Propagating the two-particle reduced-density matrix of one- and two-dimensional Hubbard systems

Stefan Donsa[1], Fabian Lackner[1], Joachim Burgdörfer[1], and Iva Brezinova[1]

[1]Institute for Theoretical Physics, Vienna University of Technology, Vienna, Austria, EU

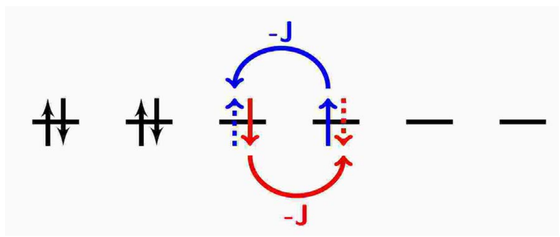
The International Max Planck Research School of Advanced Photon Science (IMPRS-APS)

Motivation

The Hubbard model is one of the simplest models for correlation in solid state physics but still beyond the scope of many theoretical methods. The advent of ultra-cold Fermi gases in optical lattices allows to investigate the Hubbard model for large systems under well-controlled conditions [1]. The time dependent two-particle reduced-density matrix method [2] is used to simulate the dynamics of finite systems from non-equilibrium initial conditions and can such help in understanding experimental results.

Hubbard model

Derived from a tight-binding approach



hopping (kinetic)

$$H = -J \sum_{\langle i,j\rangle;\sigma} a^{\dagger}_{i,\sigma} a_{j,\sigma} + a^{\dagger}_{j,\sigma} a_{i,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} + V_0 (\hat{x} - x_0)^2$$

on-site interaction

external potential

Distance from the center of the external potential

Realized with ultra cold atoms in optical lattices

Time dependent two-particle reduced-density matrix method

- Two-particle reduced-density matrix D_{12}
  - Includes two-particle correlations
  - Exact energy functional for pairwise interactions

EOM — Reconstruction $D_{123} = R[D_1, D_{12}]$

$$i\hbar \frac{\partial}{\partial t} D_{12} = [H_{12}, D_{12}] + C[D_{123}]$$

proportional to interaction U

- Reconstruction of D_{123} causes negative occupation numbers [2,3] => unphysical
- We modify D_{12} to avoid this => purification [2,4]

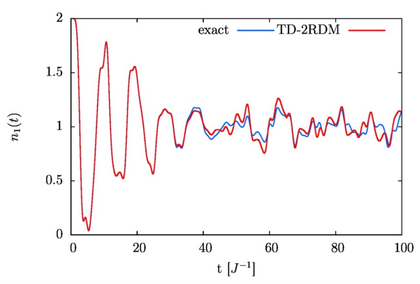
One dimensional system far from equilbrium – benchmarking for "badly chosen" systems

- Previous calculations were done for four sites with a similar method [5] and eight sites with a Green's function method [6].
- We repair stability problems observed in [5] with purification.
- Better results than similar methods but the extreme non-equilbrium condition leads to large deviations.

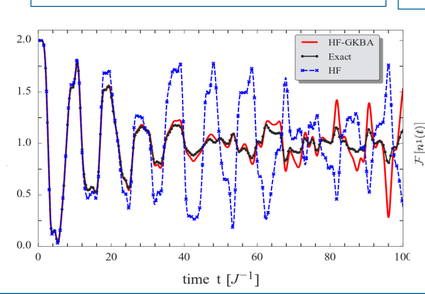
Initial condition – all particles confined to the left

=> far from equilibrium

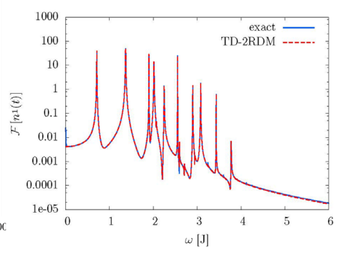
TD-2RDM calculation



Non-equilibrium Green's function method [5]

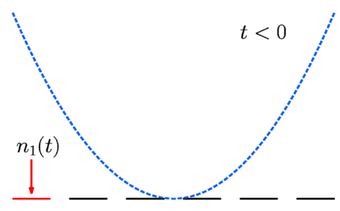


Excitation spectrum of the ground state of an eight site Hubbard cluster



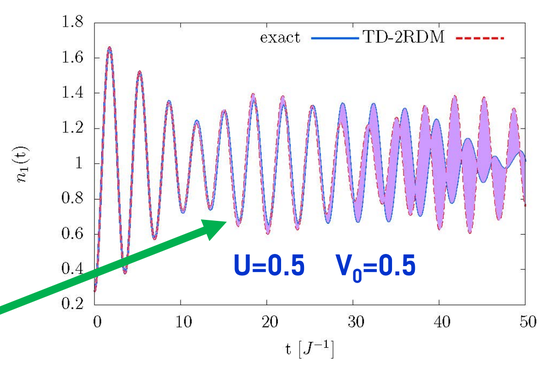
Potential quenches in 1D – limitations of the method

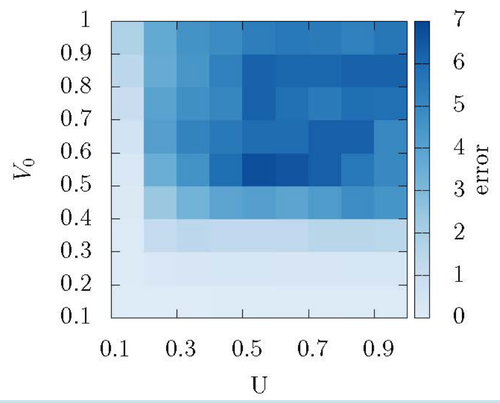
We calculate the ground state of the Hubbard model with an external potential via exact diagonalization



For t>0 we set $V_0 = 0$ and monitor the density fluctuations.

Difference between exact calculation and TD-2RDM

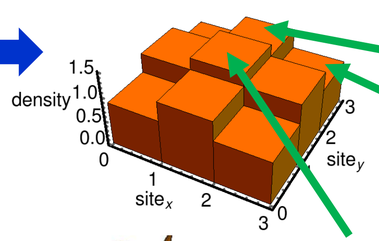




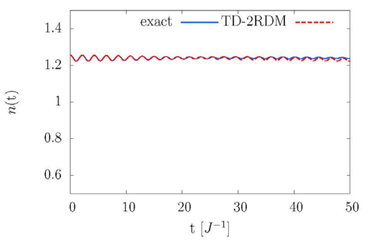
Method suitable for moderate interaction strengths and weak external potentials.

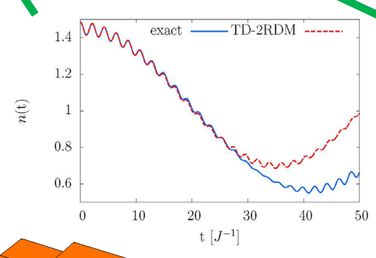
Two-dimensional system – first promising results

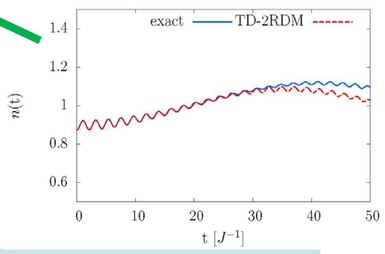
Ground state density of interacting Hubbard model + harmonic potential



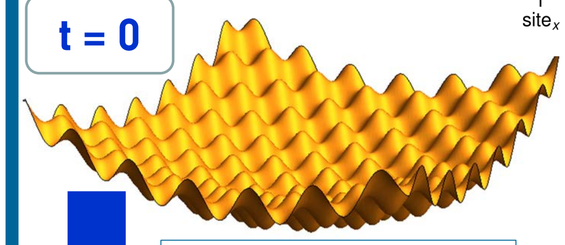
U=0.3 V_0=0.1



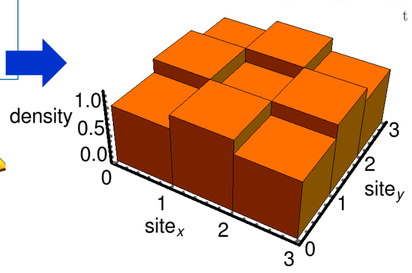


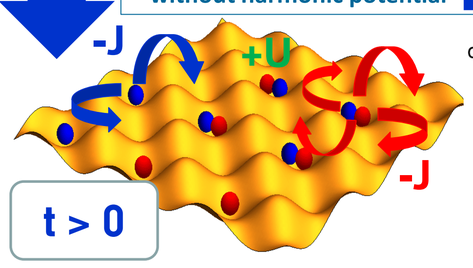


t = 0



Ground state density of interacting Hubbard model without harmonic potential





t > 0

Good agreement for moderate interactions .

No intrinsic limitations of the TD-2RDM concerning the size of the cluster

Larger clusters are possible

Summary & Outlook

- TD-2RDM method shows promising results for two-dimensional systems.
- Can be used to understand physics underlying recent experiments.
- Non-equilibrium dynamics can be accurately described.
- Method is limited to moderate interaction strengths.
- To be self-consistent, ground state calculations are needed.
- First results via adiabatic switching on of the interaction strength.

contact: stefan.donsa@tuwien.ac.at

References

[1] M. Lewenstein et al., Advances in Physics, 243, 2007.

[2] F. Lackner et al., PRA 91, 023412, 2015.

[3] K. Yasuda and H. Nakatsuji, PRL 76, 1039, 1996.

[4] D. A. Mazziotti, PRE 65, 026704, 2002.

[5] A. Akbari et al., PRB 85, 235121, 2012.

[6] S. Hermanns et al., PRB 90, 125111, 2014.

Acknowledgements:

This works has been supported by the WWTF project MA12-002, IMPRS-APS and the FWF SFB ViCoM. All calculations have been performed on the Vienna Scientific Cluster.