# Path Integral Monte Carlo calculations of atomic Bose gases

Markus Holzmann, LPMMC, CNRS UGA Grenoble

**Outline:**

- Thermodynamics of quasi 2D atomic gases
- Linear response from imaginary time dynamics
- Out-of equilibrium real time dynamics:
  Time dependent variational Monte Carlo

# Quantum Many-Body Problem

Condensed Matter

Hamiltonian:
(non relativistic)

$$H = \sum_{i=1}^{N} \left[ -\frac{\hbar^2 \nabla_i^2}{2m} + u(\mathbf{r}_i) \right] + \sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|)$$

$$H\Psi_n(\mathbf{R}) = E_n \Psi_n(\mathbf{R})$$

position/ spin variables:

$$\mathbf{R} \equiv \{\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots \mathbf{r}_N\sigma_N\}$$

Bosons: symmetric under permutations

$$\Psi_n(P\mathbf{R}) = (\pm 1)^{|P|} \Psi_n(\mathbf{R})$$

$$P\mathbf{R} \equiv \{\mathbf{r}_{P(1)}\sigma_{P(1)}, \mathbf{r}_{P(2)}\sigma_{P(2)}, \ldots\}$$

Fermions: anti-symmetric

T=0: ground state observables, e.g. energy $E_0$

$$E_0(N) \leq E_T(N) \equiv \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

finite T thermodynamics: density matrix

$$\rho(\mathbf{R}, \mathbf{R}', T) = \frac{1}{Z} \sum_n \Psi_n^*(\mathbf{R}') \Psi_n(\mathbf{R}) e^{-E_n/T}$$

electron gas (2D, 3D)
liquid $^3He$

metallic hydrogen

ultracold atomic gases

# Observation of Pair Condensation in the Quasi-2D BEC-BCS Crossover

M. G. Ries,[1,*] A. N. Wenz,[1] G. Zürn,[1] L. Bayha,[1] I. Boettcher,[2] D. Kedar,[1] P. A. Murthy,[1]
M. Neidig,[1] T. Lompe,[1,†] and S. Jochim[1]

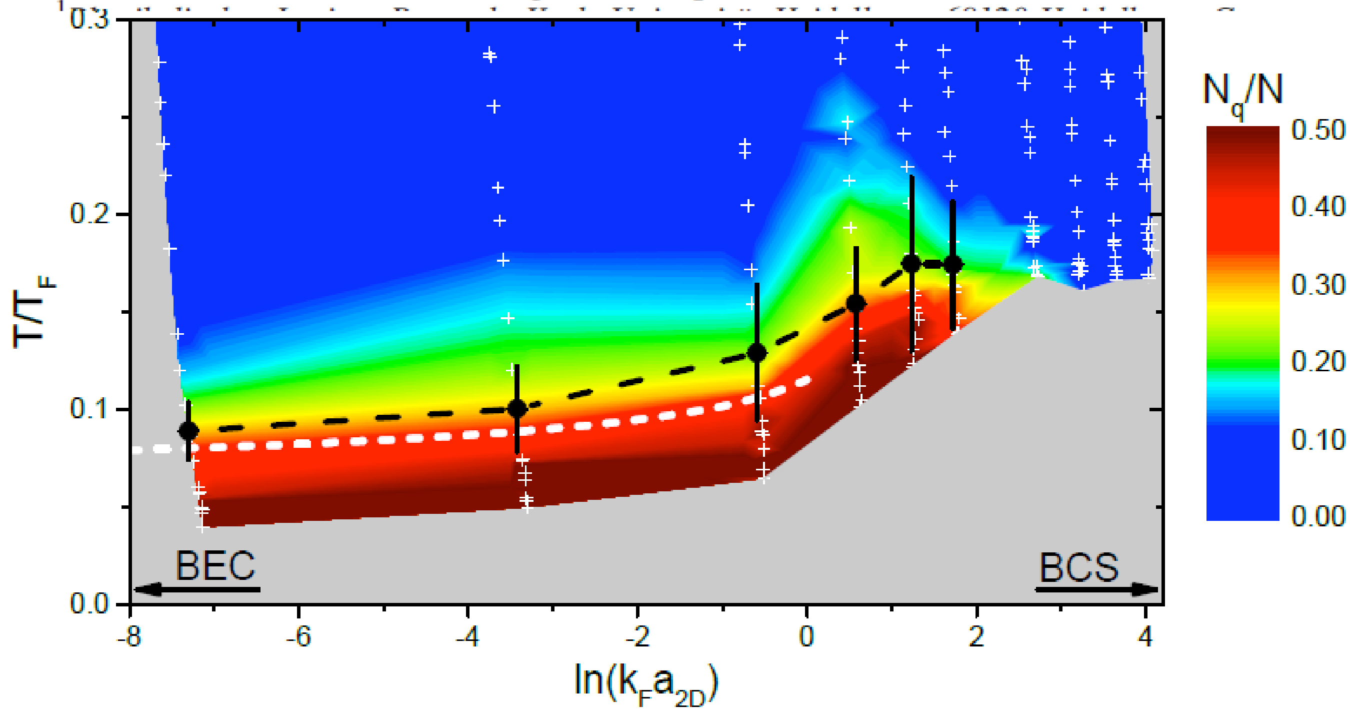



FIG. 4: **Phase diagram of the strongly interacting 2D Fermi gas.** The experimentally determined critical temperature $T_c/T_F$ is shown as black data points and the error bars indicate the statistical errors. Systematic uncertainties are discussed in detail in [27]. The color scale indicates the non-thermal fraction $N_q/N$ and is linearly interpolated between the measured data points (white crosses). Each data point is the average of about 30 measurements. The dashed white line is the theoretical prediction for the BKT transition temperature given in [40].

# Characteristics of 2D physics at T>0:

- any temperature T>0 — Mermin, Wagner, Hohenberg (1966-68)

  absence of long-range order ↔ no BEC

- low temperture $T<T_{KT}$ — Berezinskii (1971)

  algebraic correlations $g_1(r) \sim r^{-\eta}$

  T dependent exponent $\eta(T)$

  superfluidity, superfluid density $\rho_s$

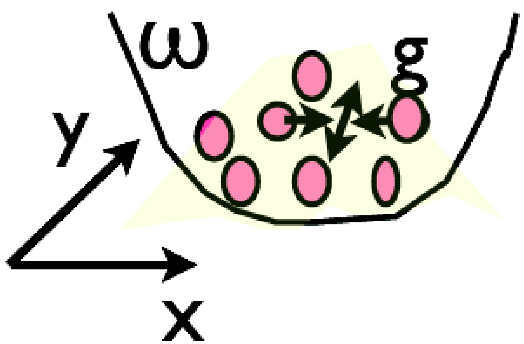
- phase transition at $T_{KT}$ — Kosterlitz, Thouless (1973)

  universal exponent: $\eta_{KT} = 1/4$

  universal jump of the superfluid density: $\rho_s = \frac{2mT_{KT}}{\pi}$

**enourmous finite size effects ⇨ macroscopic systems needed**

# Ultracold atomic gases:




$\omega$: trap frequency
g: interaction constant
N: number of Bosons

quasi2D: $\omega_z >> \omega_x \approx \omega_y$

$g \sim (\log na^2)^{-1}$ for hard disks of diameter a

- trapping potential: density variation vs algebraic order
- interaction: BEC vs KT
- confining potential: quasi2D vs anisotropic 3D
- mesoscopic atom number: small vs big
- Fermions vs Bosons: particles vs quasi-particles

cross-over between different regimes

⇨ quantitative studies needed (and possible)

# QMC simulations of Bosons: A successful story

based on Feynman's path integral representation of the N-particle density matrix

$$\rho(\mathbf{R},\mathbf{R}') = \frac{1}{Z}\langle \mathbf{R}|e^{-\beta H}|\mathbf{R}'\rangle \qquad \langle \mathbf{R}|e^{-\beta H}|\mathbf{R}'\rangle \equiv \int d\mathbf{R}_2\,\langle \mathbf{R}|e^{-\beta H/2}|\mathbf{R}_2\rangle\langle \mathbf{R}_2|e^{-\beta H/2}|\mathbf{R}'\rangle$$

Bosons: $\rho_B(\mathbf{R},\mathbf{R}') = \frac{1}{Z_B}\frac{1}{N!}\sum_P (+1)^P \rho(\mathbf{R},P(\mathbf{R}'))$ $\quad \mathbf{R} \equiv (\mathbf{r}_1,\mathbf{r}_2,\ldots \mathbf{r}_N)$

## Path Integral Monte Carlo:

use M>>1 discretizations («time slices»): $\tau = \beta/M \rightarrow 0$

use of high temperature approximation, e.g. : (position representation → positive!) $\langle R|e^{-\tau H}|R'\rangle \simeq \langle R|e^{-\tau T}|R'\rangle\, e^{-\tau V(R')}$

Do random walk in extended position space (M x d x N coordinates) and permutation space (N! permutations)

Ceperley, Pollock, Boninsegni, Svistunov, Prokof'ev,...

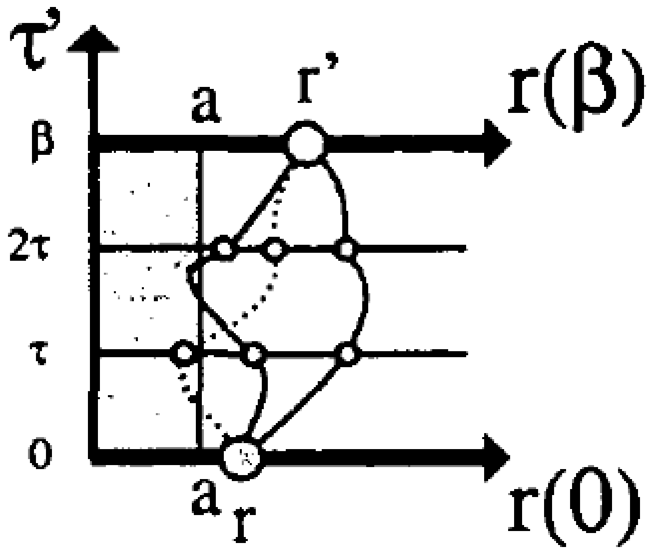
Zero temperature variants:

Ground State Path Intetgral, Diffusion, Reptation,... Monte Carlo

# Simulating dilute degenerate gas:

$$a_s n^{1/d} \sim a_s/\lambda_T \ll 1$$

Collision between 2 particles, thermal wavelength $\lambda_T$
(relative space): hard core a (= scattering length $a_s$), density: n




Path-discretization needed to see potential

$$\tau \lesssim \frac{ma^2}{\hbar^2}$$

Huge number of slices are needed for dilute gas

$$M = \frac{\beta}{\tau} \gg \frac{\lambda_T^2}{a^2} \sim 1/n^{2/d}a^2$$

How to be efficient for $a \ll n^{-1/d}$ ?

- Use soft pseudopotential $a \sim n^{-1/d}$
- Use hard pseudopotential and pair density matrix

Pre-solve 2-body problem exactly
$$g_2(\mathbf{r},\mathbf{r}',\tau) = \frac{\langle \mathbf{r}| e^{-\tau(p^2/m+V)} |\mathbf{r}'\rangle}{\langle \mathbf{r}| e^{-\tau(p^2/m)} |\mathbf{r}'\rangle}$$

Pair-particle approximation: $\langle \mathbf{R}| e^{-\tau H} |\mathbf{R}'\rangle \simeq \prod_{i=1}^{N} \rho_1(\mathbf{r}_i,\mathbf{r}'_i;\tau) \prod_{j<i} g_2(\mathbf{r}_{ij},\mathbf{r}'_{ij},\tau)$

$M \gtrsim n\lambda_T^d$  Analytical expression: M.H.,Y.Castin, EPJD 7, 425 (1999)

# Quasi2D Bose gases

direct comparison between experiment and exact QMC calculations possible

S.P. Rath, T. Yefsah, K.J. Günter, M. Cheneau, R. Desbuquois, M.H., W. Krauth, J. Dalibard,
Phys. Rev. A 82, 013609 (2010)

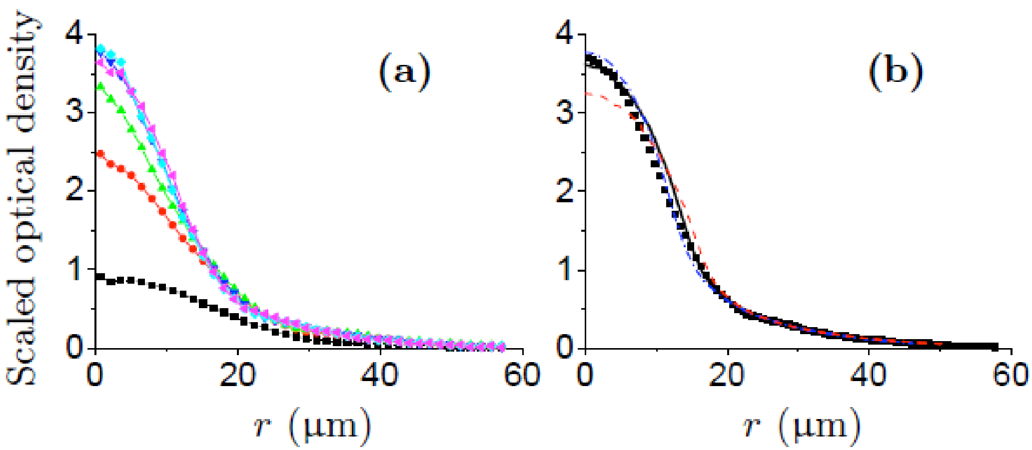



FIG. 4: (Color online) (a) Optical density profiles obtained for a TOF duration $t = 0$ (black), 3 (red), 6 (green), 10 (blue), 12 (cyan), 14 (magenta) ms and rescaled to their in-situ value according to (1). (b) Squares: Optical density profile obtained by averaging the results of (a) for $10 \leq t \leq 14$ ms, yielding fit parameters $T = 94$ nK, $\alpha = 0.36$ for $\xi = 0.63$. Lines: QMC results for the same fit parameters (continuous, $N = 42000$), and for those deduced assuming $\xi = 0.47$ [dashed red, $(T\ (\text{nK}), \alpha, N) = (104, 0.39, 57600)$] and $\xi = 0.79$ [dash-dotted blue, $(87, 0.33,\ 32100)$].

density profiles compared using scale invariance in 2D time-of-flight exapnsion

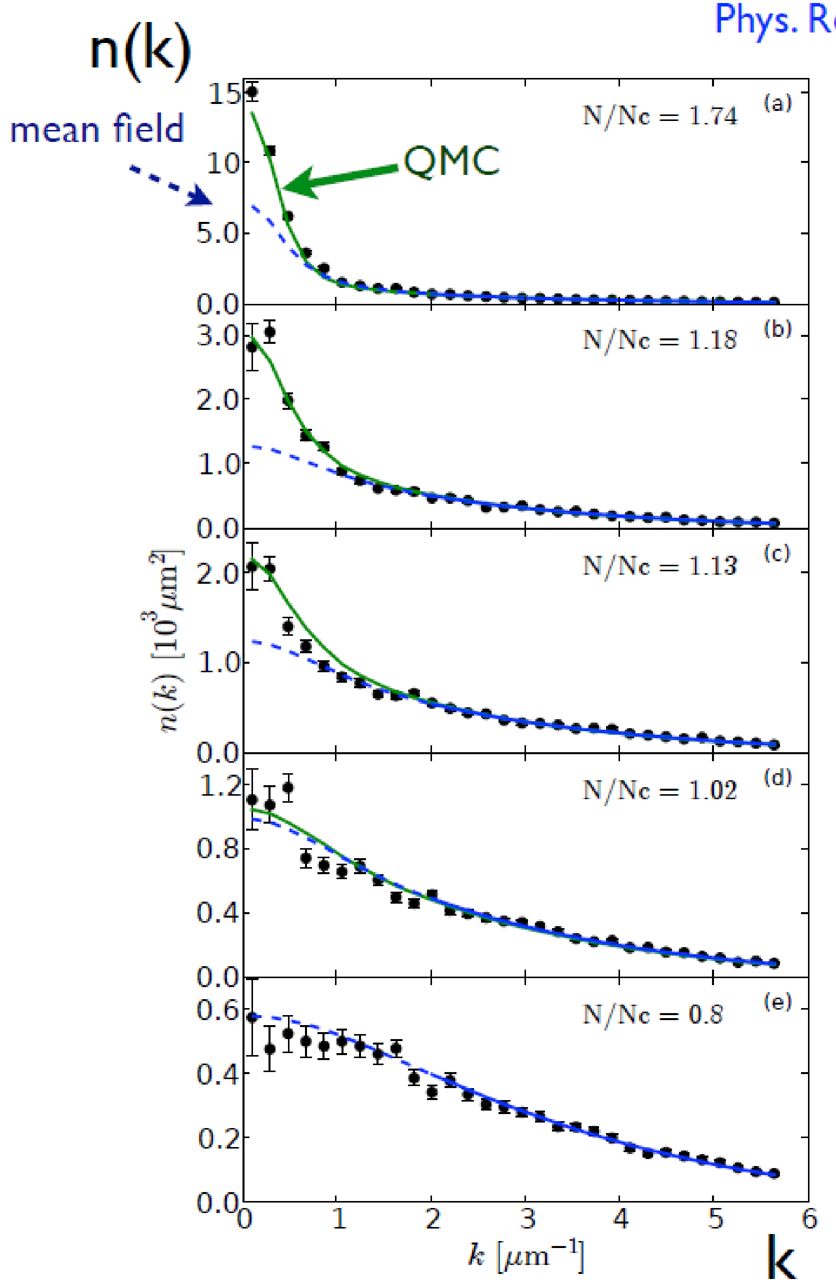
density profile after 2D time-of-flight given by scaling transform

$$n(\mathbf{r}, t) = \nu_t^2 n(\nu_t \mathbf{r})$$

$$\nu_t = (1 + \omega^2 t^2)^{-1/2}$$

# Non-local probe for: Momentum profile n(k)

T. Plisson, B. Allard, M. H., G. Salomon, A. Aspect, P. Bouyer, and T. Bourdel
Phys. Rev. A 84, 061606(R) (2011)




## 3D Time of flight expansion (TOF):

- time evolution of the density operator

$$\rho(t) = e^{-iHt/\hbar}\rho(t=0)e^{iHt/\hbar}$$

- strong confinement in z (quasi 2D)
  - ⇒ large initial momentum in z
  - ⇒ rapid expansion in z
- slow expansion for in-plane density x/y

$$H_{TOF} \approx \sum_i \frac{p_{ix}^2 + p_{iy}^2}{2m}$$

⇒ TOF density ≅ momentum dist., n(k),

for long TOF-time t

# Theory (QMC) ↔ Experiment: Coherence properties

T. Plisson, B. Allard, M. H., G. Salomon, A. Aspect, P. Bouyer, and T. Bourdel
Phys. Rev. A 84, 061606(R) (2011)

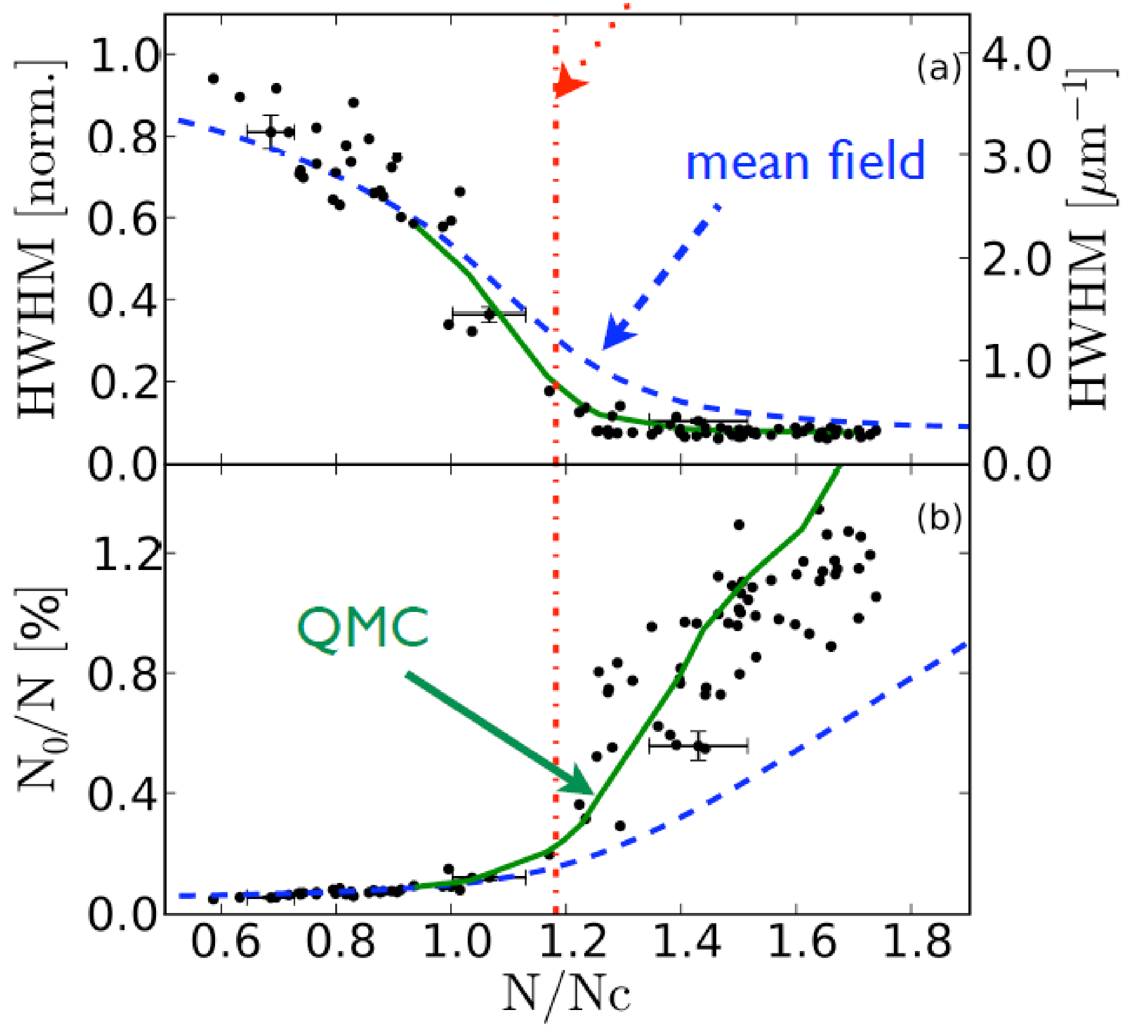
Kosterlitz-Thouless transition: $N_{KT}$

Characterization of Coherence (Peak around k=0):

Width of the peak: HWHM

Height of the peak:

Fraction of particles in k=0 peak: $N_0/N$



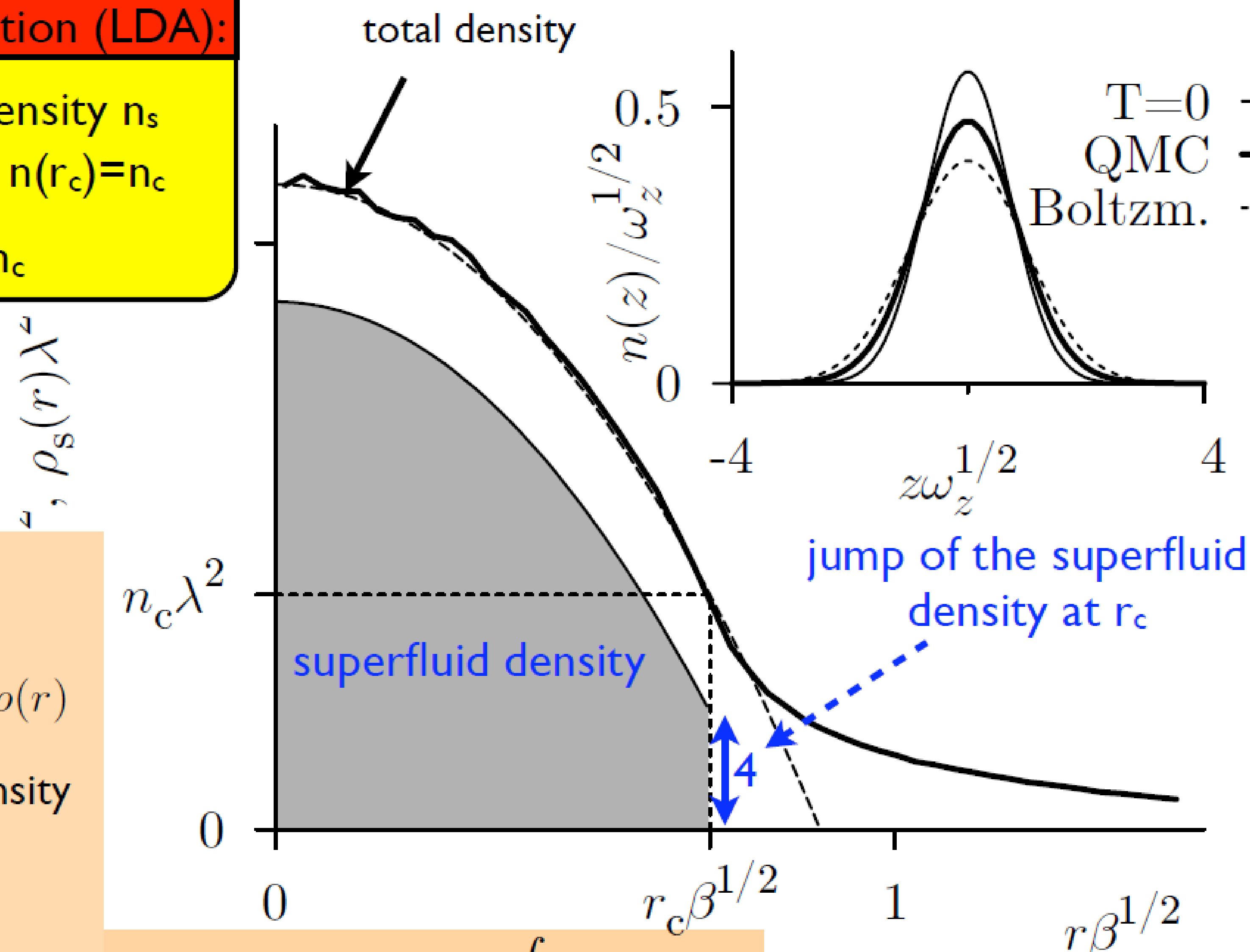

$N/N_c = (T/T_c)^{-2}$

# Superfluid properties (LDA)

**Local density approximation (LDA):**

jump in the superfluid density $n_s$ where density is critical $n(r_c)=n_c$

KT: $n_s\lambda^2 = 4$ at $n_c$




moment of inertia I:

classical: $I_{cl} = \int d\mathbf{r}\, r^2 \rho(r)$

below $T_c$: only normal density

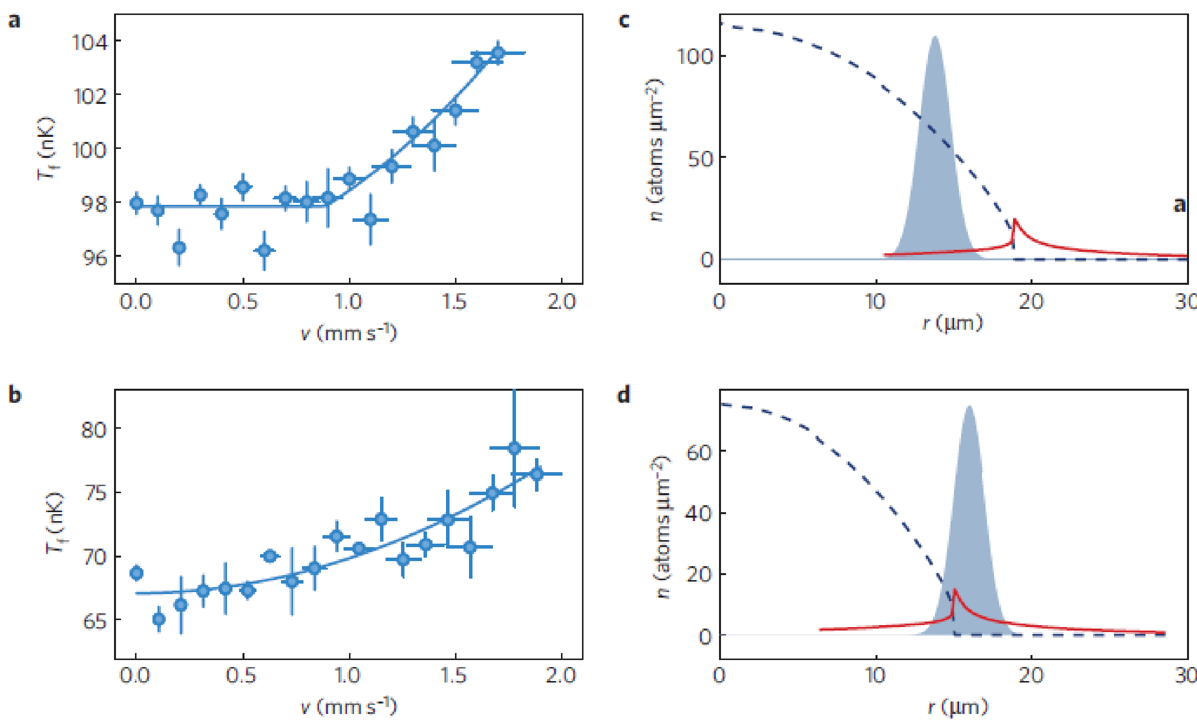
$$I = \int d\mathbf{r}\, r^2 \rho_n(r)$$

non-classical moment of Inertia (NCMI): $I_{cl} - I = \int d\mathbf{r}\, r^2 \rho_s(r)$

M. H., W. Krauth, PRL 100, 190402 (2008)

# Local superfluid probe: stirring experiment

R. Desbuquois, L. Chomaz, T. Yefsah, J. Léonard, J. Beugnon, C. Weitenberg, and J. Dalibard,
Nature Physics 8, 645 (2012)




Step-like behavior in the local critical velocity as a function of the local chem. potential

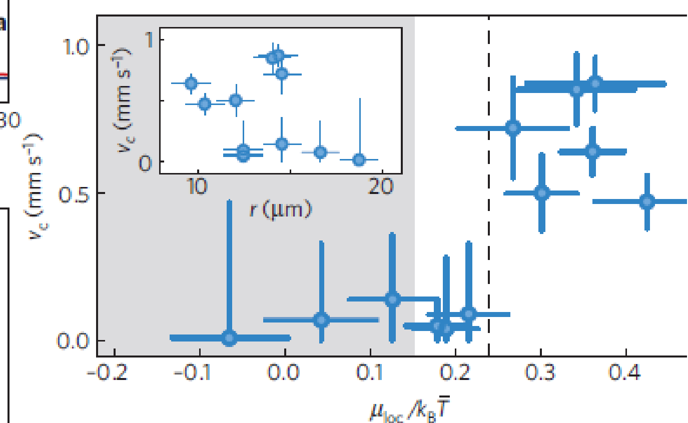


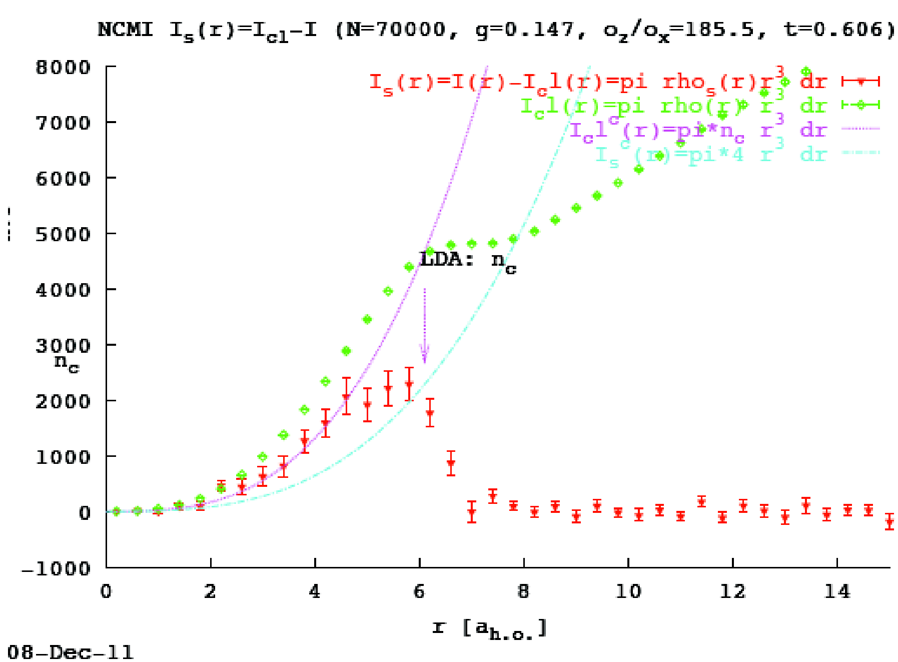

**Figure 2 | Evidence for a critical velocity.** Two typical curves of the temperature after stirring the laser beam at varying velocities. **a**, In the superfluid regime, we observe a critical velocity (here $v_c = 0.87(9)$ mm s$^{-1}$), below which there is no dissipation. **b**, In the normal regime, the heating is quadratic in the velocity. The fitted heating coefficients are $\kappa = 18(3)$ nK s mm$^{-2}$ and $\kappa = 26(3)$ nK s mm$^{-2}$ in **a** and **b**, respectively. The experimental parameters are $(N, \bar{T}, \mu, r) = (87{,}000, 89\text{ nK}, k_B \times 59\text{ nK}, 14.4\text{ µm})$ and $(38{,}000, 67\text{ nK}, k_B \times 39\text{ nK}, 16.6\text{ µm})$ for **a** and **b**, respectively, yielding $\mu_{loc}/k_B\bar{T} = 0.36$ and $\mu_{loc}/k_B\bar{T} = 0.04$. The data points are the average of typically ten shots. The $y$ error bars show the standard deviation. The $x$ error bars denote the spread of velocities along the size of the stirring beam ($1/\sqrt{e}$ radius). The solid line is a fit to the data according to equation (1). The stirring time is 0.2 s for all data points. Note that the three low-lying data points in **a** correspond to the completion of an odd number of half turns. For these data points, where we see a downshift of the temperature by approximately 1.5 nK, we also observe a displacement of the centre of mass of the cloud by a few micrometres. **c**,**d**, Calculated radial density distribution for the clouds in **a** and **b**, respectively. The dashed blue curve shows the superfluid density, the solid red curve shows the normal density. The stirring beam potential is indicated by the grey shaded area (in arbitrary units). The densities are calculated via the local density approximation from the prediction for an infinite uniform system[16]. The jump of the superfluid density from zero to a universal value of $4/\lambda_{dB}^2$ (where $\lambda_{dB}$ is the thermal de Broglie wavelength) is a prominent feature of the BKT transition. The normal density makes a corresponding jump to keep the total density continuous.

# Local superfluid density: QMC

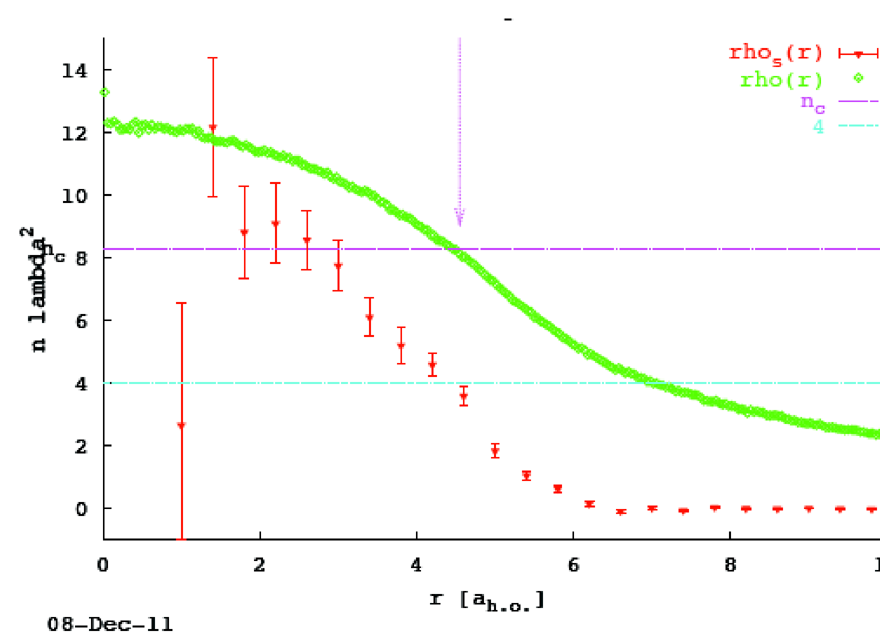
«local» moment of inertia I(r)
from linear response to local field coupled to momentum density

classical «local» moment of intertia $I_{cl}(r)$ from local total density

non-classical «local» moment of intertia $I_{ncmi}(r)=I_{cl}(r)-I(r)$



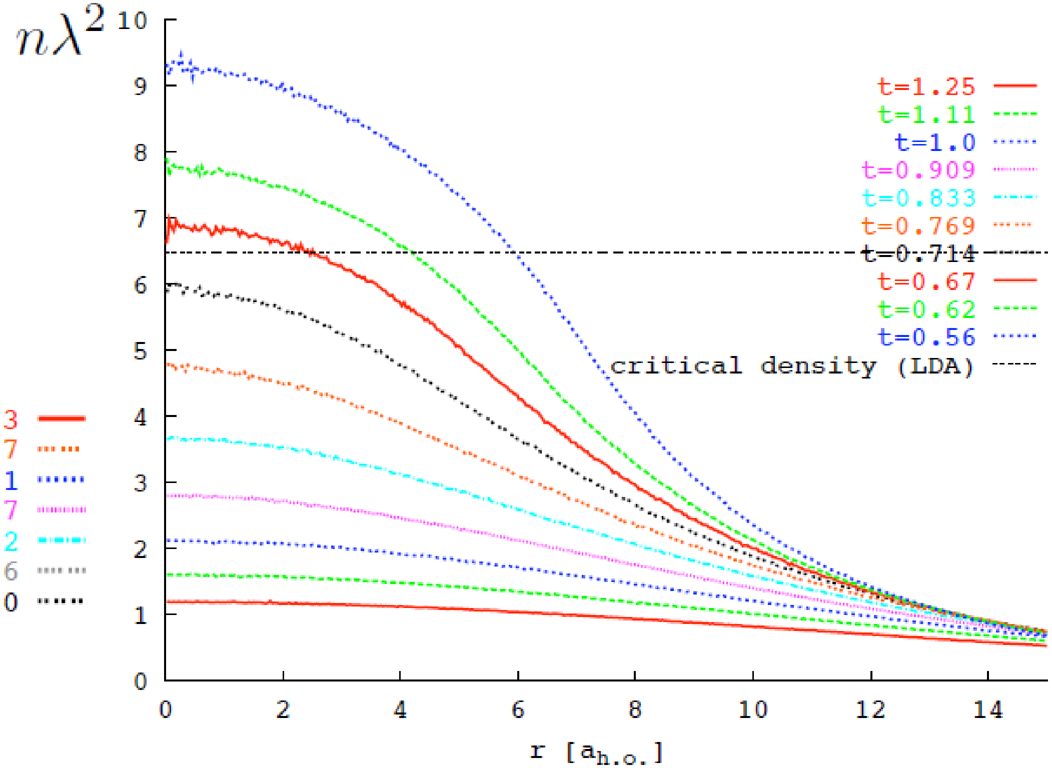

«local» superfluid density
from $I_{ncmi}(r)= n_s(r)\ r^2$



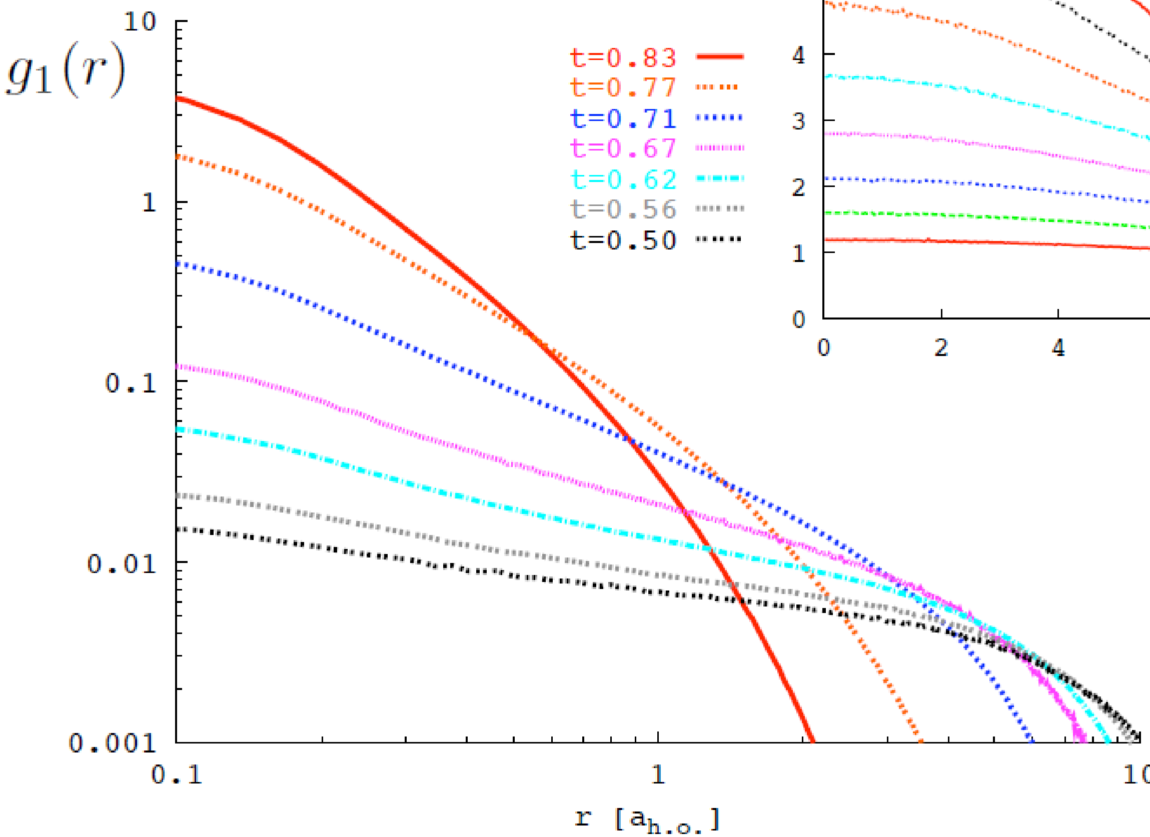
# Kosterlitz-Thouless: algebraic order

- density profile: $T_{KT}$ from phase space density + LDA

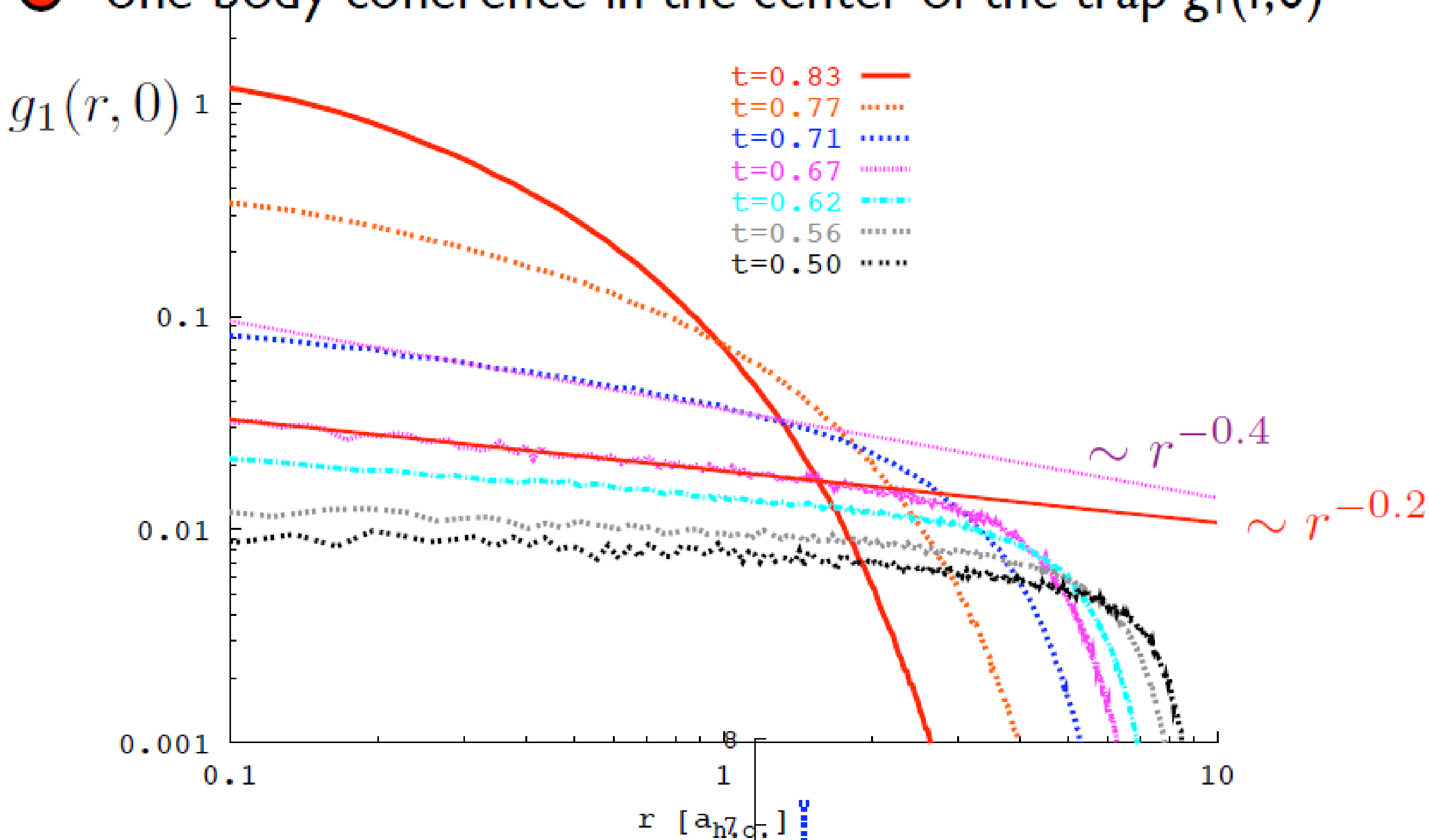
$$N = 29500, \quad \tilde{g} = 0.60, \quad \omega_z/\omega = 310$$



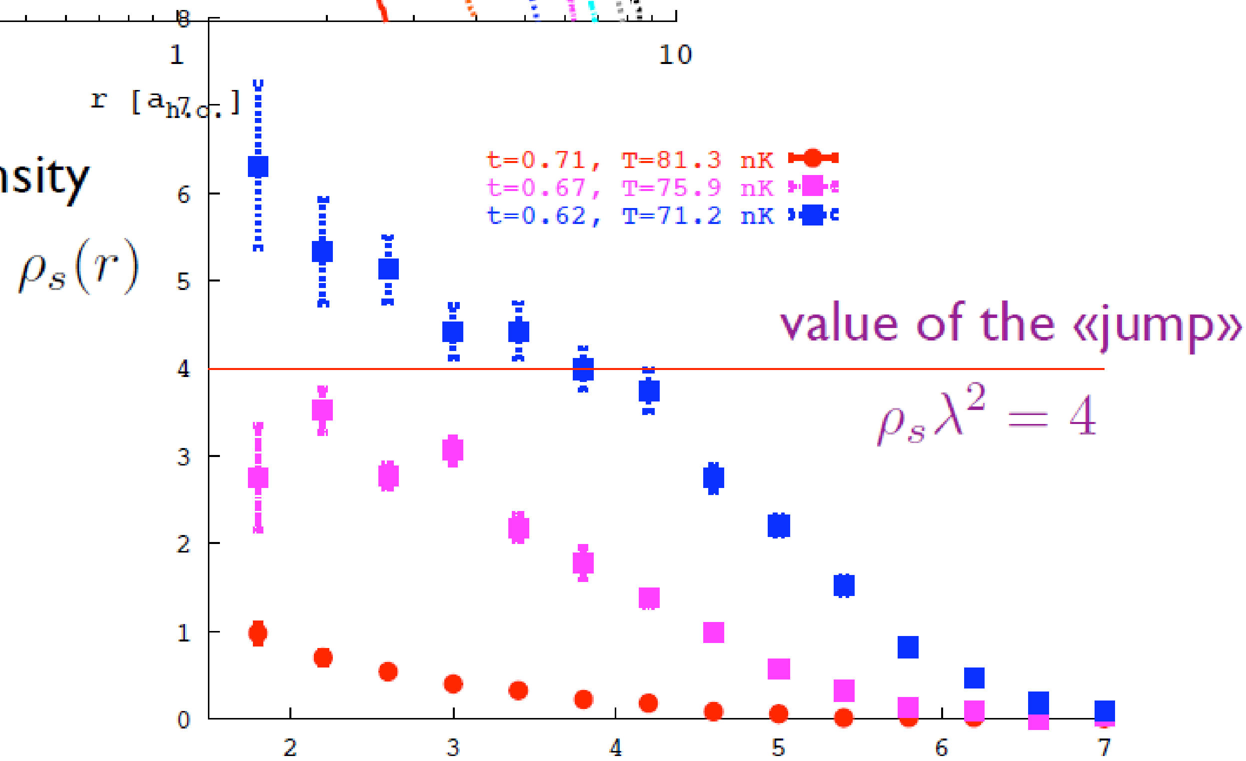

- one-body coherence (trap averaged)



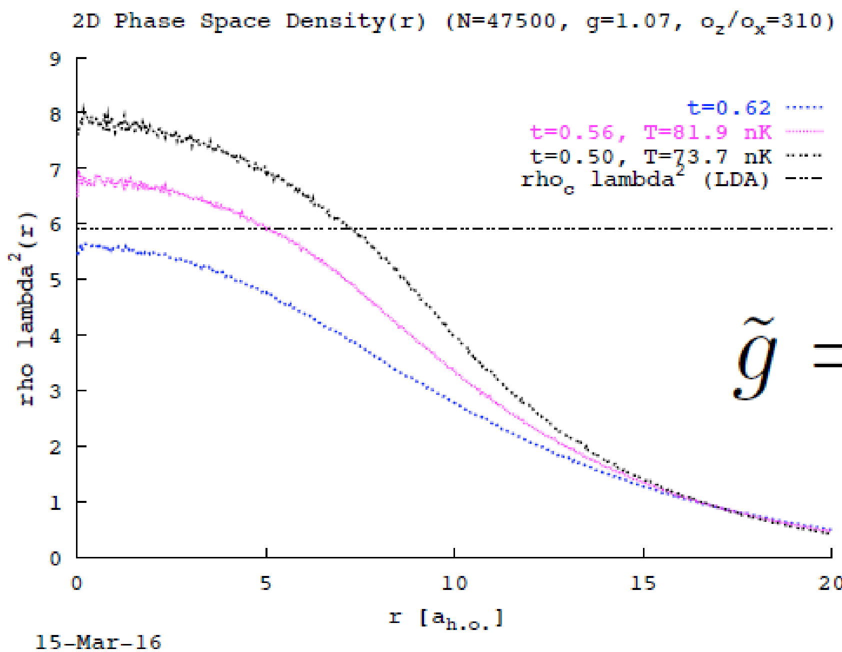
- one-body coherence in the center of the trap $g_1(r,0)$



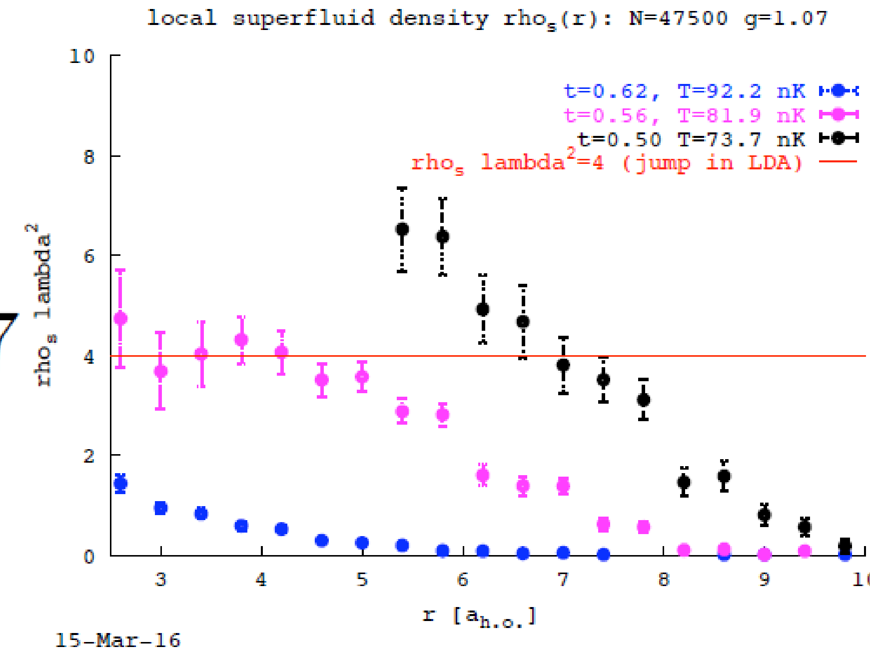

- local superfluid density

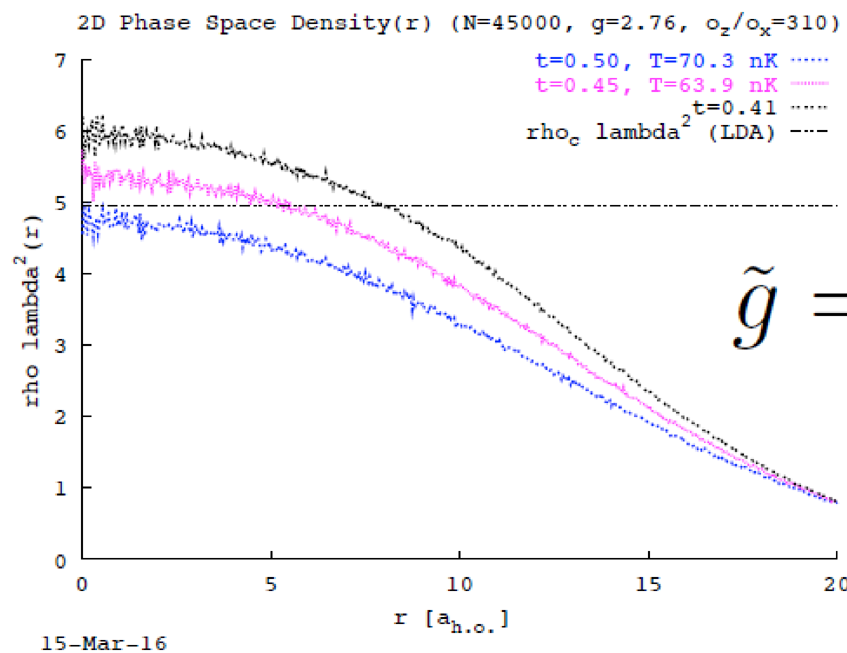


# towards stronger interactions....

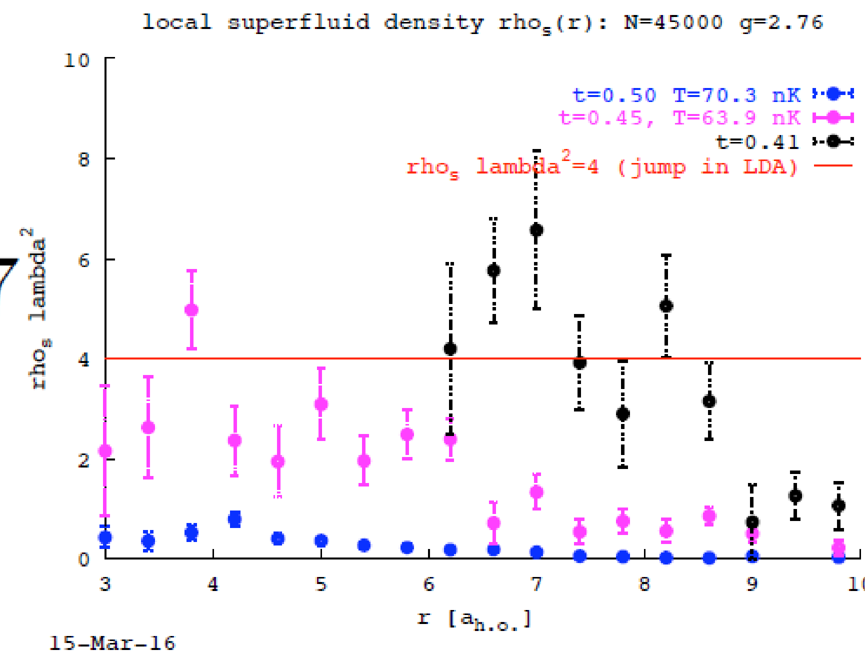



$$\tilde{g} = 1.07$$



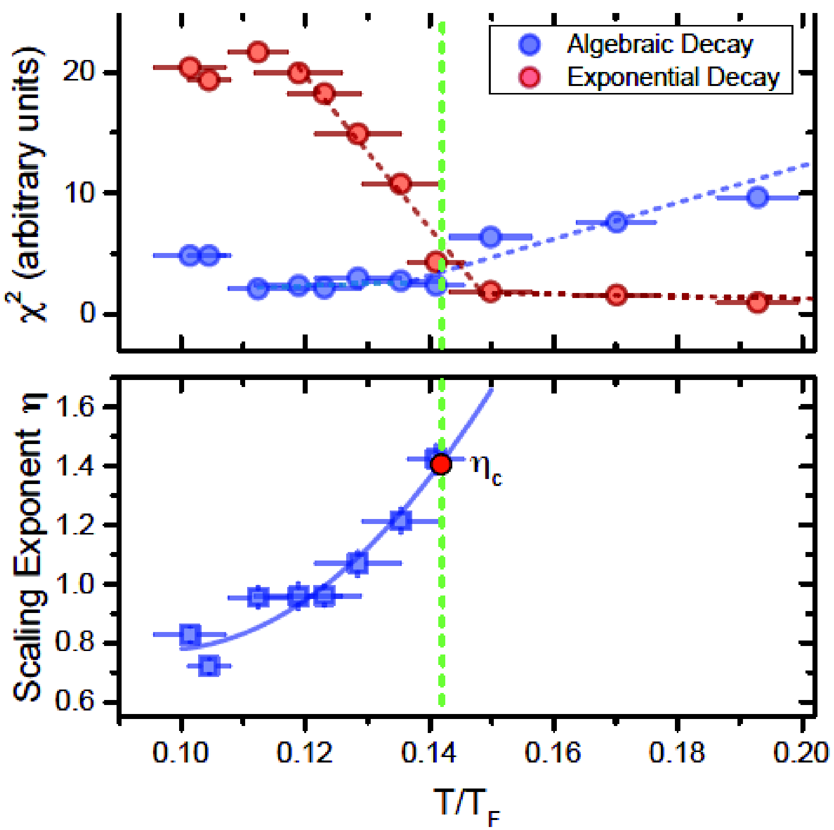




$$\tilde{g} = 2.67$$



# Algebraic decay in trap

P.A. Murthy, I. Boettcher, L. Bayha, M.H., D. Kedar, M. Neidig, M.G. Ries, A.N. Wenz, G. Zürn, S. Jochim,
Phys. Rev. Lett. 115, 010401 (2015).




apparent exponent of algebraic decay in trap

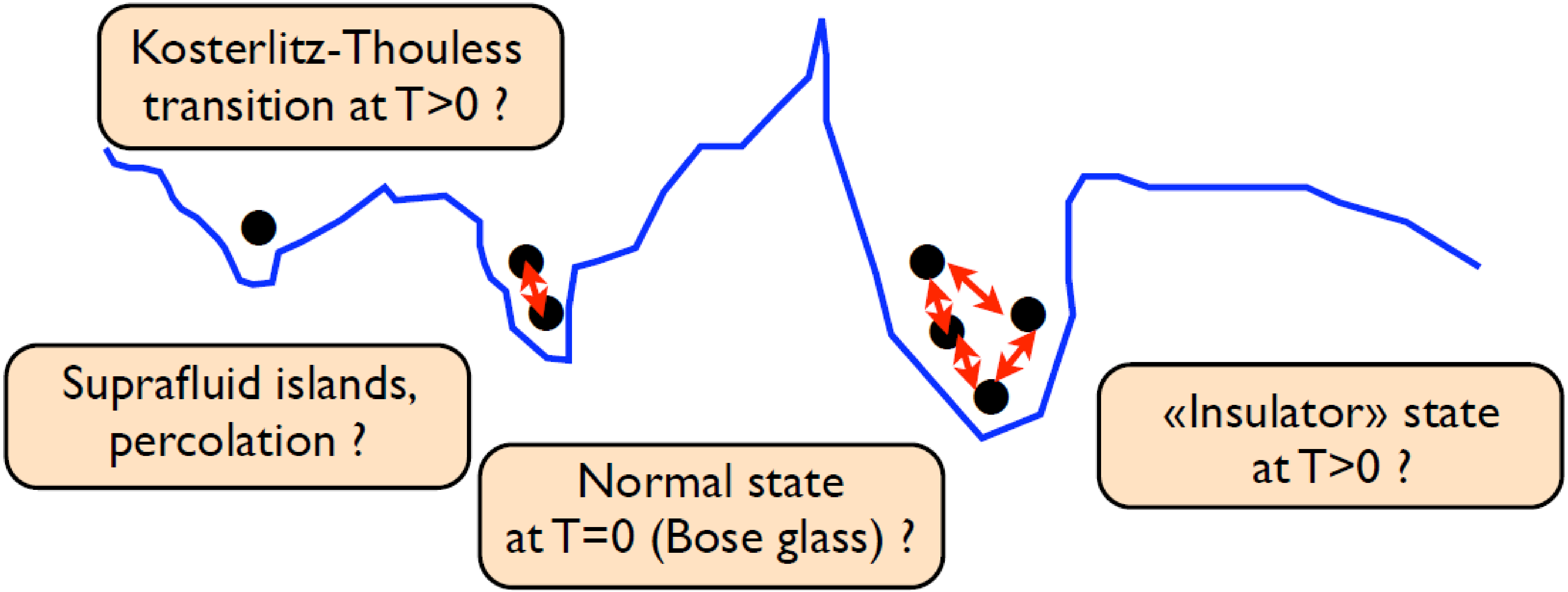
$$\eta_c(trap) \simeq 1.4 \gg 1/4$$

analytical description based on phase fluctuations (spin-wave approximation):

I. Boettcher, M.H.,
Phys. Rev. A 94, 011602(R) (2016).

# Dirty Boson Problem (2 Dimensions)

Competition between interaction (g) and disorder (V)




Experimental realizations:

- suprafluid transition of $^4$Helium in vycor,
- superconductor-insulator transition in high Tc
- ✖ trapped ultracold atoms with artificial disorder (2D)

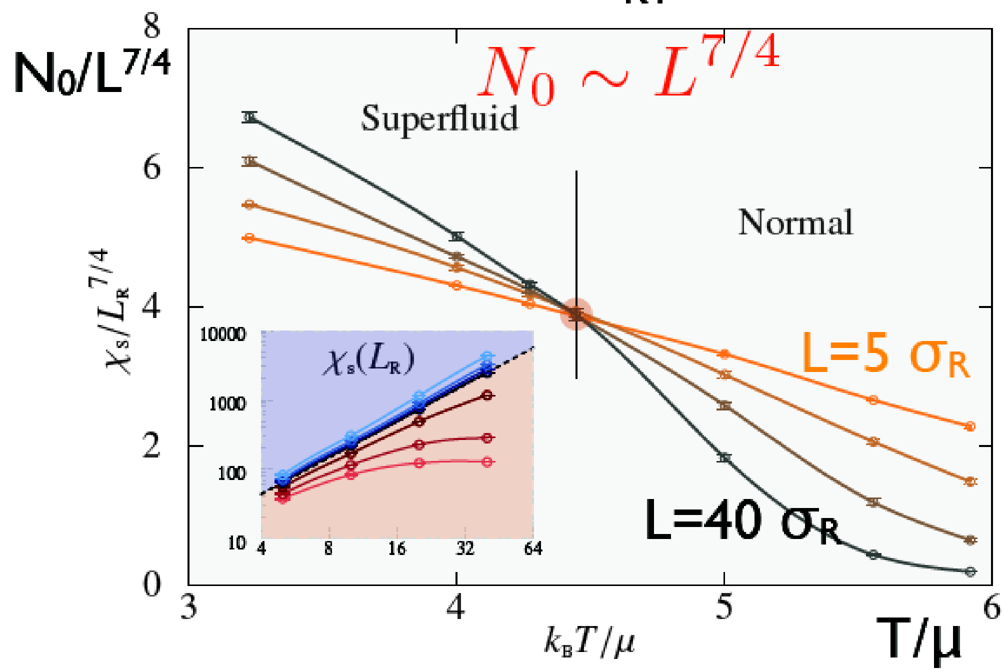
# Dirty Bosons: Suprafluid transition

Number of condensed particles $N_0$ at fixed disorder amplitude $V_R$

at $T_{KT}$

superfluid phase:

$N_0 \sim L^{2-\eta(T)}$




normal phase:

$N_0 = \mathcal{O}(1)$

Suprafluid transition remains in Kosterlitz-Thouless universality class
up to high disorder amplitude
(Harris criterium: small amplitude)

# Dirty Bosons in two dimensions: Phase diagram

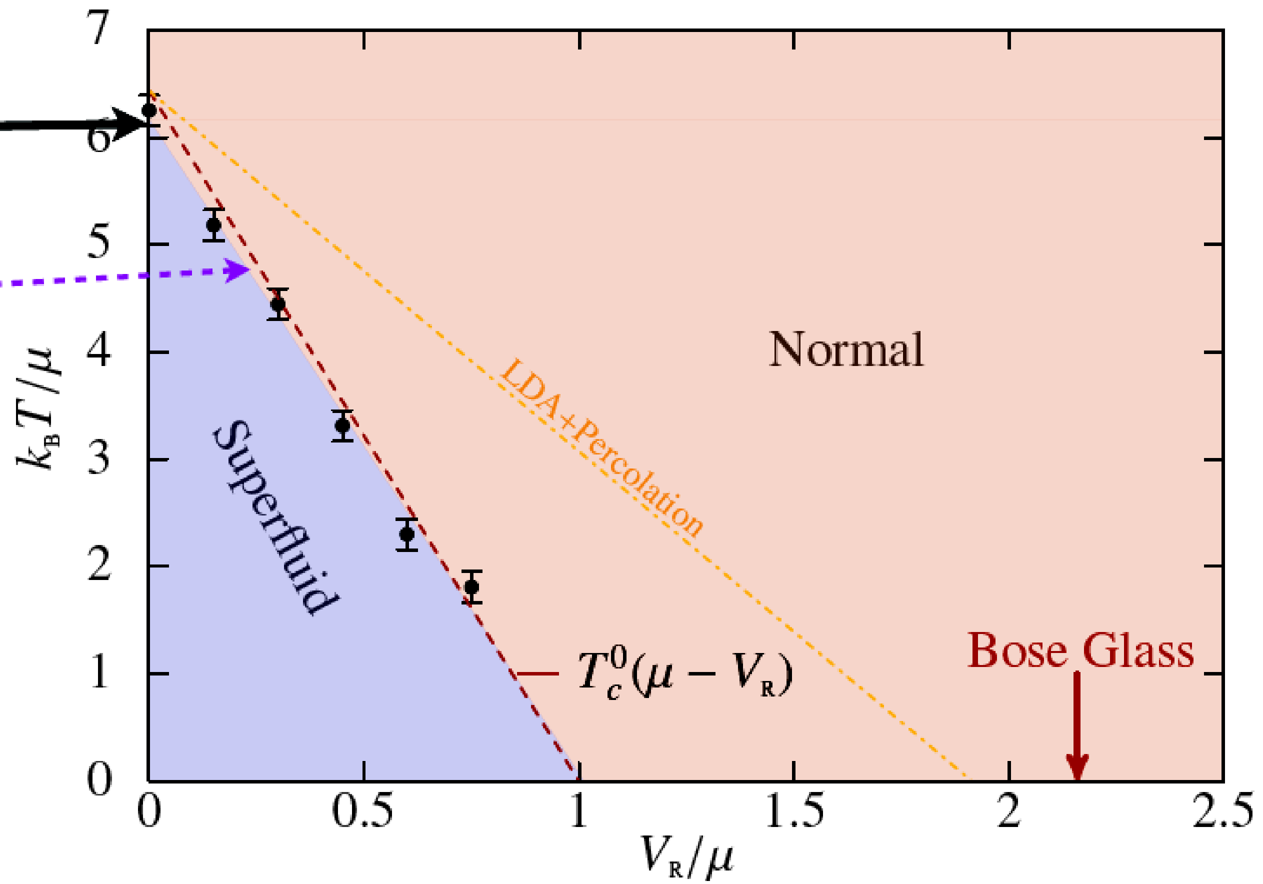
Phase diagram as a function of temperature T and disorder amplitude $V_R$

$2m\sigma^2\mu=5$ fixed

$$T_c^0(\mu)$$

Kosterlitz-Thouless universality class

(different from Percolation transition!)




$$T_c(V_R) \approx T_c^0(V_R - \mu)$$

renormalization of μ compared to clean system

# Transport : Conductance from QMC (homogenous)

G. Carleo, G. Boéris, M. Holzmann, and L. Sanchez-Palencia, Phys. Rev. Lett. 111, 037203 (2013)

current-correlations in imaginary time:

$$\langle J_\alpha(\mathbf{q},\tau) J_\alpha(-\mathbf{q},0)\rangle \equiv \frac{1}{Z}\mathrm{Tr}\left[e^{-(\beta-\tau)H} J_\alpha(\mathbf{q}) e^{-\tau H} J_\alpha(-\mathbf{q})\right]$$

conductance G(0) from inverse Laplace transform:

$$\lim_{q\to 0}\langle J_\alpha(\mathbf{q},\tau) J_\alpha(-\mathbf{q},0)\rangle = 2\int_{-\infty}^{\infty} d\omega \frac{\omega \exp(-\tau\omega)}{1-\exp(-\beta\omega)} G(\omega)$$

direct computations of current-correlations: large errors!

improved QMC estimator: large reduction of variance!

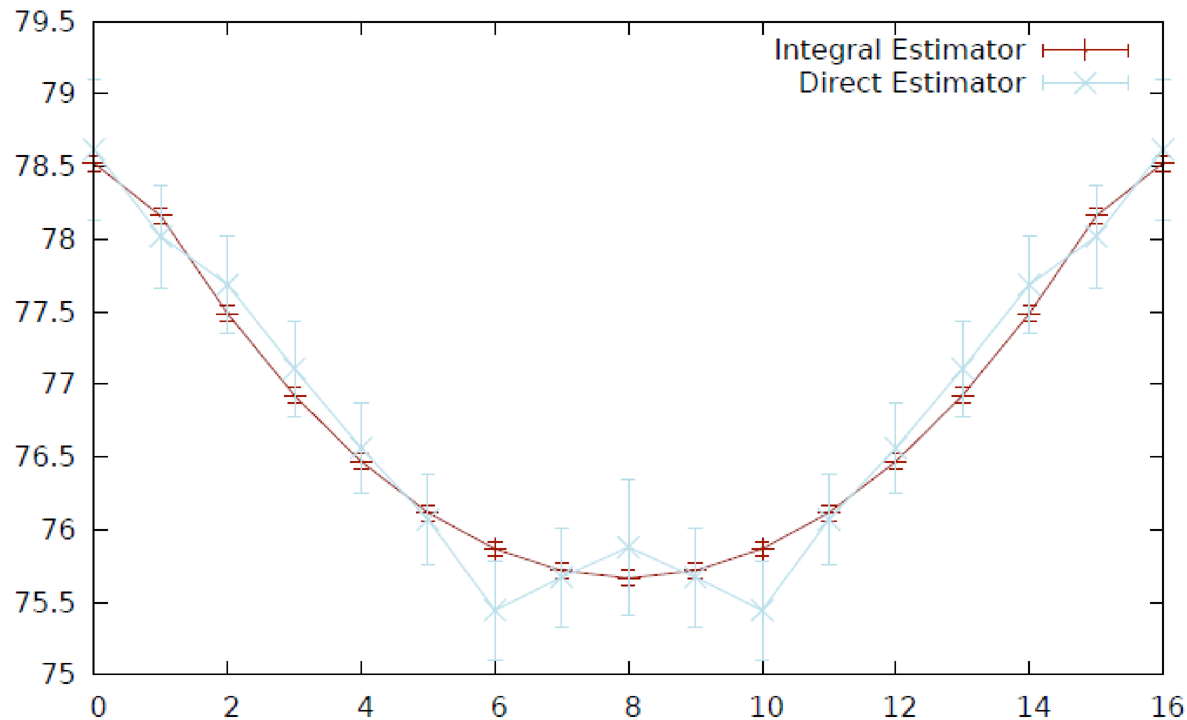


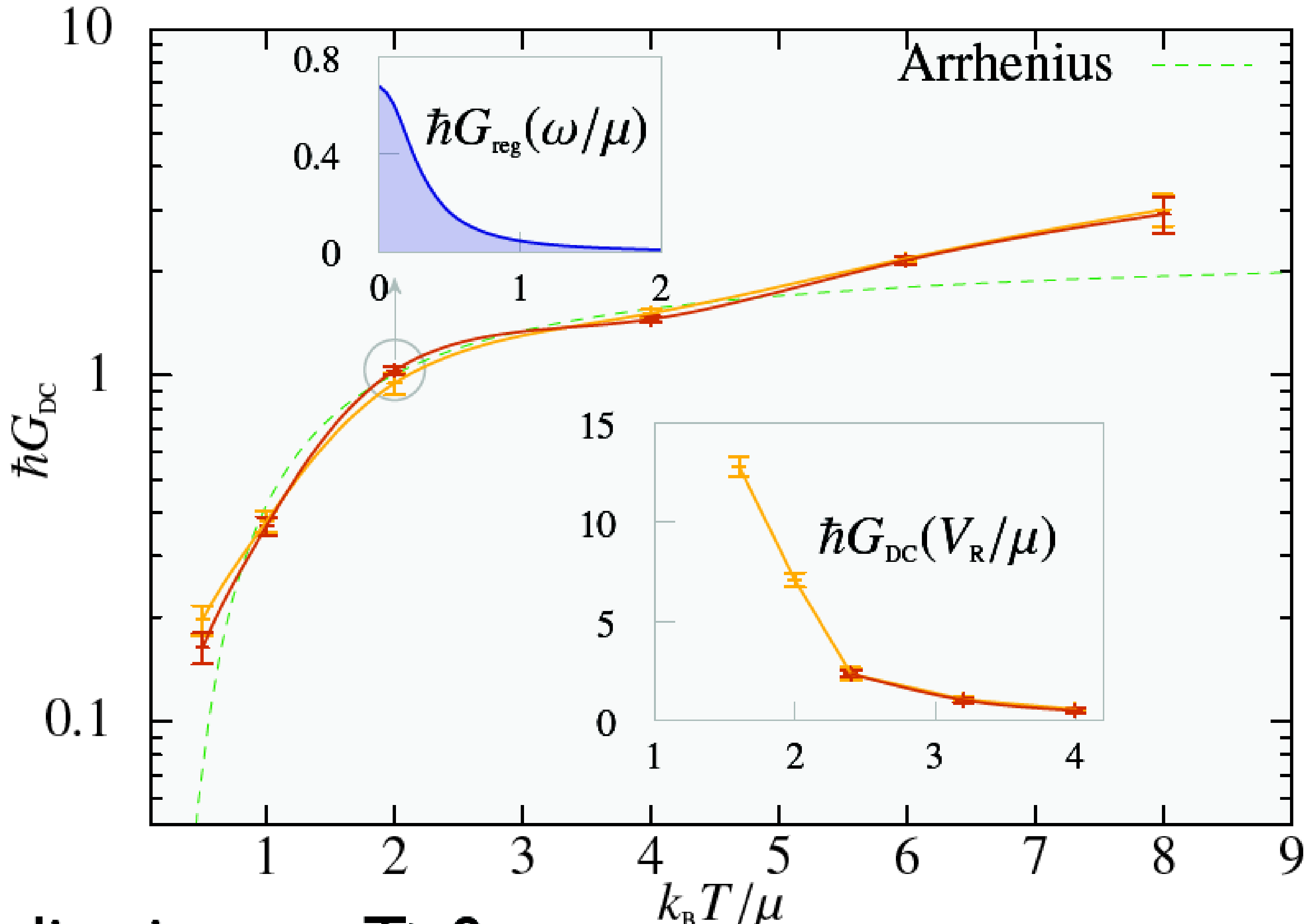

Figure 1: Current-current correlations deep in the disordered phase

# Dirty Bosons: transport properties

«Conductance» $G_{DC}$ at $V_R$=2.4μ

$$G_{DC} \sim e^{-\Delta/T}$$

no indication of localized phase at T>0




## Many-Body «delocalization» at T>0:

Perturbation theory around non-interacting localized phase diverges for continuum systems + correlated disorder

R. Nandkishore, cond-mat 1408.6235 (2014).

# Accessing Out-Of-Equilibrium-Dynamics:
# Time-Dependent Variational Monte Carlo

- Action priciple for time-dependent Schrödinger equation

$$S = \int dt \int d\mathbf{R} \Psi^*(\mathbf{R}, t) \left(-i\hbar\partial_t + H\right) \Psi(\mathbf{R}, t)$$

$$\frac{\delta S}{\delta \Psi^*(\mathbf{R}, t)} = 0 \quad \Rightarrow \quad i\hbar\partial_t \Psi(\mathbf{R}, t) = H\Psi(\mathbf{R}, t)$$

- Ansatz with correlated many-body wavefunction with time-dependent parameters

$$\Psi_T(\mathbf{R}, t) = \exp\left[-U^{(2)}(\mathbf{R}, t) - U^{(3)}(\mathbf{R}, t) - \cdots\right]$$

$$U^{(2)}(\mathbf{R}, t) = \sum_{i<j} u_2(\mathbf{r}_i, \mathbf{r}_j; t) \quad U^{(3)}(\mathbf{R}, t) = \sum_{i<j<k} u_2(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k; t)$$

→ First implementation using two-body Jastrow VMC for 1D lattice system:

G. Carleo, F. Becca, M. Schiro, and M. Fabrizio, Scientific Reports 2, 243 (2012).

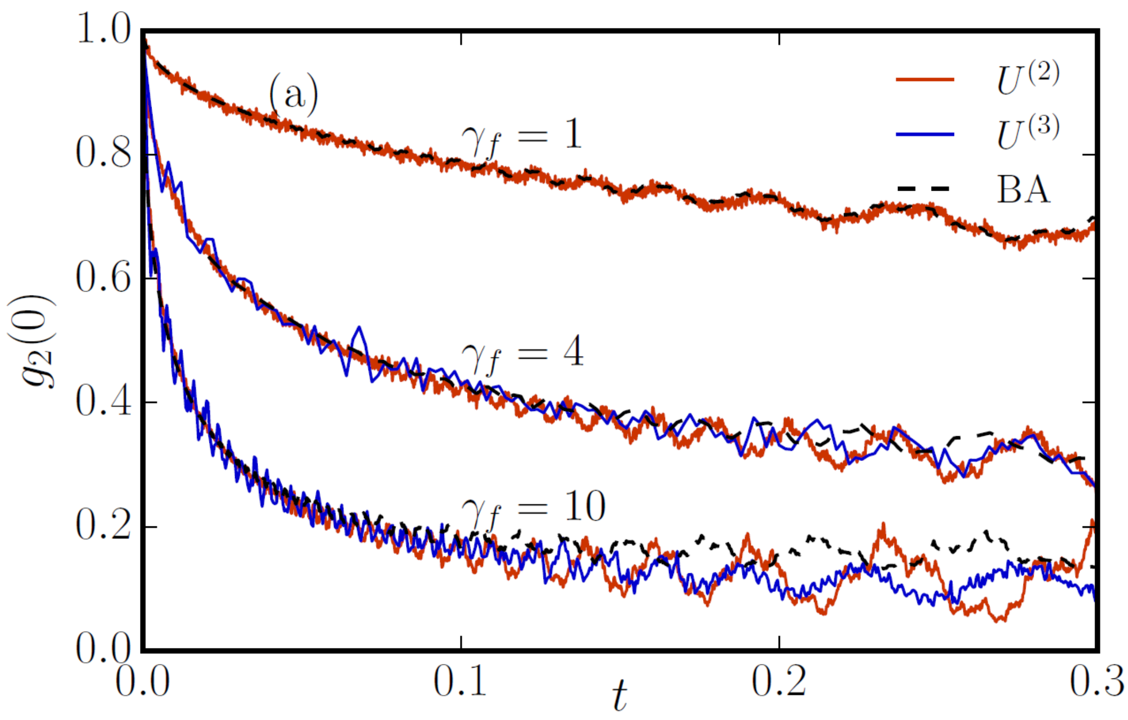
# Quench-Dynamics for Lieb-Liniger 1D Bosons: Time-Dependent VMC in continuum space

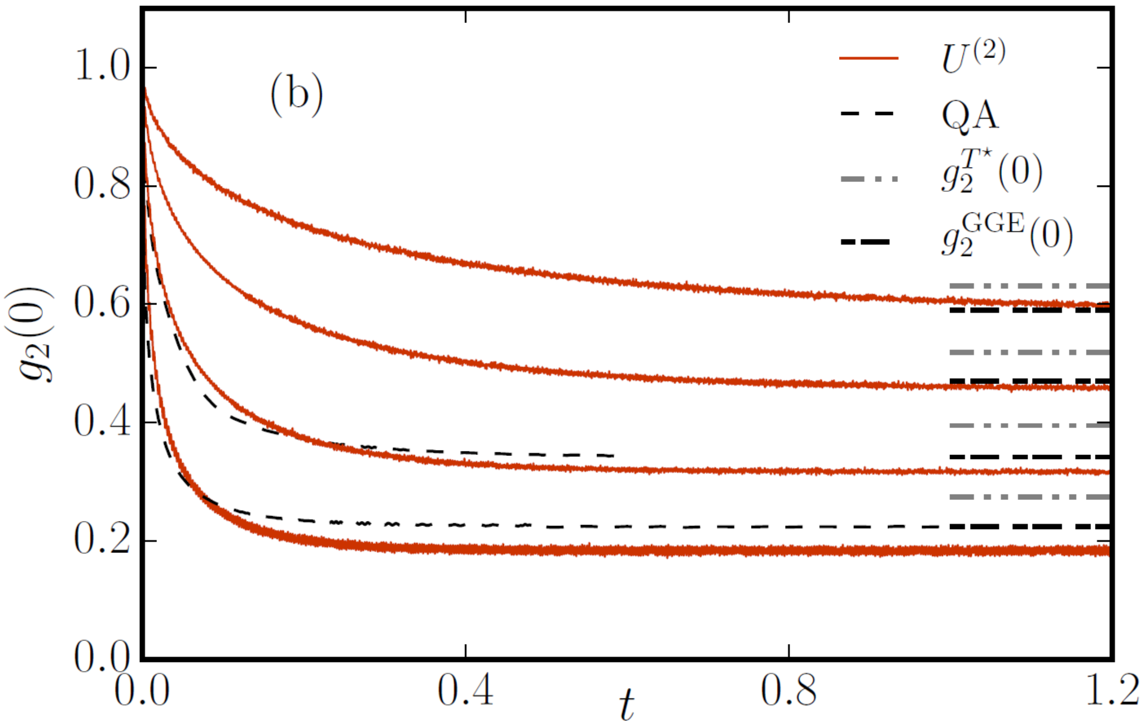
G. Carleo, L. Cevolani, L. Sanchez-Palencia, and M. H., cond-mat/1612.06392

- 1D Bosons with δ-interaction: $v_2(x, y) = g\delta(x - y)$ $\gamma = mg/\hbar^2 n$
- Sudden quench of interaction strength from g=0 to $g=g_f$ at t=0
- Correlated wave function with 2-body $U^{(2)}$ and 3-body $U^{(3)}$ Jastrow function

Comparison for N=6-11 Bosons With Bethe-Ansatz (BA) results

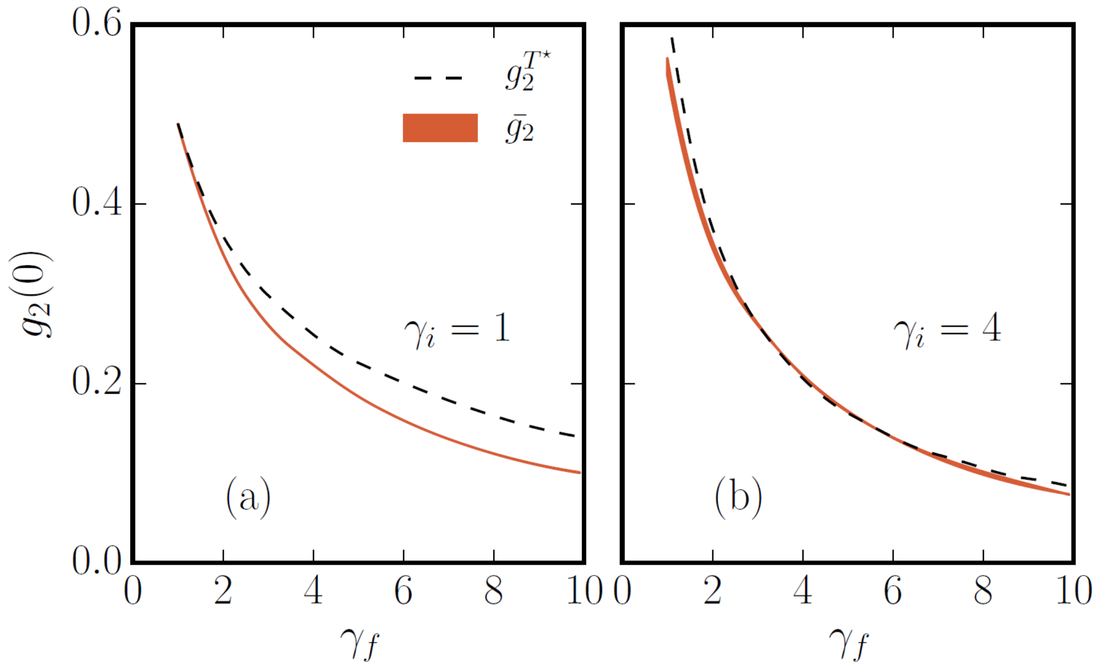
Pair-correlation function at zero distance $g_2(0)$





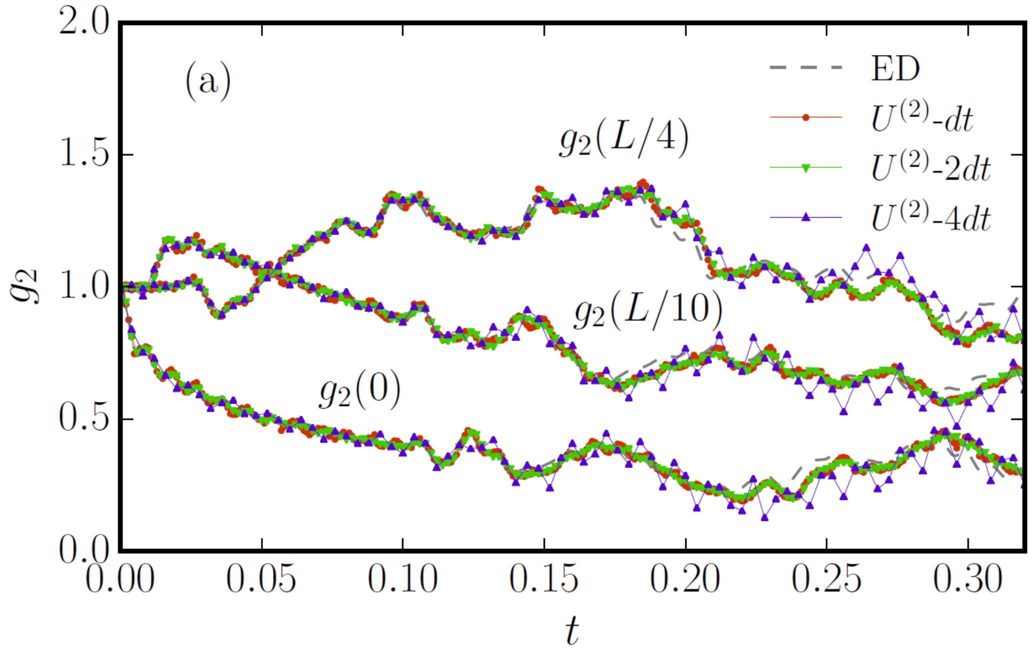

Large systems (N=100)

General quenches:
from interacting initial state $g_i$



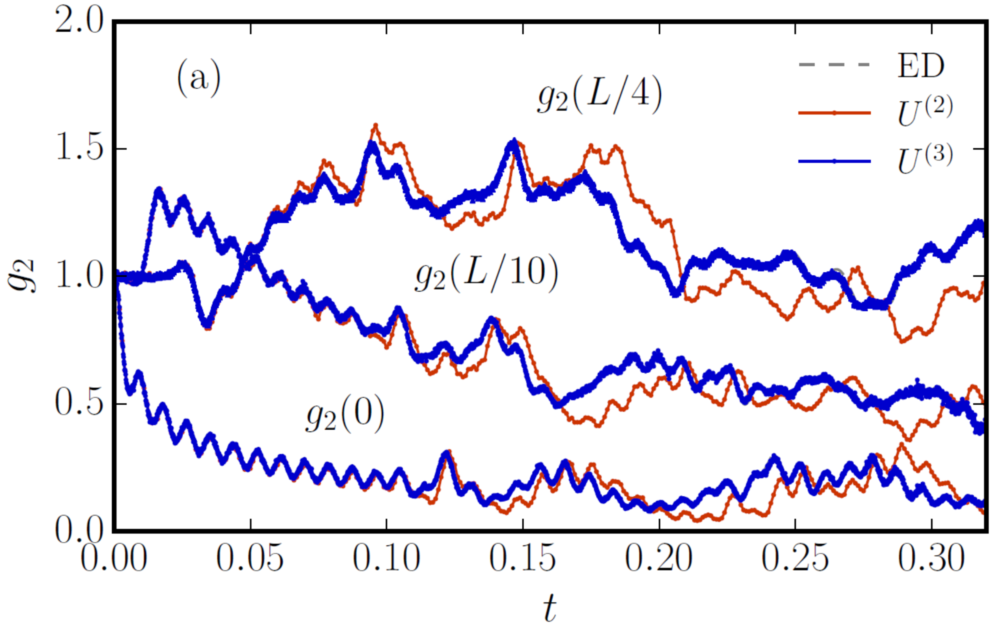
# Tests against exact diagonalization with N=3:

Time-discretization error

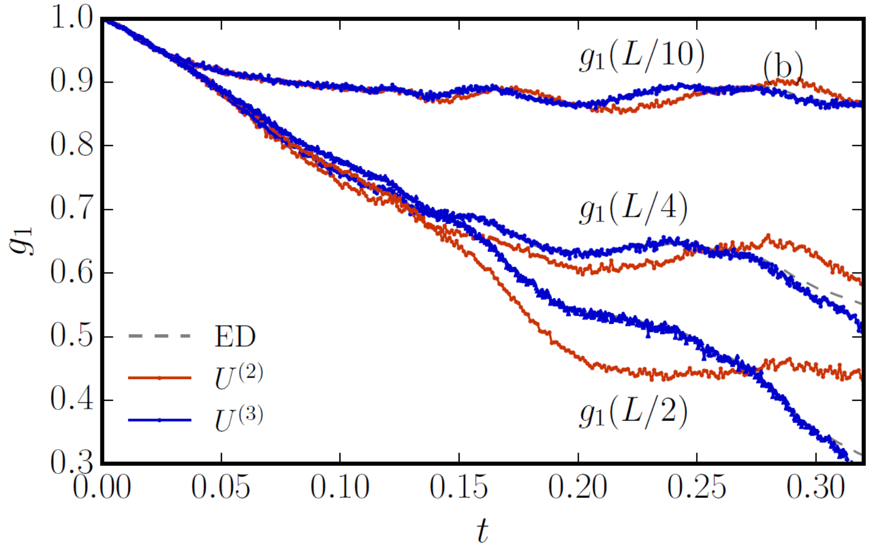



Quench from g=0 to $g_f$=8

Pair correlation at finite distance




One-body correlation function



# Perspectives:

- Fermions
  - Better variational wave functions (iterated backflow)
  - Variational density matrix ($\rightarrow$ B.Clark)
  - Imaginary time dynamics ($\rightarrow$ J.Boronat)
- spectral quantities?
  - Dynamic structure factor ($\rightarrow$ D.Galli, G.Bertaina,N.Prokof'ev)
  - conductivity
- Time dependence for 3D quantum gases/ liquids

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