Critical Stability 2014

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Monte Carlo simulations of the unitary Bose gas

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outline

- Bose gas in unitary regime
  - <u>quick</u> experimental overview
  - <u>quick</u> theoretical overview

- "Variational" Monte Carlo simulations for the homogenous gas
  - construction of the many-body wave function - I
  - **cut-off condition**
  - construction of the many-body wave function – II
  - energy per particle
  - condensate fraction

- Density Functional Theory for the non-homogeneous gas
  - comparison of static properties with VMC
  - comparison with GPE
  - monopole and quadrupole frequencies
  - momentum distribution: comparison with experiment

- conclusions

Unitary regime

s-wave scattering length $a \to \infty$

effective range $r_e \to 0$

- The length scale is fixed by r_0, the average distance among particles
- Expected universal properties depending only on the density

Unitary Fermi gas largely investigated [see book by Zwenger (Springer, 2012)]
Unitary Bose gas only marginally studied…

problem Unitary Bose gas is experimentally inaccessible [Ho, PRL 2004]

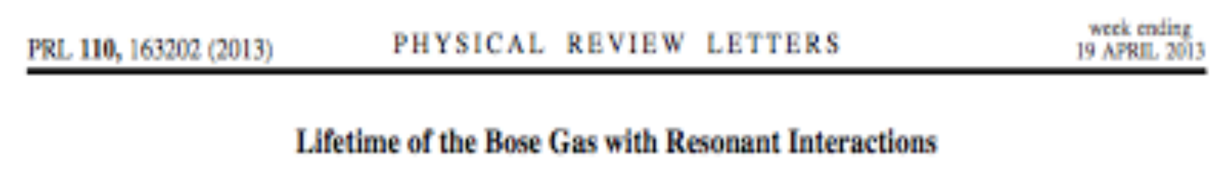
- Positive diverging a means a bound state in the potential well
- No Pauli's exclusion principle for Bosons

The Bose gas is mechanically unstable at low T

- particles tend to form bound couples and triplets (3 particle loss) [Li & Ho, PRL 2012]
- self-bound ground state (cluster formation or Thomson collapse)

no hope?

Experimental overview

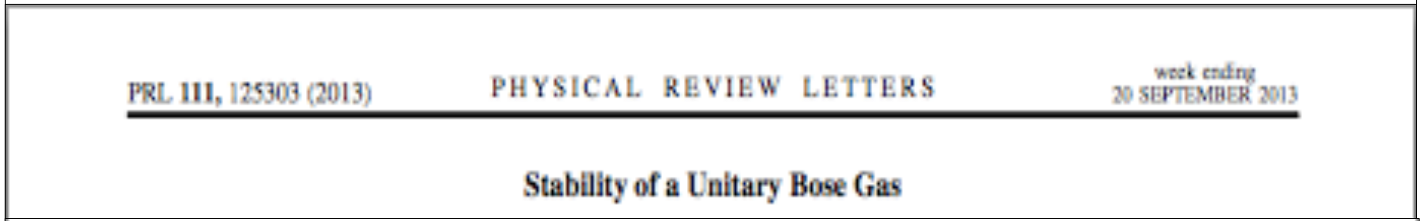

PRL 110, 163202 (2013) PHYSICAL REVIEW LETTERS week ending 19 APRIL 2013

Lifetime of the Bose Gas with Resonant Interactions

^{7}Li: $L_3 \propto L^{-2}$

$\gamma_3/\gamma_2 \propto \zeta$

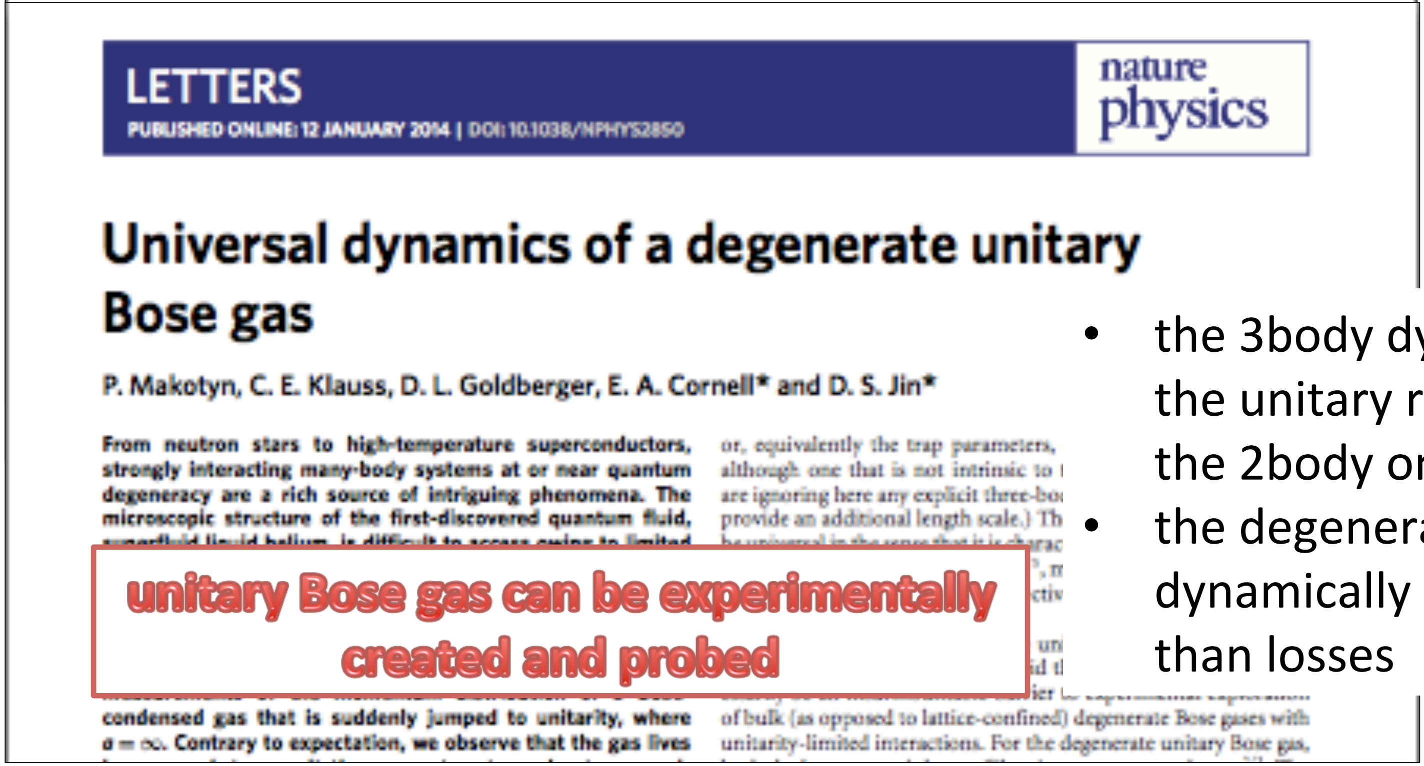
$\zeta = 0.9$


PRL 111, 125303 (2013) PHYSICAL REVIEW LETTERS week ending 20 SEPTEMBER 2013

Stability of a Unitary Bose Gas

^{39}K: $L_3 \propto L^{-1.7}$

$\zeta = 0.3$


LETTERS

PUBLISHED ONLINE: 12 JANUARY 2014 | DOI: 10.1038/NPHYS2850

nature physics

Universal dynamics of a degenerate unitary Bose gas

P. Makotyn, C. E. Klauss, D. L. Goldberger, E. A. Cornell* and D. S. Jin*

From neutron stars to high-temperature superconductors, strongly interacting many-body systems at or near quantum degeneracy are a rich source of intriguing phenomena. The microscopic structure of the first-discovered quantum fluid,

condensed gas that is suddenly jumped to unitarity, where $a = \infty$. Contrary to expectation, we observe that the gas lives

or, equivalently the trap parameters, although one that is not intrinsic to are ignoring here any explicit three-bo provide an additional length scale.) Th

of bulk (as opposed to lattice-confined) degenerate Bose gases with unitarity-limited interactions. For the degenerate unitary Bose gas,

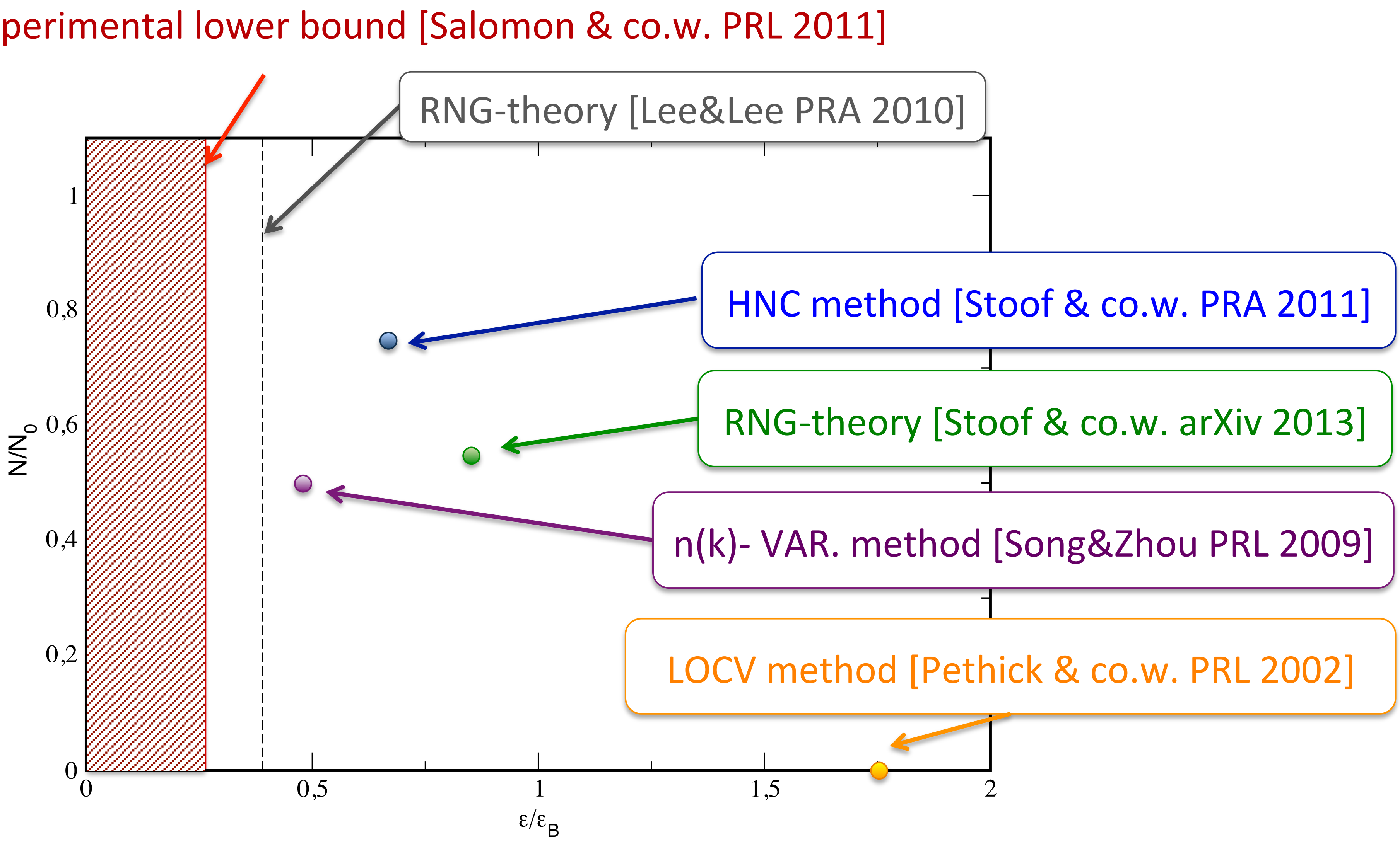
unitary Bose gas can be experimentally created and probed

^{85}Rb

- the 3body dynamics that spoils the unitary regime is slower than the 2body one
- the degenerate Bose gas evolves dynamically on a fast time scale than losses

the unitary Bose gas is a metastable state!

Theoretical overview



Experimental lower bound [Salomon & co.w. PRL 2011]

RNG-theory [Lee&Lee PRA 2010]

HNC method [Stoof & co.w. PRA 2011]

RNG-theory [Stoof & co.w. arXiv 2013]

n(k)- VAR. method [Song&Zhou PRL 2009]

LOCV method [Pethick & co.w. PRL 2002]

$$\varepsilon_B = \frac{\hbar^2}{2m}(6\pi^2 n)^{2/3} \qquad n = \frac{3}{4\pi r_0^3}$$

question

why results are so scattered?

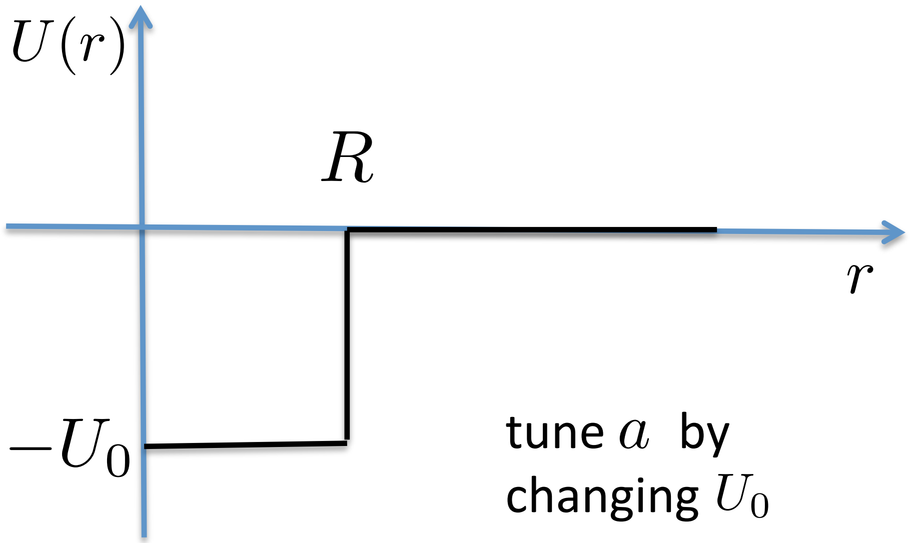
No standard technique to face **metastable states**: results will depends on how the phases space is restricted!

problems

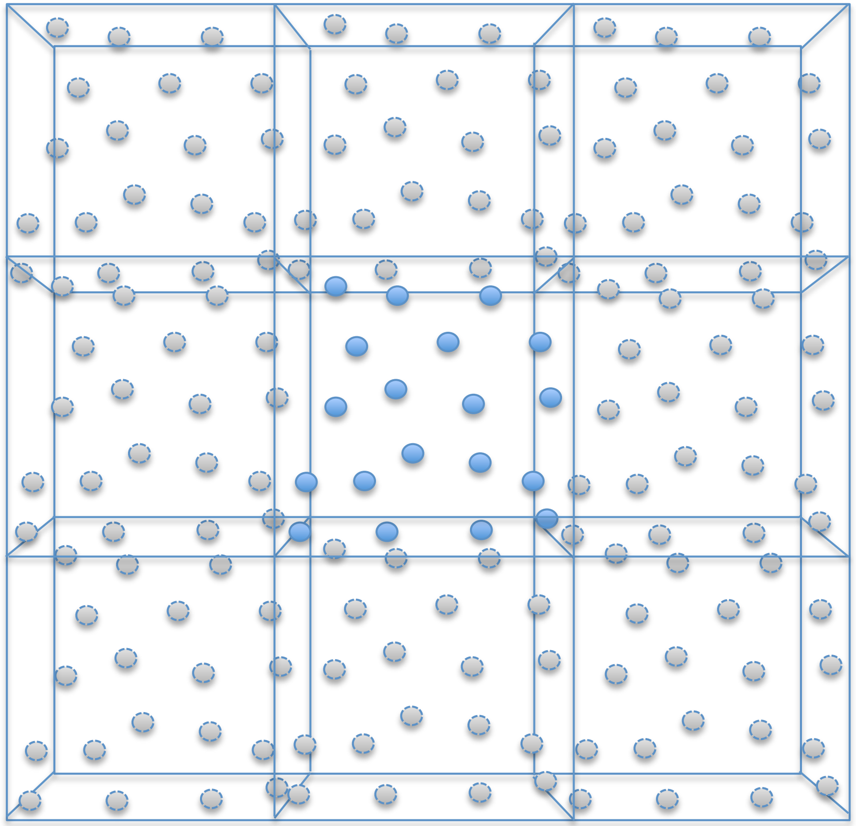
- strong interactions rule out mean-field approaches
- metastability calls for “adjustments” in standard equilibrium techniques

M. Rossi, L. Salasnich, F. Ancilotto & F. Toigo, PRA **89**, 041602(R) (2014)

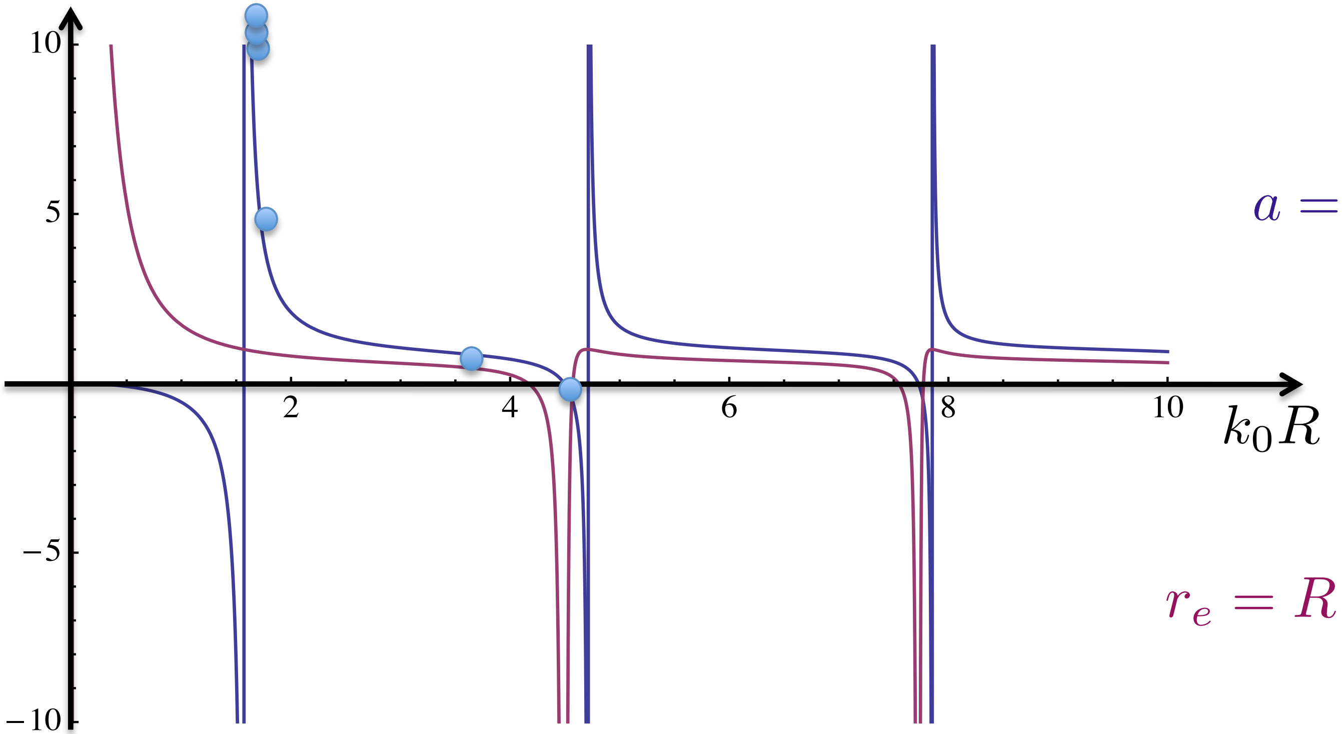
direct Monte Carlo (MC) simulation of N = 500 bosons in a cubic box with periodic boundary conditions interacting via a square well potential



tune a by changing U_0



square well potential



$$a = R\left[1 - \frac{\tan(k_0R)}{k_0R}\right]$$

$$k_0 = \sqrt{U_0}$$

$$r_e = R\left[1 - \frac{R^2}{3a^2} - \frac{R}{k_0^2aR}\right]$$

In our simulations $\frac{R}{r_0} < 0.01$ & $10^{-3} < \frac{a}{r_0} < 10^4$

so that we explore also the unitary regime $r_e \ll r_0 \ll a$

many-body wave function - I

- T = 0 K
- the system is dilute

→

only 2 body correlations are retained:
standard Jastrow – Feenberg ansatz

$$\psi_J(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = \prod_{i<j} f(|\vec{r}_i - \vec{r}_j|)$$

- f is the exact solution of the 2 body problem f_2 with energy $\varepsilon = \dfrac{\hbar^2 k^2}{2m} > 0$

$$r f_2(r) = \begin{cases} A \sin(\kappa r) & 0 < r < R \\ B \sin(kr + \delta) & r > R \end{cases}$$

$$\kappa^2 = k^2 + k_0^2$$
$$\delta = \arctan\left(\tfrac{k}{\kappa}\tan(\kappa R)\right) + kR$$
$$A = B\frac{\sin(kR+\delta)}{sin(\kappa R)}$$

in the $R \to 0$ limit the interaction potential can be replaced by the boundary condition
[Bethe & Peierls Proc.R.Soc.London A 1935]

$$\lim_{r\to 0} \frac{[r f_2(r)]'}{r f_2(r)} = -\frac{1}{a}$$

$$r f_2(r) = A \sin(rk + \delta)$$

$$\delta = \arctan(ka)$$

many-body wave function - I

- in order to account for many-body effects and for periodic boundary conditions f_2 is smoothly joined with a constant at a certain distance R_m

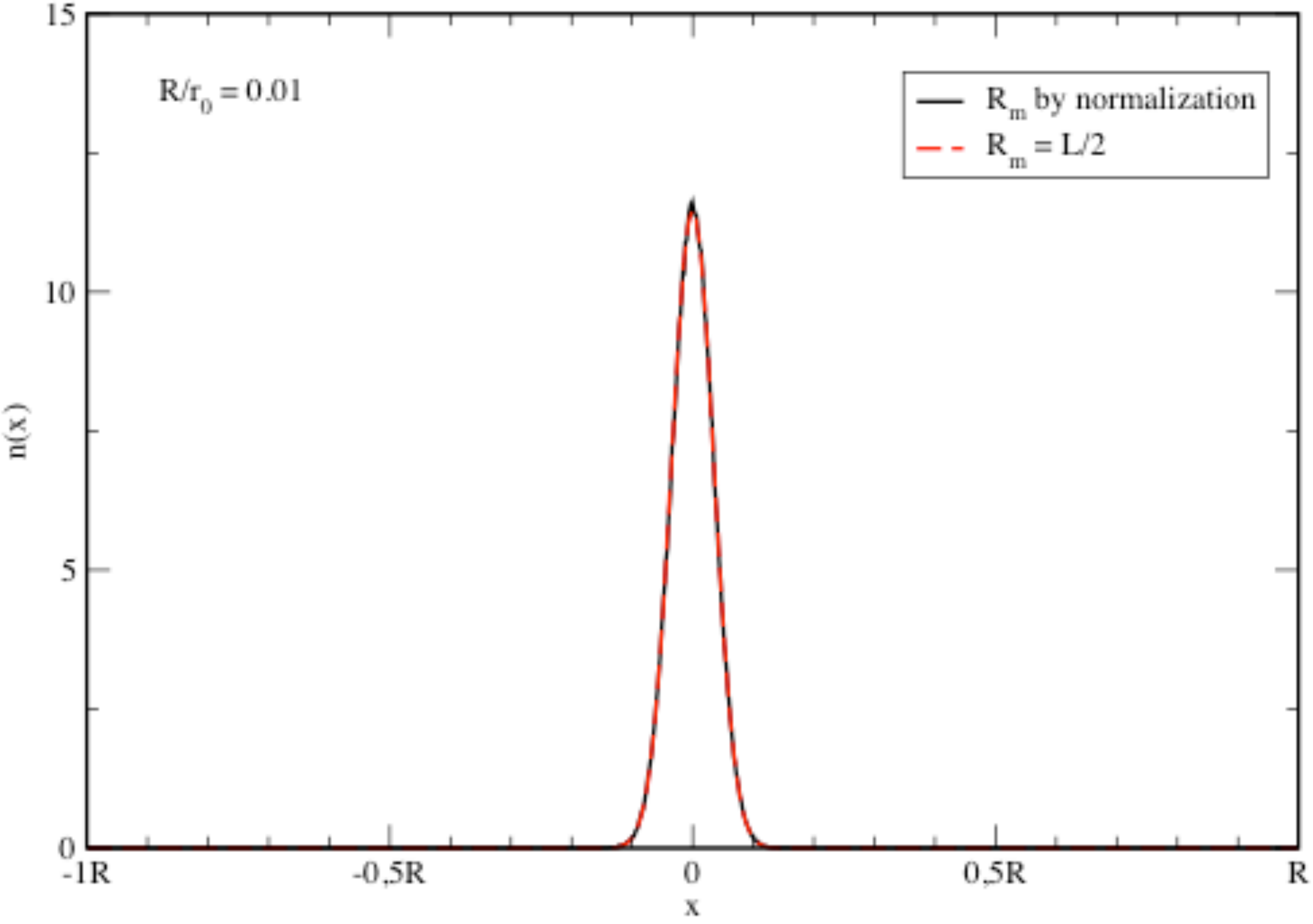
$$f(r) = \begin{cases} f_2(r) & 0 < r < R_m \\ 1 & r > R_m \end{cases}$$

the only parameter left is R_m, which cannot be fixed via a variational approach (undesired energy minimum for $R_m = 0$)

- standard QMC choice $$R_m = L/2$$
- standard LOCV method choice $$4\pi n \int_0^{R_m} f_2^2(r) r^2 dr = 1$$

[Cowell et al. PRL 2002]

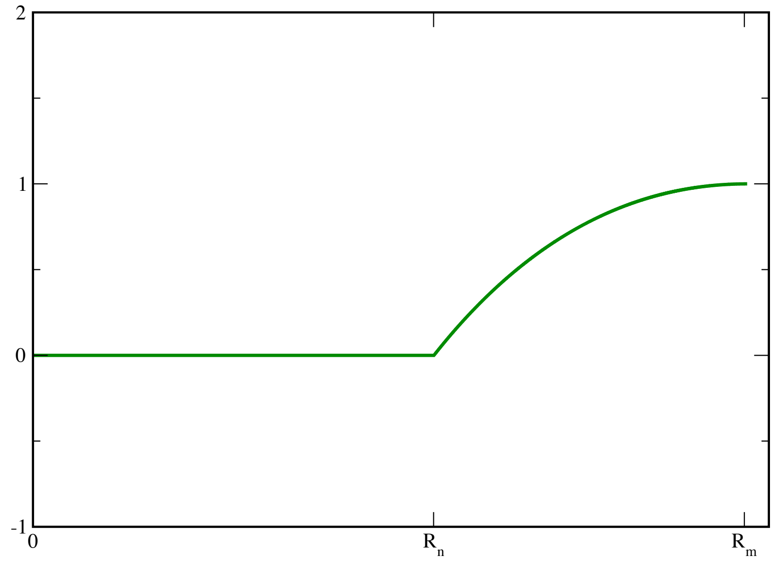
…unfortunately when a diverges the equilibrium configuration is not the desired uniform gas, but rather a compact cluster



the extreme compactness is due to the unphysical lack of hard core repulsion in the interaction potential

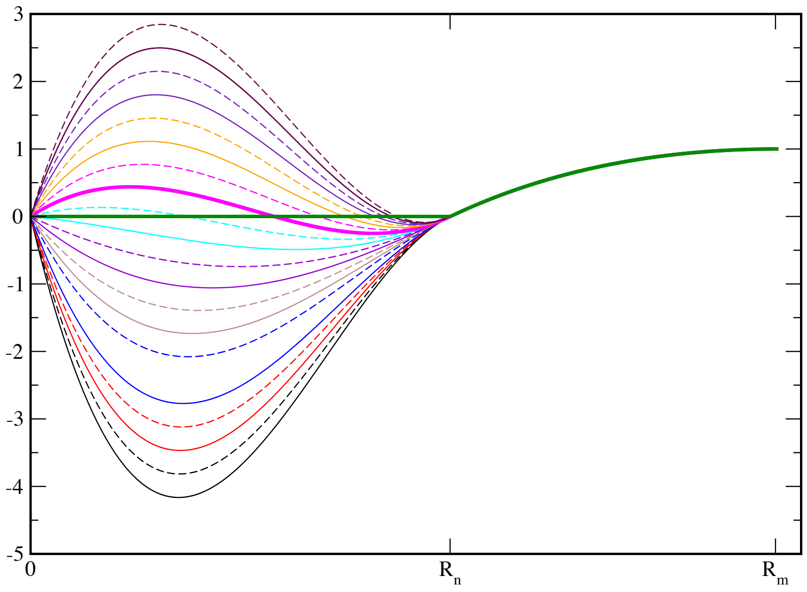
many-body wave function - II

we must correct the wave function to prevent particles to fall too close each other: we introduce a cut off:



$$f(r) = \begin{cases} 0 & 0 < r < R_n \\ f_2(r) & R_n < r < R_m \\ 1 & r > R_m \end{cases}$$

R_n is the outermost node of $f_2(r)$



- we tried also a smoother cutoff, but the energy increases
- the variationally optimized f is as flat as possible in $0 < r < R_n$
- to avoid that $R_n > r_0$, R_m is fixed via the normalization condition

thus our many-body wave function:

1. provides the long range correlations dictated by the scattering length
2. keeps the density uniform preventing the formation of clusters
3. keeps the nodes and the normalization of the actual 2body scattering wave function

this seems reasonable since, due to the extreme diluteness of the gas, the particle pairs should experience only the tails of f

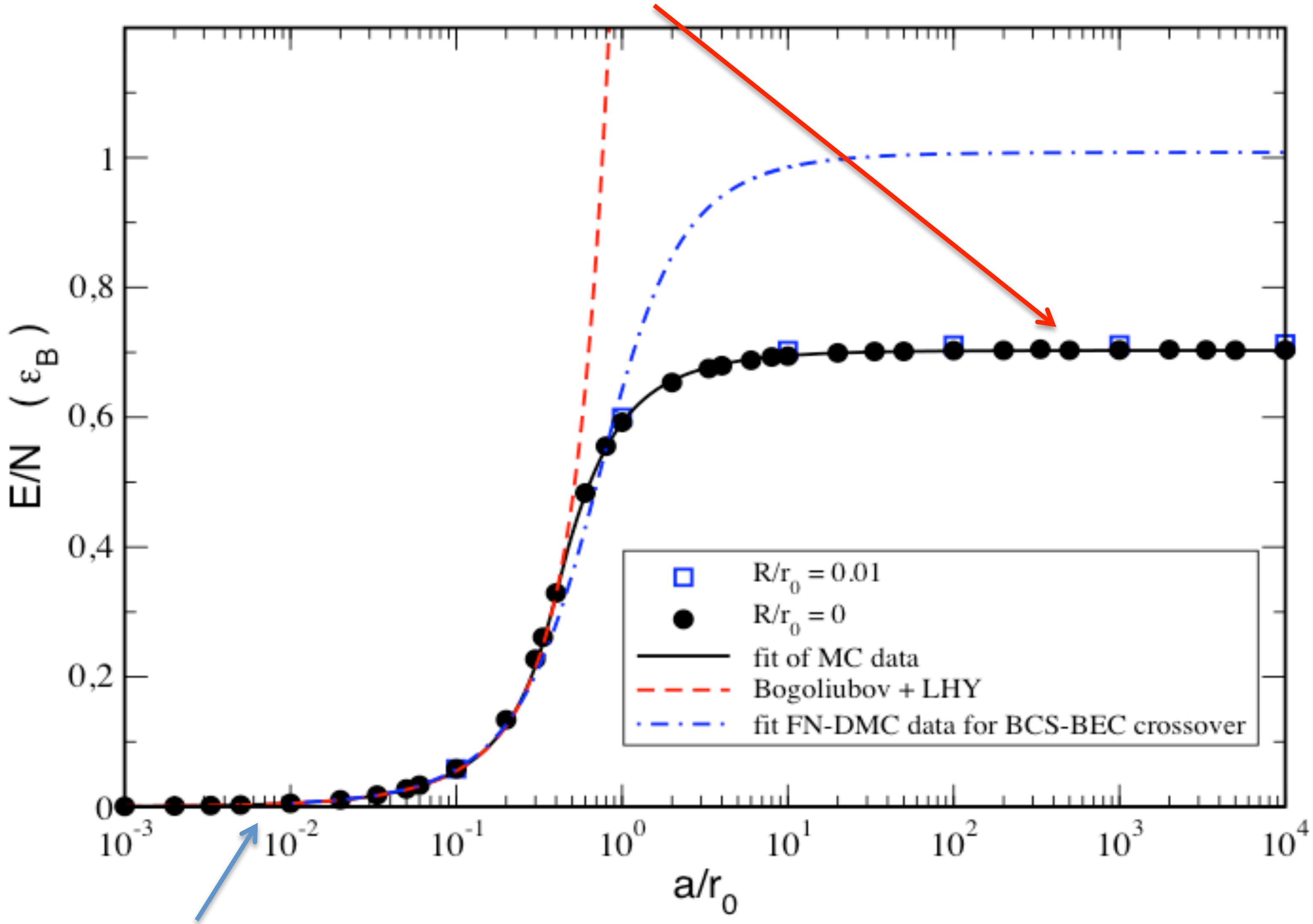
given the many-body wave function we have direct access to:

- the energy per particle $$\varepsilon = \frac{E}{N} = \frac{1}{N} \frac{\langle \psi_J | \hat{H} | \psi_J \rangle}{\langle \psi_J | \psi_J \rangle}$$
- the condensate fraction $$\frac{N_0}{N} = \lim_{|\vec{r}-\vec{r}'|\to\infty} \rho_1(|\vec{r}-\vec{r}'|)$$

$$\rho_1(|\vec{r}-\vec{r}'|) = \int d\vec{r}_2 ... d\vec{r}_N \psi_J^*(\vec{r}', \vec{r}_2, ..., \vec{r}_N) \psi_J(\vec{r}, \vec{r}_2, ..., \vec{r}_N)$$

Energy per particle

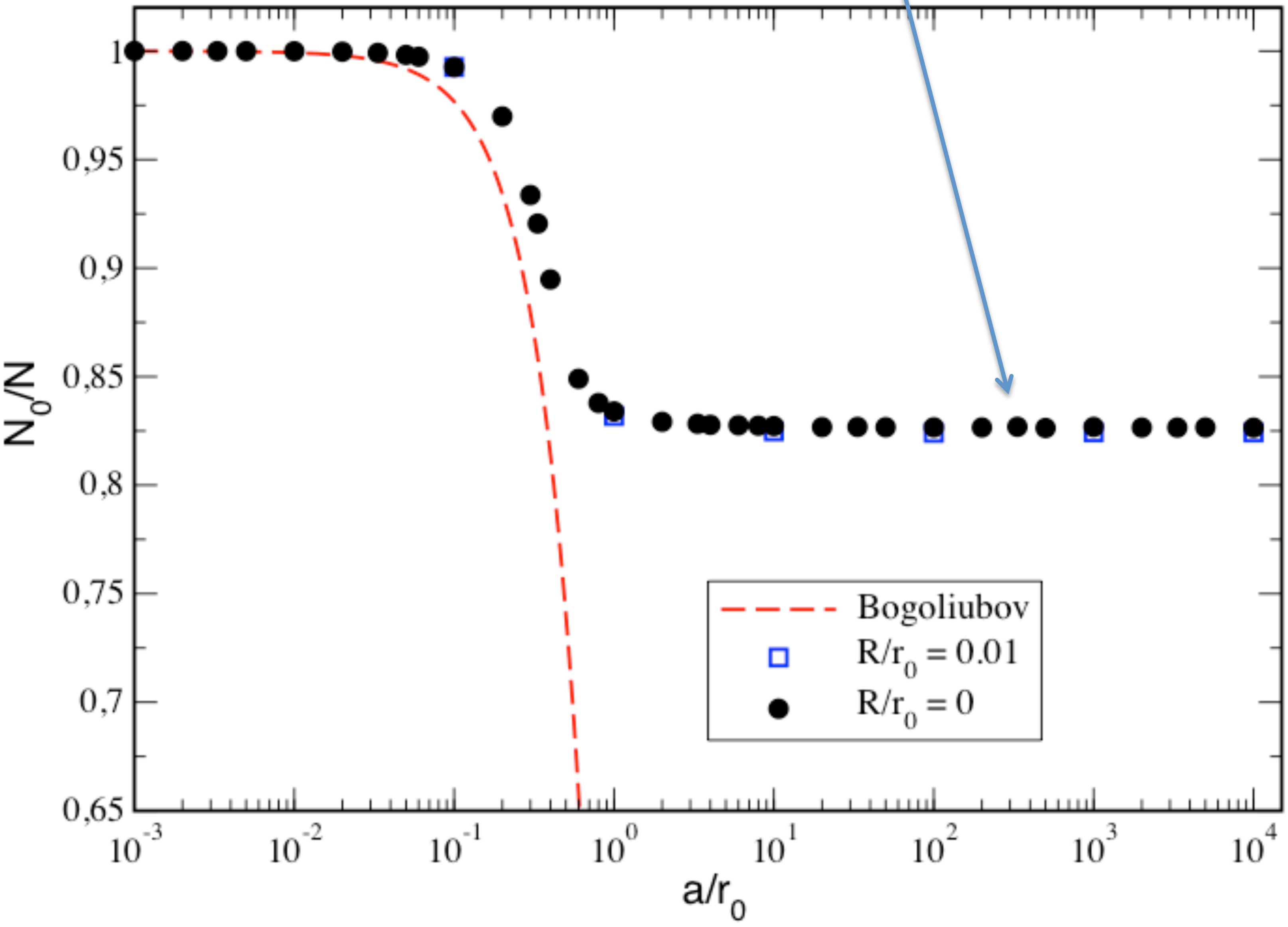
it converges to the constant value of 0.70 ε_B as $a \longrightarrow \infty$: signature of **universal behavior**



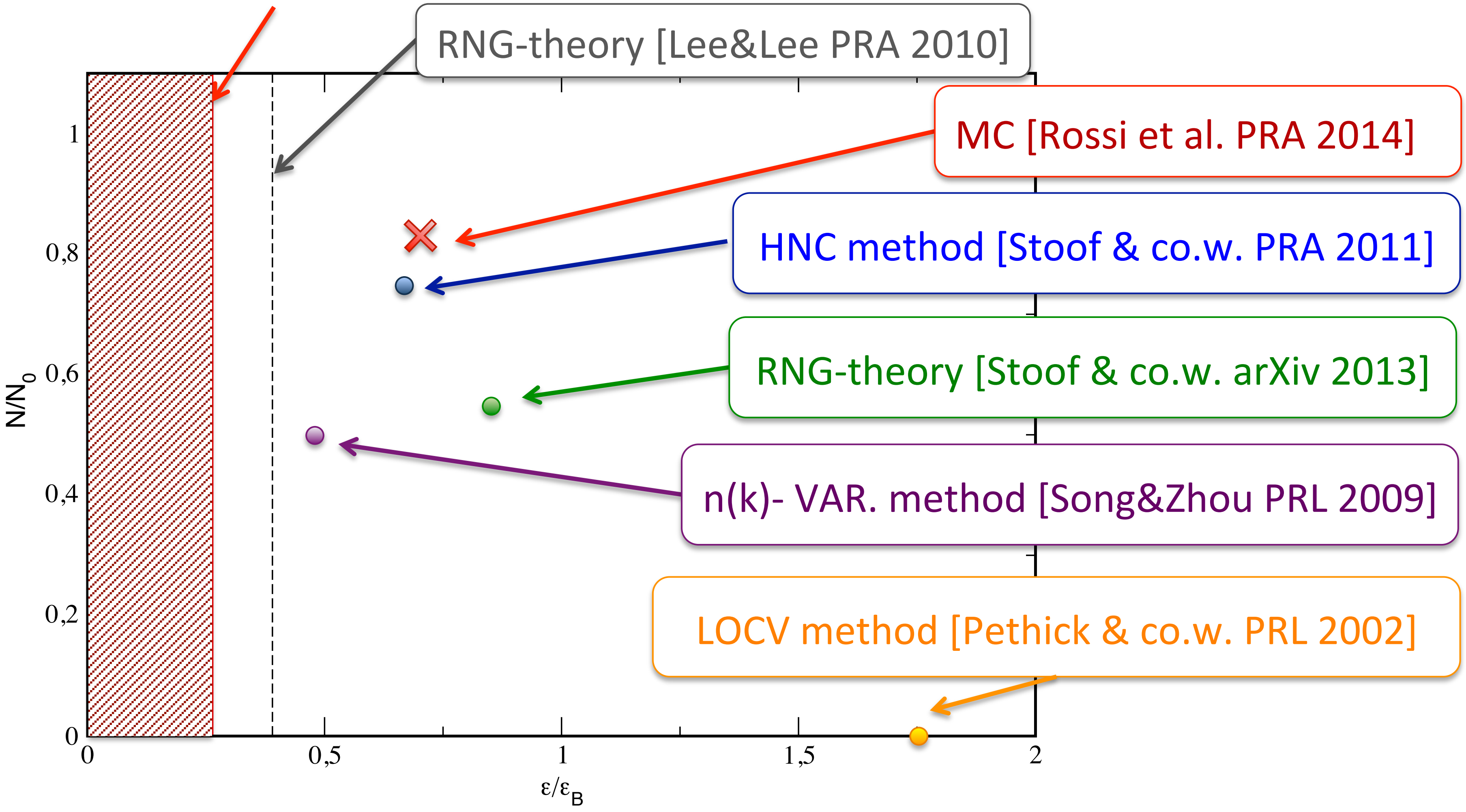
in the weakly interacting regime we recover the universal Bogoliubov prediction ε_{LHY}

condensate fraction

it converges to the constant value of 0.83



Theoretical overview



Experimental lower bound [Salomon & co.w. PRL 2011]

RNG-theory [Lee&Lee PRA 2010]

MC [Rossi et al. PRA 2014]

HNC method [Stoof & co.w. PRA 2011]

RNG-theory [Stoof & co.w. arXiv 2013]

n(k)- VAR. method [Song&Zhou PRL 2009]

LOCV method [Pethick & co.w. PRL 2002]

$$\varepsilon_B = \frac{\hbar^2}{2m}(6\pi^2 n)^{2/3} \qquad n = \frac{3}{4\pi r_0^3}$$

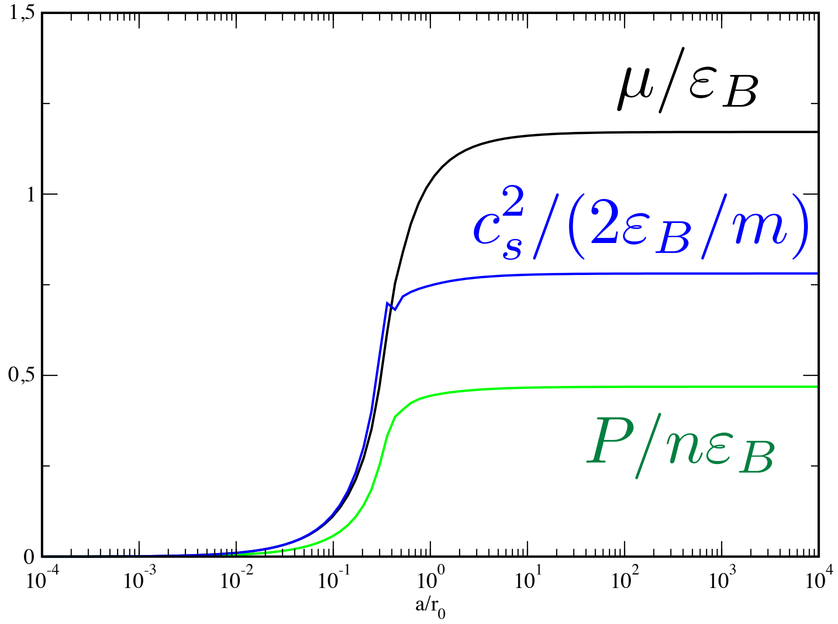
MC data can be fitted with the function ($x = a/r_0$)

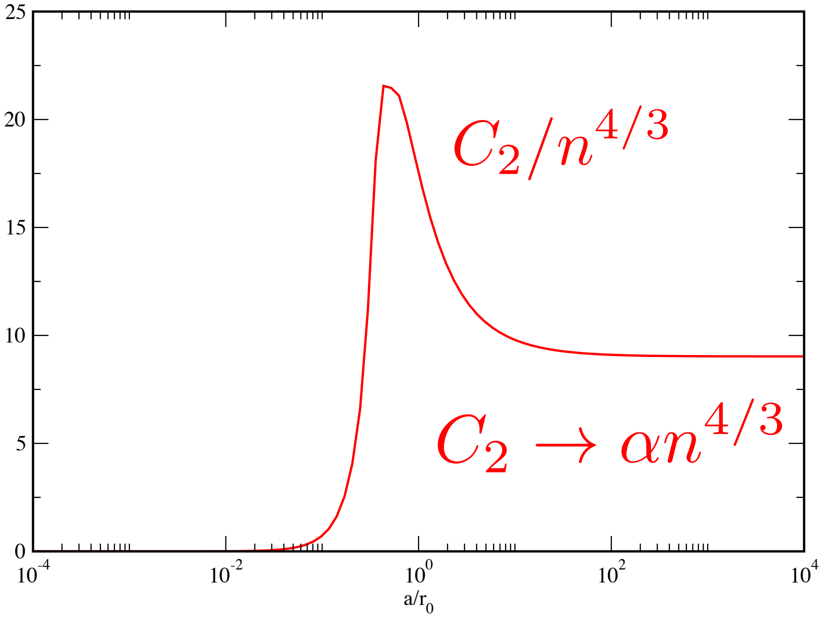
$$\varepsilon(x)/\varepsilon_B = \begin{cases} \varepsilon_{\rm LHY}(x) + a_3 x^3 & x < 0.3 \\ c_7x^7 + c_6x^6 + c_5x^5 + c_4x^4 + c_3x^3 + c_2x^2 + c_1x + c_0 & 0.3 < x < 0.5 \\ b_0 + b_1 \tanh(b_2/x + 1) & x > 0.5 \end{cases}$$

that allows the computation of other useful quantities via thermodynamic relations

- chemical potential $\mu = \partial_n(n\varepsilon)$
- pressure $P = n^2\partial_n\varepsilon$
- sound velocity $c_s^2 = n/m\ \partial_n\mu$

- Tan’s 2body contact density
  $C_2 = (8\pi n m a^2/\hbar^2) d\varepsilon/da$





α = 9.02 compares acceptably well with previous theoretical estimates

[Stoof et al. PRA 2011, arXiv 2013; Sykes et al PRA 2014]

Density Functional theory of a trapped Bose gas with tunable *a*

M. Rossi, F. Ancilotto, L. Salasnich & F. Toigo arXiv:1408.3925

time-dependent Density Functional Theory for an inhomogeneous system of interacting Bosons at zero temperature within the **local density approximation**

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2M} + U(\mathbf{r}) + \frac{\partial(n\varepsilon_a)}{\partial n}\right]\Psi(\mathbf{r},t)$$

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

$\varepsilon_a(n)$ energy per atom of a homogeneous system with density n and scattering length a

$U(\mathbf{r}) = \frac{1}{2}m\omega_H^2(x^2+y^2+z^2)$ external confinement

total energy functional

$$E = \int d^3\mathbf{r}\left\{\frac{\hbar^2}{2M}|\nabla\Psi(\mathbf{r})|^2 + n(\mathbf{r})\varepsilon_a(n(\mathbf{r})) + n(\mathbf{r})U(\mathbf{r})\right\}$$

as $\varepsilon_a(n)$ we take the MC equation of state

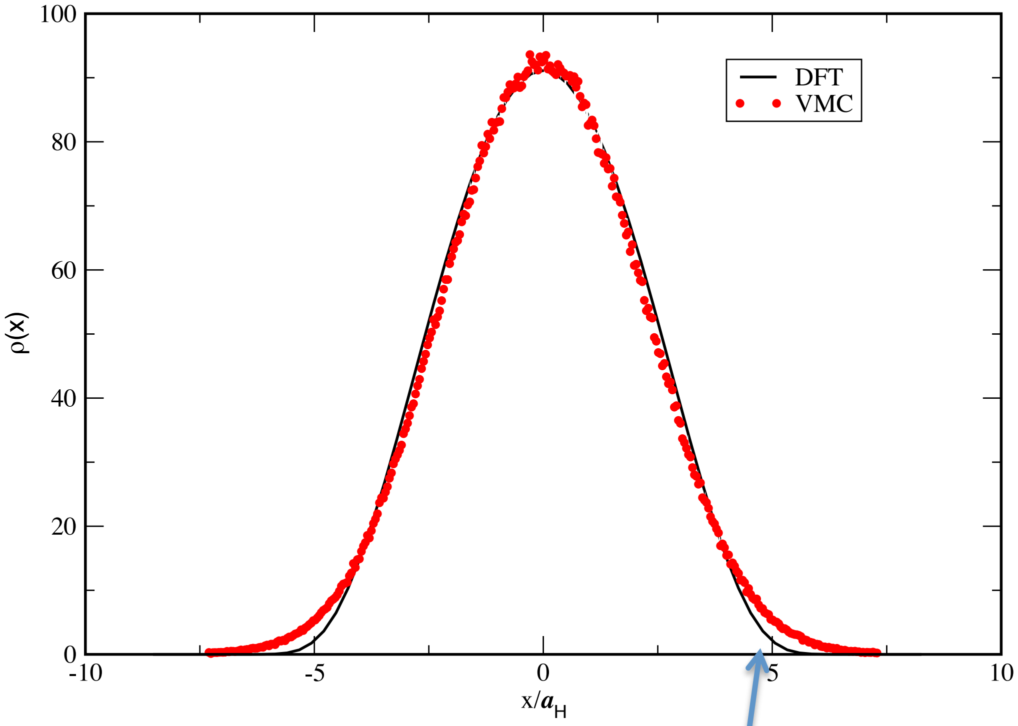
static properties: comparison with MC

integrated density profile $\rho(x) = \int dydz\ n(x,y,z)$

$N = 500$

$a = 10^4 a_0$

$a_H = \sqrt{\hbar/(m\omega_H)}$



DFT: obtained by imaginary time propagation

VMC: obtained by adding a 1 body term to the wave function

[BuBois & Glyde, PRA 2001]

$$\psi(\vec{r}_1, ..., \vec{r}_N) = \psi_J(\vec{r}_1, ..., \vec{r}_N) \prod_{i=1}^{N} e^{-\alpha r_i^2}$$

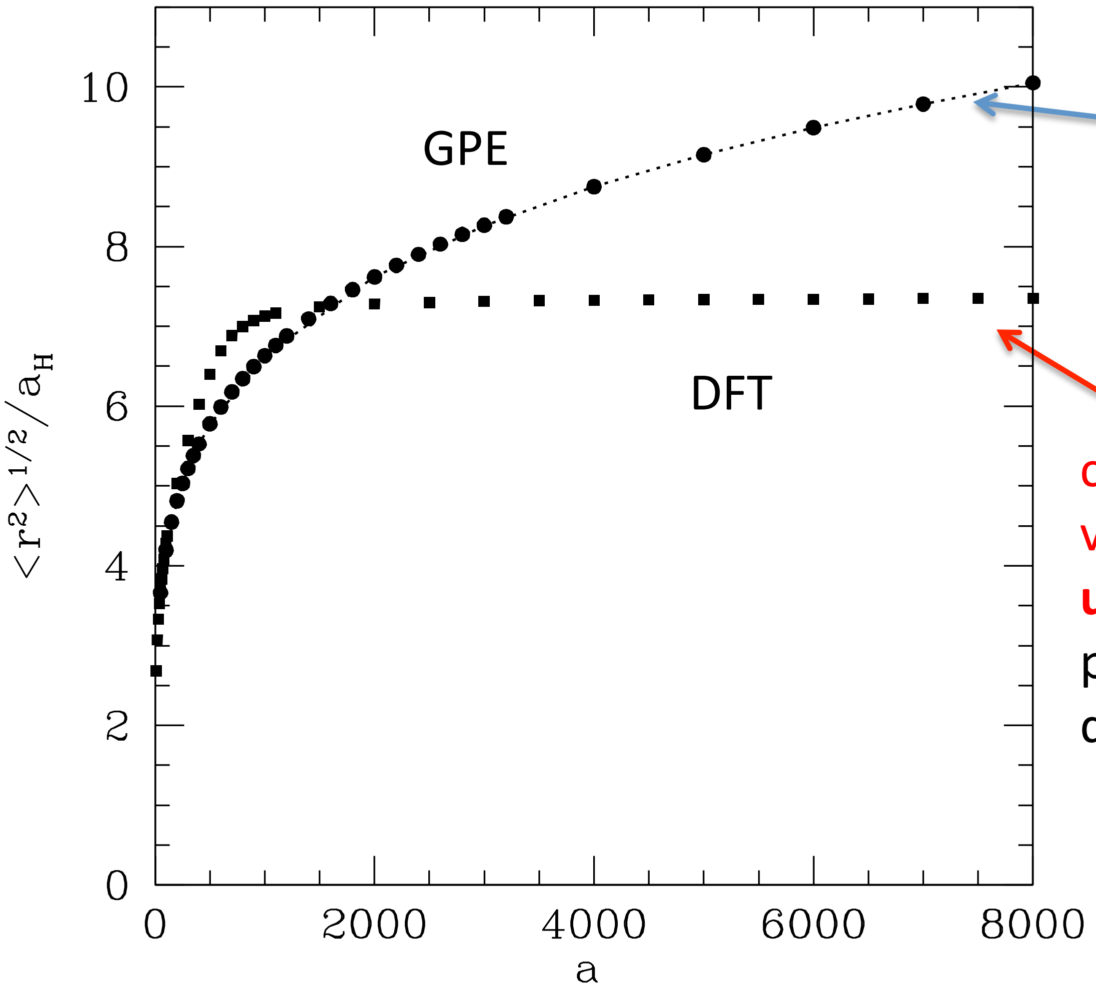
good agreement except near the surface

mainly due to the form of the 1body term, the value of a is “dominated” by the central region.

static properties: comparison with GPE

if $\varepsilon_a(n) = \dfrac{2\pi\hbar^2}{m} a n^2$ DFT reduces to Gross-Piatevskii Equation

average radius of the trapped gas



TF limit
$< r^2 >^{1/2} \propto a^{1/5}$

convergence to a constant value is expected for the **unitary regime** where the properties of the system depends only on the density

dynamical properties: mono- and quadru -pole frequencies

monopole (breathing or compressional) mode frequencies are obtained by slightly changing ω_H

quadrupole (surface) mode frequencies are obtained by using the initial state

$$\Psi(\mathbf{r}, t=0) = e^{i\eta Q}\Psi_0(\mathbf{r})$$

small parameter

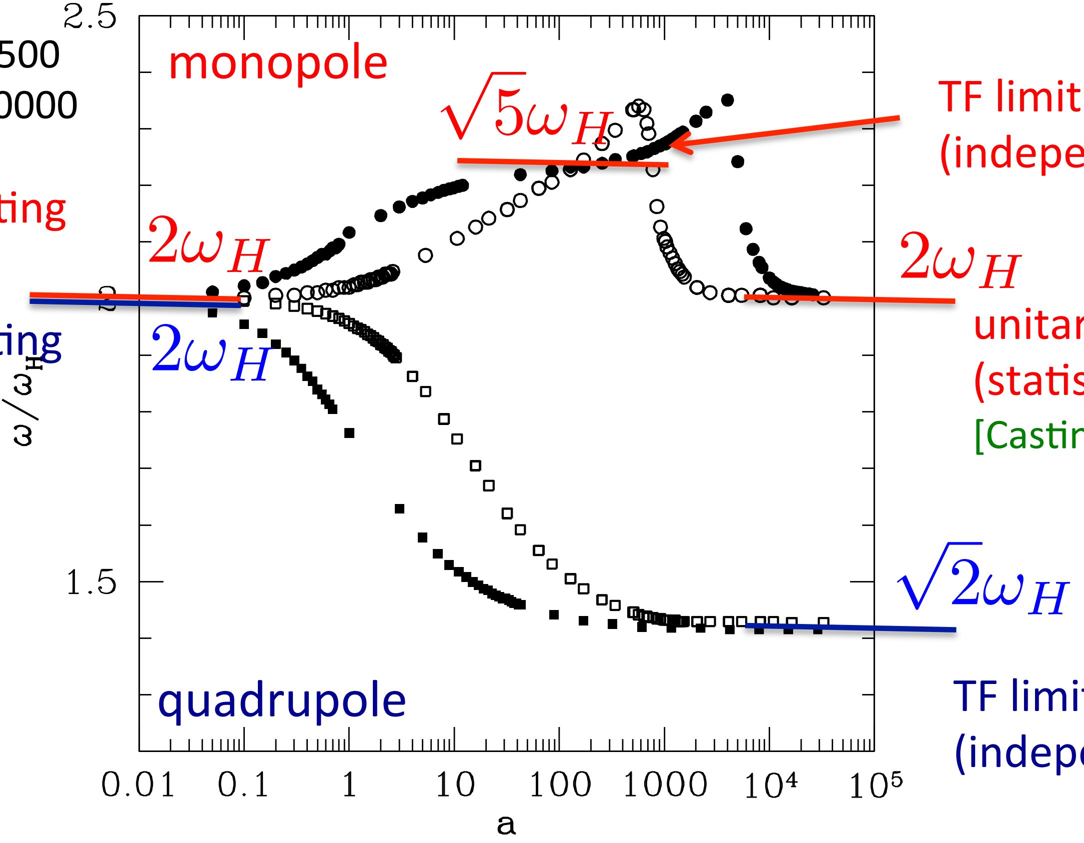
ground state wave function

$Q = 2z^2 - x^2 - y^2$ standard quadrupole operator

empty sym. : N = 500
filled sym. : N = 80000

non interacting regime

non interacting regime



TF limit
(independent of *a*)

unitary limit
(statistic independent)
[Castin CRP 2004]

TF limit
(independent of *a*)

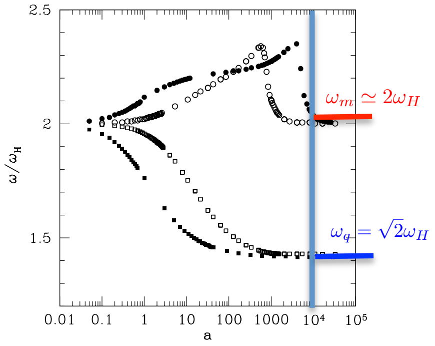
TF regime:

$$\frac{Na}{a_H} \gg 1$$

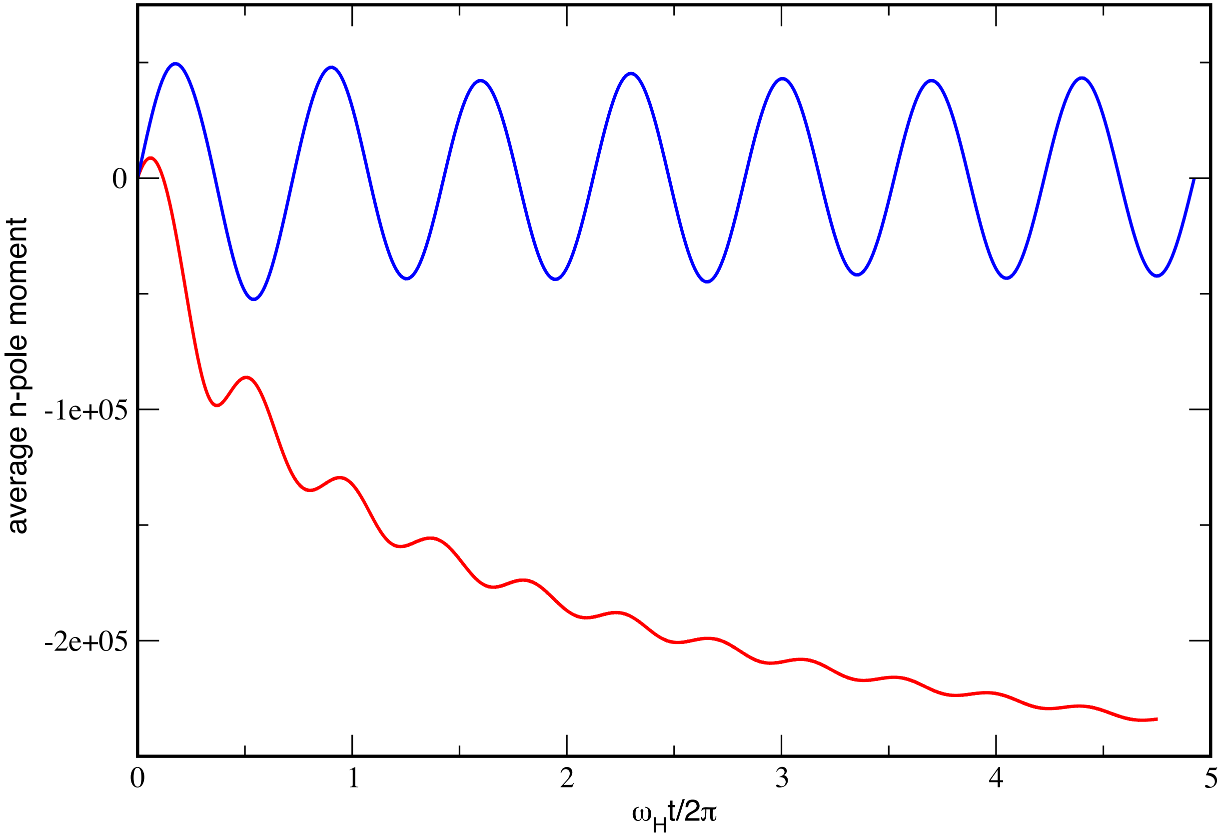
dynamical properties: 3 body losses

3 body losses can be accounted including the standard term

$$-i\hbar L_3 n^2(\mathbf{r},t)\Psi(\mathbf{r},t)$$



we can investigate the effects on the collective excitations



$$\omega_q = \sqrt{2}\omega_H$$

surface mode
only slightly
affected by
3body losses

$$\omega_m \simeq 2\omega_H$$

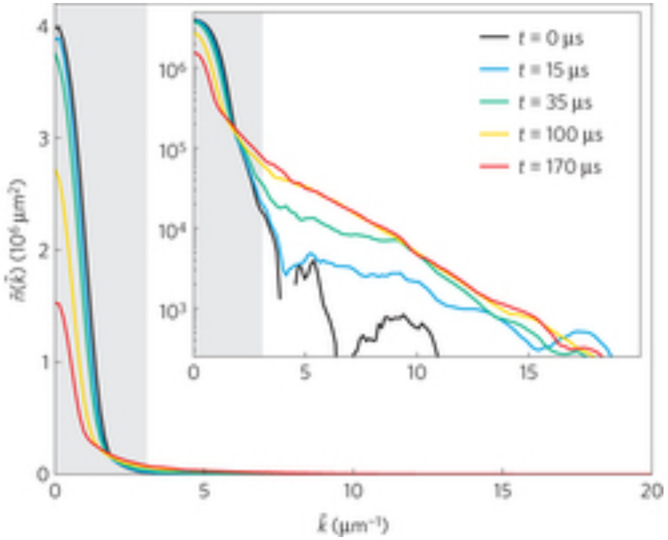
$a = 10^4 a_0$

$N = 80000$

the monopole mode follows the evolution of the average radius
with superimposed oscillations at the expected frequency

dynamical properties: momentum distribution

few experimental data to compare with: one is the momentum distribution after a sudden quench to unitary [Conell & co.w. Nat.Phys. 2014]

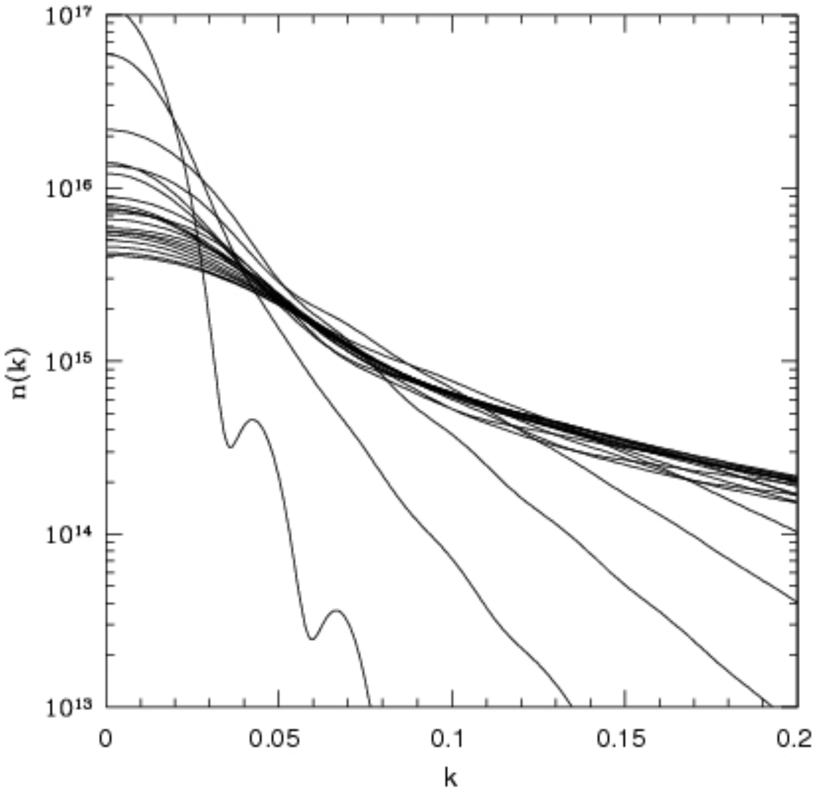


$$a = 140 \rightarrow a = 500000$$

A quasi-steady-state distribution is reach

TDDFT

$$n(\mathbf{k},t) = N \left| \int d\mathbf{r}\ \Psi(\mathbf{r},t) e^{i\mathbf{k}\cdot\mathbf{r}} \right|^2$$



quite similar behavior!
Our distribution still evolves on large time scales as already noted with a disspipative GPE approach

[Rançon & Levin PRA 2014]

conclusions

- we have studied the zero temperature **unitary Bose gas** via a Jastrow ansatz on the many-body wave function that avoids the formation of the self-bound ground state. We have computed the energy per particle ε and the condensate fraction n_0
  - in the weakly interacting regime we recover the Bogoliubov predictions
  - in the **unitary** regime both ε and n_0 converge to a **finite value**: signature of the **universal behavior**

- MC data can be used to extract also other useful information
  - via standard thermodynamic relations (μ, P, c_s, C_2…)
  - by constructing a **density functional theory**

- **TDDFT** based on the MC equation of state provides also **dynamical properties**
  - monopole mode: fulfills the expected limiting values
  - quadrupole mode
  - effect of **3body losses** can be included
  - (qualitative) comparison with the experimental momentum distribution evolution after a sudden quench

Thank you for your attention