U < 0$)

Strong coupling: T-matrix selfenergy

- to access strong coupling: use T-matrix selfenergy (sum entire Born series)
- for Hubbard model simplification[15]

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

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



- T-matrix: well defined and conserving strong coupling approximation
- limitation: low density (binary collision approximation)
- numerical optimization: large systems, long propagation feasible[16]
- no free parameters

---

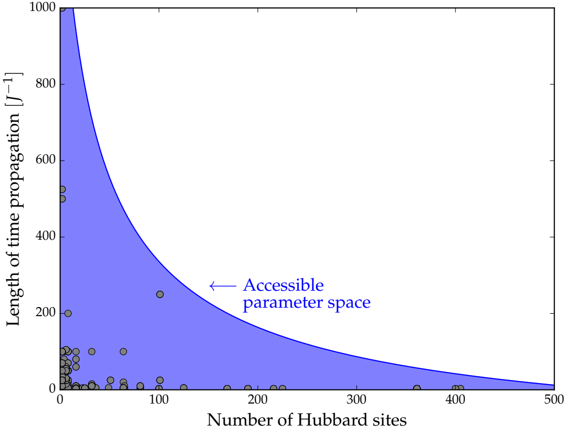
[15] P. von Friesen, C. Verdozzi, and C.O. Almbladh, Phys. Rev. B **82**, 155108 (2010)

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

Numerical capabilities (approximate)

Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

- 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.[17]
- inhomogeneous systems of any dimensionality and geometry

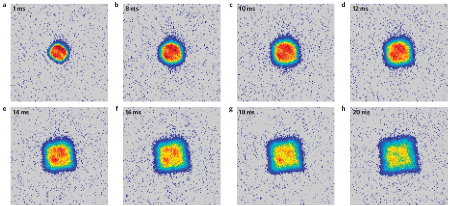


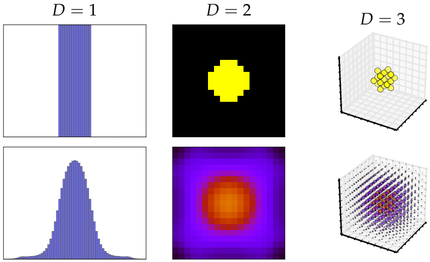
[17] Work of S. Herrmanns, N. Schlünzen and C. Hinz

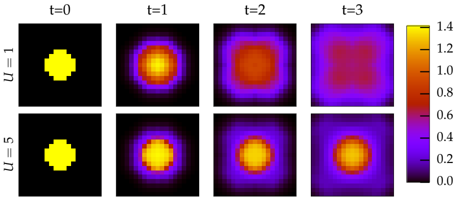
Fermion expansion and doublon decay

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

Experimental results ($U = 0$)

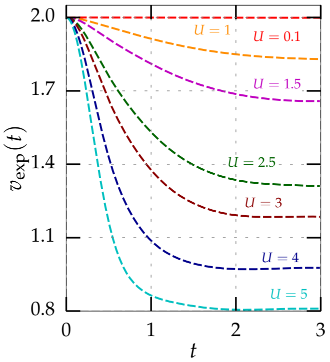






[1] U. Schneider *et al.*, Nature Physics **8**, 213-218 (2012)

Evolution of the expansion velocity



- $N = 58$ fermions in 2D

Diffusion quantities

- **mean squared displacement**

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

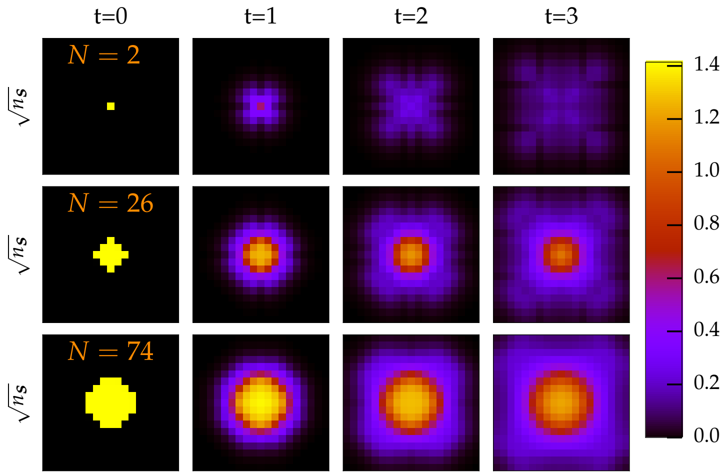
$\boldsymbol{s}_0$: center of the system

- 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**

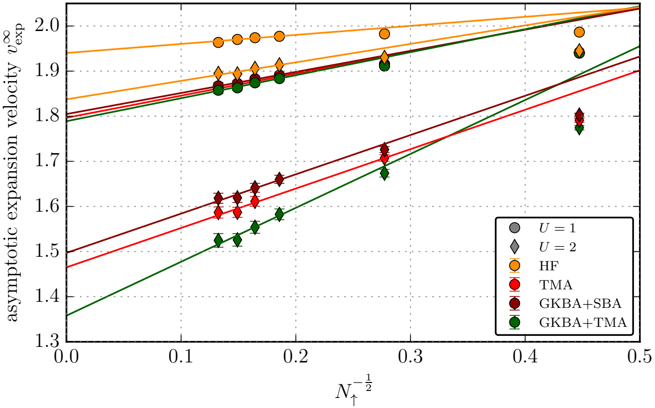
$$v_{\mathrm{exp}}^{\infty} = \lim_{t\to\infty} v_{\mathrm{exp}}(t)$$

Expansion for different particle numbers

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



Asymptotic expansion velocity: 1D–3D

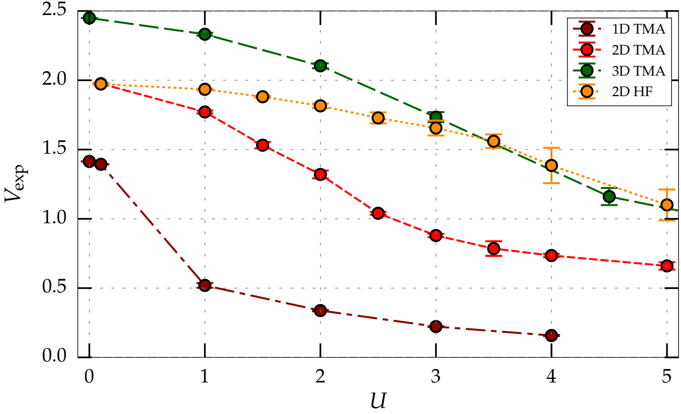


- universal scaling allows for extrapolation to macroscopic limit $V_{\mathrm{exp}}(U, D)$:

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

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

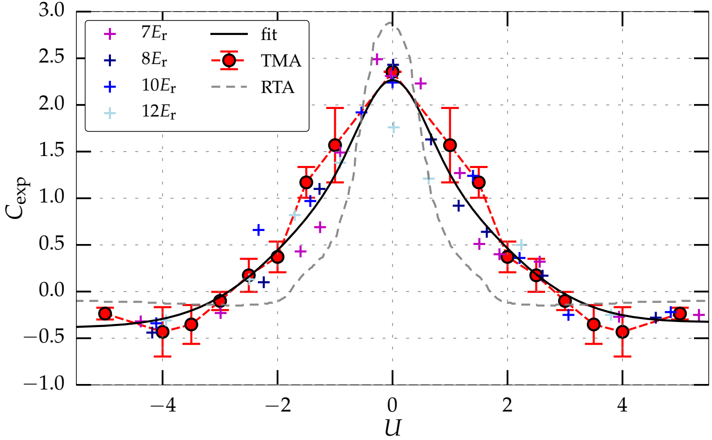
Extrapolated expansion velocity: 1D–3D



- noninteracting limit, $V_{\mathrm{exp}} = \sqrt{2D} = \sqrt{2},\ 2,\ \sqrt{6}$ in 1D-3D reproduced
- similar trend of $V_{\mathrm{exp}}(U)$ in all dimensions
- mean field (HF) fails: proper treatment of correlations crucial

"Core expansion velocity": Expt. vs. NEGF

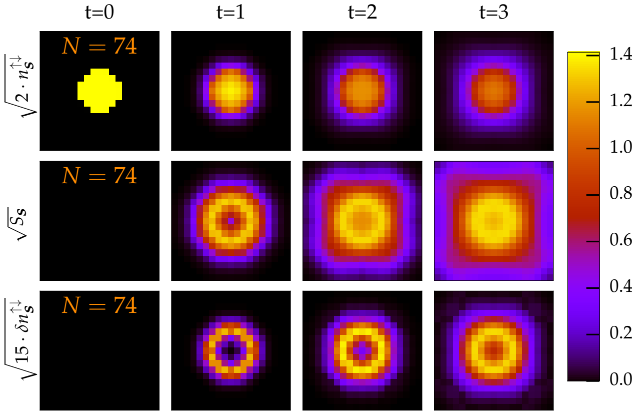
- Measured HWHM of density distribution[18], NEGF: *ab initio*, no free parameters[19]



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

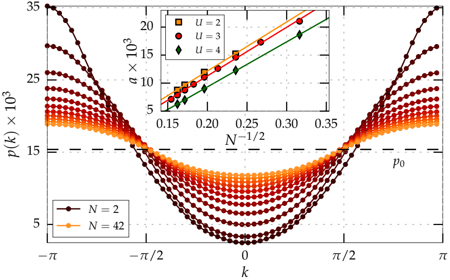
[19] N. Schlünzen *et al.*, Phys. Rev. B **93**, 035107 (2016)

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

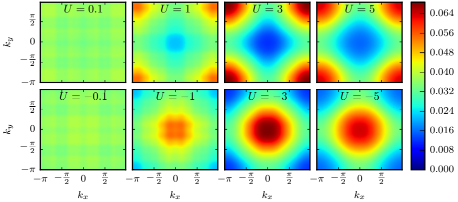


- insights into the early expansion phase
- measurable in recently developed quantum atom microscopes

1D:



2D:

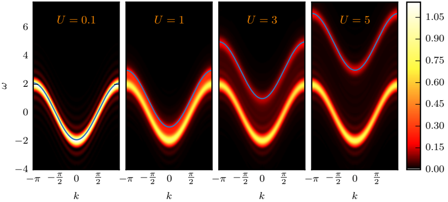


- momentum distribution

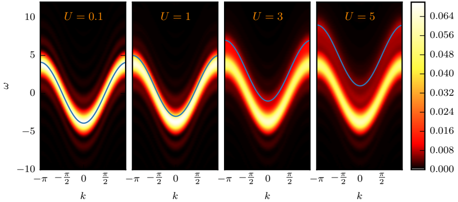
$$n_{\boldsymbol{k}}(t) \quad = \quad \frac{1}{N_s}\sum_{\boldsymbol{ss'}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}(\boldsymbol{s}-\boldsymbol{s'})} n_{\boldsymbol{ss'}}(t),$$

- positive U: occupation of large energies
- negative U: occupation of small energies

1D:



2D:



- spectral function

$$A(\omega, \boldsymbol{k}) \quad = \quad \frac{\mathrm{i}\hbar}{N_s N_t} \sum_{\boldsymbol{ss'}\, tt'} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}(\boldsymbol{s}-\boldsymbol{s}')} \mathrm{e}^{-\mathrm{i}\omega(t-t')} \left[G^{>}_{\boldsymbol{ss'}}(t,t') - G^{<}_{\boldsymbol{ss'}}(t,t') \right]$$

- separation in two energy bands: single-particle states and doublons
- doublon dispersion shifted proportional to interaction strength U

Conclusions and outlook

1. **Correlated fermions**: nontrivial nonequilibrium transport
   - slowing down of expansion with coupling
   - Separation in free/paired ("doublons") components. Symmetry $U \to -U$.
2. **Conclusions for non-equilibrium theory**: failure of
   - semiclassical approaches, including Boltzmann-type kinetic equations, RTA
   - mean-field-type approximations (quantum Vlasov, Hartee-Fock)
3. **NEGF**: pure and mixed states, conserving, advantageous scaling[20]
   1. long simulations, strong excitation possible
   2. can treat 2D, 3D, inhomogeneous/finite systems
   3. strong correlations accessible via T-matrix selfenergy (low density)
   4. further efficiency gain via GKBA or completed collision approx.
   5. excellent agreement with 2D experiments

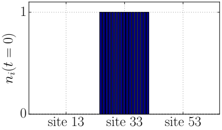
[20] No exponential scaling with N, limitation: basis size

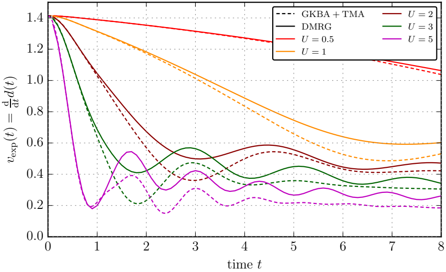
for details: N. Schlünzen and MB, Contrib. Plasma Phys. **56**, 5-91 (2016)

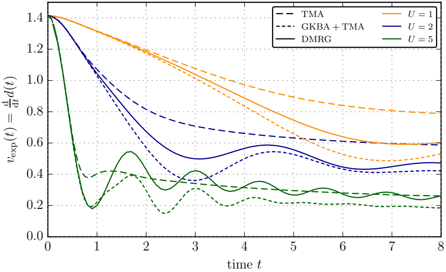
Benchmarks of NEGF against DMRG (1D)[21]

Expansion dynamics

large 1D system ($N_s = 65$)



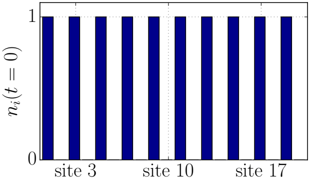


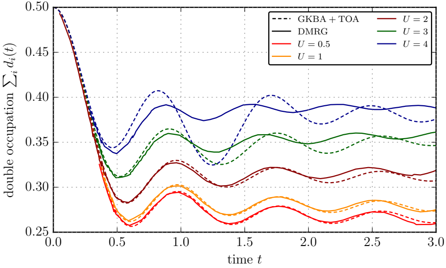


- confirm accurate asymptotic expansion velocities from NEGF T-matrix (within error bars)
- exact result bracketed by T-matrix and GKBA+T
- T misses transient oscillations, improves for large U

[21] N. Schlünzen, J.-P. Joost, F. Heidrich-Meisner, and M. Bonitz, to be published

Initial state:
charge density wave





- sensitive observable: total double occupation
- Accurate long-time behavior of GKBA+T-matrix
- good quality transients NEGF up to $U \simeq$ bandwidth

[22] N. Schlünzen, J.-P. Joost, F. Heidrich-Meisner, and M. Bonitz, to be published

Conclusions and outlook

1. **Correlated fermions**: nontrivial nonequilibrium transport
   - slowing down of expansion with coupling
   - Separation in free/paired ("doublons") components. Symmetry $U \to -U$.

2. **Conclusions for non-equilibrium theory**: failure of
   - semiclassical approaches, including Boltzmann-type kinetic equations, RTA
   - mean-field-type approximations (quantum Vlasov, Hartee-Fock)

3. **NEGF**: pure and mixed states, conserving, advantageous scaling[23]
   1. long simulations, strong excitation possible
   2. can treat 2D, 3D, inhomogeneous/finite systems
   3. strong correlations accessible via T-matrix selfenergy (low density)
   4. further efficiency gain via GKBA or completed collision approx.
   5. *excellent agreement with 2D experiments and DMRG (1D)*
      $\Rightarrow$ *Predictive capability*. Improved approximations in progress

4. Interesting prospects for ab initio plasma-surface interaction simulations

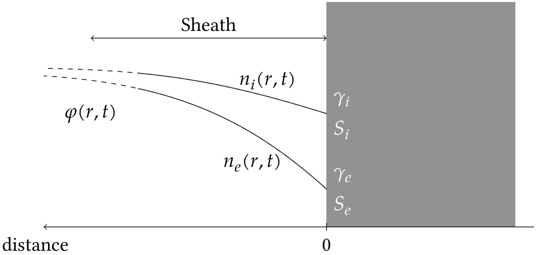
[23] No exponential scaling with N, limitation: basis size

for details: N. Schlünzen and MB, Contrib. Plasma Phys. **56**, 5-91 (2016)

4. Extending NEGF to Plasma-Surface interaction

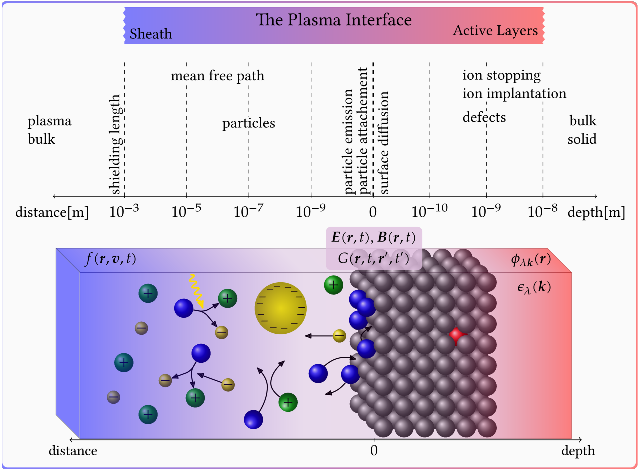
Low-temperature, low pressure plasma: 300 K, few Pa to 1at
important for applications, technology: sputtering, atomic layer deposition, coating etc.

- ionized gas of electrons, (various) ions, neutrals
- externally driven (AC voltage, f ~ 13 MHz), ions far from equilibrium
- non-neutral close to surface ("sheath")



Currently common approach: empirical treatment of solid

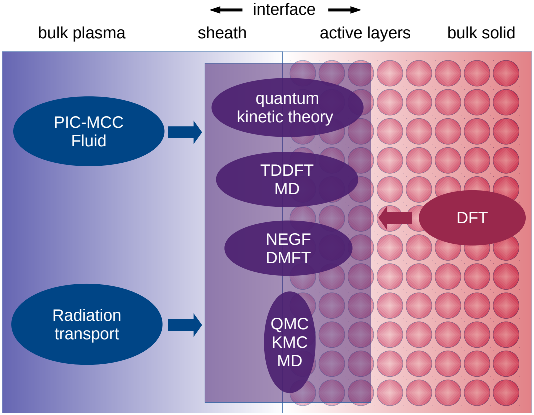
Plasma-Surface interaction–towards *in situ* experiments and selfconsistent simulations[24]



[24] New SFB/CRC initiative in Kiel

Simulating Plasma-Surface interaction: combination of methods required

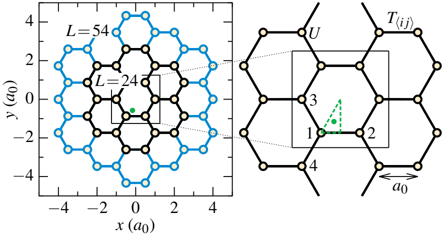
Challenges: - tremendously different density, length and time scales
- coexistence of classical and quantum behavior, bound and free electrons
- open system, out of equilibrium



Ion stopping in strongly correlated materials[26]

DFT problematic. $\Rightarrow$ first test of NEGF approach

- consider lattice model: appropriate for correlated materials
- one example: graphene. Use 2D honeycomb lattice, vary size L



$$H_{\mathsf{e}} = -\sum_{\langle i,j\rangle,\sigma} T_{\langle ij\rangle}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i (n_{i\uparrow} - \tfrac{1}{2})(n_{i\downarrow} - \tfrac{1}{2}) - \frac{Z_{\mathsf{p}} e^2}{4\pi\epsilon_0} \sum_i \frac{\mathsf{e}^{-\kappa|\vec{r}_{\mathsf{p}} - \vec{R}_i|}}{|\vec{r}_{\mathsf{p}} - \vec{R}_i|}$$

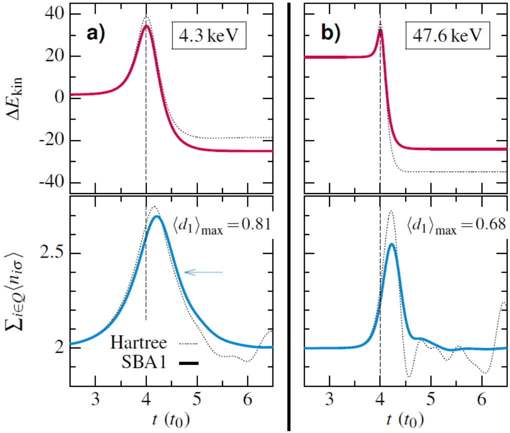
- simple projectile (proton, α), treated classically [$Z_p, \mathbf{r}_p(t)$, Ehrenfest dynamics]
- parameters[25]: $a_0 = 1.42$Å, $\mathbf{r}_p(t)/a_0 = \{-1/6, -\sqrt{3}/3, -z(t)\}$, artificial screening

[25] TDDFT: Zhao *et al.*, J. Phys.: Cond.Matt. **27**, 025401 (2015)

[26] K. Balzer, and M. Bonitz, submitted for publication, arXiv:1602.06928

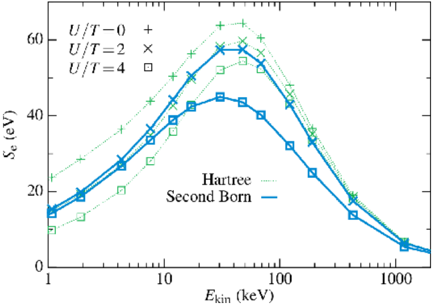
Proton stopping. $U/T_0 = 4, \quad L = 54$

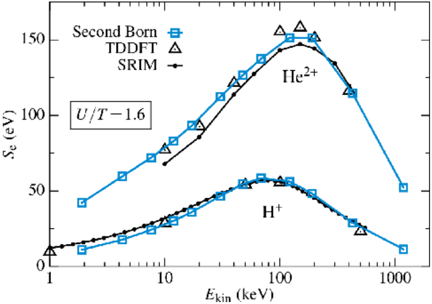
- **Top**: proton energy change. Uncorrelated (dots) vs. correlated (full line)
- **Bottom**: electron density (4 sites adjacent to projectile)



- Mean field approximation (dots) inaccurate, wrong trends

- **Left**: Relevance of correlation effects. **Right**: Model comparison for graphene



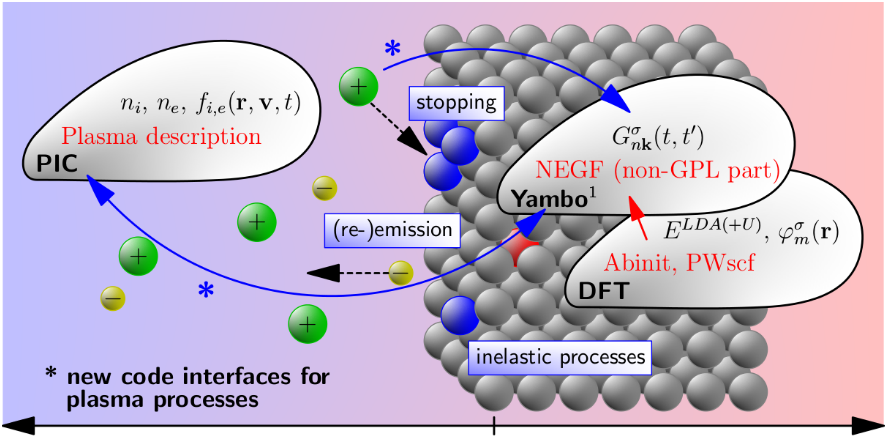


- **Work in progress**:
  - include impact ionization and nuclear dynamics (phonons)
  - extension to eV-range (longer simulations)
  - include projectile sticking and re-emission
  - extend to lattice models for surfaces

[27] K. Balzer, and M. Bonitz, submitted for publication, arXiv:1602.06928

Beyond lattice models: *Ab initio NEGF*[28]

- use Kohn-Sham basis as input for NEGF
  in collaboration with A. Marini, using Yambo



[1] A. Marini, C. Hogan, M. Gruening, and D. Varsano, Comp. Phys. Comm. **180**, 1392 (2009)

[28] e.g. Pedro Miguel M. C. de Melo and Andrea Marini Phys. Rev. B **93**, 155102 (2016)

Thank you for your attention!

Christian-Albrechts-Universität zu Kiel
Mathematisch-Naturwissenschaftliche Fakultät

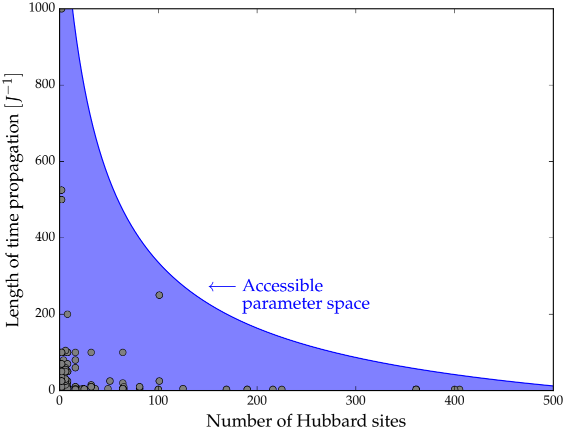
References

- N. Schlünzen and MB, Contrib. Plasma Phys. **56**, 5-91 (2016)
- M. Bonitz, *Quantum Kinetic Theory*, 2nd ed. Springer (2016)
- K. Balzer, and M. Bonitz, Springer Lect. Not. Phys. **867** (2013)
- M. Bonitz and D. Semkat, *Introduction to Computational Methods in Many-Body Physics*, Rinton Press, Princeton (2006)

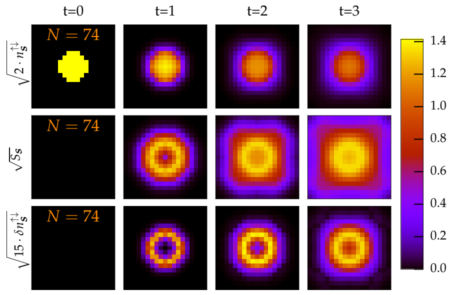
- www.itap.uni-kiel.de/theo-physik/bonitz

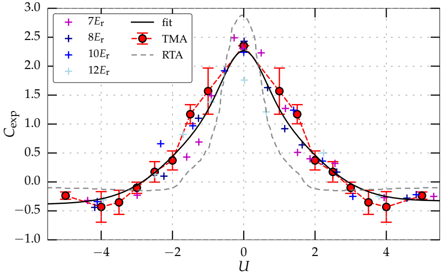
Numerical capabilities (approximate)

- dramatic progress compared to earlier NEGF results with full two-time T-matrix
- up to $N_\mathsf{s} = 1000$, up to $T = 1000 J^{-1}$, due to optimization, GPU hardware etc.



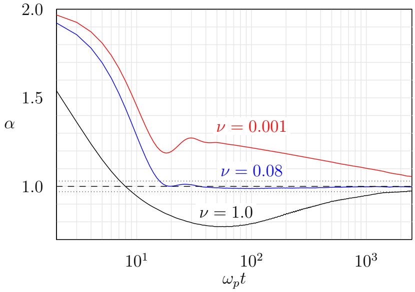
- quantum dynamics for finite systems, size dependence
- single-site resolution, any geometry/dimension
- access arbitrary time scales, arbitrary initial state
- captures correlation (and screening) buildup, doublon formation etc.
- predictive capability for novel nonequilibrium scenarios, quenches

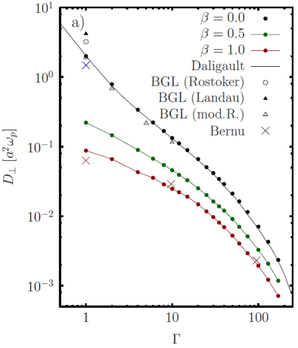




Recall effect of correlations (Γ) in classical plasmas:

1. diffusion remains "normal"[29]: $\langle(\mathbf{r}(t) - \mathbf{r}(0))^2\rangle \sim D\, t^{\alpha(t)}$, $\quad \lim_{t\to\infty} \alpha(t) = 1$
2. reduction of (asymptotic) mobility[30]





[29] T. Ott, and MB, Phys. Rev. Lett. **103**, 195001 (2009)

[30] T. Ott, and MB, Phys. Rev. Lett. **107**, 135003 (2011)