Time-evolving block decimation: application to one-dimensional fermions

Vesa Apaja
Deparment of Physics
Nanoscience Center
University of Jyväskylä, Finland

Collaboration:

Robert vanLeeuwen
Petri Myöhänen
Adrian Stan
Gianluca Stefanucci
Matti Manninen
Mikko Leskinen
Päivi Törmä

Outline

Matrix Product States and Hubbard model

TEBD algorithm by Guifre Vidal

Time Evolving Block Decimation

Algorithm to optimize MPS; related to DMRG

Local imaginary/real time evolution
operator on a MPS and forcing it back to MPS

Applications:

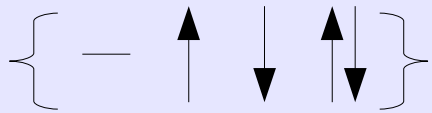
- Measuring pairing gap with RF pulse
- Time dependent quantum transport

Matrix product states

Ordinary many-body state expression in product basis

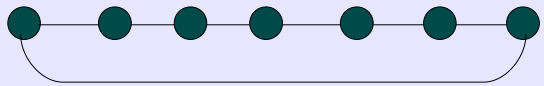
$$|\Psi\rangle = \sum_{i_1 \ldots i_N} c(i_1 \ldots i_N) |i_1 \ldots i_N\rangle$$

Single-site basis:



Matrix product state (periodic boundaries)

$$\begin{aligned} |\Psi\rangle &= \sum_{i_1 \ldots i_N} \mathrm{Tr}(A^{i_1} A^{i_2} \ldots A^{i_N}) |i_1 \ldots i_N\rangle \\ &= \sum_{i_1 \ldots i_N} A^{i_1}_{\alpha\beta} A^{i_2}_{\beta\gamma} \ldots A^{i_{N-1}}_{\epsilon\delta} A^{i_N}_{\delta\alpha} |i_1 \ldots i_N\rangle \end{aligned}$$

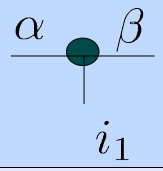


Any state can be expressed as an MPS
if you take big enough matrices
(G. Vidal, *Phys. Rev. Lett.* **93**, 040502 (2003))

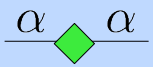
$$c(i_1,...,i_N) = \Gamma^{[1]i_1}_{\alpha_1} \lambda^{[1]}_{\alpha_1} \Gamma^{[2]i_2}_{\alpha_1\alpha_2} \lambda^{[2]}_{\alpha_2} ... \Gamma^{[N]i_N}_{\alpha_{N-1}}$$

Diagrammatic notation

$\Gamma^{[1]i_1}_{\alpha\beta}$ (*DxD* matrix)



λ_α



Systematically better variational wave function with increasing matrix dimension *D*

Unitary changes to subsystems don't change
the Schmidt decomposition elsewhere => Local updates

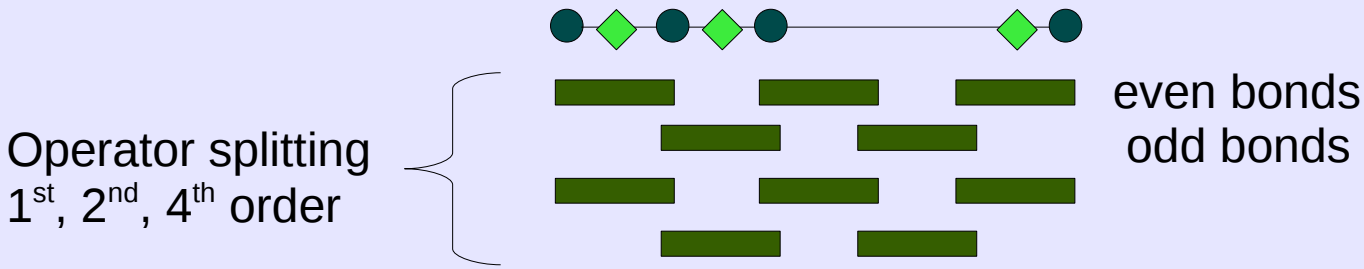
Hubbard Hamiltonian

Hopping between nearest neighbours and on-site repulsion

Apply real/imaginary time evolution to even and odd bonds separately:

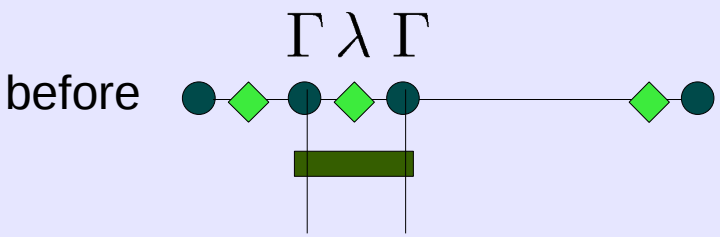
$$\hat{H} = \sum_{k(even)}^{bonds} \hat{h}_k + \sum_{k(odd)}^{bonds} \hat{h}_k$$

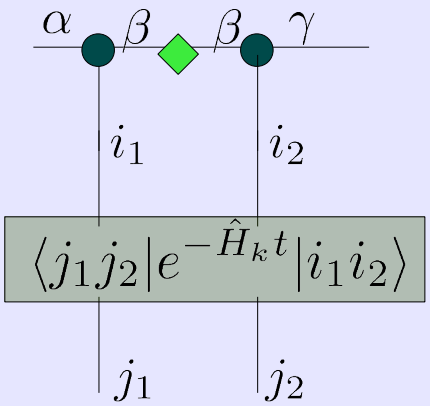
$e^{i\hat{h}_k t/\hbar}$ or $e^{-\hat{h}_k t/\hbar}$



MPS ➡ local update ➡ MPS

Hubbard Hamiltonian couples two nearest neighbor sites





SVD

$$= \Theta_{(\alpha,j_1),(\gamma,j_2)} = A_{(\alpha,j_1)m}\lambda_m B_{m,(\gamma,j_2)}$$

often m > D

Block decimation:
Truncate, keeping only D largest singular values

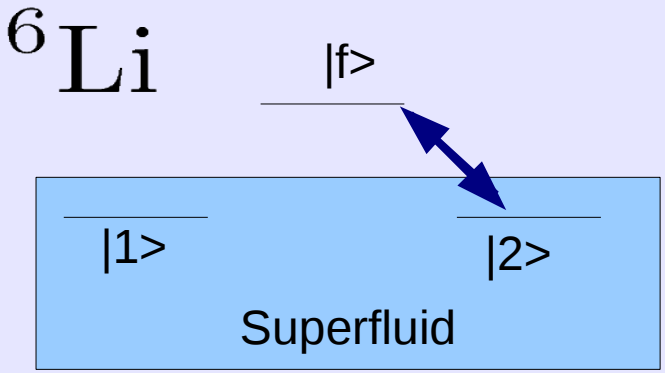
$$\approx \Gamma^{j_1}_{\alpha,\beta}\lambda_\beta\Gamma^{j_2}_{\beta,\gamma}$$

Insert back to Ψ

Measuring pairing gap with RF pulse

Chin et al. *Science 305, 1128 (2004)*

"*Observation of the Pairing Gap in a Strongly Interacting Fermi Gas*"



RF offset (detuning)

$$\delta = \omega_{RF} - (w_f - w_2)$$

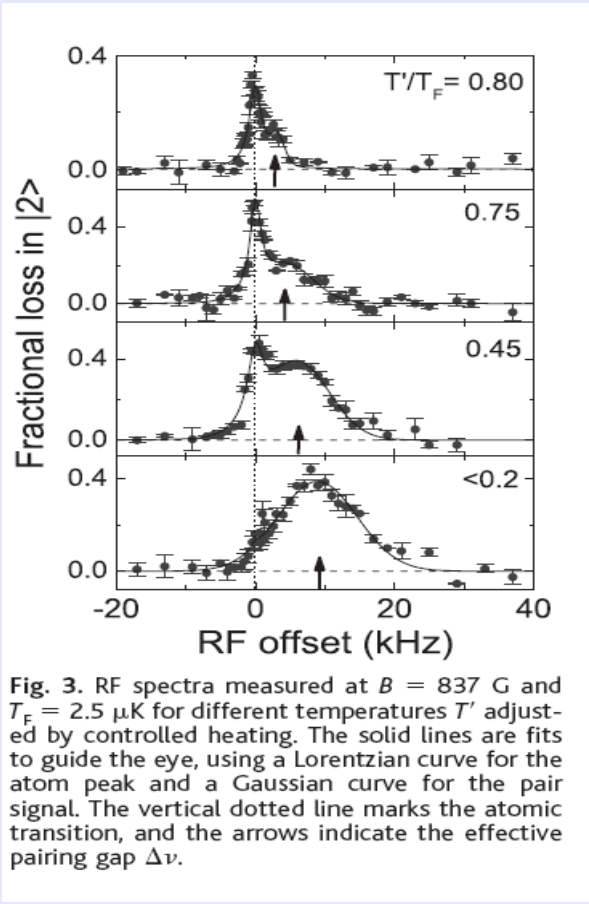
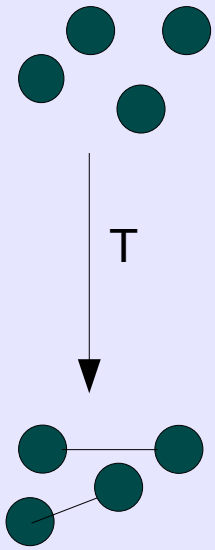


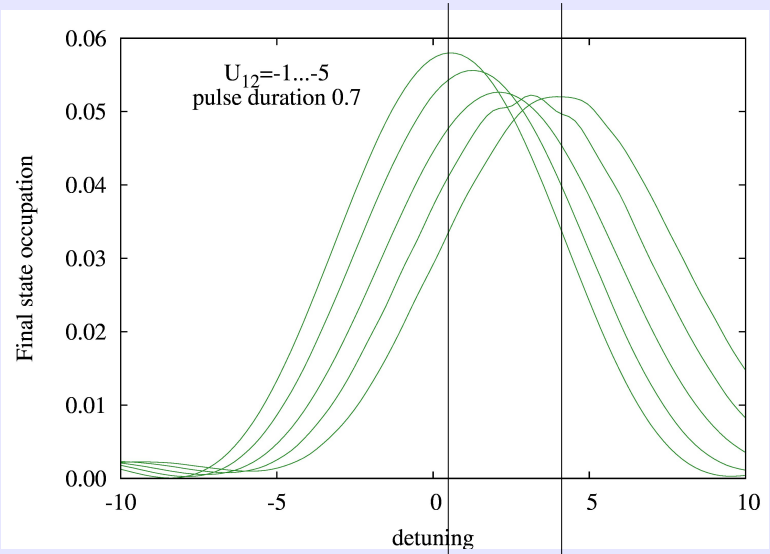
Fig. 3. RF spectra measured at $B = 837$ G and $T_F = 2.5$ μK for different temperatures T' adjusted by controlled heating. The solid lines are fits to guide the eye, using a Lorentzian curve for the atom peak and a Gaussian curve for the pair signal. The vertical dotted line marks the atomic transition, and the arrows indicate the effective pairing gap $\Delta\nu$.

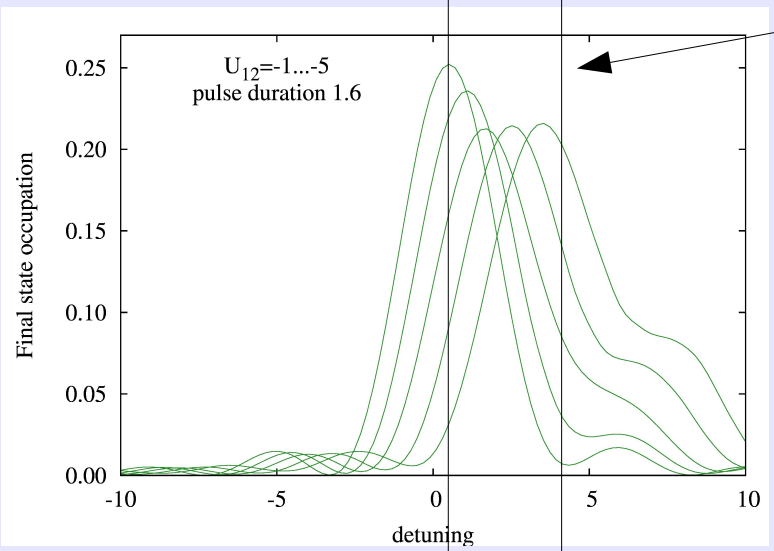


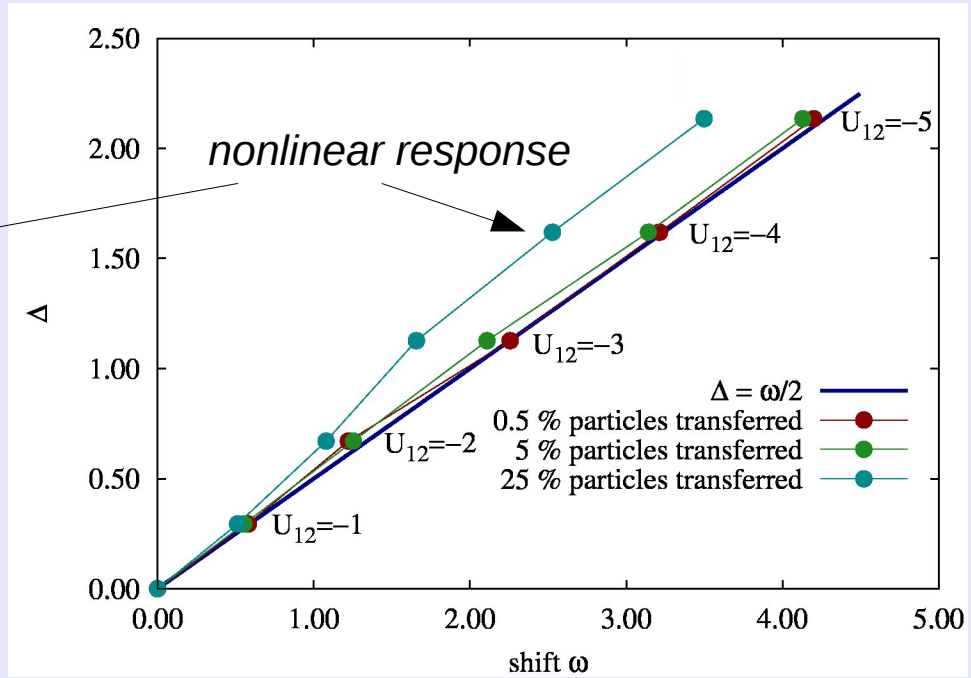
Attractive-U Hubbard model, $U_{12} < 0, |U_{12}| \sim \Delta$

Relation RF-shift – gap is nonlinear for long pulses

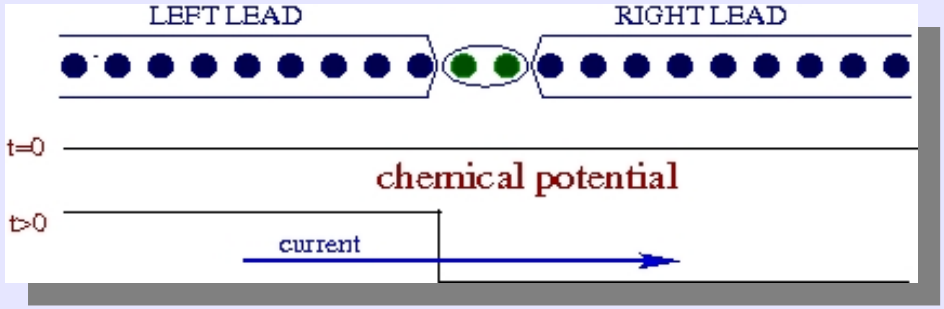
M. J. Leskinen, V. A., J. Kajala, and P. Törmä , *Phys. Rev.* ***A 78****, 023602* (2008)







Time-dependent quantum transport

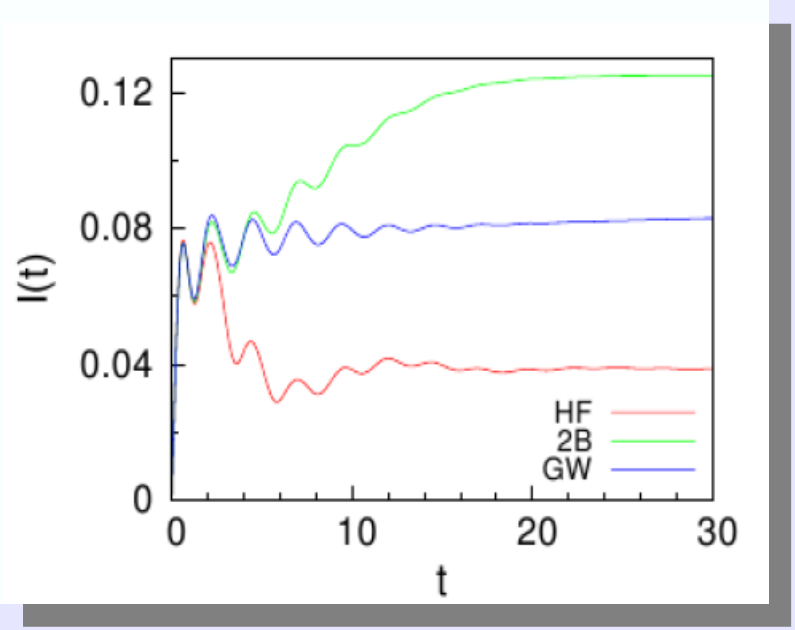


Many-body effects have a large impact on currents

K. S. Thygesen *(Phys.Rev.Lett. 100 166804 (2008)*
P. Myöhänen *et al. (Europhys. Lett. 84, 67001 (2008), cond-mat: arXiv: 0808.3483 (2008))*

Many-body approximations give
different transient and steady state currents

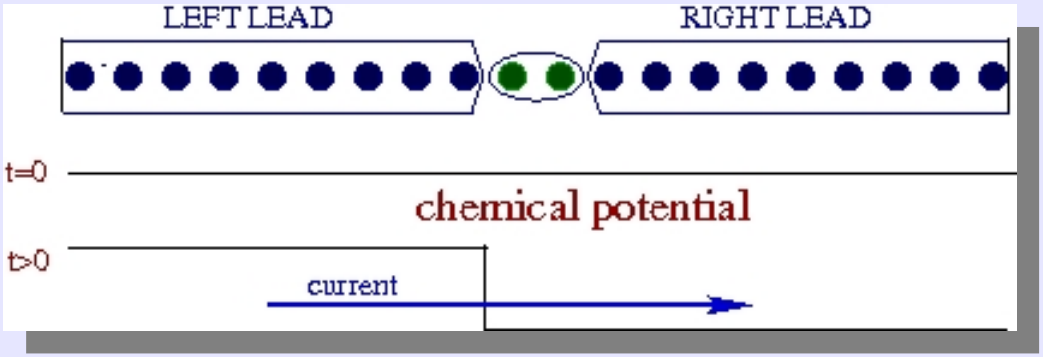
For example:



Self-energy approximations:
HF = Hartree-Fock
2B = 2nd Born
GW = GW

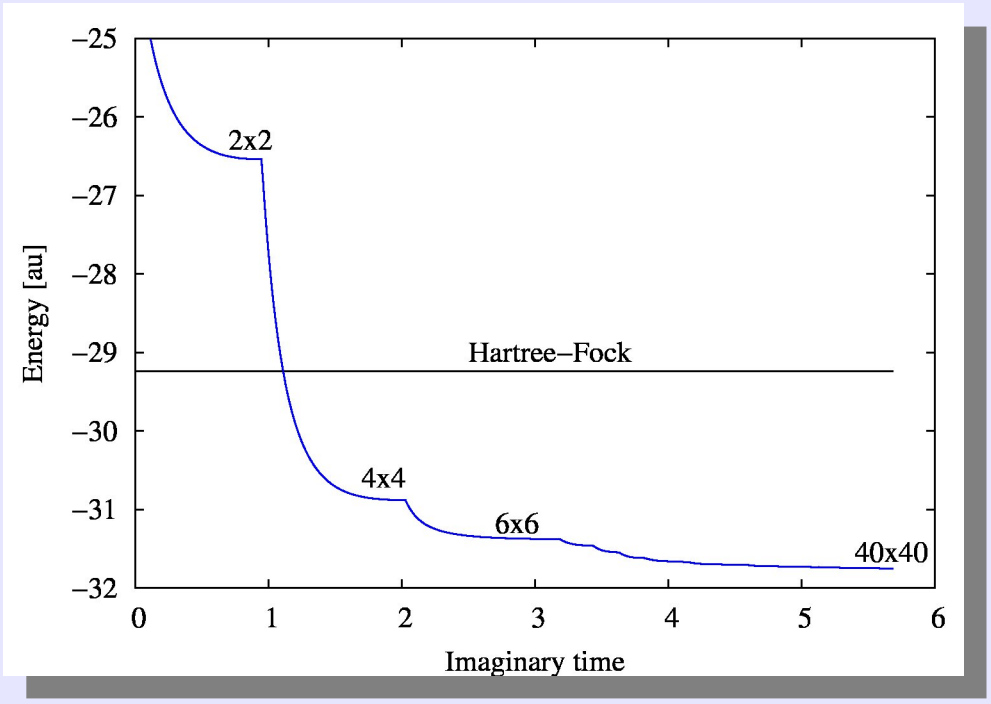
Which one is the best?

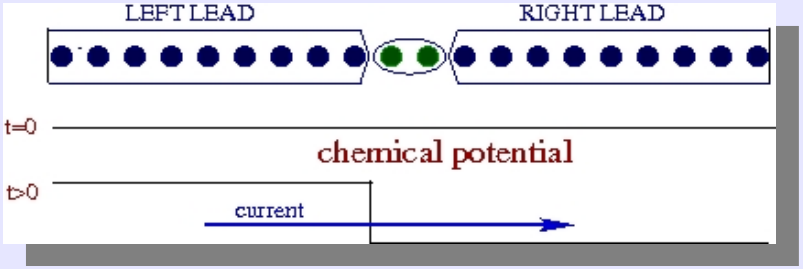
Simple model system

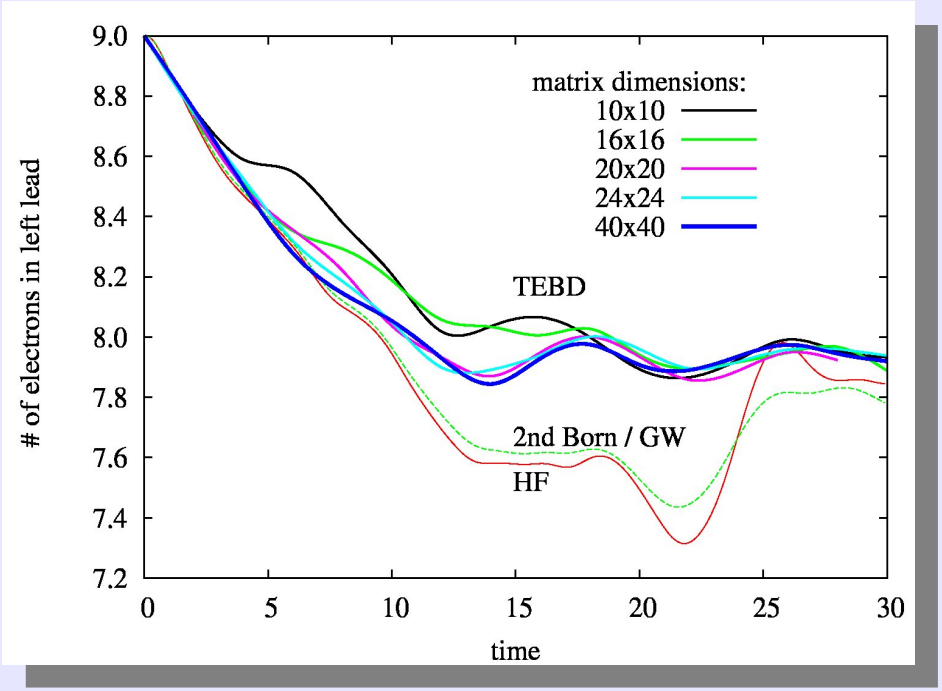


On-site repulsion U = 0.5
Hopping t = -1.5 in leads
-0.5 between leads and center atoms
-1.0 between center atoms

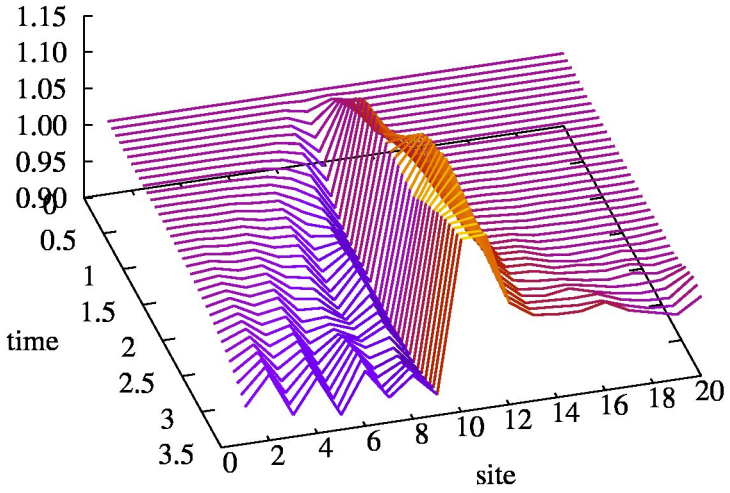
Ground state at constant chemical potential

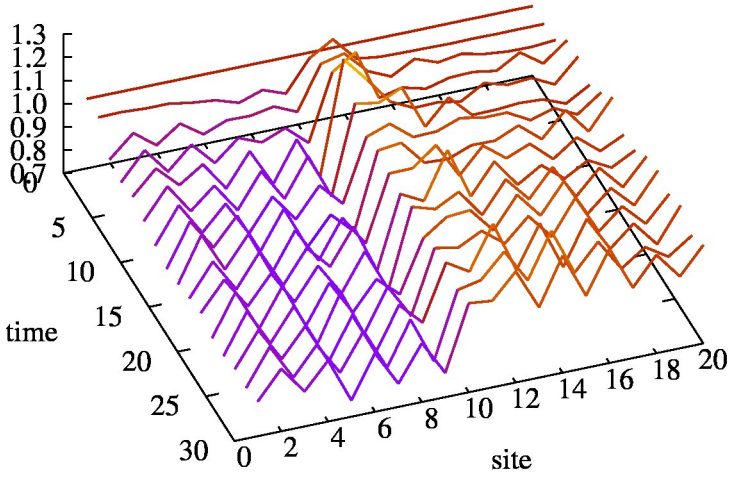






Local density





Thank You!

Hubbard model in 1D

$$\hat{H} = -J \sum_{\langle i,j \rangle} (\hat{a}_i^\dagger \hat{a}_j + h.c.) + \sum_i \mu \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)$$

Tunnel matrix element : nearest neighbor site-to-site hopping

$$J = J_{ij} = -\int d^3x w(\mathbf{x} - \mathbf{x}_i) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{lat}(\mathbf{x}) \right) w(\mathbf{x} - \mathbf{x}_j)$$

On-site interaction matrix element

$$U = \frac{4\pi\hbar^2 a}{m} \int d^3 |w(\mathbf{x})|^4$$

μ Is the chemical potential
a is the scattering length

Localized Wannier wave functions

Field operator in Wannier basis

$$\hat{\psi}(\mathbf{x}) = \sum_i \hat{a}_i w(\mathbf{x} - \mathbf{x}_i)$$

Current conserving approximations: