
**Universitat Politècnica de Catalunya, Barcelona, Spain**

# Diffusion Monte Carlo: symmetric trial wave function for a solid and pure estimators for one-body density matrix.

**G.E. Astrakharchik**

**Seattle, 1st of August, 2013**

Classical Monte Carlo simulations:

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"Thermal and quantum fluctuations in low dimensional dipolar chains", J. Phys. B: At. Mol. Opt. Phys. **42**, 154026 (2009)

Metropolis sampling of an exact wave function
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Bachelor thesis "Quantum simulation of mesoscopic cluisters" (2000);
O. N. Osychenko, GEA, Y. Lutsyshyn, Yu. E. Lozovik, and J. Boronat "Phase diagram of Rydberg atoms with repulsive van der Waals interaction" PRA **84**, 063621 (2011)

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## - Weakly interacting Bose gas / short-range bosons

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D.S. Petrov, GEA, C. Salomon, G.V. Shlyapnikov, "Crystalline phase of strongly interacting Fermi mixtures", PRL **99**, 130407 (2007)

GEA, J. Boronat, I. L. Kurbakov, Yu. E. Lozovik, and F. Mazzanti, "Low-dimensional weakly interacting Bose gases: Nonuniversal equations of state", PRA **81**, 013612 (2010)

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## - Dipolar gases

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Diffusion Monte Carlo simulations:

-One dimensional systems:

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GEA and S. Giorgini "Correlation functions of a Lieb-Liniger Bose gas" J. Phys. B: At. Mol. Opt. Phys. **39** S1 (2006)

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F. Mazzanti, GEA, J.Boronat, and J. Casulleras,"Ground-state properties of a one-dimensional system of Hard Rods", PRL **100**, 020401 (2008); F. Mazzanti, GEA, J.Boronat, and J. Casulleras,"Off-diagonal ground-state properties of a one-dimensional gas of Fermi hard rods" PRA **77**, 043632 (2008);

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- Liquid & solid $^4$He

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Y. Lutsyshyn, C. Cazorla, GEA, and J. Boronat, "Properties of vacancy formation in hcp 4He crystals at zero temperature and fixed pressure", PRB 82, 180506 (R) (2010)

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GEA, R. Combescot, X. Leyronas and S. Stringari "Equation of state and collective frequencies of a trapped Fermi gas along the BEC-unitarity crossover", PRL **95**, 030404 (2005);

GEA, S. Giorgini, J. Boronat "Stability of resonantly interacting heavy-light Fermi mixtures", PRB **86**, 174518 (2012)

A. Golomedov, AGE, J. Boronat "A Quantum Monte Carlo study of exciton formation in two component Coulomb gas" to appear soon

# MOTIVATION

Some technical details of diffusion Monte Carlo (DMC) method will be discussed

- Symmetric trial w.f. for a solid phase
- Algorithm with linear complexity in number of particles $N$
- Calculation of pure estimators in DMC

# CRYSTAL: NONSYMMETRIC W.F



The easiest (*de facto* standard) way to introduce the symmetry of a crystal is to multiply the Jastrow two-body correlation terms by a Nosanow one-body term $f_1^1(\mathbf{r}_i, \mathbf{r}_i^{latt.})$ which localizes a particle $\mathbf{r}_i$ at its corresponding lattice site $\mathbf{r}_i^{latt.}$:

$$\psi(\mathbf{r}_1, ..., \mathbf{r}_N) = \prod_{i=1}^{N} f_1^1(\mathbf{r}_i, \mathbf{r}_i^{latt.}) \times \prod_{j<k}^{N} f_2(\mathbf{r}_j, \mathbf{r}_k)$$

The lower index in $f()$ denotes how many particles are involved (one-body, two-body correlation terms) and the upper index shows number of lattice sites involved. The standard choice for the one-body term is the a Gaussian localization

$$f_1^1(\mathbf{r}_i, \mathbf{r}_i^{latt.}) = \exp\{-\alpha(\mathbf{r}_i - \mathbf{r}_i^{latt.})^2\}$$

with the strength $\alpha$ being a variational parameter.

# NON-SYMMETRIC W.F.



The advantages of the Nosanow-Jastrow function are

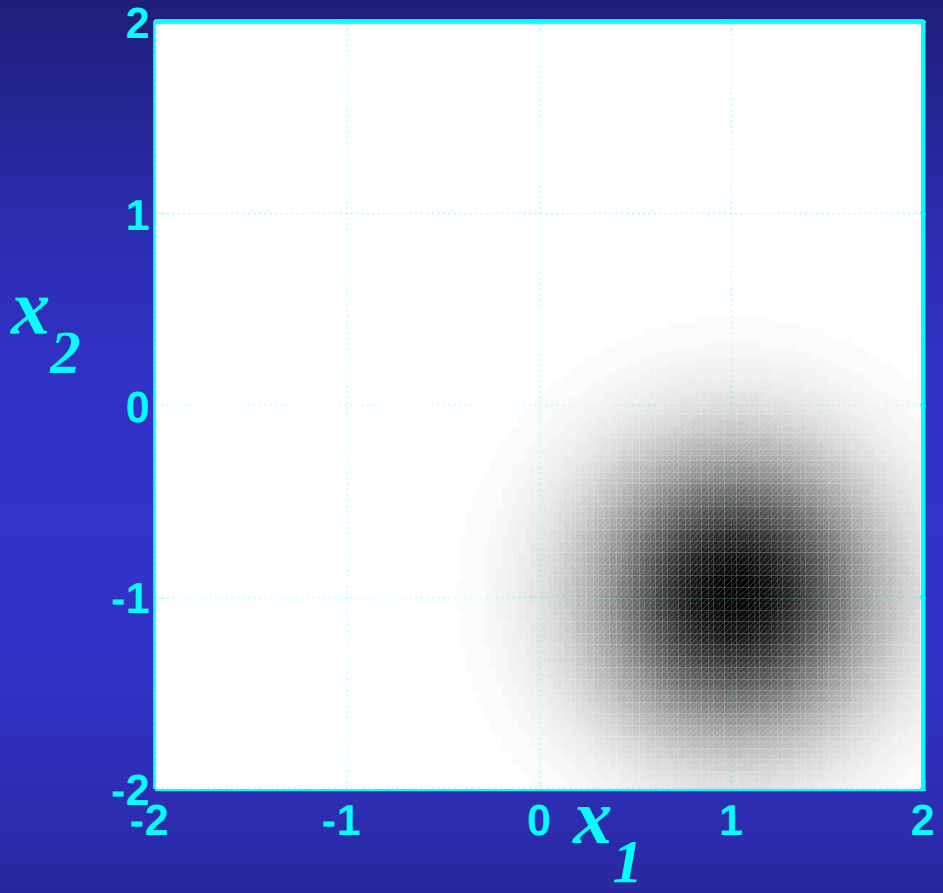
- properly describes the limit of strong localiztion
- where the w.f. is Gaussian close to position of the minimum
- provides good estimate for the energy in the crystal state

The disadvantages of the Nosanow-Jastrow function are

- has symmetry of distinguishable particles
- i.e. for bosons the wave function should be symmetric under exchange
- not able to describe off-diagonal properties: ODLRO? superfluid?

# EXAMPLE: TWO PARTICLE SYSTEM






Schematic representation of the w.f. for one-dimensional system of $N = 2$ particles $|\psi(x_1, x_2)|^2$. Positions of lattice sites are $x^{latt.} = 1$ and $x^{latt.} = -1$.

# CRYSTAL: SYMMETRIC ONE-BODY W.F



A simple way to construct a symmetric w.f. is to use a one-body term

$$\psi(\mathbf{r}_1,...,\mathbf{r}_N) = \prod_{i=1}^{N} f_1^N(\mathbf{r}_i, \mathbf{r}_1^{latt.},...,\mathbf{r}_N^{latt.}) \times \prod_{j<k}^{N} f_2(\mathbf{r}_j,\mathbf{r}_k)$$

[1] For example, for a Gaussian localization

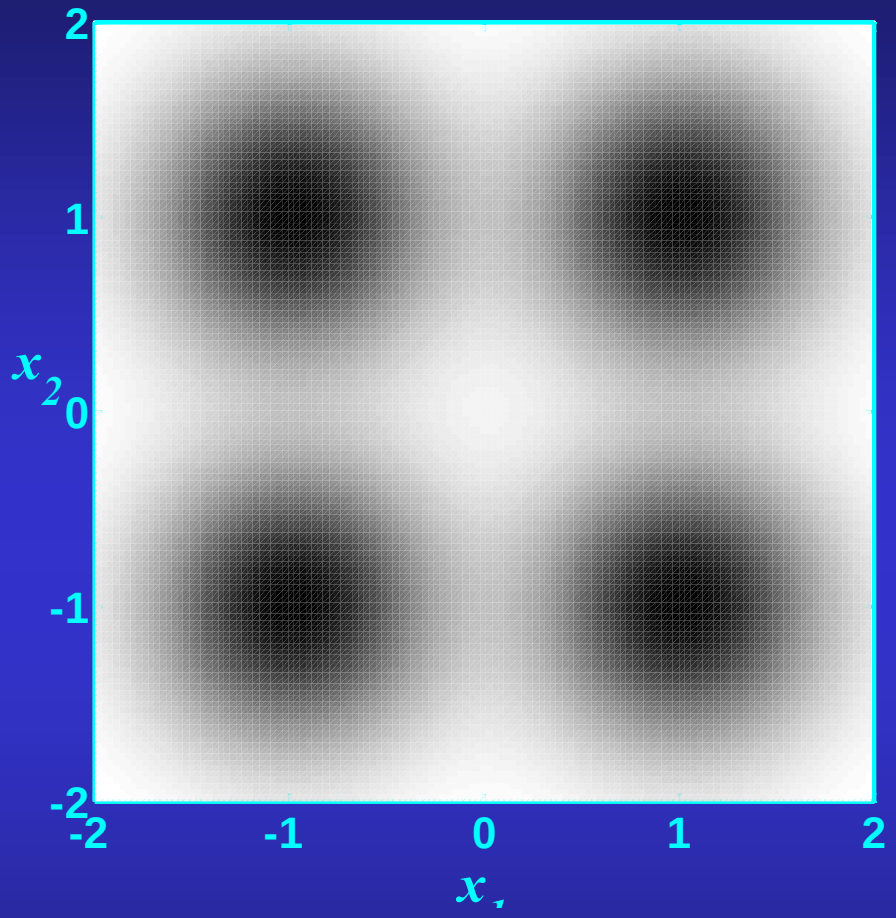
$$f_1^N(\mathbf{r}_i, \mathbf{r}_1^{latt.},...,\mathbf{r}_N^{latt.}) = \sum_{l=1}^{N} \exp\{-\alpha(\mathbf{r}_i,\mathbf{r}_l^{latt.})^2\}$$

[2] Another way to generate symmetric one-body term is to use a periodic function, e.g.

$$f_1^N(\mathbf{r}_i, \mathbf{r}_1^{latt.},...,\mathbf{r}_N^{latt.}) = \cos^2[2\pi(x_i a_1 + y_i a_2 + z_i a_3)]$$

# EXAMPLE: TWO PARTICLE SYSTEM






Schematic representation of the w.f. for one-dimensional system of $N = 2$ particles $|\psi(x_1, x_2)|^2$. Positions of lattice sites are $x^{latt.} = 1$ and $x^{latt.} = -1$.

# CRYSTAL: SYMMETRIC ONE-BODY W.F

Instead of the previous one-body example,

$$\psi(\mathbf{r}_1,...,\mathbf{r}_N)=\prod_{i=1}^{N}\left(\sum_{l=1}^{N_{latt.}}\exp\{-\alpha(\mathbf{r}_i-\mathbf{r}_l^{latt.})^2\}\right)\times\prod_{j<k}^{N}f_2(\mathbf{r}_j,\mathbf{r}_k)$$

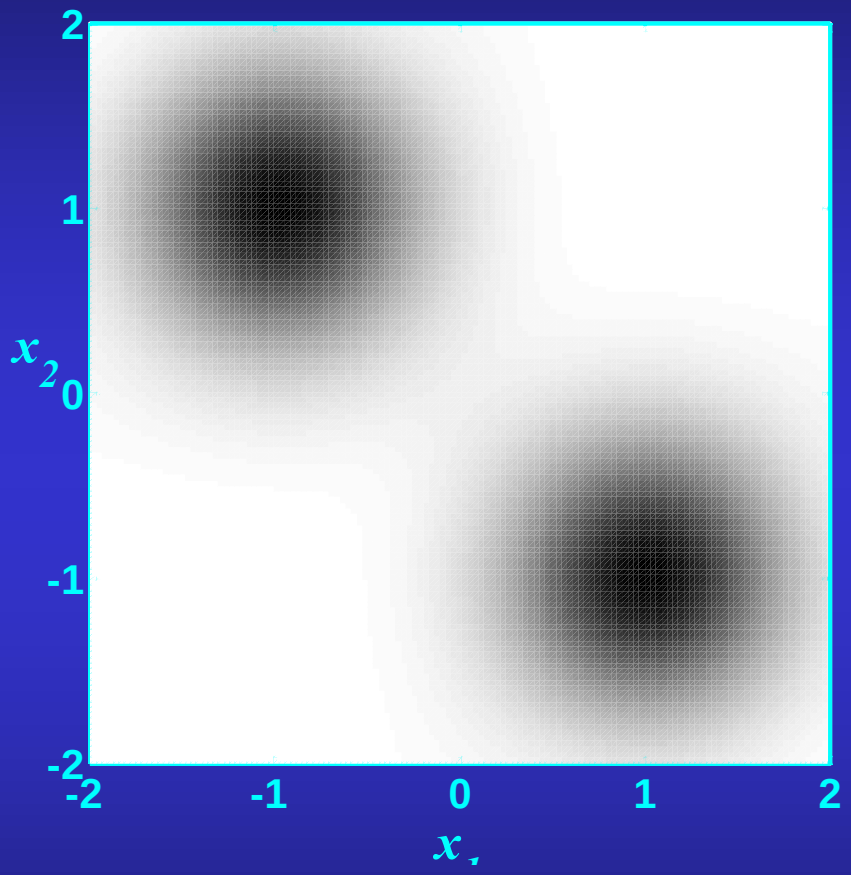
we propose to construct the trial wave function in the following form:

$$\psi(\mathbf{r}_1,...,\mathbf{r}_N)=\prod_{l=1}^{N_{latt}}\left(\sum_{i=1}^{N}\exp\{-\alpha(\mathbf{r}_i-\mathbf{r}_l^{latt.})^2\}\right)\times\prod_{j<k}^{N}f_2(\mathbf{r}_j,\mathbf{r}_k)$$

which differs by the indices of the summation.

# EXAMPLE: TWO PARTICLE SYSTEM






Schematic representation of the w.f. for one-dimensional system of $N = 2$ particles $|\psi(x_1, x_2)|^2$. Positions of lattice sites are $x^{latt.} = 1$ and $x^{latt.} = -1$.

# SYMMETRIC W.F.

The symmetrized w.f. of a crystal

- has a proper symmetry for a quantum system
- is symmetric under exchange of two particles
- is not a one-body or two-body term, but a $N$-body term
- permits evaluation of off-diagonal long-range properties: OBDM, superfluid density
- independent choice of number of particles $N$ and lattice sites $N_{latt}$
- allows to study incommensurate geometry/defects: vacancies $N < N_{latt}$.

# EX: HELIUM LIQUID-SOLID TRANSITION



We use the following w.f. for a study of liquid-solid phase transition in $^4$He

$$\psi_{\mathrm{SNJ}} = \underbrace{\left( \prod_{i,j}^{N} f_2(r_{ij}) \right)}_{\text{pair correlations}} \times \underbrace{\left( \prod_{k}^{N_{latt}} \sum_{i}^{N} f(|\boldsymbol{r}_i - \boldsymbol{l}_k|) \right)}_{\text{lattice confinement}} \qquad (1)$$

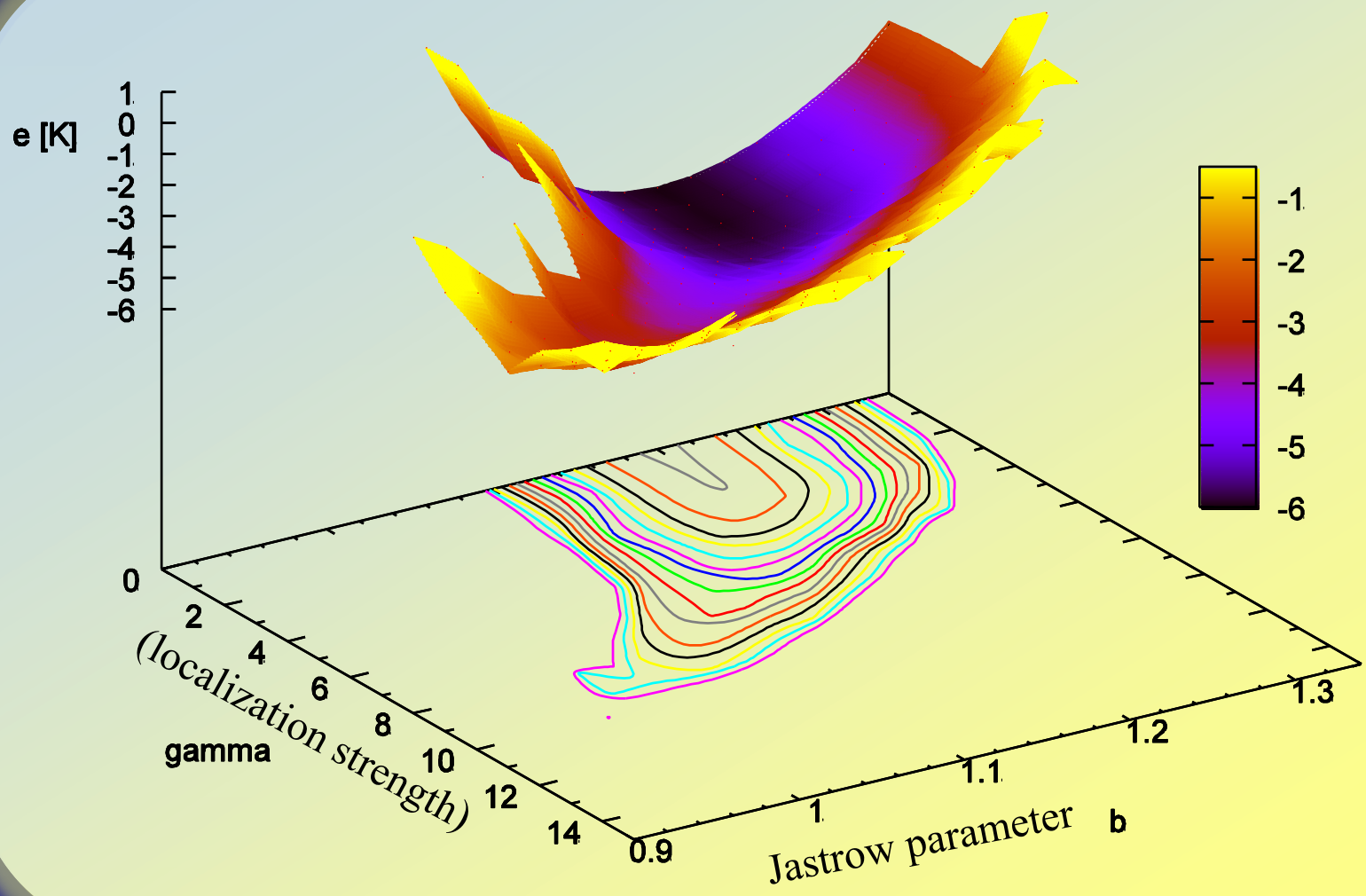
where

| | |
|---|---|
| $N$ | is the number of particles, found at $\boldsymbol{r}_i$ |
| $N_{latt}$ | is the number of lattice sites, located at $\boldsymbol{l}_k$ |
| $f_2$ | is a pair-correlation factor |
| $f_1$ | is the localization function $f_1(r) = \exp\left(-\frac{1}{2}\gamma r^2\right)$ |

[ ] Yaroslav Lutsyshyn, Dieter Bauer, Claudio Cazorla, GEA, Jordi Boronat, to appear soon

# JASTROW TWO-BODY TERMS

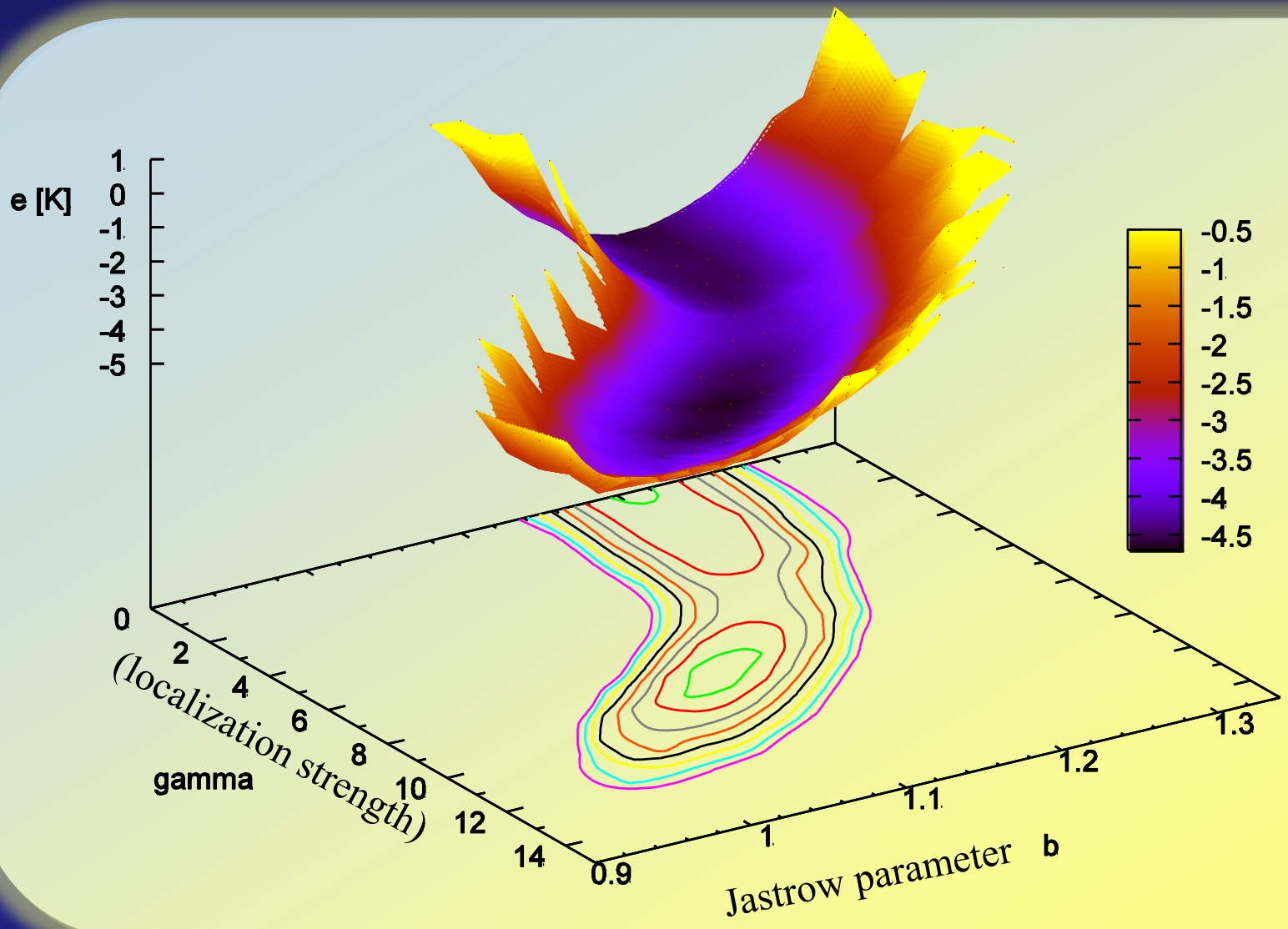





Variational energy in the optimization of the two-parameter wave function. Density $22.2\,\mathrm{nm}^{-3}$ is well below the transition

# JASTROW TWO-BODY TERMS

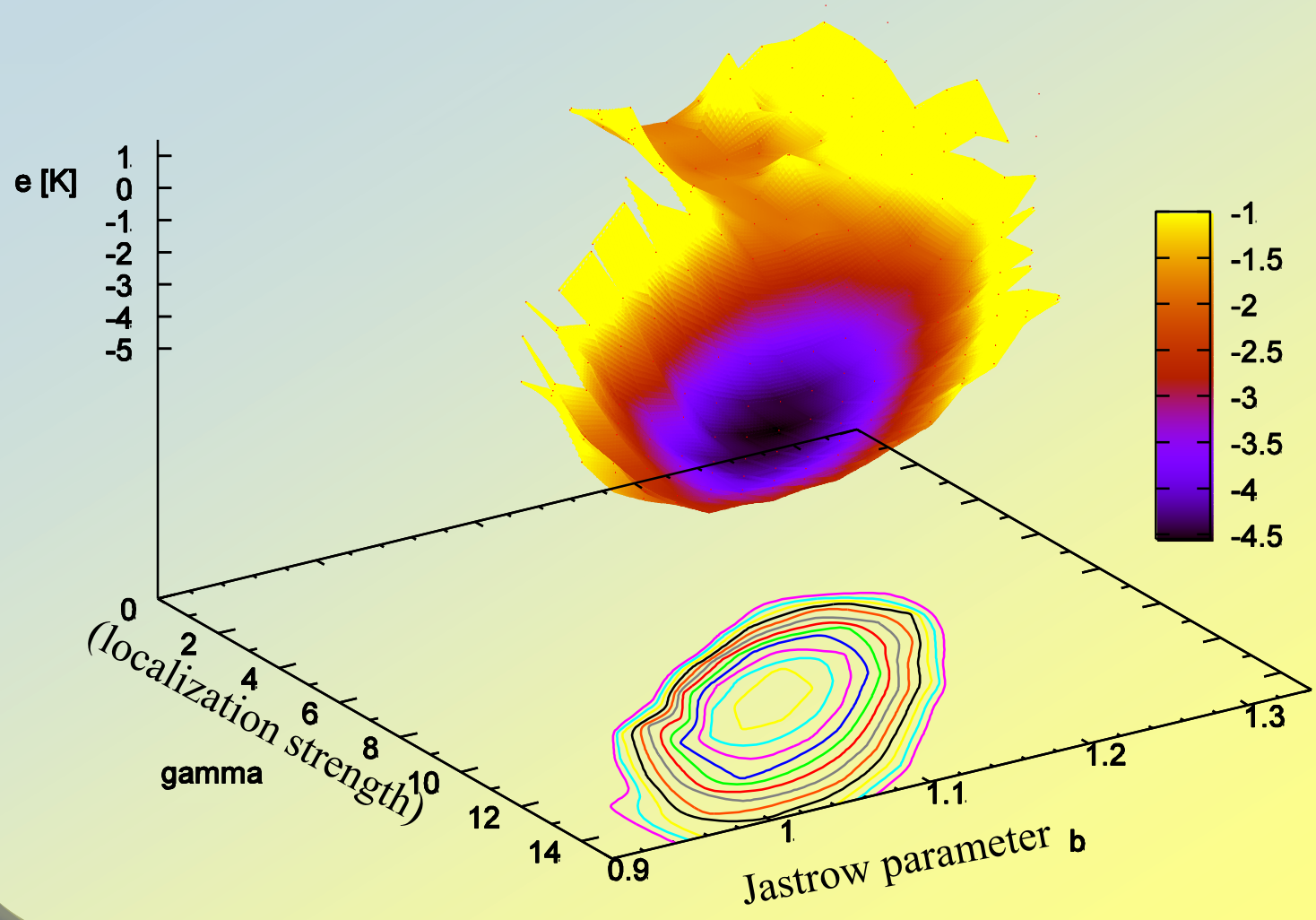





Optimization for density in the coexistence regime, $\rho = 25.8\,\mathrm{nm}^{-3}$
the energy landscape has two separated minima.

# JASTROW TWO-BODY TERMS

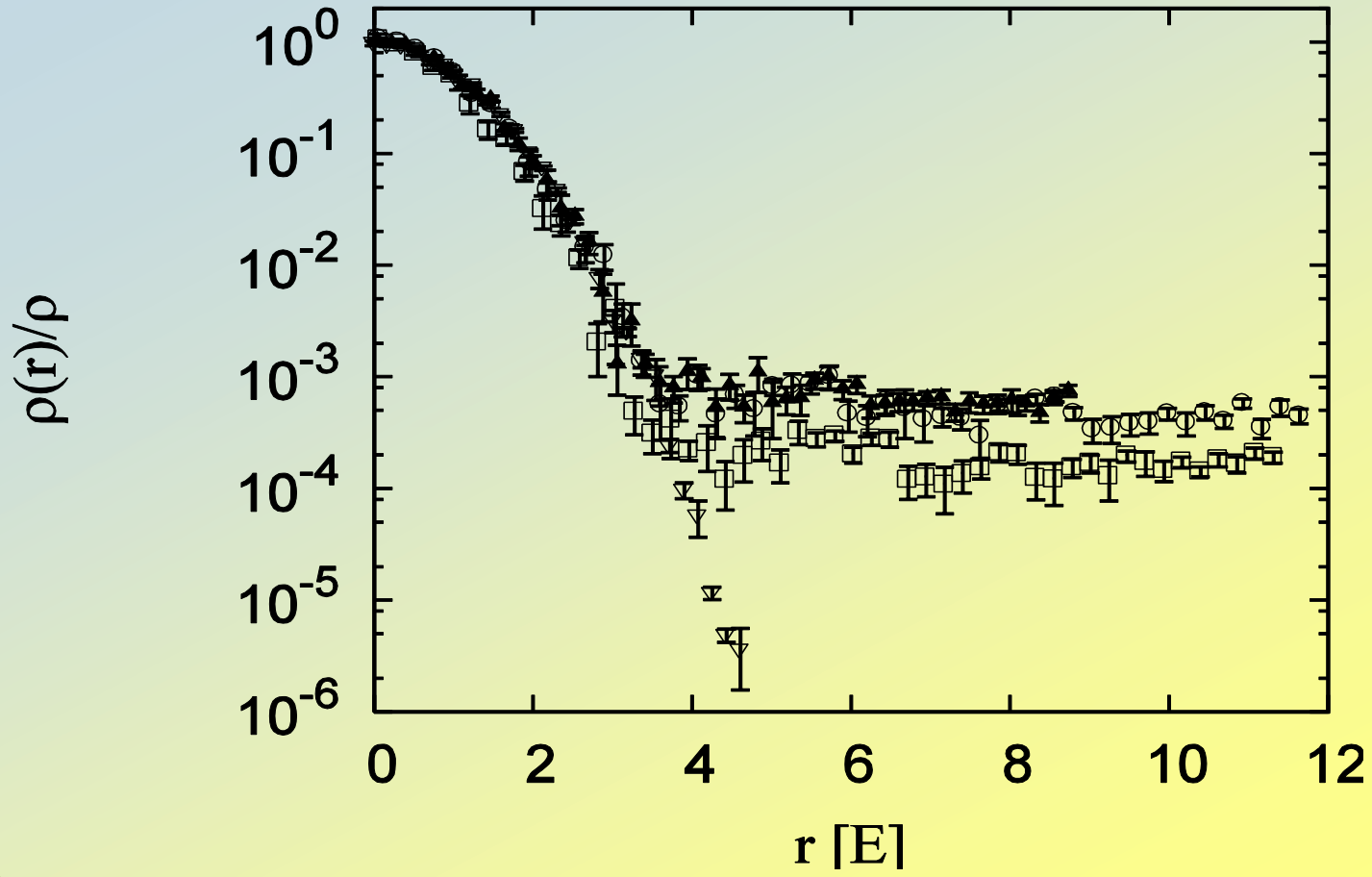





Solid phase, $\rho = 29.3\,\mathrm{nm}^{-3}$, the local minimum at $\gamma = 0$ has disappeared.

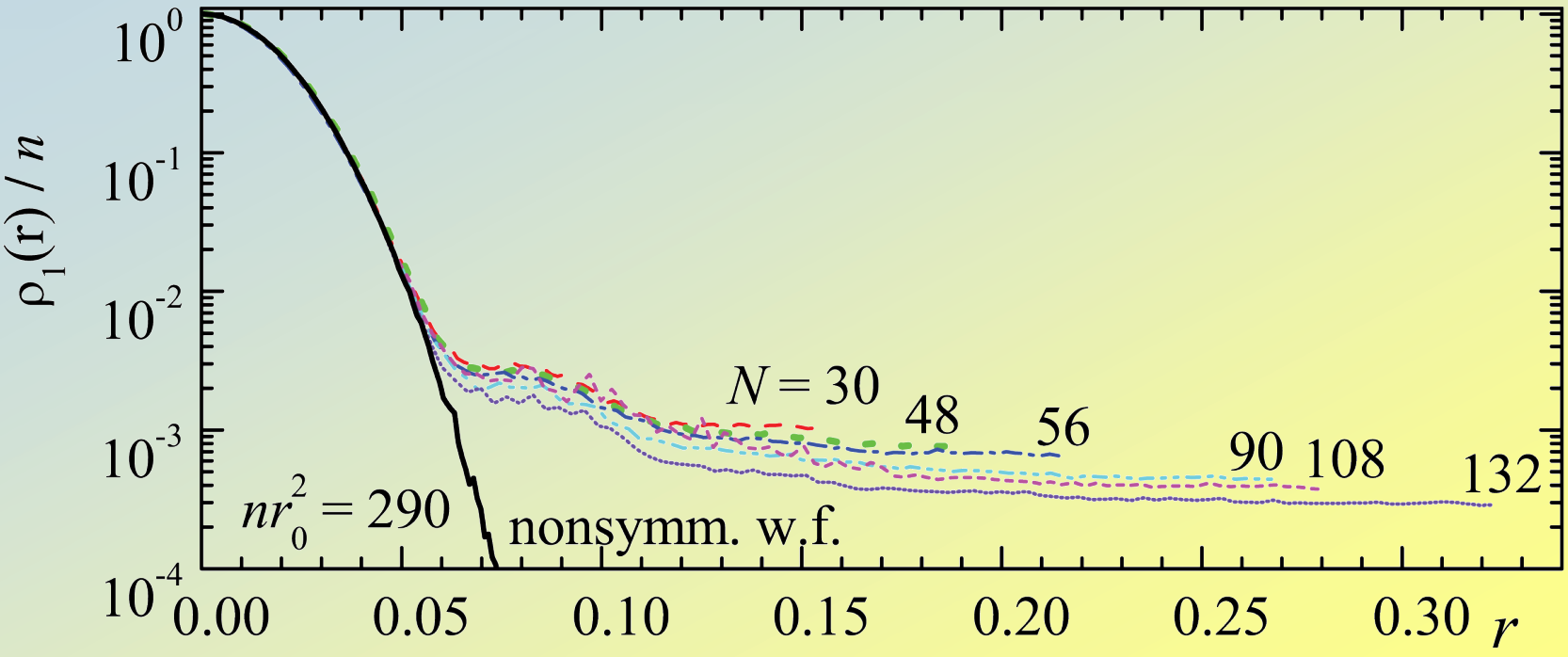
# ¿SUPERSOLID? HELIUM





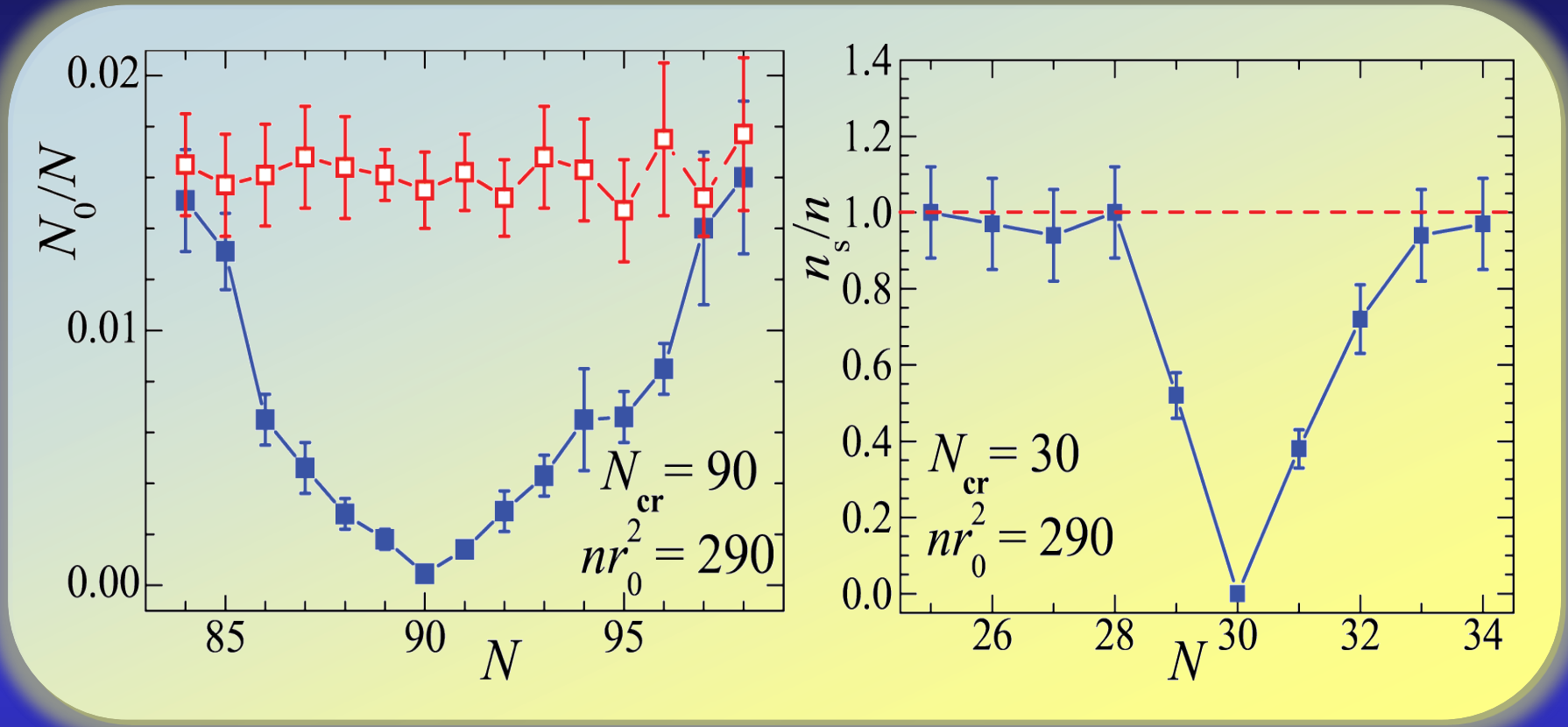

OBDM of solid $^4$He at densities $\rho = 0.491$ (circles) and $\rho = 0.535\ \sigma^{-3}$ (squares) and $N = 180$ particles. stand for a calculation at $\rho = 0.491\sigma^{-3}$ Open $\nabla$ - Nosanow w.f. C. Cazorla, GEA, J. Casulleras and J. Boronat New J. Phys. **11** 013047 (2009)

# DIPOLES ON 2D PLANE




One-body density matrix of the perfect 2D crystal at density $nr_0^2 = 290$ as a function of the number of particles $N$; the solid line – nonsymmetric trial wave function I. L. Kurbakov, Yu. E. Lozovik, AGE, and J. Boronat Phys. Rev. B **82**, 014508 (2010).

# VACANCIES




Condensate fraction (a), superfluid fraction (b) for a crystal with vacancies or interstitials ($N \neq N_{\rm cr}$) at the phase transition density $nr_0^2 = 290$. Solid ■ and open □ symbols stand for the solid and gas phases, respectively.

# CONCLUSIONS 1/3



- A simple ($N^2$ complexity) symmetric wave function can be used for describing a system of bosons
- Allows calculation of quantum long-range properties
- Describes liquid-solid phase transition
- Permits calculation of defects $N \neq N_{latt.}$, for example
  - vacancies
  - intestitials

# MOTIVATION

- Standard diffusion Monte Carlo method has $N^2$ complexity
- The quadratic dependence originates from calculations of all $N(N-1)/2$ possible pairs in the system. Such calculations are done when:
  1. Potential energy of a long-range interaction potential is calculated
  2. Two-body Jastrow terms are calculated (in calculation of Metropolis weight of a configuration, or in Drift force, or in contribution to the local energy)
- Can this be increased to permit investigation of large system sizes?
- At least for short-range interaction? For example, $\delta$-interacting gas in one dimension?

# PHONONS AND JASTROW W.F.

- two-body Jastrow term contains long-range correlations
- from hydrodynamic considerations[1], the ground-state wave function contains long-range two-body Jastrow correlations:

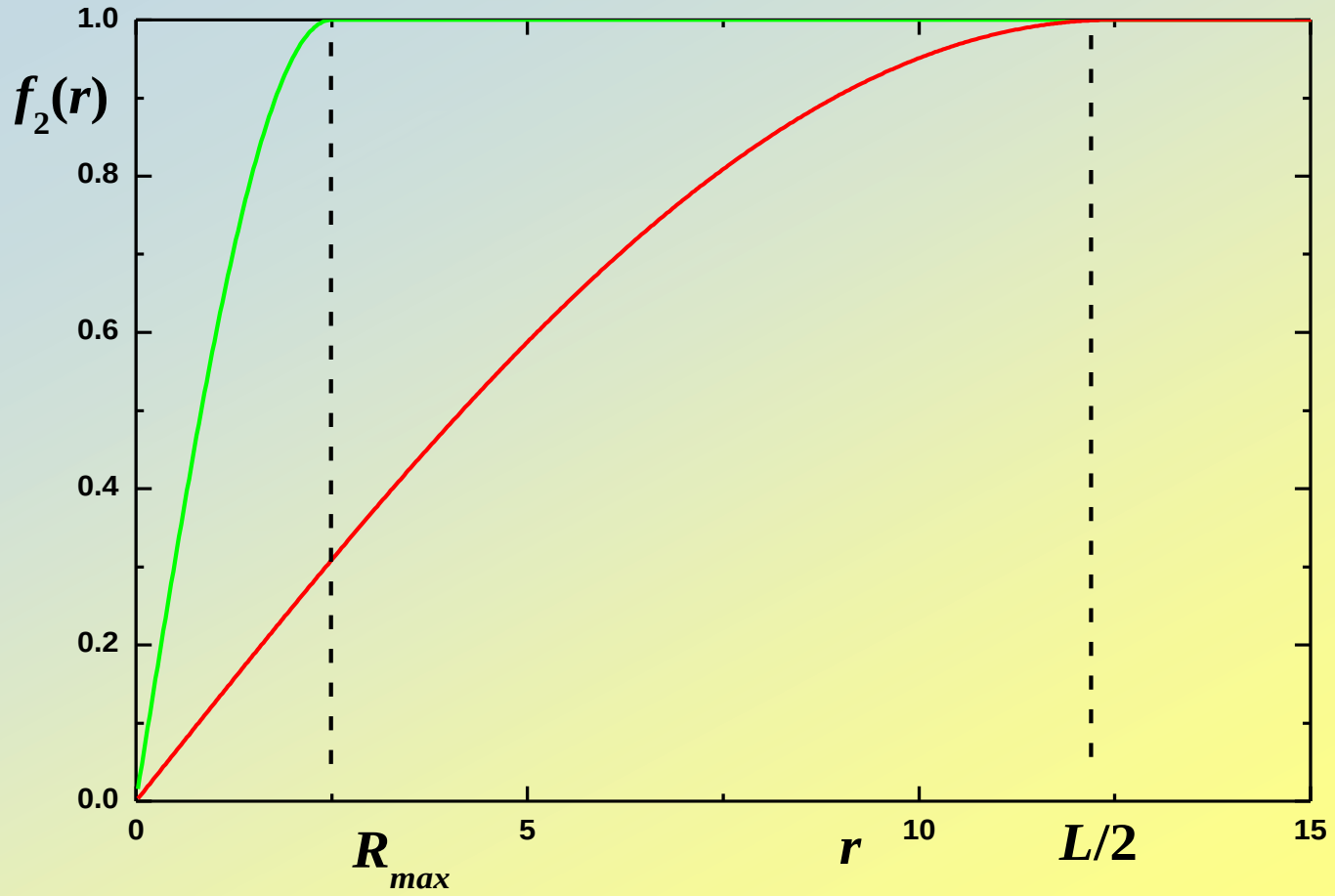
$$\begin{aligned} f_2^{3D}(r) &\propto \exp(-C_1/r^2) \\ f_2^{2D}(r) &\propto \exp\{-C_1/r\} \\ f_2^{1D}(r) &\propto \sin^{C_1}[\pi|r|/(2L)] \end{aligned}$$

where coefficient $C_1$ depends on the speed of sound.

[1] L. Reatto and G.V. Chester, Phys. Rev. **155**, 88 (1967).

# JASTROW TWO-BODY TERMS






The DMC code can be made scalable if the two-body Jastrow is truncated at some distance $R_{max} < L/2$. The complexity of the algorithm is $N(N_{neigh.} - 1)/2$, where $N_{neigh.} \approx nR_{max}^D$ is the number of neighbor particles.

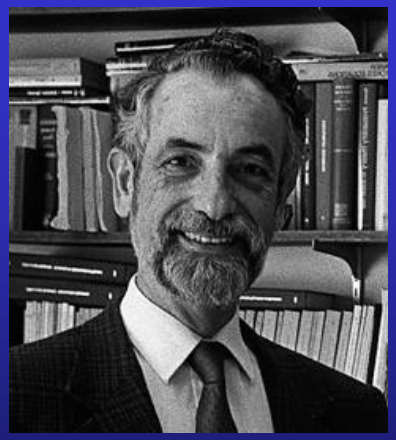
# TEST: EXACT LIEB-LINIGER MODEL

$N$ bosonic particles of mass $m$ interacting with contact $\delta$-function pseudopotential in a one dimensional system are described by the Lieb-Liniger Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial z_i^2} + g_{1D}\sum_{i<j}^{N}\delta(z_i - z_j)$$

The effective quasi-one-dimensional coupling constant is inversely proportional to the one-dimensional $s$-wave scattering length

$$g_{1D} = -\frac{2\hbar^2}{m a_{1D}}$$

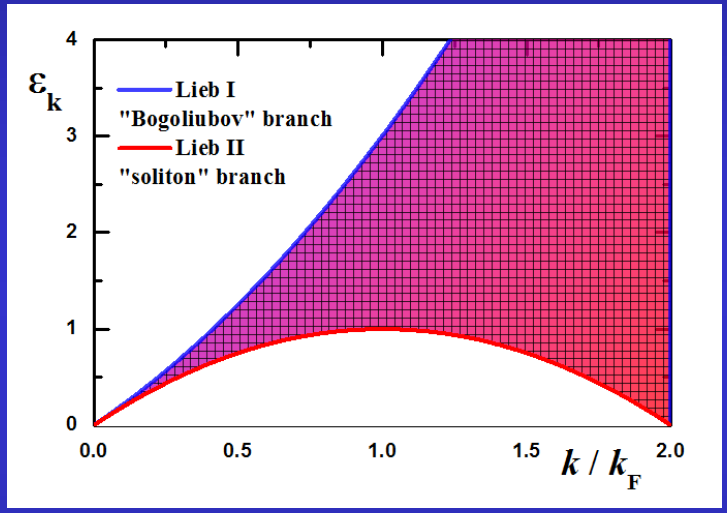


Elliott H. Lieb

The model solved exactly by
E. H. Lieb and W. Liniger in (1963)
Phys. Rev. **130**, 1605 (1963)

# DIFFERENT REGIMES

The characteristic parameter of the problem is $\gamma = c/\rho$ which defines the strength of particle-particle interactions. Here $c$ is one-dimensional couping constant and $\rho$ is the linear density.




In particular, when

- $\gamma \to 0$ interactions are weak, system behaves as a weakly interacting Bose gas (Gross-Pitaevskii regime)
- $\gamma \to \infty$ interactions are strong, system behaves as an ideal Fermi gas (Tonks-Girardeau regime)

# ONE-DIMENSIONAL FERMI GAS



The Slater determinant of one-dimensional plane waves $\varphi_l(z) = e^{i\frac{2\pi}{L}z}$ can be writen in form of a Vandermonde matrix.

$$\Psi(z_1,...,z_N) = \begin{vmatrix} \varphi_1(z_1) & \dots & \varphi_N(z_1) \\ \vdots & \ddots & \vdots \\ \varphi_1(z_1) & \dots & \varphi_N(z_N) \end{vmatrix} = \begin{vmatrix} 1 & e^{i\frac{2\pi}{L}z_1} & \dots & (e^{i\frac{2\pi}{L}z_1})^{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & e^{i\frac{2\pi}{L}z_N} & \dots & (e^{i\frac{2\pi}{L}z_N})^{N-1} \end{vmatrix} = \prod_{i<j}(e^{i\frac{2\pi}{L}z_i} - e^{i\frac{2\pi}{L}z_j})$$

$$= \prod_{i<j}\mathrm{sign}(z_i - z_j)\prod_{i<j}|\sin\tfrac{\pi}{L}(z_i - z_j)| = \mathcal{A}(z_1,...,z_N)\prod_{i<j}|\sin\tfrac{\pi}{L}(z_i - z_j)|$$

- The wave function of an ideal Fermi gas simplifies into a pair product of $|\sin\frac{\pi}{L}(z_i - z_j)|$ terms with antisymmetric multiplier $\mathcal{A}$
- The parity of given configuration can be written in a very simple form: $(-1)^{\mathcal{P}} = \prod_{i<j}^{N}\mathrm{sign}(z_i - z_j)$
- Fermionic $N^3$ problem is reduced to $N^2$ bosonic complexity!

# BOSONS: MAPPING OF THE WAVE FUNCTION



Apart from the symmetrizing $\mathcal{A}$ factor wave function of a one-dimensional ideal Fermi gas looks like a wave function of a Bose system

$$\Psi(z_1, ..., z_N) = \mathcal{A}(z_1, ..., z_N) \prod_{i<j} |\sin \tfrac{\pi}{L}(z_i - z_j)|$$

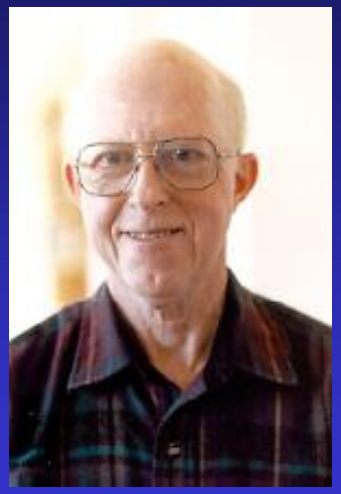
Here enter special properties of one-dimensional geometry:

- The only way to exchange two particles is to pass drag one particle through the other.
- Pauli exclusion principle can be mimicked by a strong short-range repulsion

# TONKS-GIRARDEAU GAS: WF

The absolute value of the wave function of an ideal Fermi gas is exactly the same as the wave function of Bose particles interacting via infinitely strong short-range interaction (Girardeau 1960)

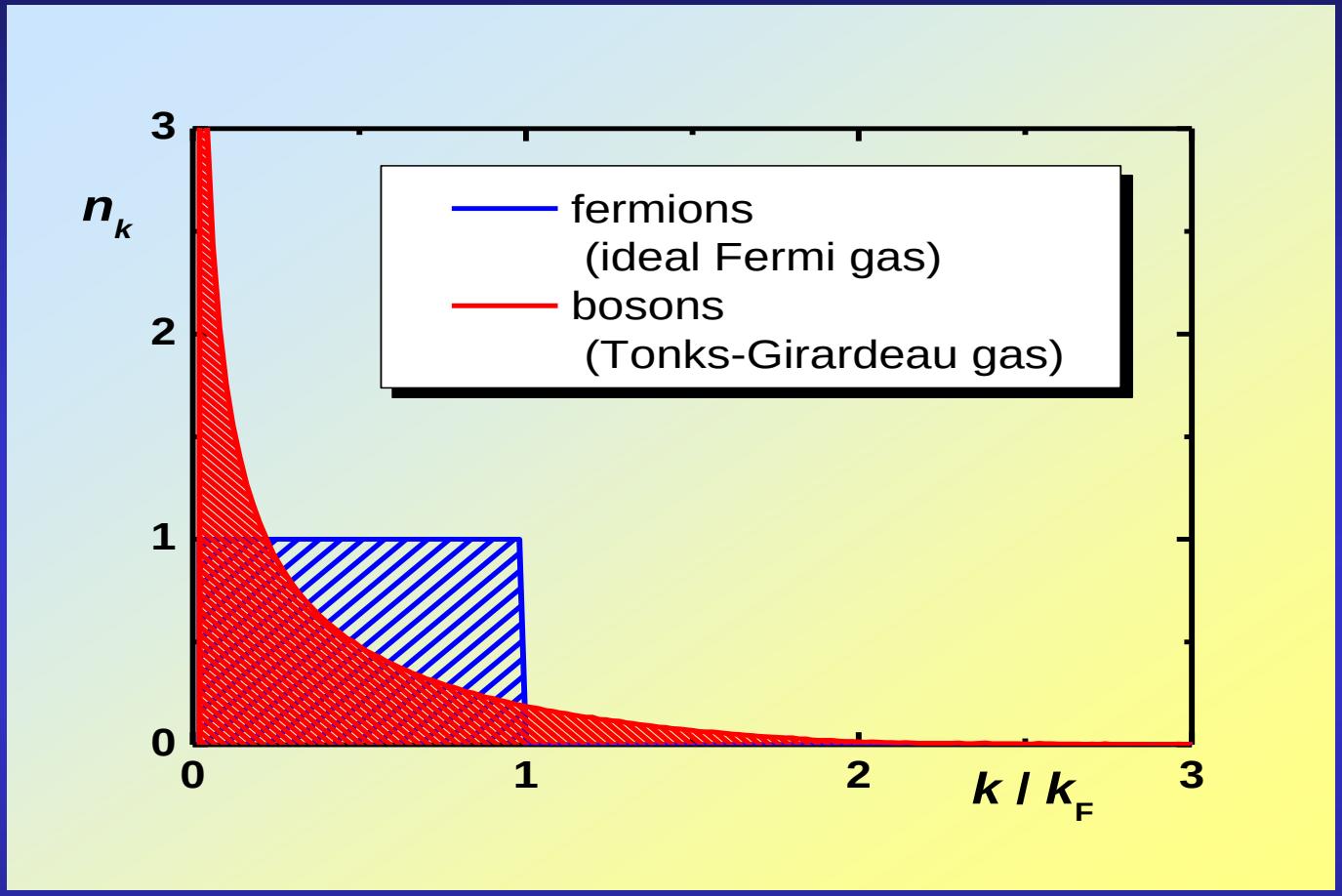
$$\Psi_B(z_1, ..., z_N) = |\Psi_F(z_1, ..., z_N)|$$



- All diagonal properies (density profile, pair distribution function, etc) are exactly the same
- Energies and chemical potential are exactly the same $\mu = \frac{\hbar^2 k_F^2}{2m}$
- Non-diagonal properties (one-body density matrix, momentum distribution, etc) are different

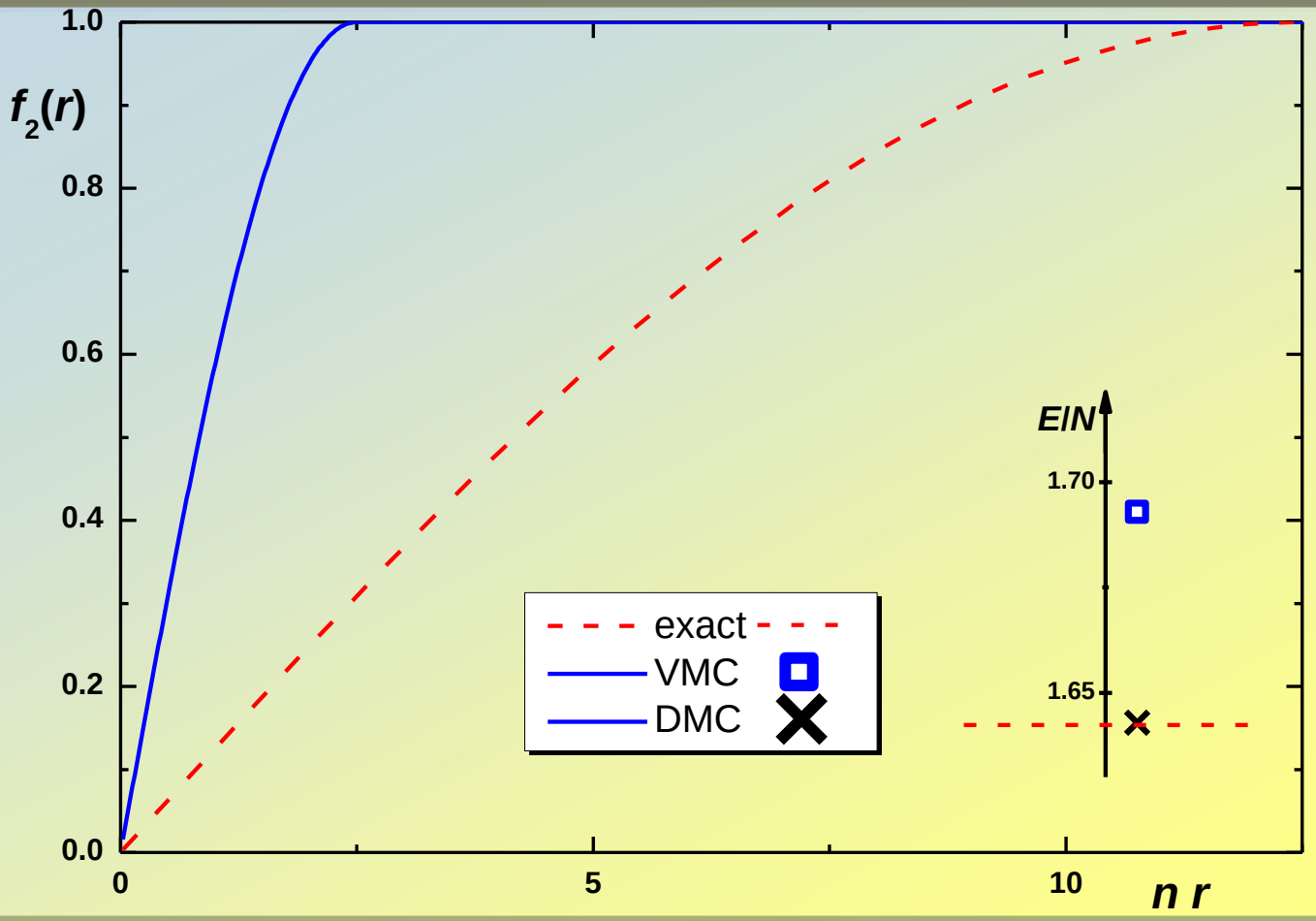
# TG GAS: MOMENTUM DISTRIBUTION






Momentum distribution $n_k$ of a homogeneous ideal Fermi gas and Tonks-Girardeau gas Here $k_F = \pi n$ is the Fermi momentum.

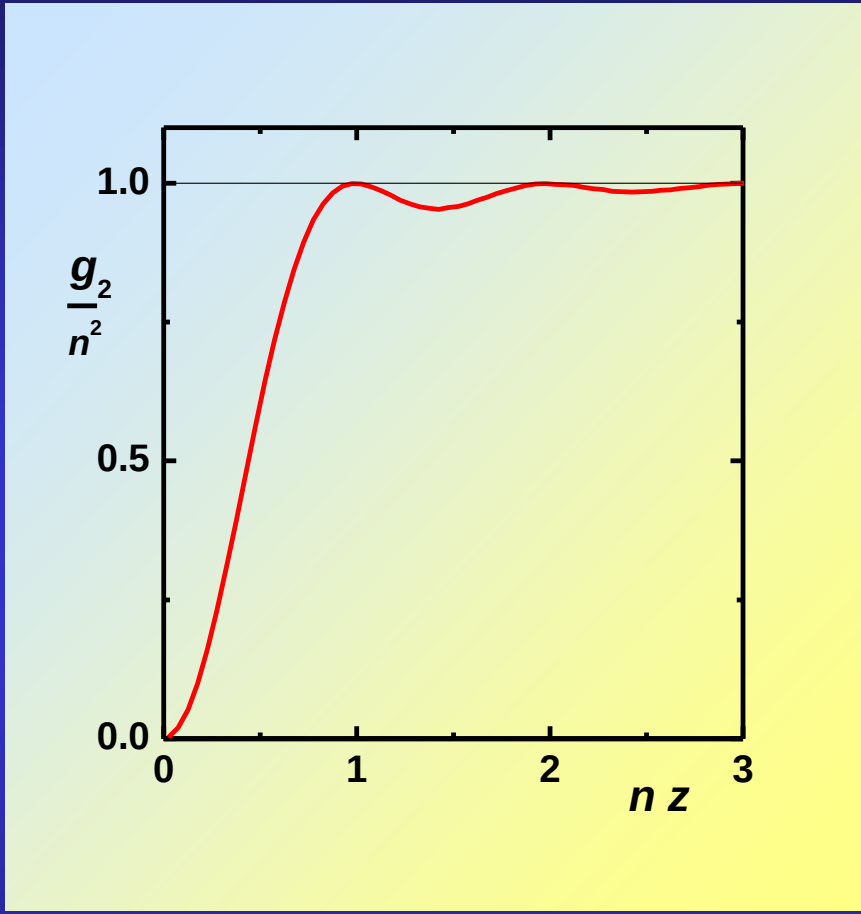
# TESTING THE ENERGY

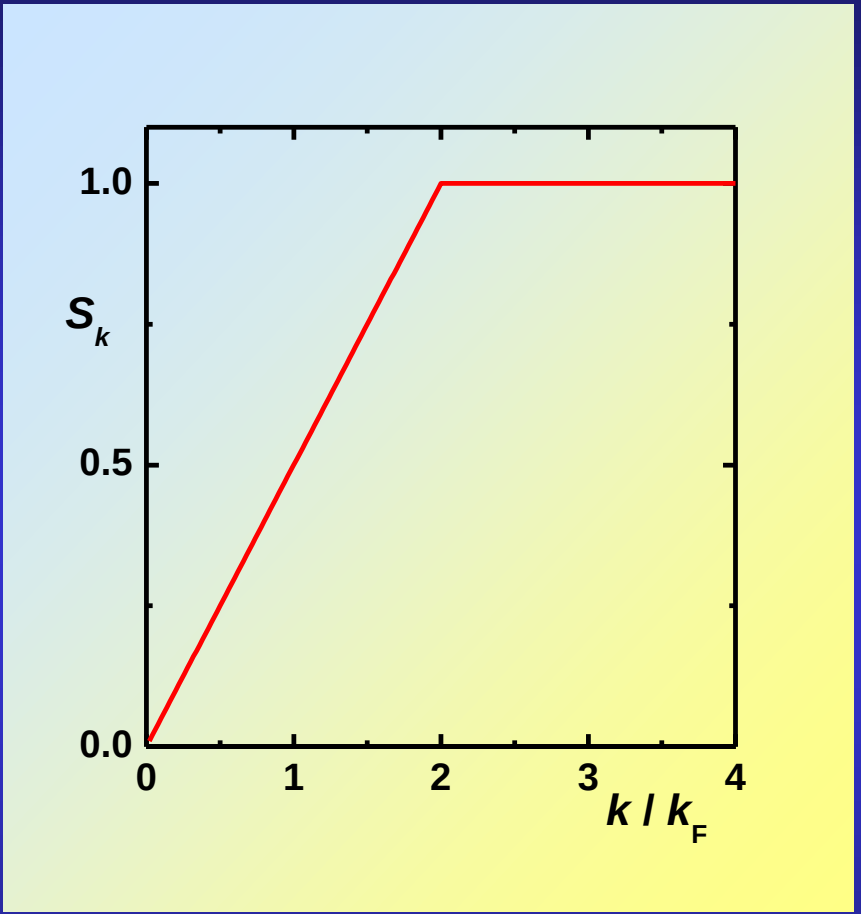



The DMC code can be made scalable if the two-body Jastrow is truncated at some distance $R_{max} < L/2$. The complexity of the algorithm is $N(N_{neigh.} - 1)/2$, where $N_{neigh.} \approx nR_{max}^D$ is the number of neighbor particles.

# CORRELATION FUNCTIONS (EXACT)



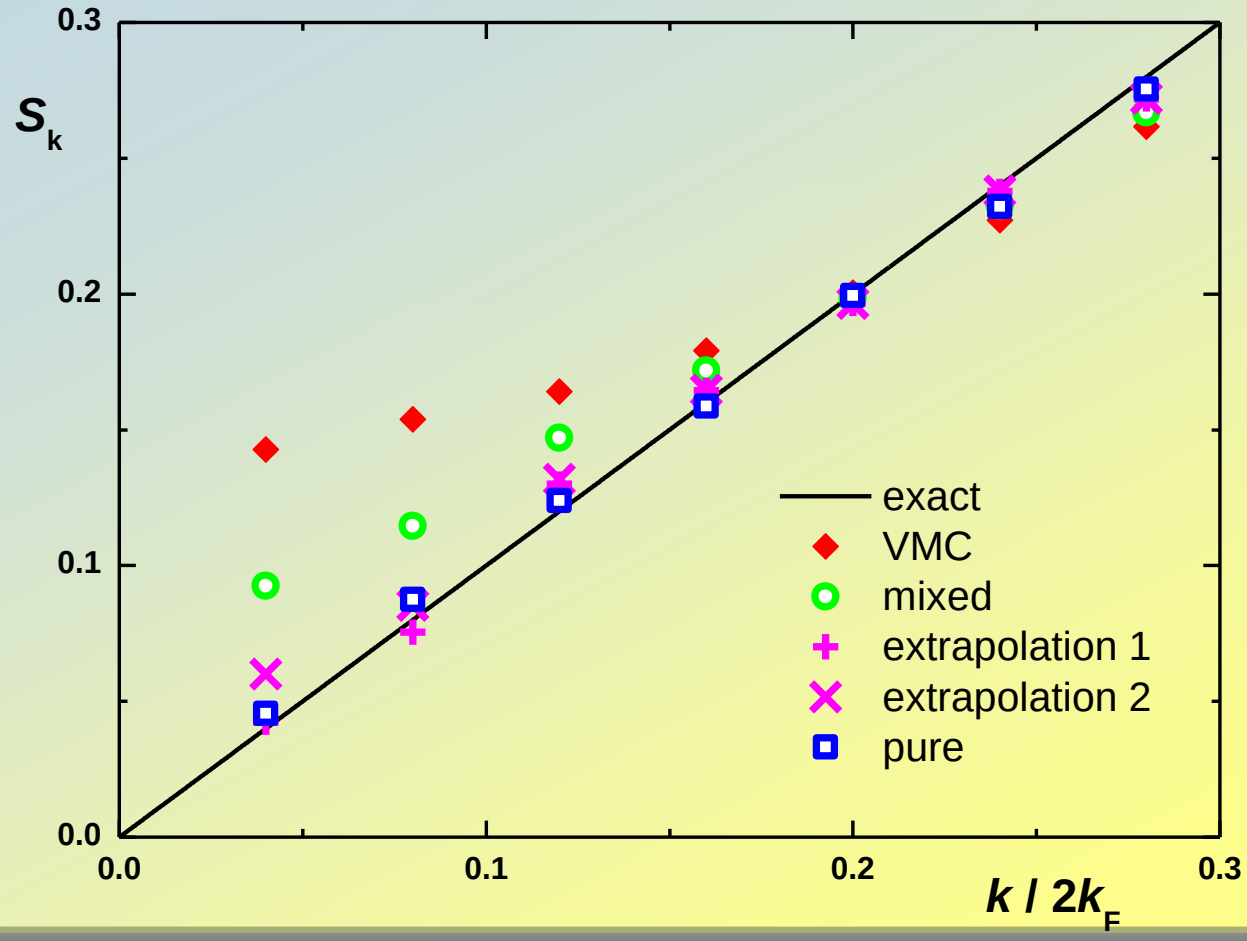



(left) Density-density pair distribution function $g_2(z)$ (right) and static structure factor $S_k$.

# TEST: STATIC STRUCTURE FACTOR






Low-momentum part of the static structure factor. Solid line - exact thermodynamic result; Monte Carlo results with $N = 25$ particles, estimators: diamonds - variational, circles - mixed, pluses and crosses - extrapolation 1 and 2, squares - pure

# OPEN PROBLEM



good Linear in $N$ complexity can be achieved ($NN_{neighb}$) - calculation at a single step

bad Long-range / phononic correlations are spoiled

good Pure estimators fix it

bad Not the end of the story, DMC time step should be adjusted as $N$ is increased

# SCHRÖDINGER EQUATION

Imaginary time evolution is governed by Schrödinger equation

$$-\frac{\partial}{\partial \tau}\varphi(\mathbf{R},\tau) = (\hat{H} - E)\varphi(\mathbf{R},\tau),$$

The formal solution $\psi(\mathbf{R},\tau) = e^{-(\hat{H}-E)\tau}\psi(\mathbf{R},0)$ can be expanded in eigenstate functions of the Hamiltonian $\hat{H}\phi_n = E_n\phi_n$, ordered as $E_0 < E_1 < ...$

$$\psi(\mathbf{R},\tau) = \sum_{n=0}^{\infty} c_n\phi_n(\mathbf{R},\tau) = \sum_{n=0}^{\infty} c_n\phi_n(\mathbf{R},0)e^{-(E_n-E)\,\tau}$$

- For large times $\psi(\mathbf{R},\tau) \to c_0\ \phi_0(\mathbf{R},0)\ e^{-(E_0-E)\,\tau}$
- In the long time limit the wave function is projected to the ground state and $E$ approaches $E_0$

# IMPORTANCE SAMPLING

- The efficiency is improved by sampling $f(\mathbf{R},\tau) = \psi_T(\mathbf{R})\psi(\mathbf{R},\tau)$ where $\psi_T(\mathbf{R})$ is a known trial w.f.

- The equivalent differential equation is

$$-\frac{\partial}{\partial\tau} f(\mathbf{R},\tau) = -D\Delta_{\mathbf{R}} f(\mathbf{R},\tau) + D\nabla_{\mathbf{R}}(\mathbf{F} f(\mathbf{R},\tau)) + (E^{loc}(\mathbf{R}) - E) f(\mathbf{R},\tau),$$

- The *local energy* $E^{loc}(\mathbf{R}) = \psi_T^{-1}(\mathbf{R})\hat{H}\psi_T(\mathbf{R})$

- The *drift force* $\mathbf{F} = \frac{2}{\psi_T(\mathbf{R})}\nabla_{\mathbf{R}}\psi_T(\mathbf{R})$

# DMC ALGORITHM

- Non-negative $f(\mathbf{R},\tau)$ is interpreted as population density distribution $f(\mathbf{R},\tau) = \sum_{i=1}^{N_W} C\delta(\mathbf{R}-\mathbf{R_i}(\tau))$ of *walkers* with coordinates $\mathbf{R_i}(\tau)$

- DMC algorithm for a primitive time propagation:

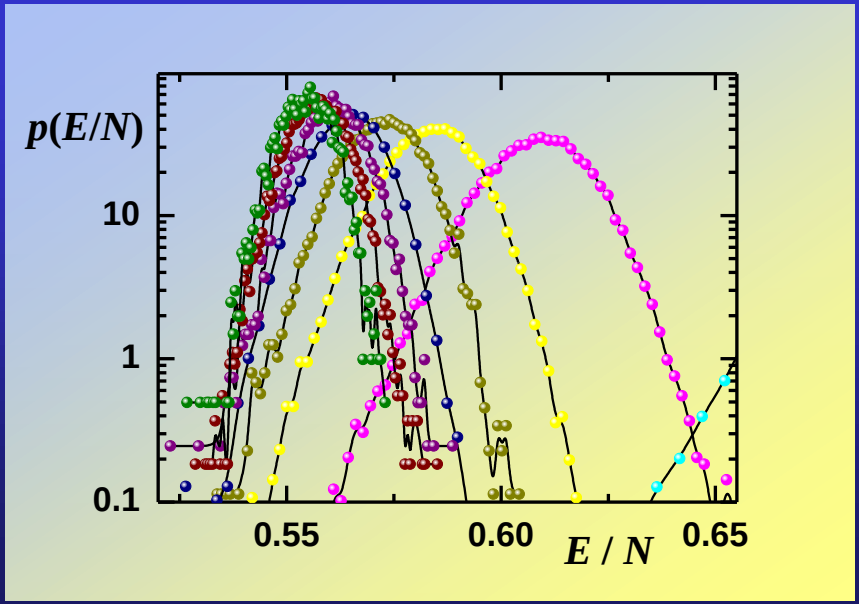
1 *Diffusion* delocalizes according to the kinetic part $\mathbf{R^{(1)}}(t+\Delta\tau) = \mathbf{R}(\tau) + \chi$, with $\chi$ random value having a gaussian distribution $\exp\{-\chi^2/(4D\Delta\tau)\}$

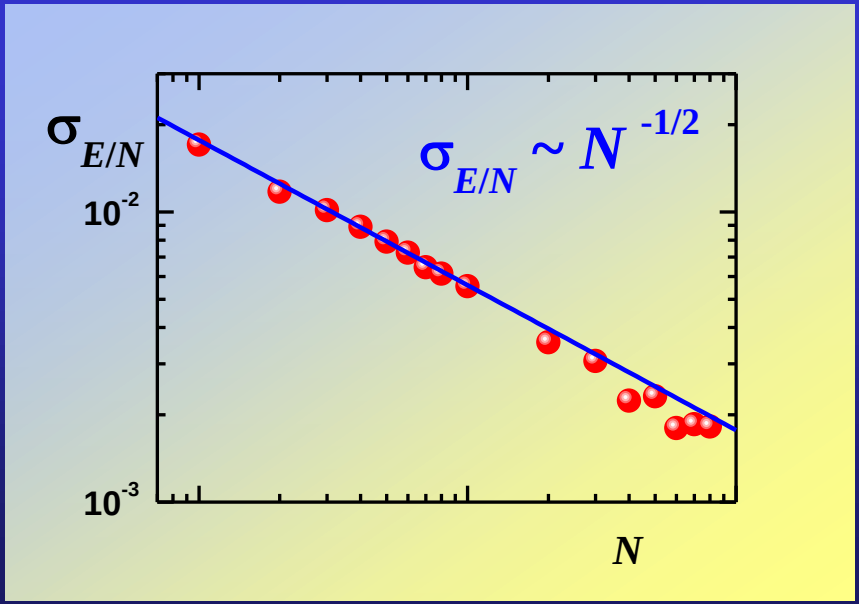
2 Drift force pushes the walkers to most important areas of the phase space $\mathbf{R^{(2)}}(t+\Delta\tau) = \mathbf{R}(\tau) + DF(\mathbf{R})\Delta\tau$

3 *Branching* corrects the trial w.f. and does the projection $f^{(3)}(\mathbf{R},\tau+\Delta\tau) = \exp\{-(E^{loc}(\mathbf{R}) - E)\,\Delta\tau\}\; f(\mathbf{R},\tau)$

# TIMESTEP SLOWDOWN

- The branching term $f^{(3)}(\mathbf{R}, \tau + \Delta\tau) = \exp\{-(E^{loc}(\mathbf{R}) - E)\,\Delta\tau\}\; f(\mathbf{R}, \tau)$
- The short time expansion requires $\sigma_E \Delta\tau \ll 1$
- Typical variance of the *total* energy $\sigma_E \propto N^{1/2}$
- Limitation on the timestep $\Delta\tau \propto N^{-1/2}$



# CONCLUSIONS 2/3



- Linear in $N$ complexity can be achieved ($NN_{neighb}$) - calculation at a single step
- Long-range / phononic correlations are spoiled
- Pure estimators fixes it
- Additionally, an effective $N^{+1/2}$ order is added due to time step limitations, leading to
  - effective $N^{2.5}$ order in a standard formulation,
  - effective $N^{1.5}N_{neighb}$ order for short-range potential & Jastrow.

# PURE ESTIMATORS



Diffusion Monte Carlo method has advantages of being:

- exact (at least conceptually) for calculation of the ground-state energy
- able to calculate in a pure way local properties (e.g. potential energy, pair distribution function, static structure factor, density profile, etc.)

Still DMC suffers from the following disadvantages:

- non-local correlation functions are obtained as a mixed estimator (one-body density matrix, momentum distribution, etc.)
- Extrapolation technique can be used with no guarantee, e.g. zero/finite condensate fraction.
- Other Monte Carlo methods overcome this problem (e.g. PIMC, PIGS, ...)

Is it possible to calculate OBDM in a pure way?

# OBDM

The one-body density matrix $\rho_1(|\mathbf{r}_1 - \mathbf{r}_2|)$ is a non-local quantity and is related to the probability of inserting a particle at position $\mathbf{r}_2$ after destroying a particle at position $\mathbf{r}_1$ while keeping coordinates of all other particles fixed
In terms of the ground-state wave function $\phi_0(\mathbf{R})$ the one-body density matrix is defined as

$$\rho_1(|\mathbf{r}|) = \frac{\int \phi_0(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, ..., \mathbf{r}_N)\phi_0(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)\, \mathbf{dr}_1 ... \mathbf{dr}_N}{\int |\phi_0(\mathbf{r}_1, ..., \mathbf{r}_N)|^2\, \mathbf{dr}_1 ... \mathbf{dr}_N}$$

for convenience we consider a homogeneous system, so that $\rho_1$ depends on one argument $r = |\mathbf{r}_1 - \mathbf{r}_2|$.

# PURE ESTIMATOR FOR OBDM 1/3

The *pure* expression for the one-body density matrix can be written as

$$\rho_1(|\mathbf{r}|) = \frac{\int \frac{\psi_T(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)}{\psi_T(\ \mathbf{r}_1\ ,\mathbf{r}_2,..,\mathbf{r}_N)} \frac{\phi_0(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)}{\psi_T(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)} \psi_T(\mathbf{R})\phi_0(\mathbf{R})\, \mathbf{dr}_1..\mathbf{dr}_N}{\int \frac{\phi_0(\mathbf{R})}{\psi_T(\mathbf{R})} f(\mathbf{R})\, \mathbf{dr}_1...\mathbf{dr}_N}$$

- For long times of integration, the DMC procedure generates a series of configurations satisfying the probability distribution $f(\mathbf{R}) = \psi_T(\mathbf{R})\phi_0(\mathbf{R})$.
- last term corresponds to sampling over distribution $f(\mathbf{R})$

# PURE ESTIMATOR FOR OBDM 2/3

The *pure* expression for the one-body density matrix can be written as

$$\rho_1(|\mathbf{r}|) = \frac{\int \frac{\psi_T(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)}{\psi_T(\mathbf{r}_1,\mathbf{r}_2,..,\mathbf{r}_N)} \frac{\phi_0(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)}{\psi_T(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)} \psi_T(\mathbf{R})\phi_0(\mathbf{R})\, \mathbf{dr}_1..\mathbf{dr}_N}{\int \frac{\phi_0(\mathbf{R})}{\psi_T(\mathbf{R})} f(\mathbf{R})\, \mathbf{dr}_1...\mathbf{dr}_N}$$

- Another piece is calculated directly from the known trial wave function $\psi_T(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,...,\mathbf{r}_N)/\psi_T(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N)$
- Average of this term alone over $f(\mathbf{R})$ would provide a mixed estimator.

# PURE ESTIMATOR FOR OBDM 3/3

The *pure* expression for the one-body density matrix can be written as

$$\rho_1(|\mathbf{r}|) = \frac{\int \frac{\psi_T(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)}{\psi_T(\mathbf{r}_1,\mathbf{r}_2,..,\mathbf{r}_N)} \frac{\phi_0(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)}{\psi_T(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,..,\mathbf{r}_N)} \psi_T(\mathbf{R})\phi_0(\mathbf{R})\, \mathbf{dr}_1..\mathbf{dr}_N}{\int \frac{\phi_0(\mathbf{R})}{\psi_T(\mathbf{R})} f(\mathbf{R})\, \mathbf{dr}_1...\mathbf{dr}_N}$$

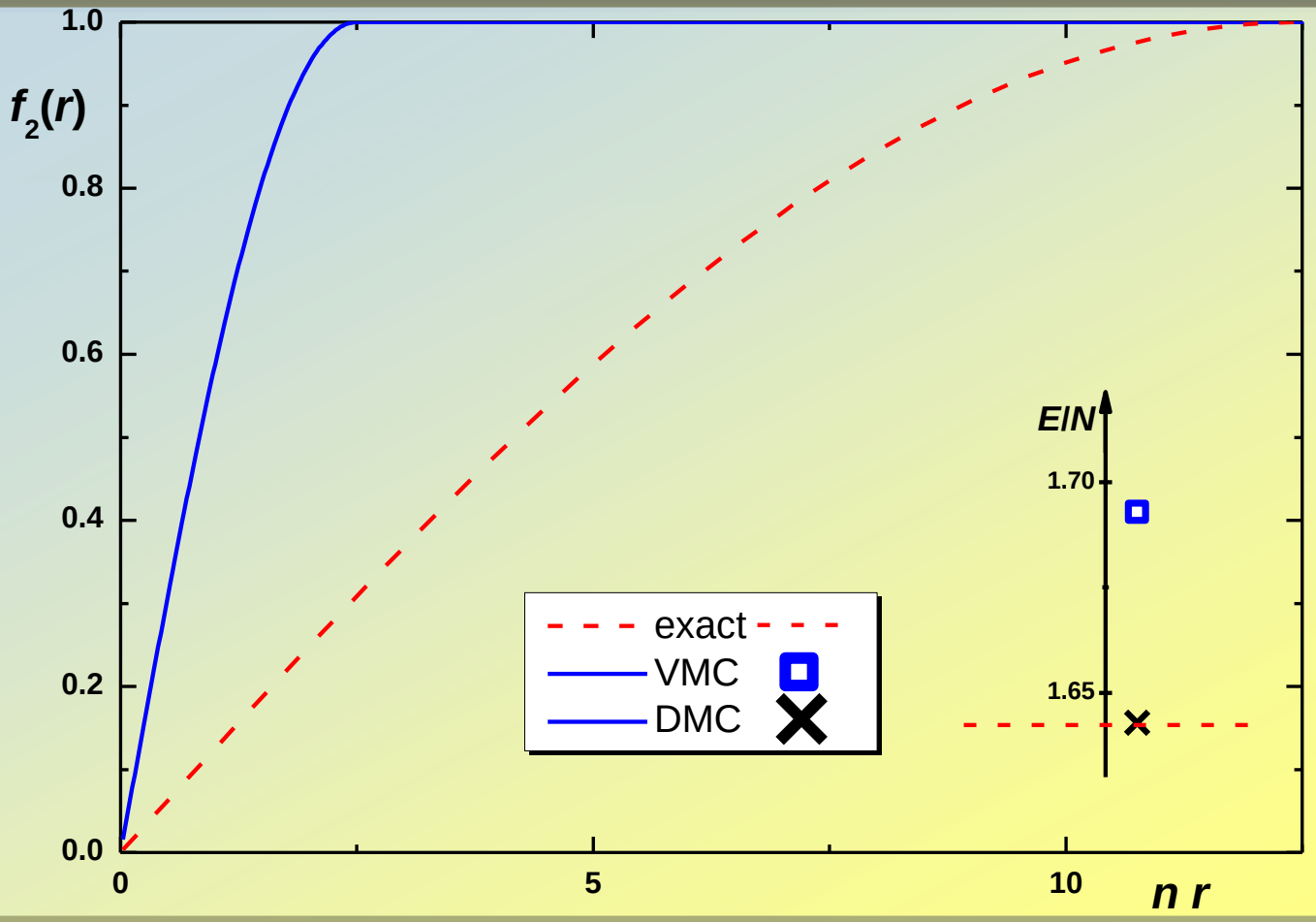
- The third piece is the ratio of ground state and trial wave functions at a displaced position $\phi_0(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,...,\mathbf{r}_N)/\psi_T(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,...,\mathbf{r}_N)$.
- It was shown in [1] that for a non-displaced position the ratio can be obtained as a number of sons of the walker $W(\mathbf{R}) = W(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N) = \phi_0(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N)/\psi_T(\mathbf{r}_1,\mathbf{r}_2,...,$
- The problem is that there is no walker in $(\mathbf{r}_1+\mathbf{r},\mathbf{r}_2,...,\mathbf{r}_N)$

[1] K. S. Liu, M. H. Kalos, G. V. Chester PRA **10**, 303 (1974)

# VIRTUAL WALKER

- For local quantities ($\mathbf{r} = 0$) number of sons $W(\mathbf{R})$ are obtained by following the walker in imaginary time $\phi_0(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)/\psi_T(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \rightarrow W(\mathbf{R}, \tau), \tau \rightarrow \infty$
- For non-local quantities, we introduce a *virtual walker* with artificially displaced coordinates $\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, ..., \mathbf{r}_N$ and accumulate its weight in the branching process. $\phi_0(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, ..., \mathbf{r}_N)/\psi_T(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, ..., \mathbf{r}_N) \rightarrow W(\mathbf{R}', \tau), \tau \rightarrow \infty$
- The walker is virtual in the sense that it does not contribute to any other observable.

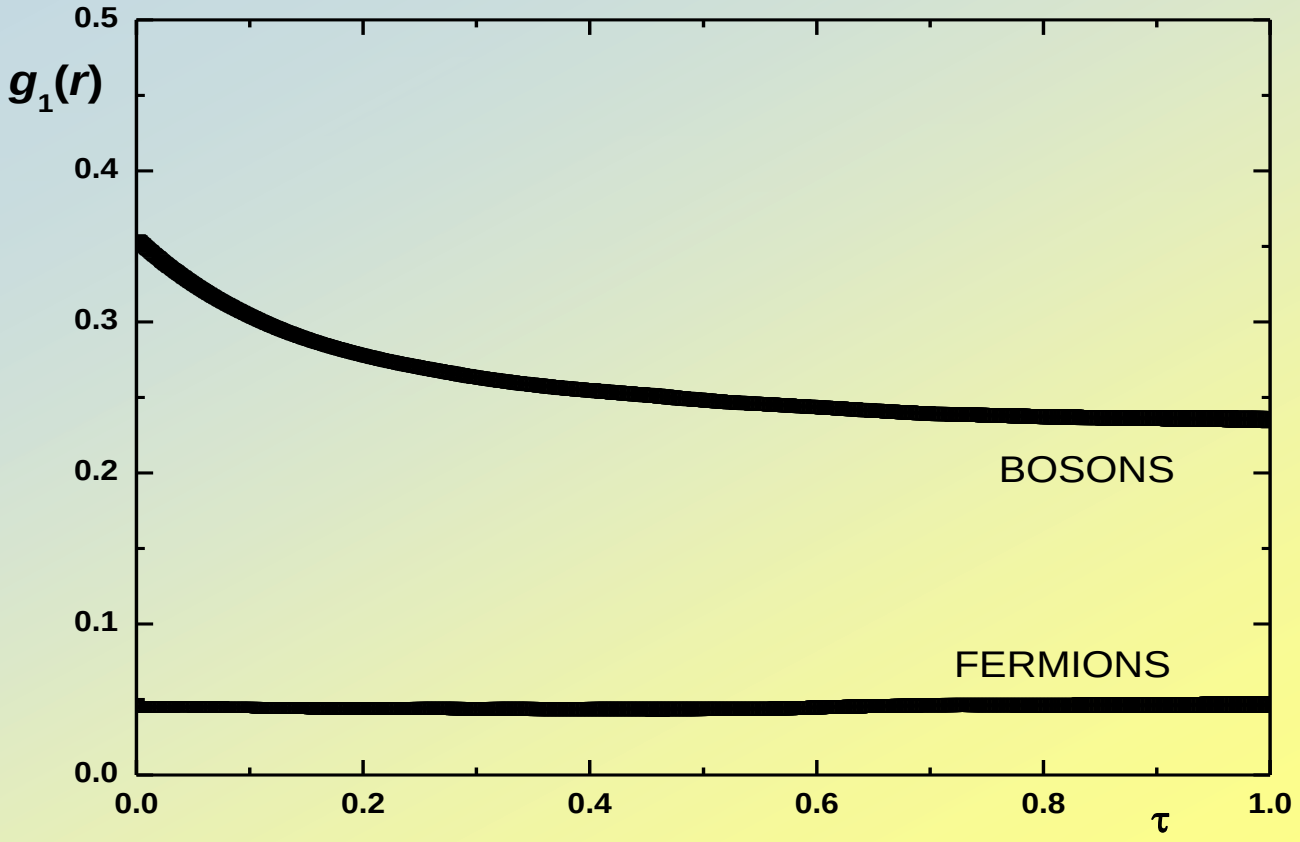
# JASTROW TWO-BODY TERMS




In order to verify the pure estimators we heavily spoil the wave function.

# OBDM: imaginary-time convergence

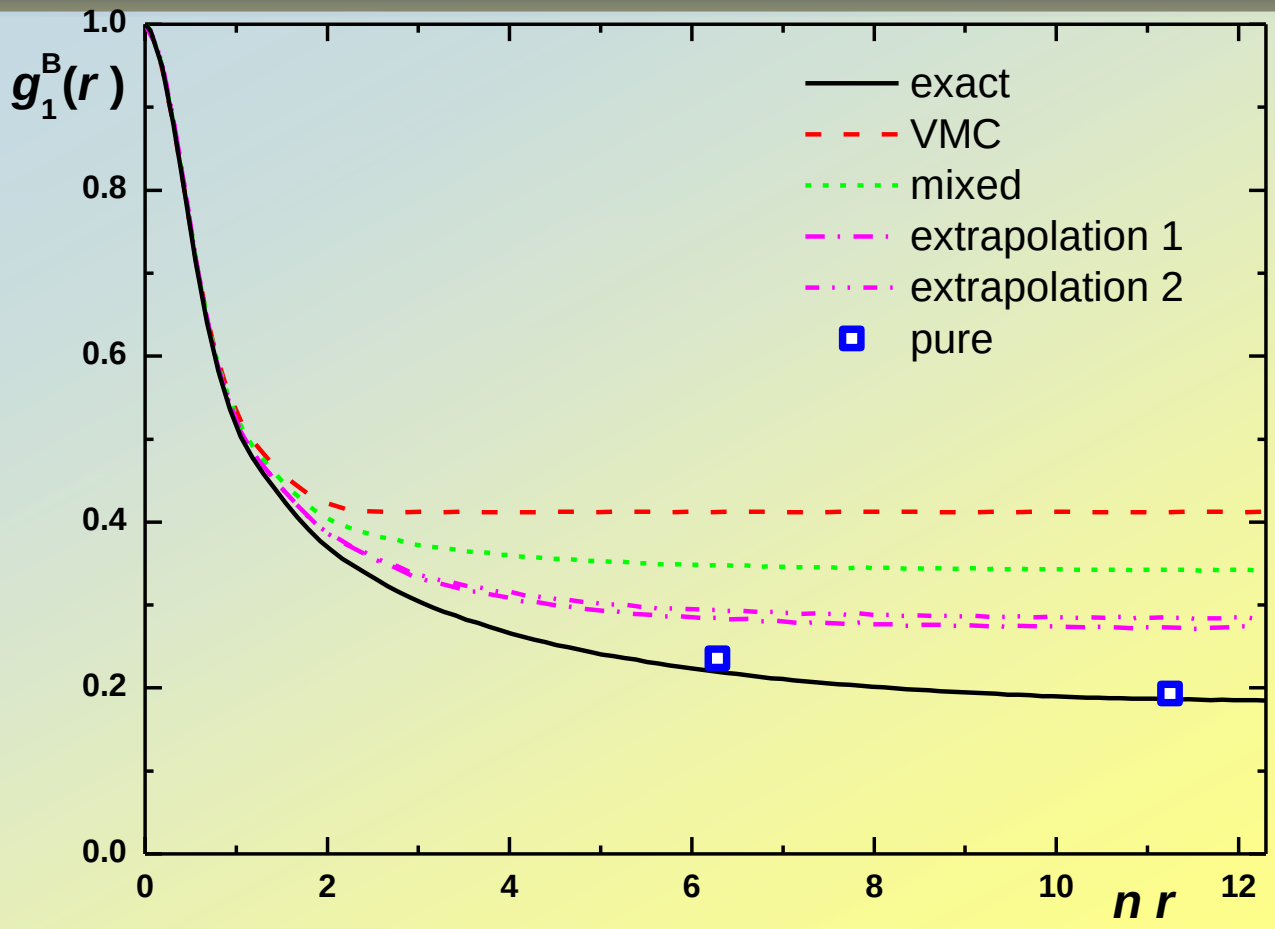





The average "number of sons" $\langle W(\mathbf{R}')\rangle_{f(\mathbf{R})}$ of a virtual walker
Zero imaginary time - mixed estimator, infinite imaginary time - pure estimator.

# OBDM: bosons

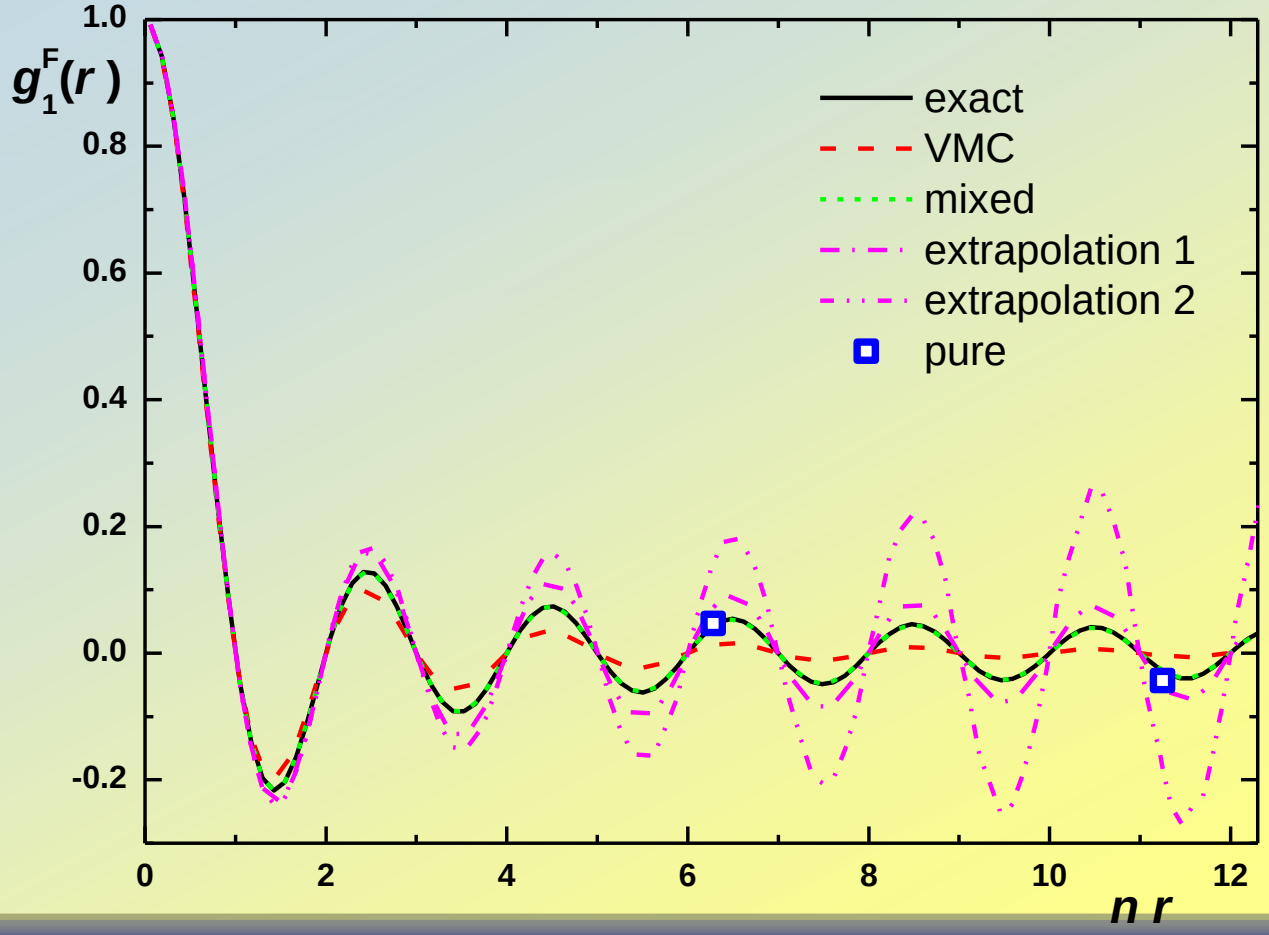





Bosonic one-body density matrix. Solid line - exact wave function, long-dashed line - variational estimator, short-dashed line - mixed estimator, dash-dot and dash-dot-dot - extrapolations 1 and 2, square symbols - pure estimator

# OBDM: fermions






Fermionic one-body density matrix. Solid line - exact wave function, long-dashed line - variational estimator, short-dashed line - mixed estimator, dash-dot and dash-dot-dot - extrapolations 1 and 2, square symbols - pure estimator

# CONCLUSIONS 3/3



- Pure estimators of local quantities can be obtained by following imaginary-time evolution of walkers
- Pure estimators of non-local quantities can be obtained by following imaginary-time evolution of virtual walkers

THANK YOU VERY MUCH
FOR YOUR ATTENTION!

# CONDITION FOR ONE-DIMENSIONALITY



The gas behaves dynamically as one-dimensional when the excitations of the levels of the transverse confinement are not possible:

- Condition for the energy

$$\frac{E}{N} - \frac{1}{2}\hbar\omega_{\mathrm{osc}} \ll \hbar\omega_{\mathrm{osc}}$$

- Condition for the temperature

$$k_B T \ll \hbar\omega_{\mathrm{osc}}$$

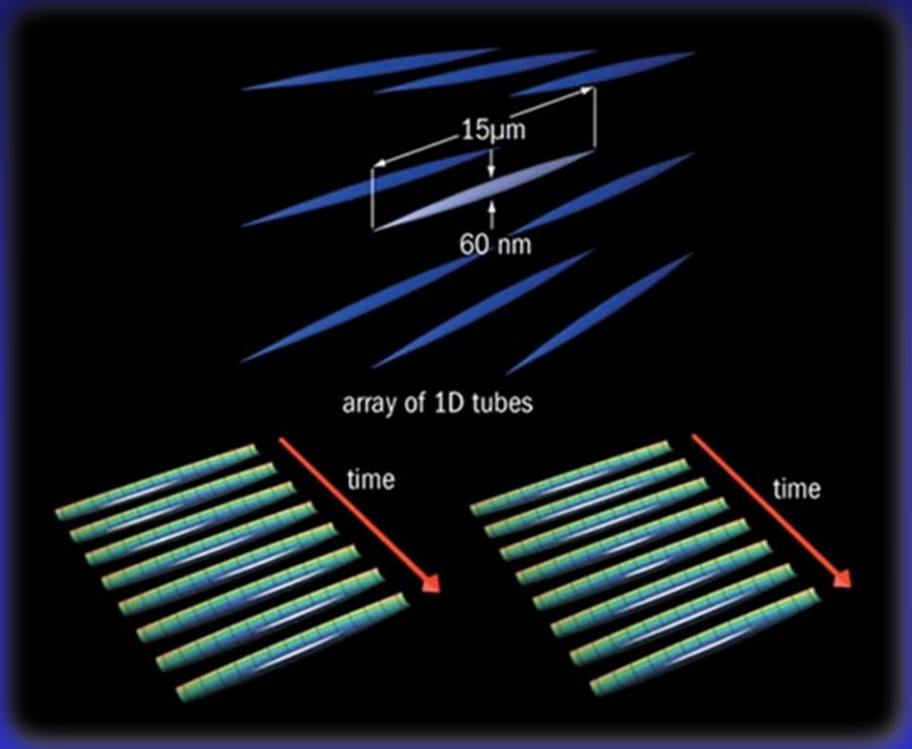
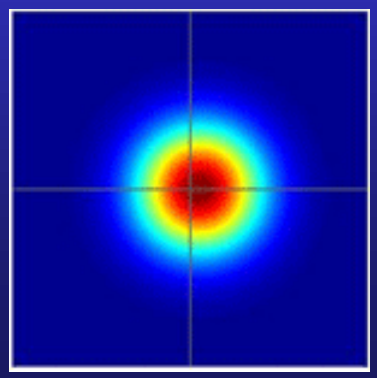
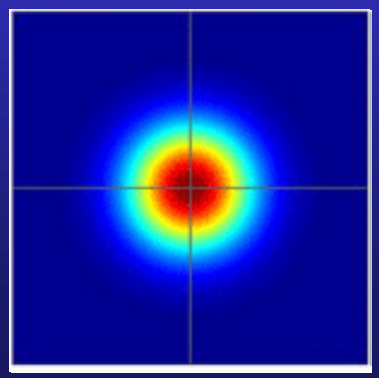



Figure is taken from
T.Esslinger et al./Zurich





Comparison of the frequencies of the dipole and breathing modes confirms the achievement of the quasi-one-dimensional regime.

# CORRELATION FUNCTIONS

- The one-body density matrix quantifies correlations of the field-operator between two points in space
$g_1(x) = \langle \hat{\Psi}^\dagger(x)\hat{\Psi}(0)\rangle = \frac{N}{n}\frac{\int \Psi_0^*(x_1+x,\ldots,x_N)\Psi_0(x_1,\ldots,x_N)\,dx_2\ldots dx_N}{\int |\Psi_0(x_1,\ldots,x_N)|^2\,dx_1\ldots dx_N}$

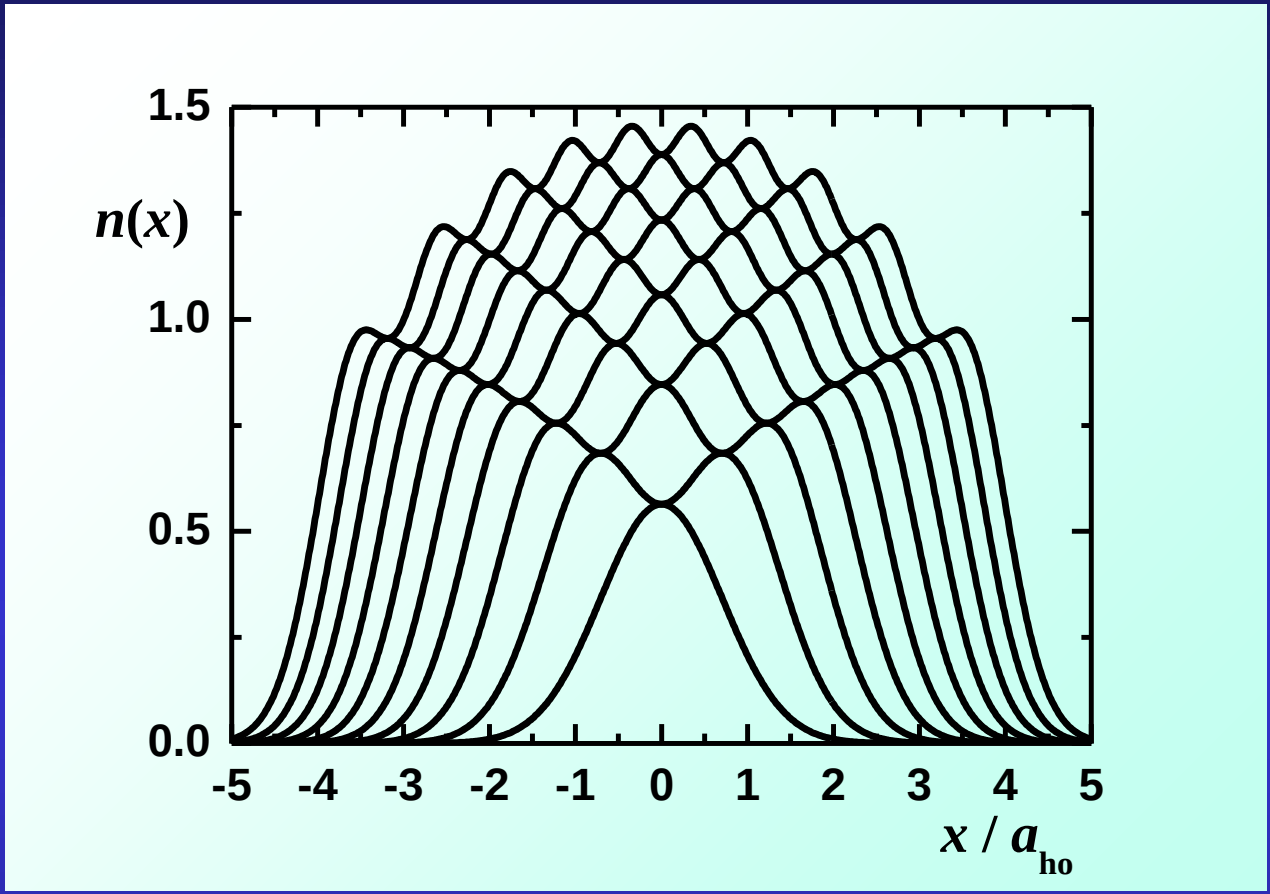
- The pair distribution function gives the possibility to find a particle at a distance $x$ from another particle
$g_2(x) = \langle \hat{\Psi}^\dagger(0)\Psi^\dagger(x)\hat{\Psi}(x)\hat{\Psi}(0)\rangle = \frac{N(N-1)}{n^2}\frac{\int |\Psi_0(x,0,x_3,\ldots,x_N)|^2\,dx_3\ldots dx_N}{\int |\Psi_0(x_1,\ldots,x_N)|^2\,dx_1\ldots dx_N}$

- The static structure factor is related to the Fourier transform of the pair distribution function $S(k) = 1 + n\int e^{ikx}(g_2(x)-1)\,dx$

- The momentum distribution is the Fourier transform of the one-body density matrix $n(k) = n\int e^{ikx} g_1(x)\,dx$

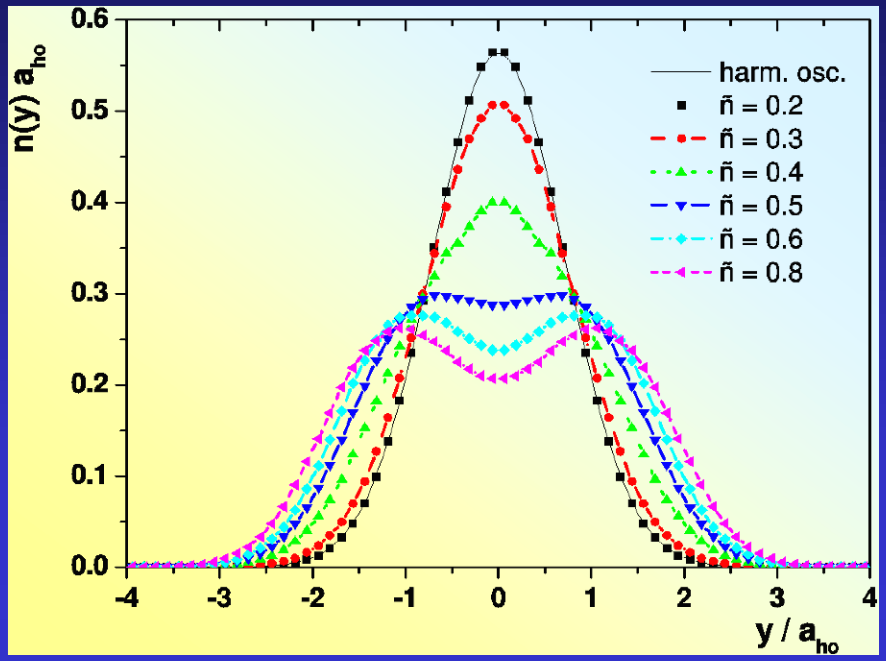
- The value at zero distance of the three-body correlation function gives the probability of finding three particles at the same position in space $g_3(0) = \frac{N(N-1)(N-2)}{n^3}\frac{\int |\Psi_0(0,0,0,x_4,\ldots,x_N)|^2\,dx_4\ldots dx_N}{\int |\Psi_0(x_1,\ldots,x_N)|^2\,dx_1\ldots dx_N}$

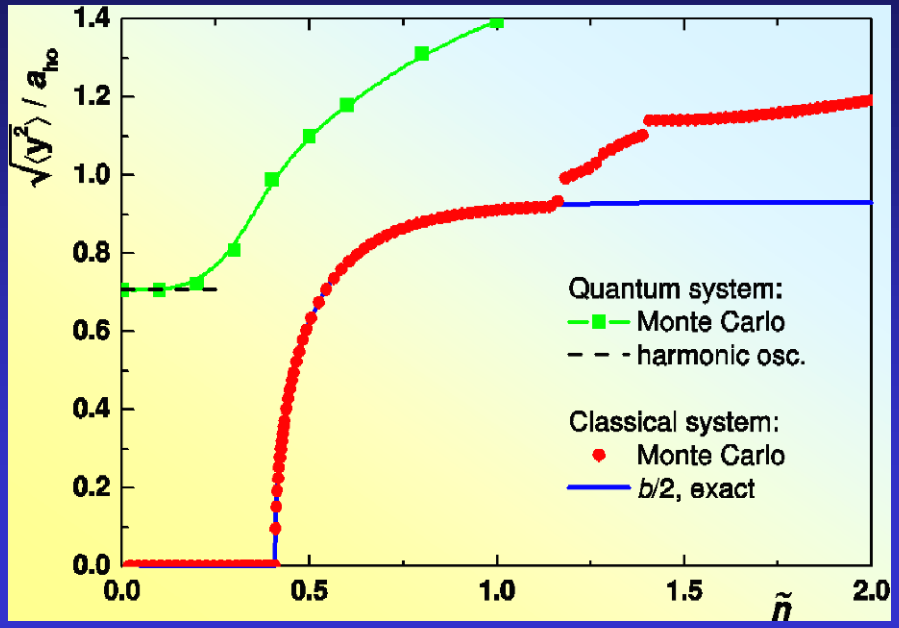
# TRAPPED IDEAL FERMI / TONKS-GIRARDEAU GAS

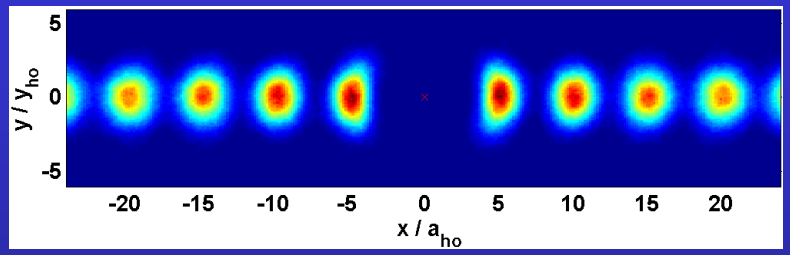


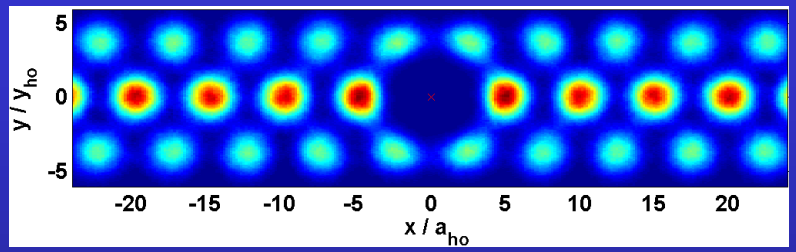

- Known exactly: $n(x) = \sum_{i=0}^{N-1} |\phi_i(x)|^2$ , with $\phi_n(x) = \frac{1}{\sqrt{\pi^{1/2} 2^n n!}} e^{-\frac{x^2}{2a_{ho}^2}} H_n(x)$
- Show oscillations (shell structure)
- Some non-trivial features: maxima for $N$ particles coincide exactly with minima of $N+1$ particles.

# ZIG-ZAG 2ND ORDER PHASE TRANSITION:1D DIPOLES




GEA, Giovanna Morigi, Gabriele De Chiara, and J. Boronat Ground state of low-dimensional dipolar gases Linear and zigzag chains Phys. Rev. A **78**, 063622 (2008); GEA. Astrakharchik, G. De Chiara, Giovanna Morigi and J. Boronat, Thermal and quantum fluctuations in low dimensional dipolar chains, J. Phys. B **42**, 154026 (2009)