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SCHOOL ON QUANTUM PHASE TRANSITIONS
AND
NON-EQUILIBRIUM PHENOMENA IN COLD ATOMIC GASES

11 - 22 July 2005

Numerical studies of low dimensional ultracold atoms

Presented by:

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Numerical studies of low dimensional ultracold atoms

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- **Motivation: ultracold atoms in optical lattices: strongly correlated limit**
  - **Quantum criticality**
  - **Universalities**
  - **Nonequilibrium dynamics**

- **Technique: Numerical methods**
  - **Quantum Monte Carlo simulations (equilibrium)**
  - **Exact numerics for hard core bosons in 1 dimension (ground-state and nonequilibrum dynamics)**
  - **Lanczos time evolution with DMRG**

- **Results:**
  - **Local quantum criticality crossing to Mott-insulating domains**
  - **Universalities in hard-core bosons confined on 1-D lattices**
  - **Nonequilibrium dynamics of hard-core bosons**
  - **Collapse and revival of a Luttinger liquid**

Collaborators

- **Georges G. Batrouni** (University of Nice)
- **Peter J.H. Denteneer** (University of Leiden)
- **Salvatore Manmana** (University of Stuttgart)
- **Reinhard Noack** (University of Marburg)
- **Marcos Rigol** (University of California, Davis)
- **Valerie Rousseau** (University of Nice)
- **Richard T. Scalettar** (University of California, Davis)
- **Matthias Troyer** (ETH-Zürich)

QMC for the Bose-Hubbard model in 1D

$$H = -t \sum_i \left(b_i^\dagger b_{i+1} + h.c. \right) + U \sum_i n_i (n_i - 1) + V \sum_i \left(i - L/2 \right)^2 n_i$$

The world-line algorithm

J.E. Hirsch, R. L. Sugar, D. J. Scalapino, and R. Blankenbecler, Phys. Rev. B **26**, 5033 (1982).

Consider a 1-D system with nearest neighbor terms

$$H = \sum_i H_{i,i+1}$$

Partition function

$$\begin{aligned} Z &= \mathrm{Tr}\; \mathrm{e}^{-\beta H} = \mathrm{Tr} \prod_{\ell=1}^{L} \mathrm{e}^{-\Delta\tau H} \\ &= \sum_{\{i_\ell\}} < i_1 | \mathrm{e}^{-\Delta\tau H} | i_L >< i_L | \mathrm{e}^{-\Delta\tau H} | i_{L-1} > \cdots < i_2 | \mathrm{e}^{-\Delta\tau H} | i_1 > , \end{aligned}$$

where $\Delta\tau = \beta / L$, and $\{ | i_\ell > \}$ complete sets of states at each time slice.

Trotter-Suzuki decomposition $\longrightarrow$ $H = H_1 + H_2$.

$$e^{-\Delta\tau H} = e^{-\Delta\tau H_1} e^{-\Delta\tau H_2} + \mathcal{O}\left[(\Delta\tau)^2\right] .$$

Choose

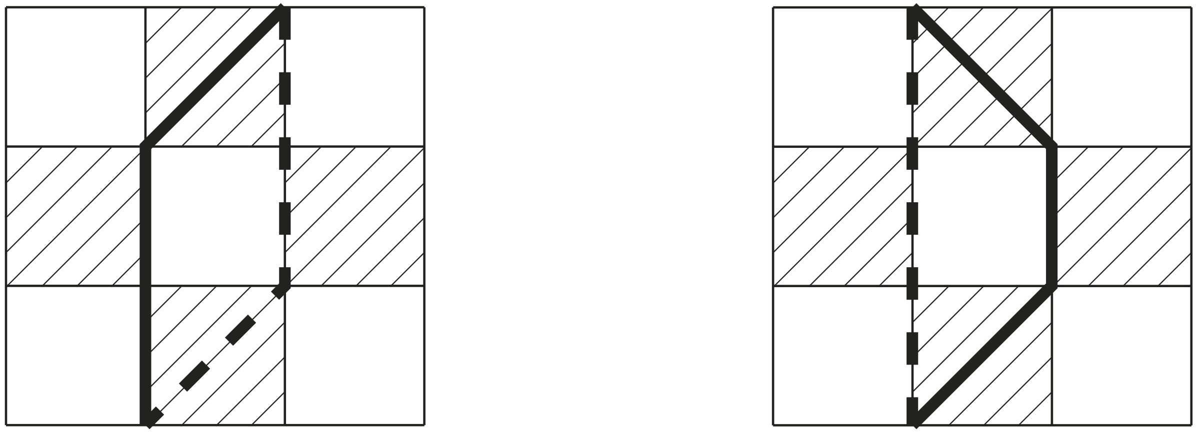
$$H_{1\,(2)} = \sum_{i\,\text{odd}\,(\text{even})} H_{i,i+1} ,$$

$\hookrightarrow$ H_1 **and** H_2 **consist each of a sum of mutually commuting pieces.**

$\hookrightarrow$ **the matrix elements are reduced to a product of two-site matrix elements:**

$$\begin{aligned} &< i_\ell \mid e^{-\Delta\tau H} \mid i_{\ell+1} > \\ &= \; < i_{2\ell} \mid e^{-\Delta\tau H_1} \mid i_{2\ell-1} >< i_{2\ell-1} \mid e^{-\Delta\tau H_2} \mid i_{2\ell-2} > + \mathcal{O}\left[(\Delta\tau)^2\right] \\ &= \; \prod_{i\,\text{odd}} < i_{2\ell} \mid e^{-\Delta\tau H_{i,i+1}} \mid i_{2\ell-1} > \\ &\qquad \times \prod_{i\,\text{even}} < i_{2\ell-1} \mid e^{-\Delta\tau H_{i,i+1}} \mid i_{2\ell-2} > + \mathcal{O}\left[(\Delta\tau)^2\right] . \end{aligned}$$

Local moves



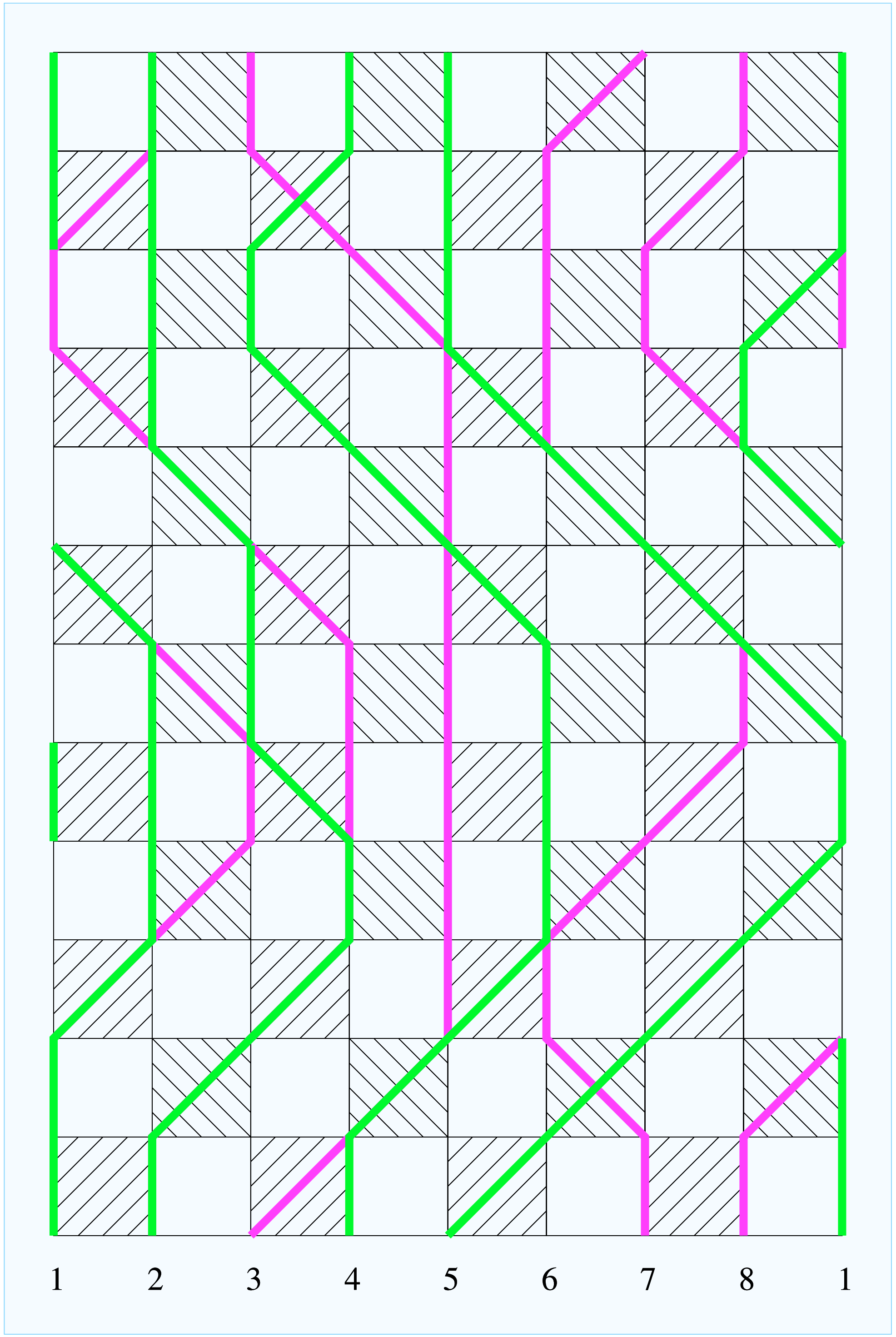
Update

$$R = \frac{W_{\text{new}}}{W_{\text{old}}} = \left[\tanh \Delta\tau J/2\right]^{su} \left[\cosh \Delta\tau J/2 \mathrm{e}^{\Delta\tau J \Delta/2}\right]^{sv}$$

with

$$\begin{aligned} s &\equiv n(i,j) + n(i,j+1) - n(i+1,j) - n(i+1,j+1)\ , \\ u &= 1 - n(i+1,j-1) - n(i+1,j+2), \\ v &= n(i-1,j) - n(i+2,j)\ . \end{aligned}$$

Simulation



initial configuration

final configuration

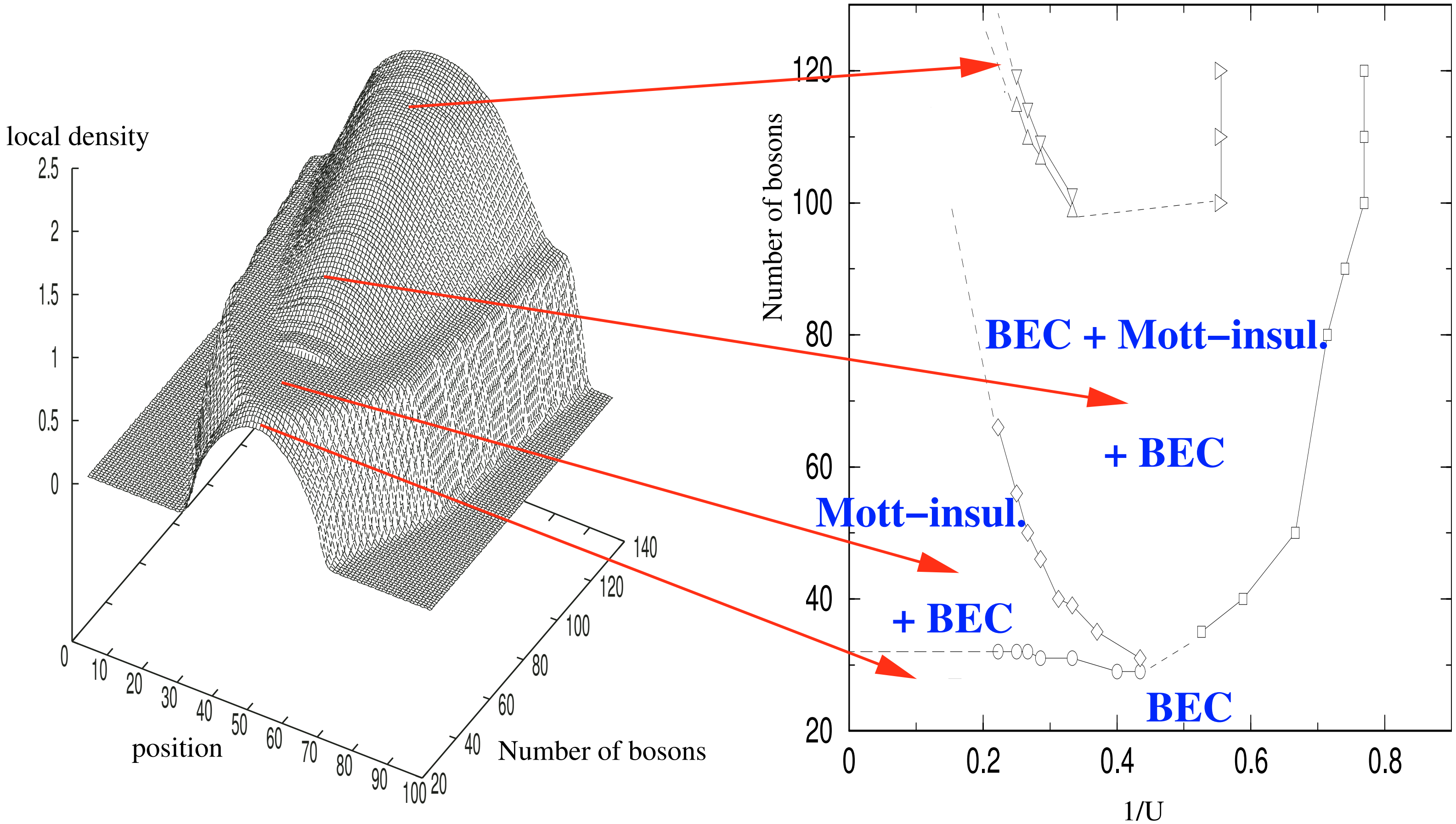
Stochastic series expansion (SSE)

S. Wessel, F. Alet, M. Troyer, and
G. Batrouni, Phys. Rev. A **70**, 053615 (2004)

Mott domains of bosons confined on optical lattices

G.G. Batrouni, V. Rousseau, R. Scalettar, M. Rigol, A. Muramatsu, P.J.H. Denteneer, and M. Troyer, Phys. Rev. Lett. **89**, 117203 (2002).

$$H = -t \sum_i \left(b_i^\dagger b_{i+1} + h.c. \right) + U \sum_i n_i(n_i - 1) + V \sum_i (i - L/2)^2 \, n_i$$



QMC for the Fermi-Hubbard model in 1D

$$H = -t \sum_{\substack{<i,j> \\ \sigma}} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i \left(i - \frac{N}{2} \right)^2 n_i$$

The projector algorithm (T=0)

G. Sugiyama and S. Koonin, Annals of Physics **168**, 1 (1986).

S. Sorella *et al.*, Int. Jour. Mod. Phys. B **1**, 993 (1988).

R. Blankenbecler, D. Scalapino, and R. Sugar, Phys. Rev. D **24**, 2278 (1981).

$$\lim_{\Theta\to\infty} \mathrm{e}^{-\Theta H} \mid \Psi_T\rangle = \lim_{\Theta\to\infty} \sum_n \mathrm{e}^{-\Theta H} \mid n\rangle\langle n \mid \Psi_T\rangle$$

$$= \lim_{\Theta\to\infty} \mathrm{e}^{-\Theta E_0} \left[\mid \Psi_G\rangle\langle\Psi_G \mid \Psi_T\rangle + \sum_{n\neq 0} \mathrm{e}^{-\Theta(E_n - E_0)} \mid n\rangle\langle n \mid \Psi_T\rangle \right]$$

Discrete Hubbard-Stratonovich transformation

J.E. Hirsch, Phys. Rev. B **28**, 4059 (1983).

$$\mathrm{e}^{-\Delta\tau U n_{i\uparrow} n_{i\downarrow}} = \frac{1}{2} \sum_{\sigma_i = \pm 1} \mathrm{e}^{2\lambda\sigma_i \left[\left(n_{i\uparrow} - \frac{1}{2}\right) - \left(n_{i\downarrow} - \frac{1}{2}\right) \right] - \frac{1}{2} U \Delta\tau \left(n_{i\uparrow} + n_{i\downarrow}\right)}$$

with $\tanh^2 \lambda = \tanh(\Delta\tau U/4)$**.**

Projection: evolution in imaginary time in the space of Slater determinants

Trial wavefunction: Slater determinant

$$| \Psi_T\rangle = \prod_{j=1}^{N_p} \sum_{i=1}^{N} P_{ij} c_i^\dagger \mid 0\rangle$$

A bilinear form transforms a Slater determinant into another one

$$| \Psi_F\rangle \quad = \quad \mathrm{e}^{-\Delta\tau \tilde{H}[\sigma_L]} \cdots \mathrm{e}^{-\Delta\tau \tilde{H}[\sigma_1]} \mid \Psi_T\rangle = \prod_{j=1}^{N_p} \sum_{i=1}^{N} P_{ij}^F c_i^\dagger \mid 0\rangle$$

Weight for an Ising-field configuration $\longrightarrow$ fermionic determinant

$$\langle \Psi_T \mid \mathrm{e}^{-\Delta\tau \tilde{H}[\sigma_L]} \cdots \mathrm{e}^{-\Delta\tau \tilde{H}[\sigma_1]} \mid \Psi_T\rangle = \det P^T P^F$$

Further reading A. Muramatsu in *Quantum Monte Carlo Methods in Physics and Chemistry*, eds.: M.P. Nightingale and C.J. Umrigar, NATO Science series, Kluwer (1999).
F.F. Assaad in *Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms*, eds.: J. Grotendorst, D. Marx, and A. Muramatsu, NIC Series, Vol. 10 (2002).

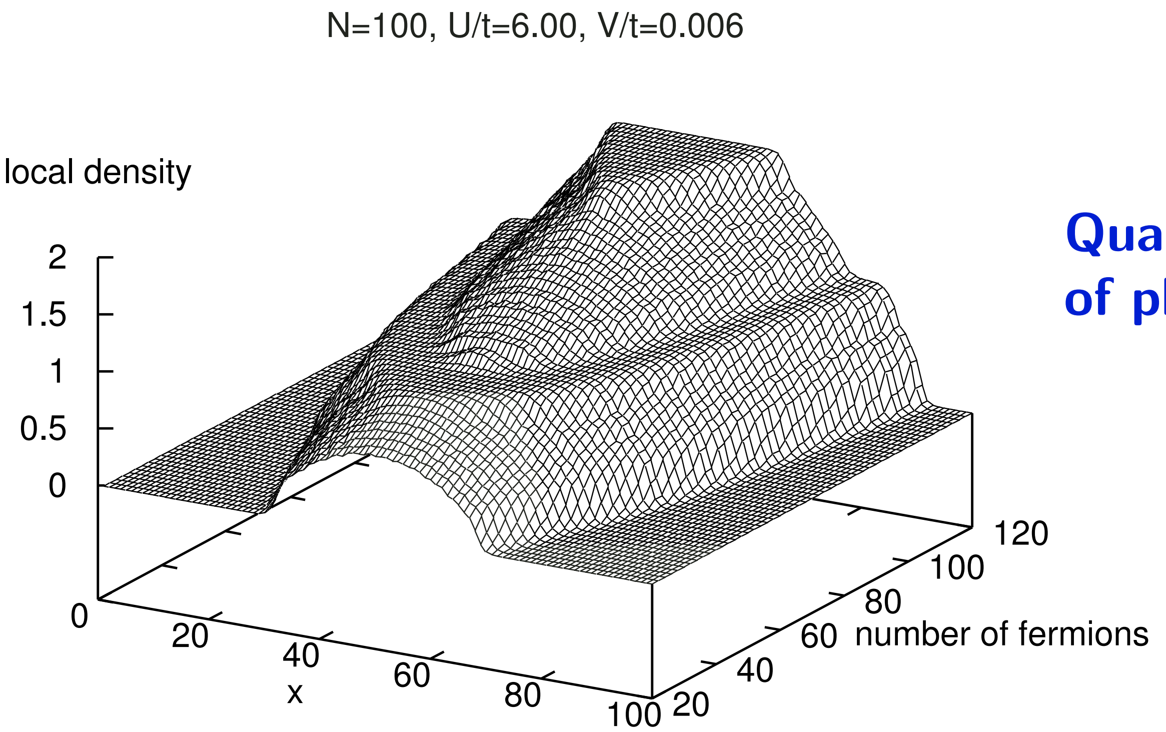
Local quantum criticality in confined fermions on optical lattices

M. Rigol, A.M., G.G. Batrouni, R.T. Scalettar, PRL **91**, 130403 (2003).

M. Rigol, A.M., Phys. Rev. A **69**, 053612 (2004).

$$H = -t \sum_{\substack{<i,j> \\ \sigma}} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{i} \left(i - \frac{N}{2} \right)^2 n_i$$

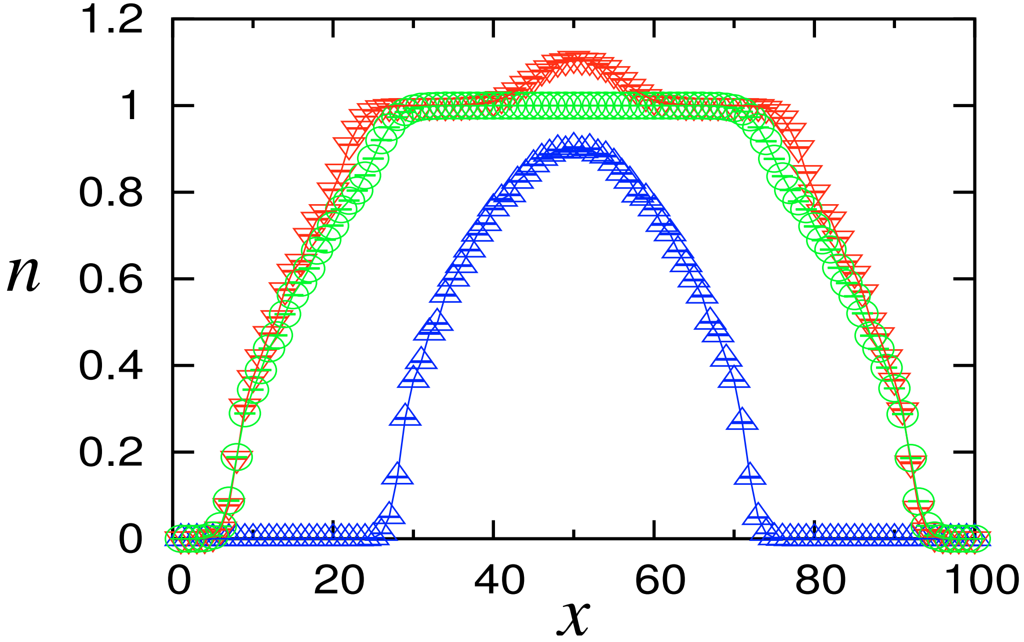
Density profile



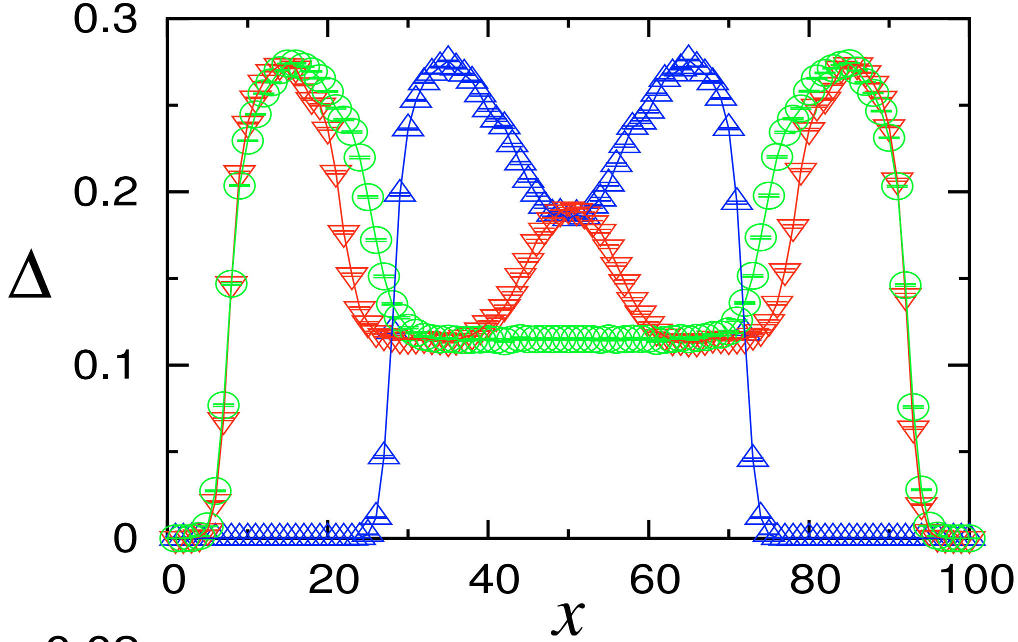
Quantitative characterization of phases?

Local order parameter

Density profile

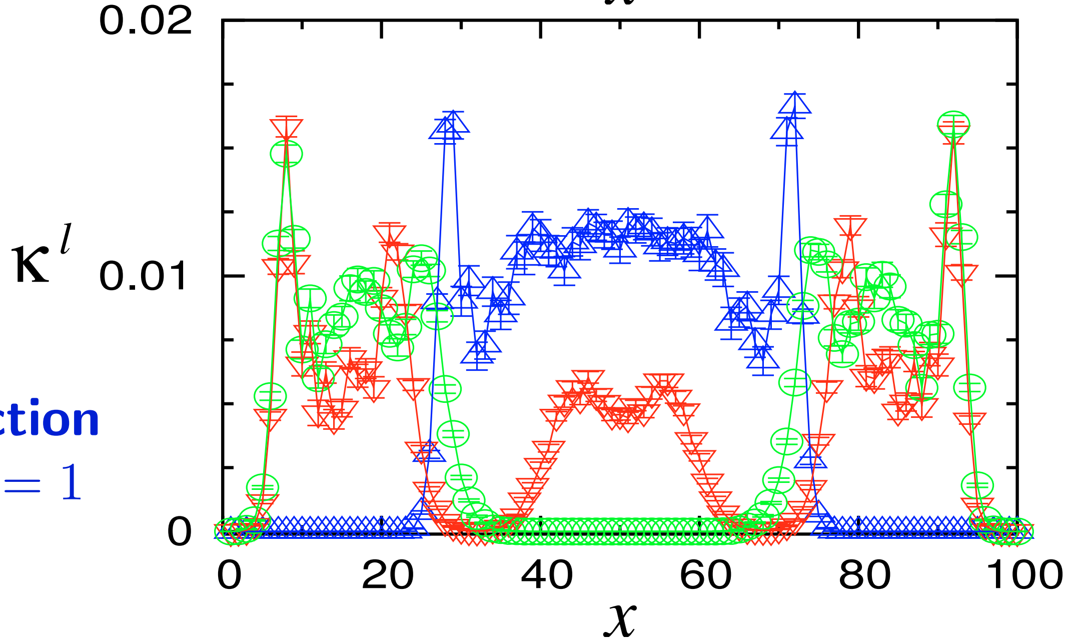


$\Delta \equiv < n^2 > - < n >^2$



Local compressibility

$$\kappa_i^\ell \equiv \sum_{|j| \leq \ell(U)} \chi_{i,i+j}$$

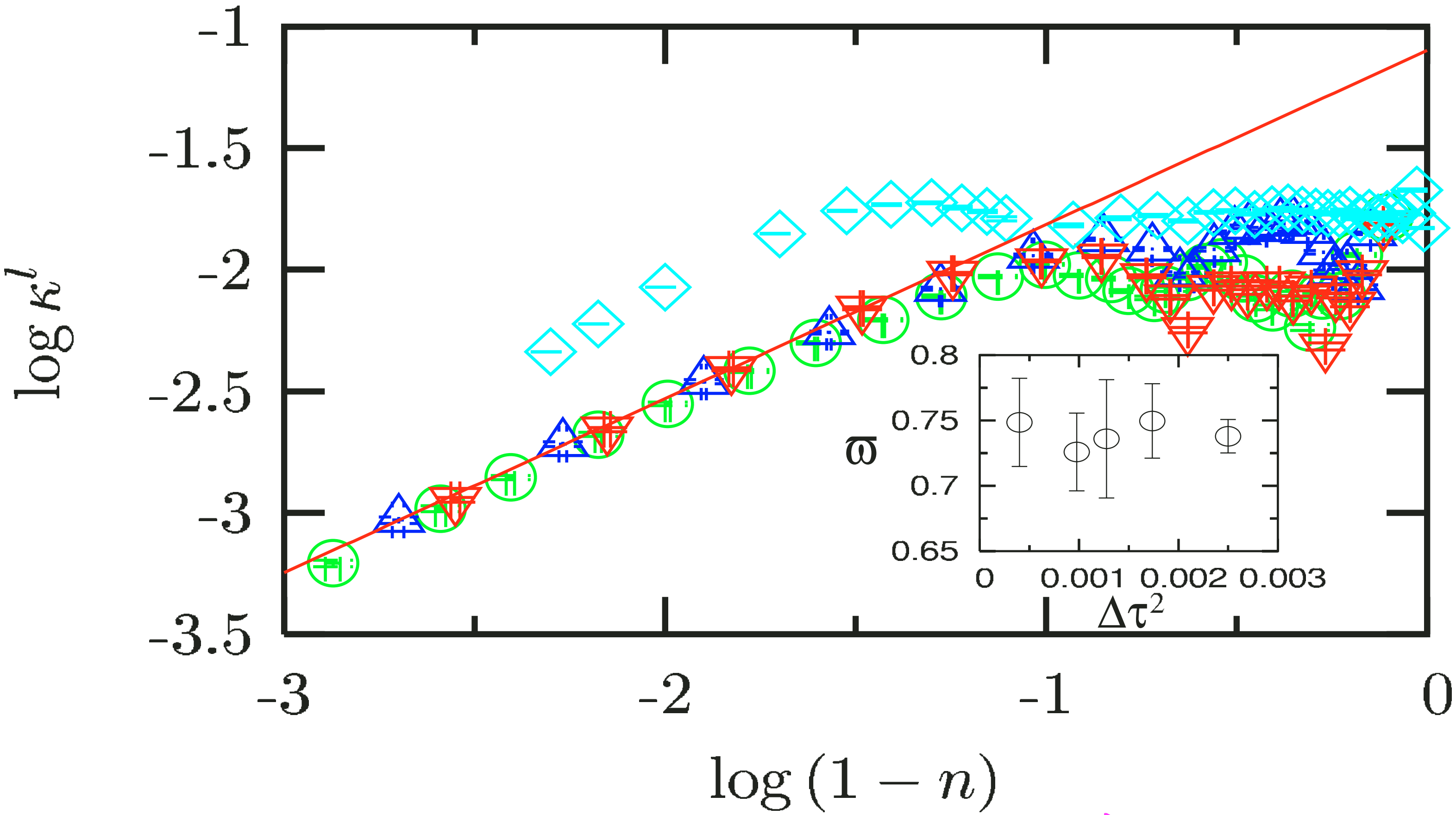


$\chi_{i,j}$: **Density-Density correlation function**

$\ell(U) \sim \xi(U)$: **Correlation length at** $n = 1$

Universality and local quantum critical behavior

Local compressibility κ^{ℓ} *vs.* $(1-n)$



△ $U = 8t$ **and** $V_2 = 0.0025t$

▽ $U = 6t$ **and** $V_2 = 0.0025t$

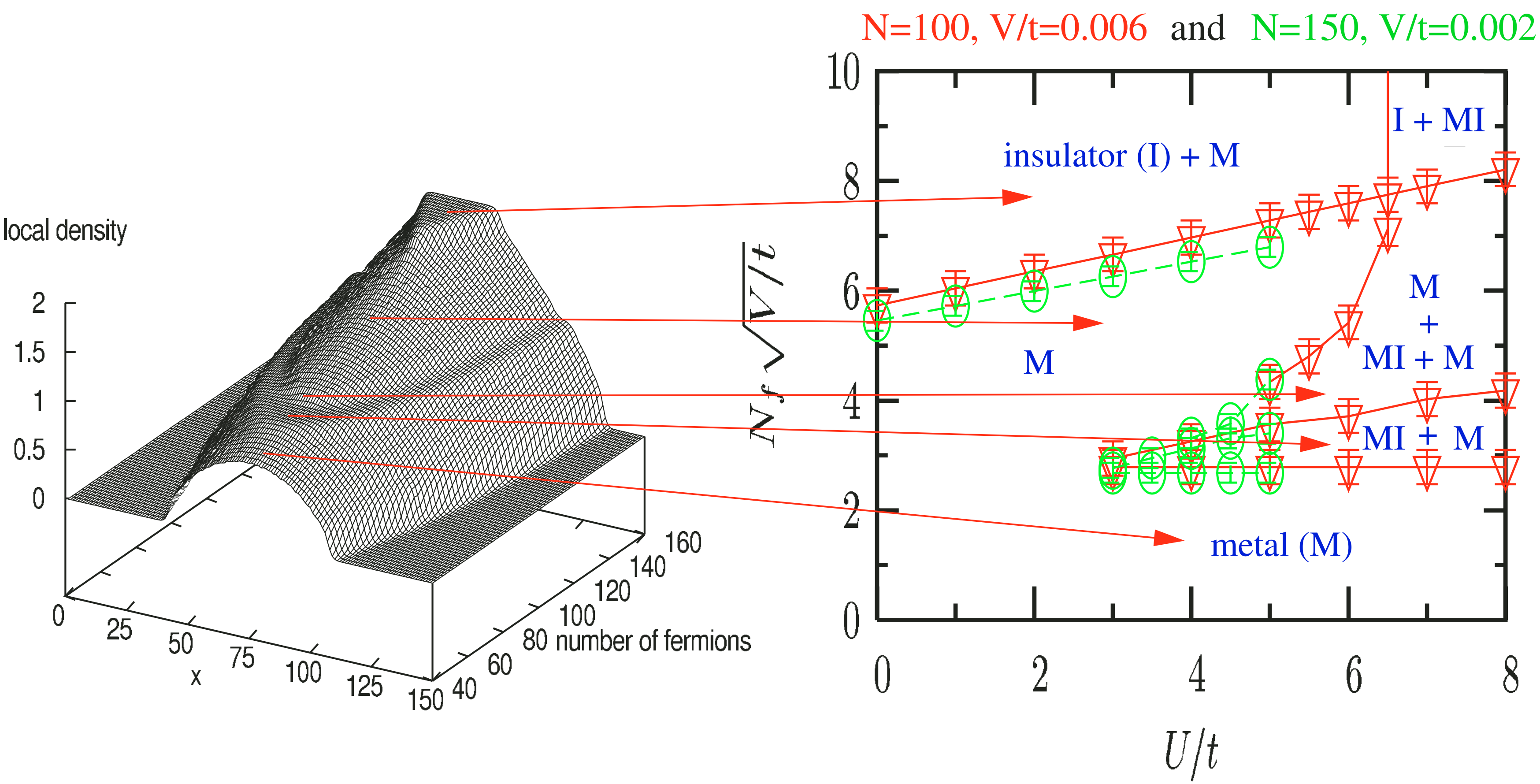
○ $U = 6t$ **and a quartic potential with** $V_4 = 10^{-6}t$

◇ **unconfined periodic system with** $U = 6t$.

$\kappa^{\ell} \sim (1-n)^{\varpi}$

where $\varpi \simeq 0.68 - 0.78$

Generic phase diagram



Characteristic density $N_f\sqrt{V/t} \longrightarrow$ generic phase diagram

Hard-core bosons in one dimension

Effective one-dimensional coupling

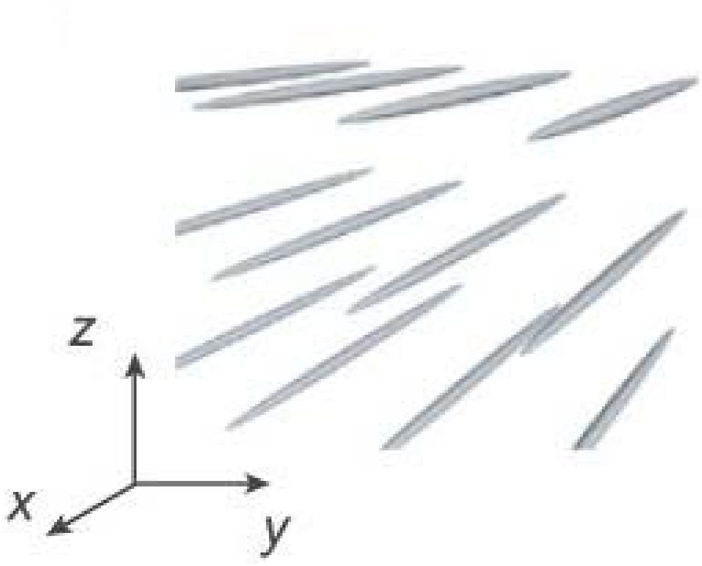
M. Olshanii, PRL **81**, 938 (1998)

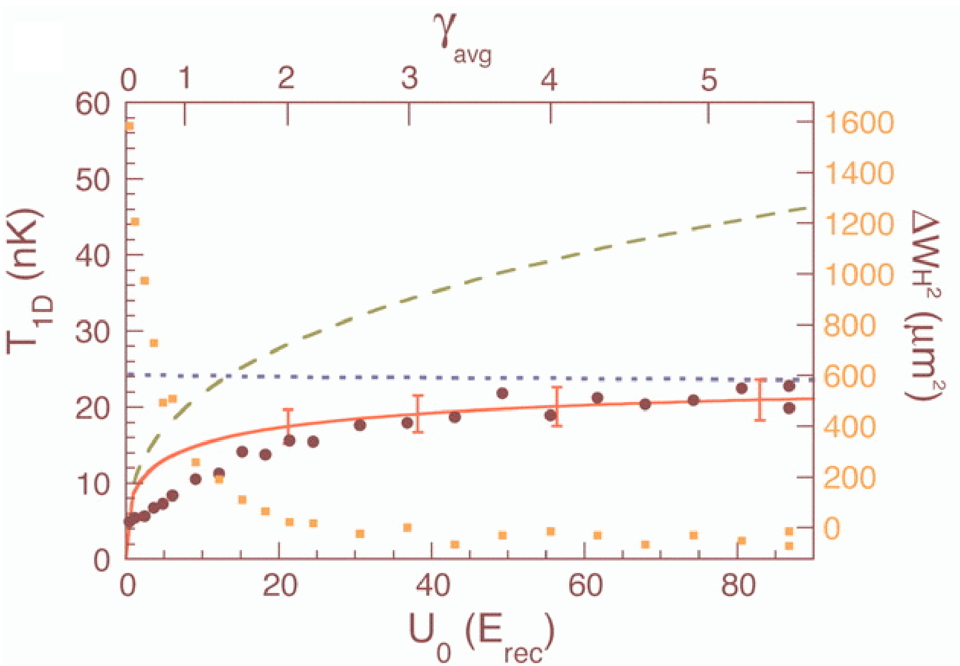
$$\gamma = \frac{E_{\rm int}}{E_{\rm kin}} = \frac{2am\omega_\perp}{n\hbar\left[1 - Ca\sqrt{\frac{m\omega_\perp}{2\hbar}}\right]}$$

Experimental realization

B. Paredes *et al.*, Nature **429**, 277 (2004)

T. Kinoshita, T. Wenger, and D.S. Weiss, Science **305**, 1125 (2004)





Exact numerics for hard-core bosons in one dimension

Hard-core bosons confined on a one-dimensional lattice

$$H = -t \sum_i \left(b_i^\dagger b_{i+1} + h.c. \right) + V_\alpha \sum_i x_i^\alpha \; n_i,$$

Bosonic operators with constraint

$$b_i^{\dagger 2} = b_i^2 = 0 \,, \quad \left[b_i, b_i^\dagger \right] = 1$$

Jordan-Wigner transformation

$$b_i^\dagger = f_i^\dagger \prod_{j=1}^{i-1} e^{-i\pi f_j^\dagger f_j} \,, \quad b_i = \prod_{j=1}^{i-1} e^{i\pi f_j^\dagger f_j} f_i \;\;,$$

Equivalent fermionic Hamiltonian

$$H = -t \sum_i \left(f_i^\dagger f_{i+1} + h.c. \right) + V_\alpha \sum_i x_i^\alpha \; n_i^f,$$

One-particle Green's function for hard-core bosons

$$G_{ij} = \langle \Psi^G_{HCB} | b_i b_j^\dagger | \Psi^G_{HCB} \rangle$$

$$= \langle \Psi^G_F | \prod_{\alpha=1}^{i-1} e^{i\pi f_\alpha^\dagger f_\alpha} f_i f_j^\dagger \prod_{\beta=1}^{j-1} e^{-i\pi f_\beta^\dagger f_\beta} | \Psi^G_F \rangle \ .$$

Evolution of a Slater determinant by a bilinear form

$$|\Psi^G_F\rangle = \prod_{\ell=1}^{N_f} \sum_{i=1}^{N} P_{i\ell} f_i^\dagger \ |0\rangle \quad \Rightarrow \quad e^{f_\alpha^\dagger A_{\alpha\beta} f_\beta} |\Psi^G_F\rangle = \prod_{\ell=1}^{N_f} \sum_{i=1}^{N} \tilde{P}_{i\ell} f_i^\dagger \ |0\rangle$$

Efficient exact evaluation of the Green's function

$$G_{ij} = \det\left[\left(\mathbf{P}'^A \right)^\dagger \mathbf{P}'^B \right] \ ,$$

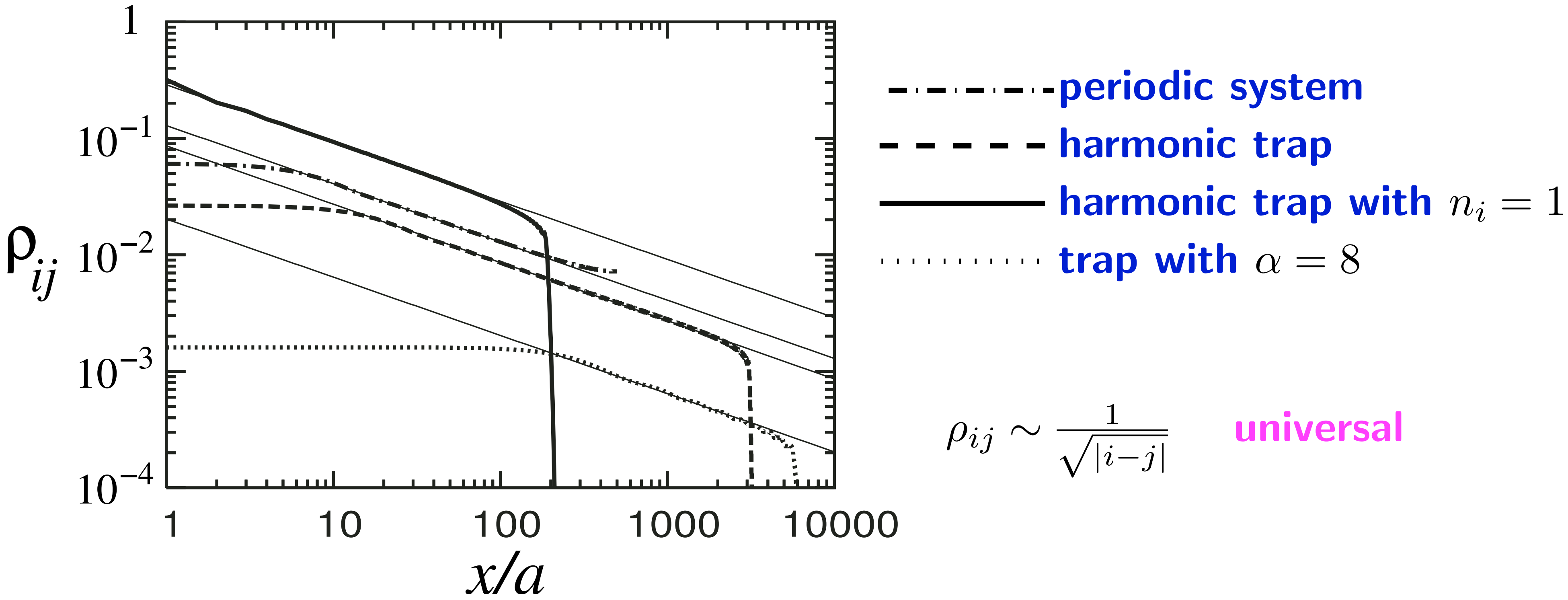
Universal properties of hard-core bosons confined on 1-D lattices

M. Rigol, A.M., Phys. Rev. A **70**, 031603(R) (2004); Phys. Rev. A **72**, 013604 (2005).

Hard-core bosons with confining potential V_α ($\alpha = 2, \ldots$)

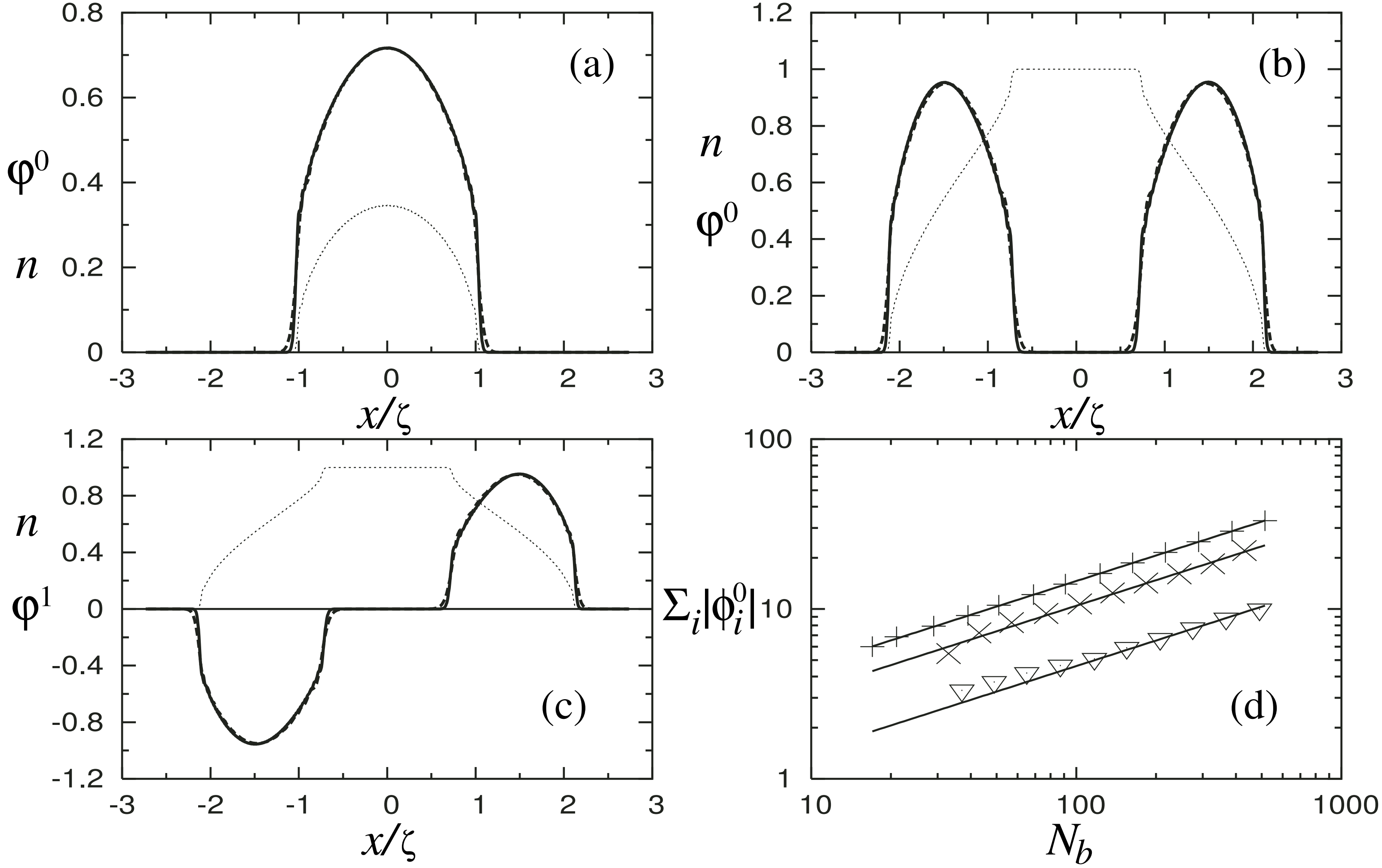
$$H = -t \sum_i \left(b_i^\dagger b_{i+1} + h.c. \right) + V_\alpha \sum_i x_i^\alpha \; n_i$$

Universal tail of the one-particle density matrix $\rho_{ij} = < b_i^\dagger b_j >$.



$\rho_{ij} \sim \frac{1}{\sqrt{|i-j|}}$ **universal**

Scaled natural orbitals and occupation of the lowest natural orbital



Scaled natural orbitals

Occupation of the lowest NO

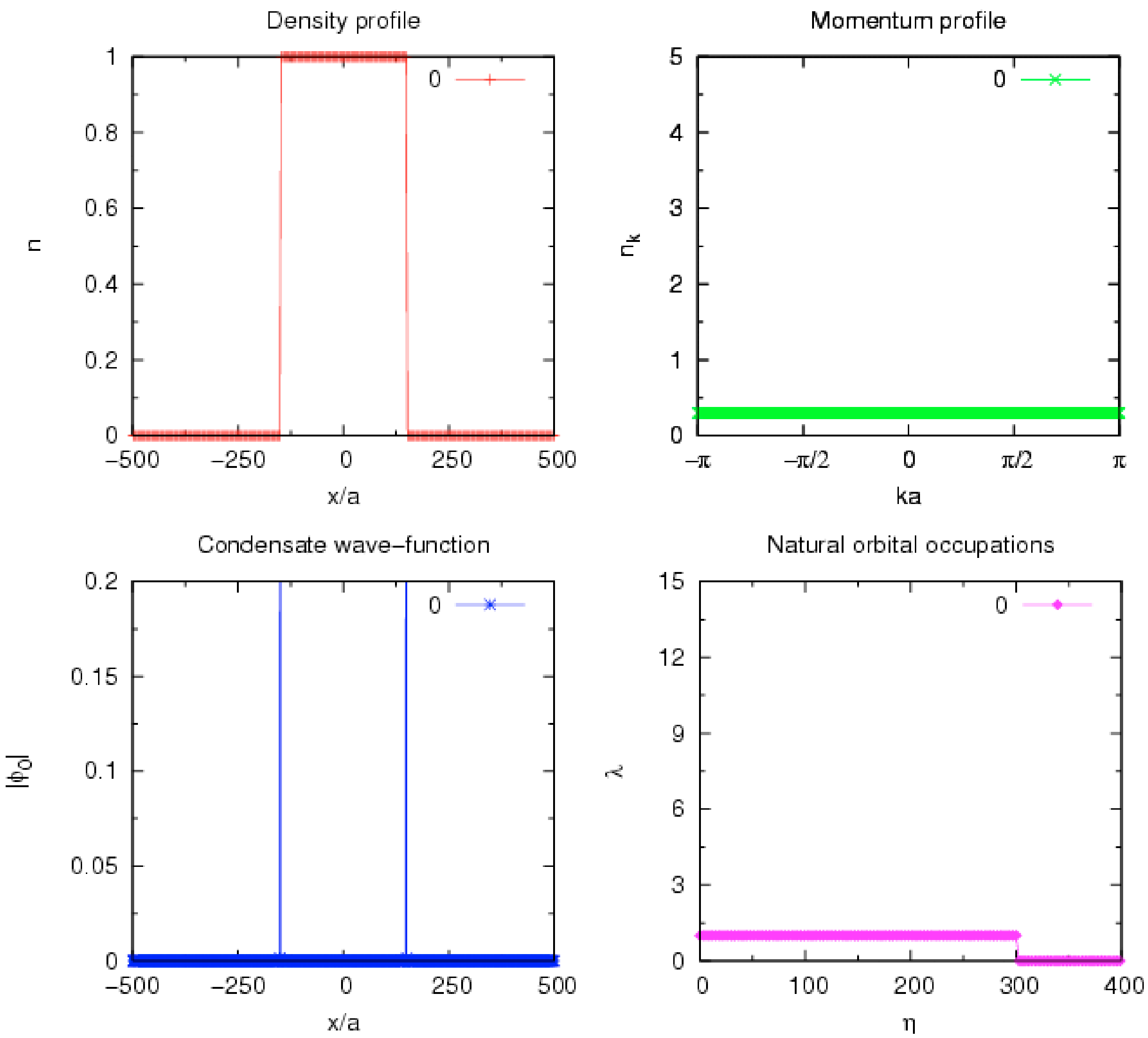
$$\varphi^0 = \left[N_b \left(V_\alpha/t\right)^{-1/\alpha}\right]^{\frac{1}{4}} \phi^0$$

$$\lambda_0 \sim \sqrt{N_b}$$

Emergence of quasi-condensates of HCB at finite momentum

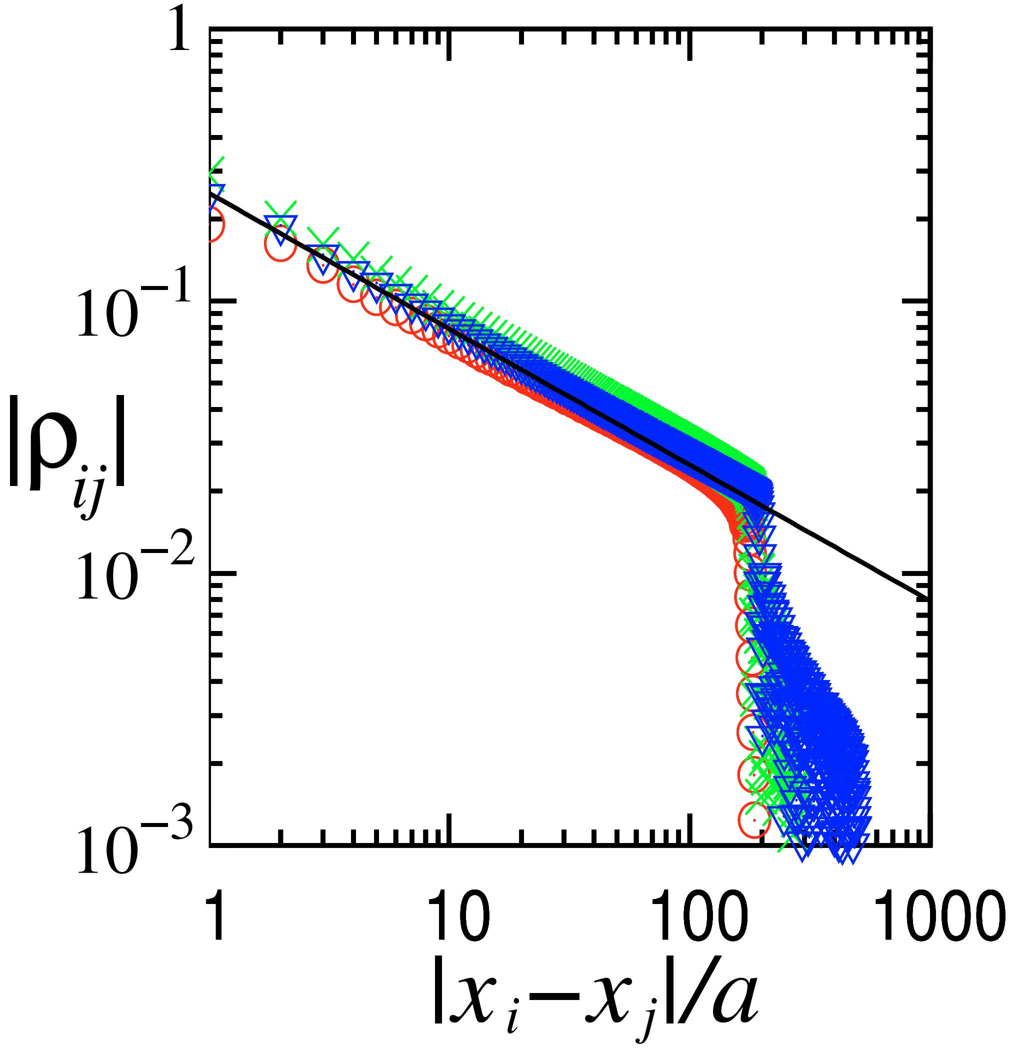
M. Rigol, A.M., Phys. Rev. Lett. **93**, 230404 (2004)

Evolution from a Fock state on a lattice



Quasi long-range order at finite momentum

Density matrix



$$\rho_{ij} \sim \frac{1}{\sqrt{|i-j|}}$$

$\Longrightarrow$ $\lambda_0 \sim \sqrt{N_b}$

$\Longrightarrow$ **Quasicondensate**

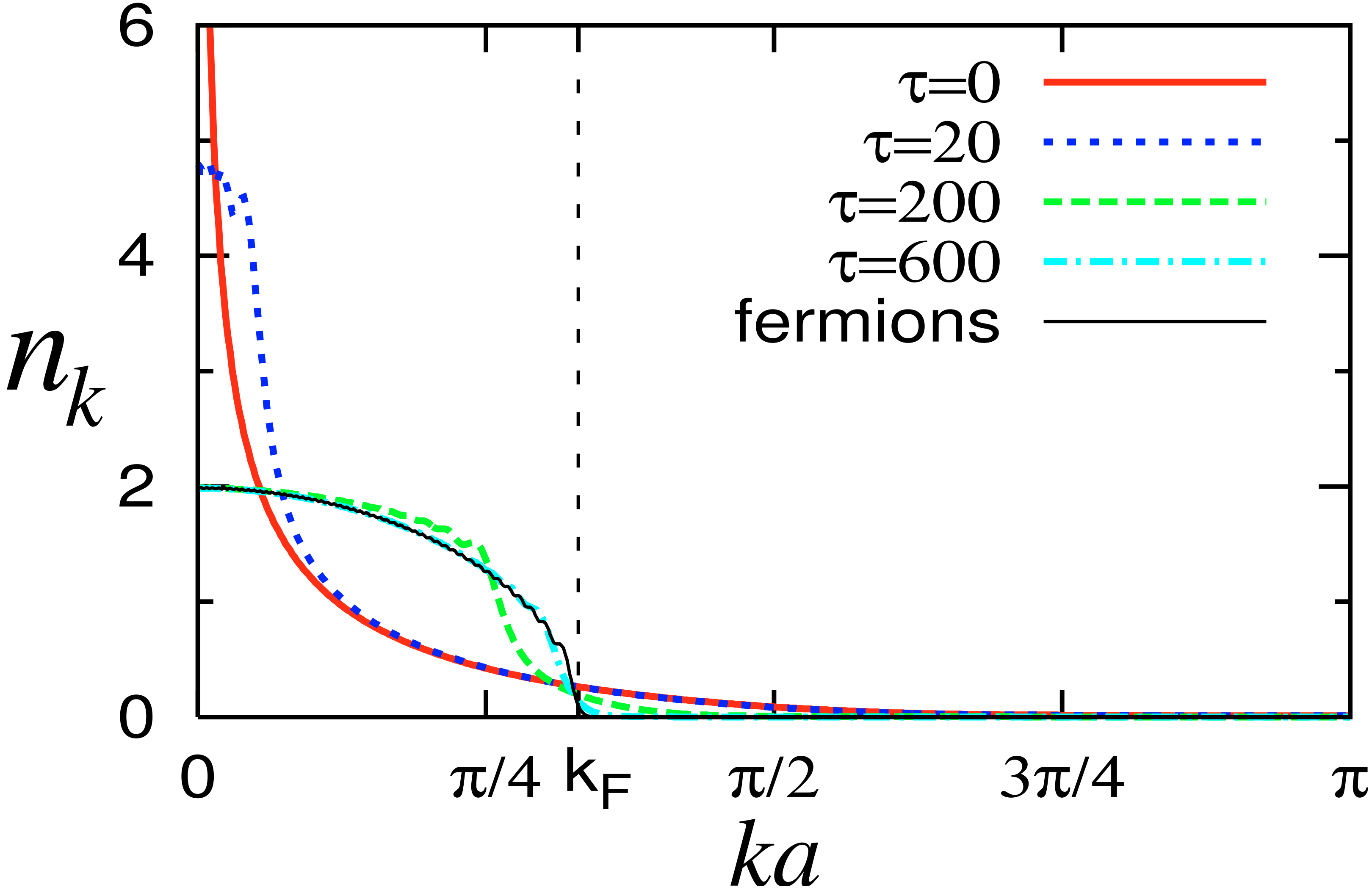
$\Downarrow$

Atomlaser

Fermionization in an expanding 1D gas of hard-core bosons

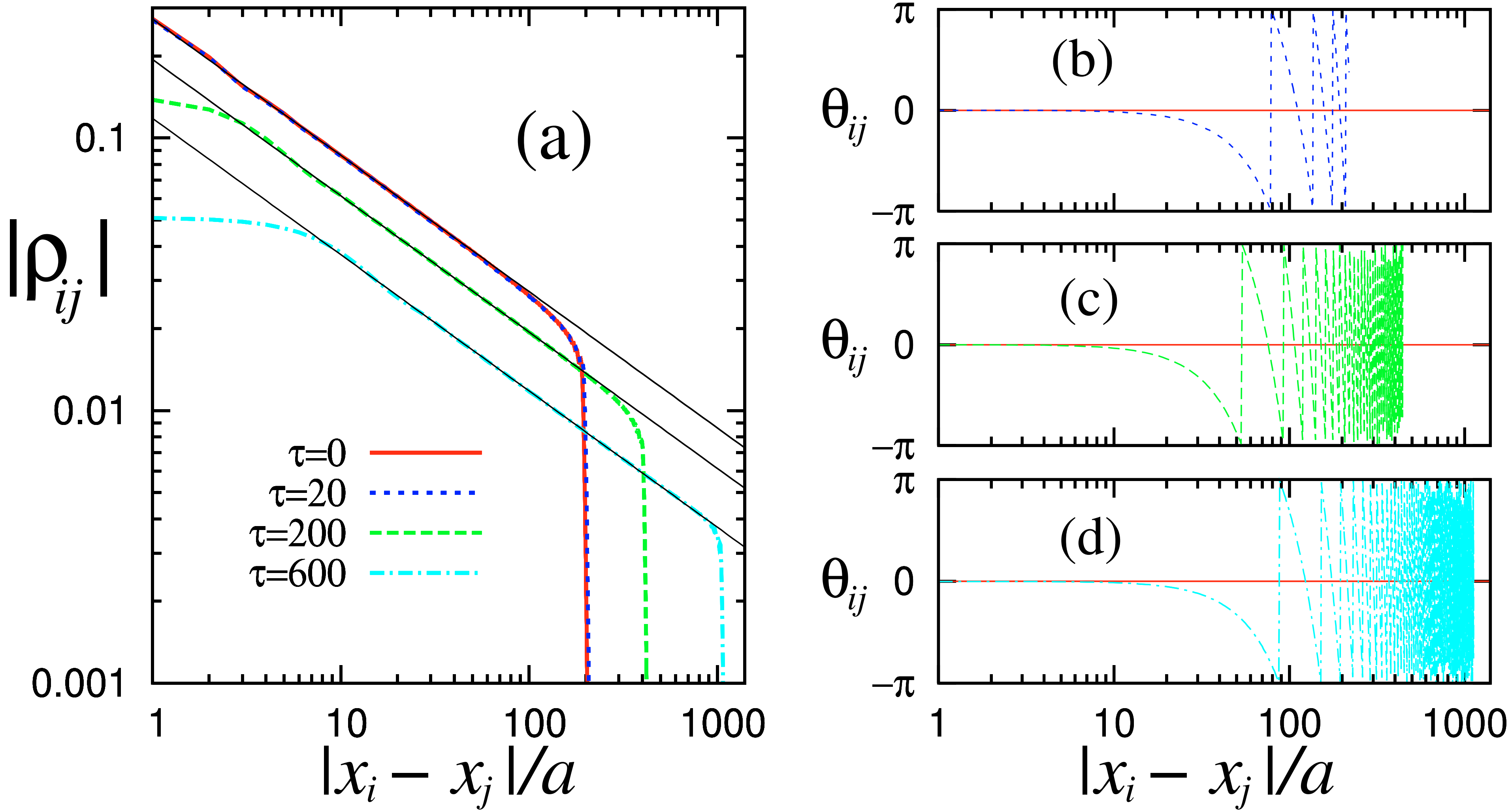
M. Rigol, A.M., Phys. Rev. Lett. **94**, 240403 (2005)

Evolution from a quasicondensate



Modulus and phase of the density matrix

Modulus **Phase**



Beyond hard-core bosons: Lanczos time evolution with DMRG

t-DMRG M.A. Cazalilla and J.B. Marston, PRL **88**, 256403 (2002).
G. Vidal, PRL **93**, 040502 (2004).
S.R. White and A.E. Feiguin, PRL **93**, 076401 (2004).
A.J. Daley, C. Kollath, U. Schollwöck, and G. Vidal, J. Stat. Mech.: Theor. Exp. P04005 (2004).
P. Schmitteckert, PR B **70**, 121302(R) (2004).

Lanczos time evolution

W: bandwidth of spectrum of H, assume $\Delta t\, W \ll 1$.

$$\hookrightarrow | \psi(t+\Delta t)\rangle = \mathrm{e}^{-iH\,\Delta t} \mid \psi(t)\rangle \simeq \sum_{n=0}^{m-1} \frac{(-i\Delta t)^n}{n!} H^n \mid \psi(t)\rangle$$

$$K_m = \mathrm{span}\left\{ | \psi(t)\rangle, H \mid \psi(t)\rangle, \ldots, H^{m-1} \mid \psi(t)\rangle \right\} \Longrightarrow$$ **Krylov subspace.**

$\hookrightarrow$ orthonormal basis $V_m = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\} \rightarrow L_m = V_m^T H V_m$ tridiagonal matrix

Time evolution

$$\mathrm{e}^{-iH\,\Delta t} \mid \psi\rangle \simeq V_m\, \mathrm{e}^{-iL_m\,\Delta t}\, V_m^T \mid \psi\rangle \equiv | \bar{\psi}\rangle$$

Exact error bound

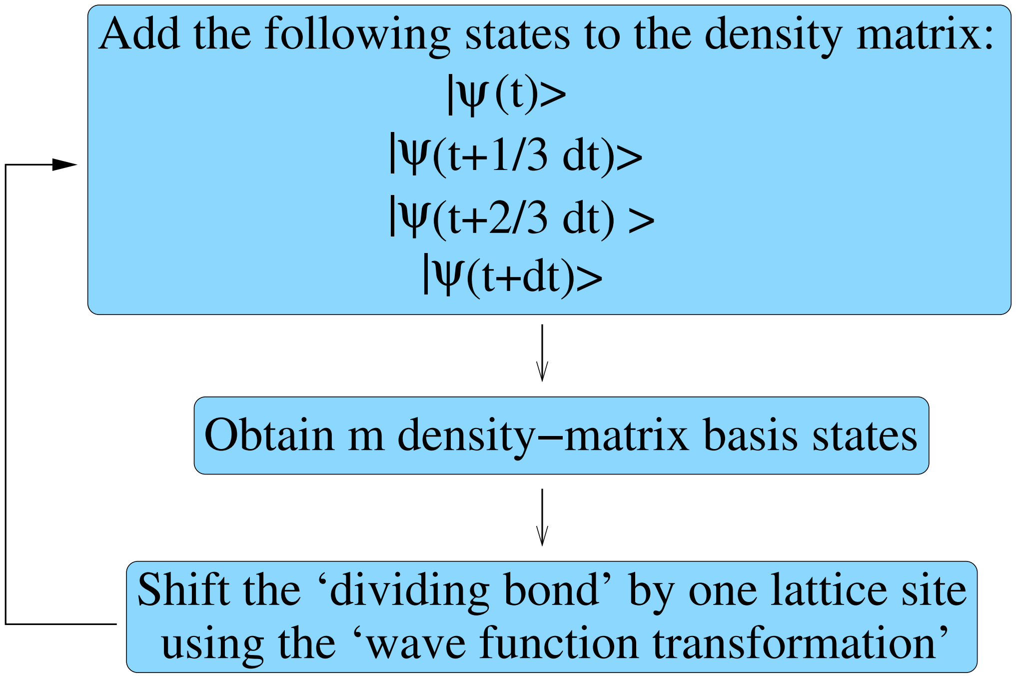
M. Hochbruck and Ch. Lubich, SIAM J. Numer. Anal. **34**, 1911 (1997)

$$\|\mathrm{e}^{-iH\,\Delta t}\mid\psi\rangle - \mid\bar{\psi}\rangle\| \leq 12\,\mathrm{e}^{-\frac{(W\,\Delta t)^2}{16m}}\left(\frac{eW\,\Delta t}{4m}\right)^m\,, \qquad m \geq \frac{W\,\Delta t}{2}$$

$\hookrightarrow$ **almost exponential convergence** $\longrightarrow\ \sim \Delta t^m$

Adaptive DMRG basis for the time evolution

A.E. Feiguin and S.R. White, cond-mat/0502475



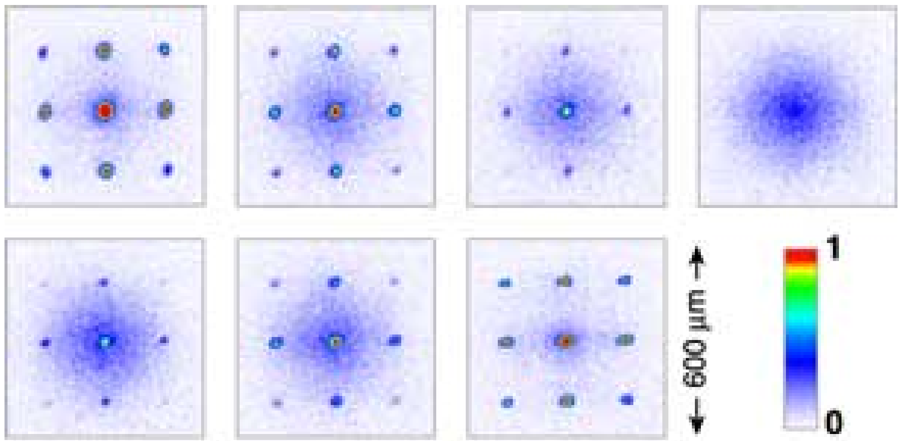
Evolution performed with Lanczos approximation

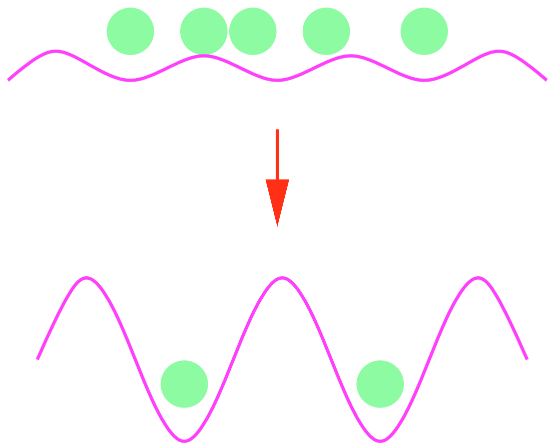
Collapse and revival of a Luttinger liquid

Motivation

Collapse and revival of a Bose-Einstein condensate

M. Greiner, O. Mandel, T.W. Hänsch, and I. Bloch, Nature **419**, 51 (2002)





For fermions

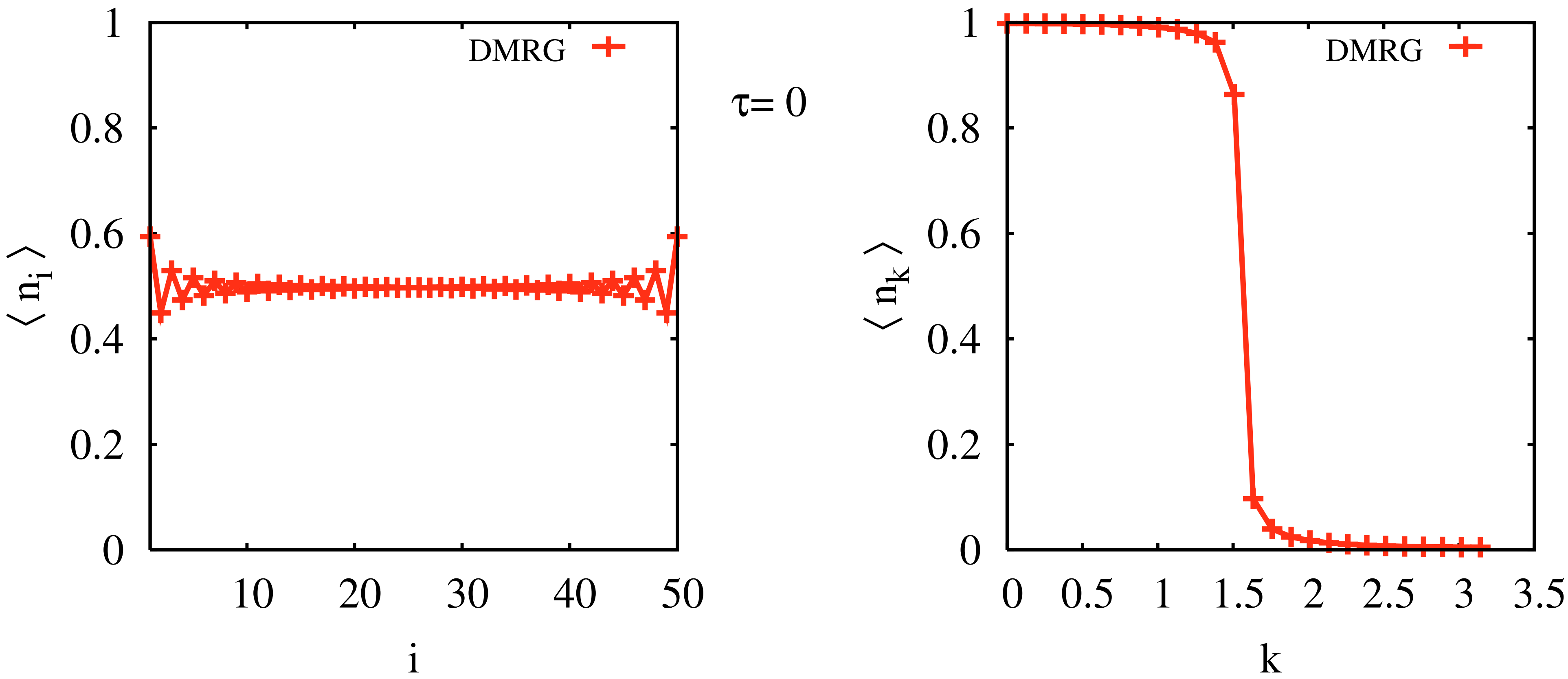
$$H = -t \sum_i \left(f_i^\dagger f_{i+1} + h.c. \right) + V \sum_i n_i n_{i+1}$$

$V < 2t \longrightarrow$ **metal,** $V > 2t \longrightarrow$ **insulator**

Time evolution with Lanczos + DMRG with basis adaption

S.R. Manmana, A.M., and R.M. Noack, cond-mat/0502396

L=50, OBC, V(τ=0) = 0.5t, V(τ>0) = 100t (DMRG with m=50 states)



Summary

Ultracold atoms confined on optical lattices

$\Downarrow$

Realizations of new states of matter

Numerical simulations for the ground-state and nonequilibrium dynamics of strongly correlated quantum systems

- **Universality and scaling in traps**
- **Emergence of coherence from a Fock state**
  $\hookrightarrow$ **Matter laser tunable through an optical lattice**
- **Fermionization through expansion**
- **Collapse and revival of coherence in quantum gases**