The legacy of Adelchi Fabrocini

Short-range correlations and structure of dilute hard- and soft – sphere gases

- Microscopic description. Hamiltonian.
- Variational approach. HNC theory.
- Optimal correlation function. Asymptotic behavior. Excitation Spectrum.
- Uniform approximation.
- Momentum distributions and condensed fraction.
- Universal behavior of the total energy


09/25/2004

We started our collaboration in 1979 with the derivation of the HNC-FHNC equations for Bose-Fermi mixtures.
Momentum distributions, impurities …

PHYSICAL REVIEW B VOLUME 33, NUMBER 9 1 MAY 1986

Microscopic calculations of the excitation spectrum of one ^{3}He impurity in liquid ^{4}He

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(Received 16 September 1985)

This paper has been rediscovered by the cold-atoms community in relation to the polaron problem.

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 50, NUMBER 6 1 AUGUST 1994-II

Effective mass of one ^{4}He atom in liquid ^{3}He

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(Received 18 March 1994)

A microscopic calculation of the effective mass of one ^{4}He impurity in homogeneous liquid ^{3}He at zero temperature is performed for an extended Jastrow-Slater wave function, including two- and three-body dynamical correlations and also backflow correlations between the ^{4}He atom and the particles in the medium. The effective mass at equilibrium density, $m_4^*/m_4=1.21$, is in very good agreement with the recent experimental determination by Edwards *et al.* The three-particle correlations appear to give a small contribution to the effective mass and different approximations for the three-particle distribution function give almost identical results for m_4^*/m_4.

PHYSICAL REVIEW A VOLUME 60, NUMBER 3 SEPTEMBER 1999

Beyond the Gross-Pitaevskii approximation: Local density versus correlated basis approach for trapped bosons

A. Fabrocini[1] and A. Polls[2]

PHYSICAL REVIEW A, VOLUME 64, 063610

Bose-Einstein condensates in the large-gas-parameter regime

A. Fabrocini[1,2] and A. Polls[3]

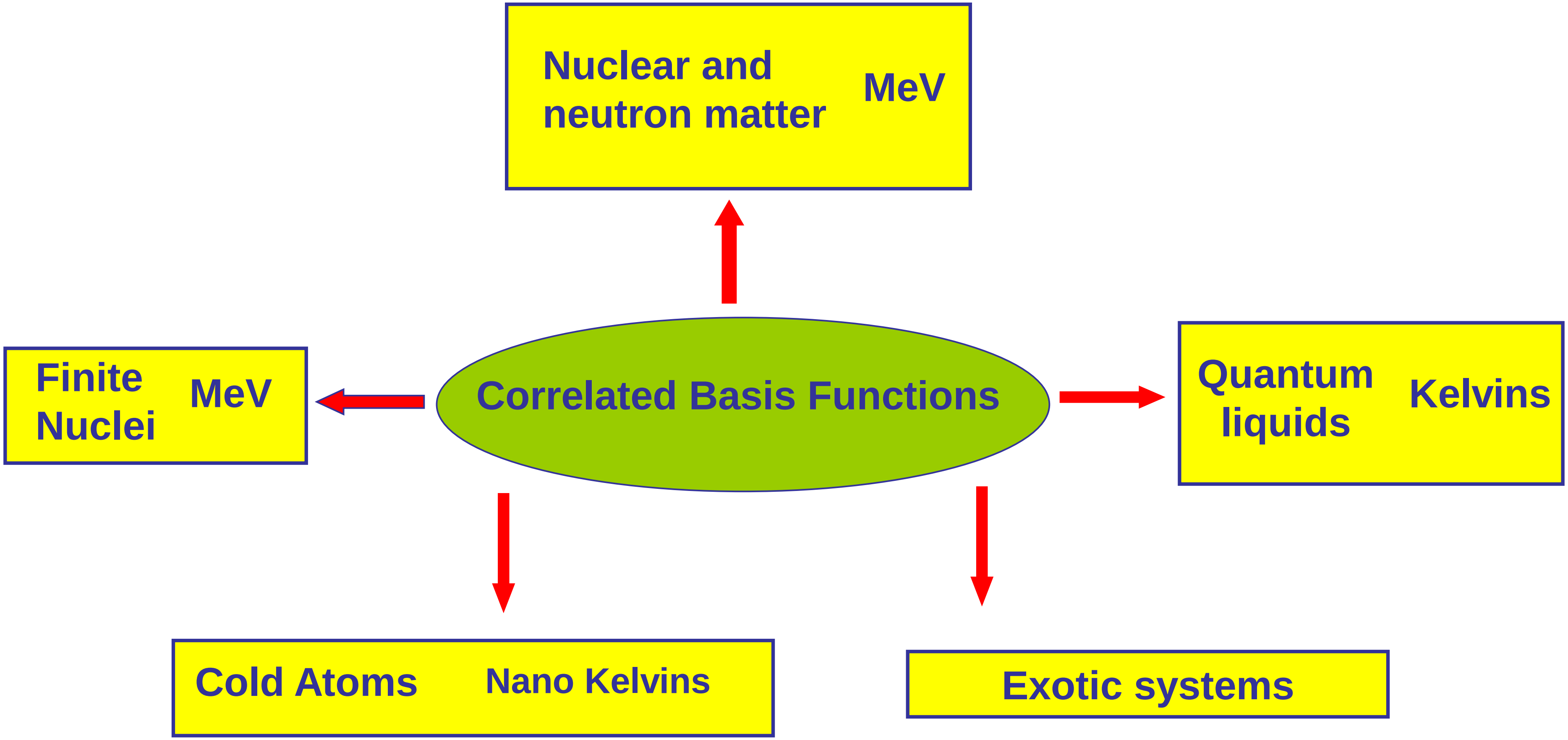
PHYSICAL REVIEW A 71, 033615 (2005)

Ground-state properties of a dilute homogeneous Bose gas of hard disks in two dimensions

F. Mazzanti,[1] A. Polls,[2] and A. Fabrocini[3]

Also very elegant!

Nearly all physics is many-body physics at the most microscopic level of understanding



Correlated wave functions

The sytems we are interested in have interactions between their constituents which can largely modify the wave function respect to the simple mean-field ansatz ➔ correlations between the constituent particles ➔ Difficult for perturbative calculations

ALTERNATIVE

Incorporate from the very begining the correlations to the wave function

$$\Psi(r_1, ..., r_n) = F(r_1, ..., r_n)\phi(r_1, ..., r_n)$$

For infinite uniform system

$$\phi(r_1, ..., r_n) = 1$$

For bosons

$$\phi(r_1, ..., r_n) \equiv FreeFermiSea$$

For fermions, normal Fermi liquid

A good starting point

$$F(r_1, ..., r_n) = \prod_{i<j} f(r_{ij})$$

Hard- and soft-sphere Bose gases

Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\nabla_j^2 + \sum_{1=i<j}^{N} V(r_{ij})$$

Interaction

$$V(r) = \begin{cases} \infty, & r<a \\ 0 & r>a, \end{cases}$$

$$V(r) = \begin{cases} V_0>0, & r<R \\ 0, & r>R, \end{cases}$$

Hard-spheres

$$a = R[1-\tanh(K_0R)/(K_0R)],$$

$$x = \rho * a^3$$

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

$$K_0^2 = V_0 m/\hbar^2$$

Soft-spheres

Variational approach

Correlated ground-state wave function

$$\Psi_0(1,2,\ldots,N) = \mathcal{F}(1,2,\ldots,N)\Phi_0(1,2,\ldots,N)$$

In the Bose case $\Phi_0(1,2,\ldots,N)$

All bosons in the zero-momentum state

$$\Phi_0 = 1$$

The exact wave function of a homogeneous, interacting Bose system can be written the product of up to N-body correlation factors

$$\Psi_0(1,2,\ldots,N) = \prod_{i<j}^{N} f_2(r_{ij}) \prod_{k<l<m}^{N} f_3(\mathbf{r}_{kl},\mathbf{r}_{km},\mathbf{r}_{lm})\cdots$$

A Jastrow correlated wave function is a good starting point

Expectation value

Also possible by Monte Carlo VMC

$$E[f_2] = \frac{\langle \Psi_0 | H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$$\frac{E}{N} = \frac{1}{2}\rho \int d\mathbf{r}_{12} g(r_{12}) \left[V(r_{12}) - \frac{\hbar^2}{2m} \nabla^2 \ln f_2(r_{12}) \right]$$

Where g(r) is the two-body radial distribution function:

$$g(r_{12}) = \frac{N(N-1)}{\rho^2} \frac{\int d\mathbf{r}_3 d\mathbf{r}_4 \cdots d\mathbf{r}_N |\Psi_0|^2}{\int d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N |\Psi_0|^2}$$

Cluster expansion, and massive sums of diagrams → HNC equations

Two options for the two-body correlation function

$$f_{SR}(r) = \begin{cases} 0, & r < 1 \\ \dfrac{d}{r}\dfrac{\sin[K(r-1)]}{\sin[K(d-1)]}, & r > 1, \end{cases}$$

where distances are in units of a, and K fulfills the equation $\cot[K(d-1)] = (Kd)^{-1}$. The latter condition ensures the healing properties: $f_{SR}(r \geqslant 1) = 1$ and $f'_{SR}(r=d) = 0$.

Optimize the functional respect to the two-body correlation function → Euler-Lagrange equation. Can be written as a minimization respect to g(r).

$$\frac{\delta E[f_2]}{\delta f_2(r)} = 0.$$

$$\frac{\delta E[g]}{\delta g(r)} = 0.$$

At the end the variations are performed respect to S(k)

The minimization leads to

$$S(k) = \frac{t(k)}{\sqrt{t^2(k) + 2V_{ph}(k)t(k)}},$$

S(k) is the static structure function,

$$S(k) = 1 + \rho \int d^3 r e^{i\vec{k}\vec{r}} [g(r) - 1]$$

with $t(k) = \hbar^2 k^2 / 2m$

and

$$V_{ph}(r) = g(r)V(r) + \frac{\hbar^2}{m} |\nabla \sqrt{g(r)}|^2 + [g(r) - 1]\omega_I(r)$$

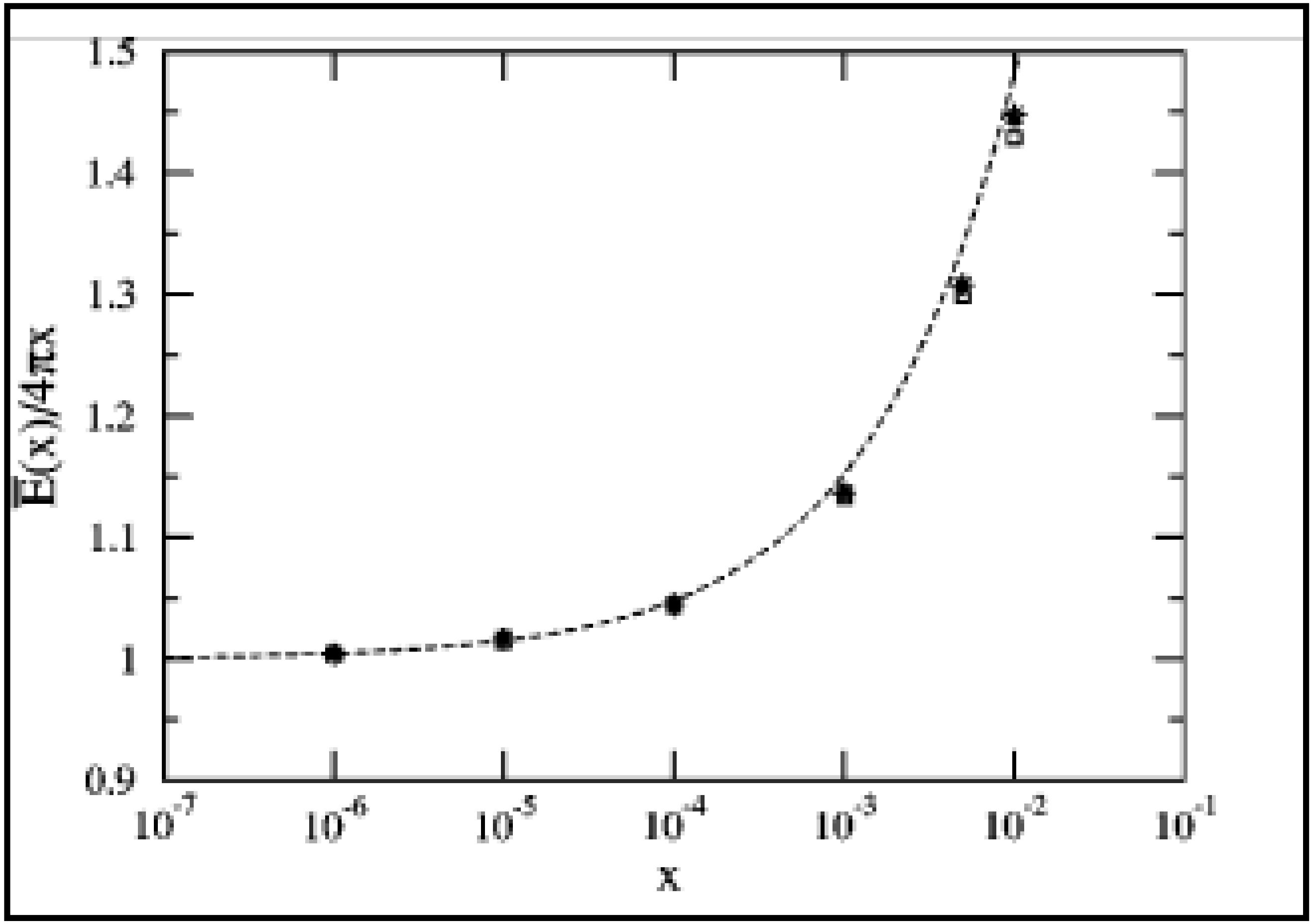
where

$$\omega_I(k) = -\frac{1}{2} t(k) \frac{[2S(k)+1][S(k)-1]^2}{S^2(k)}.$$

Is the induced interaction

$$\frac{E}{N} = \left(\frac{\hbar^2}{2ma^2}\right) 4\pi x \left[1 + \frac{128}{15}\sqrt{\frac{x}{\pi}}\right].$$

Low density expansion of Lee and Yang



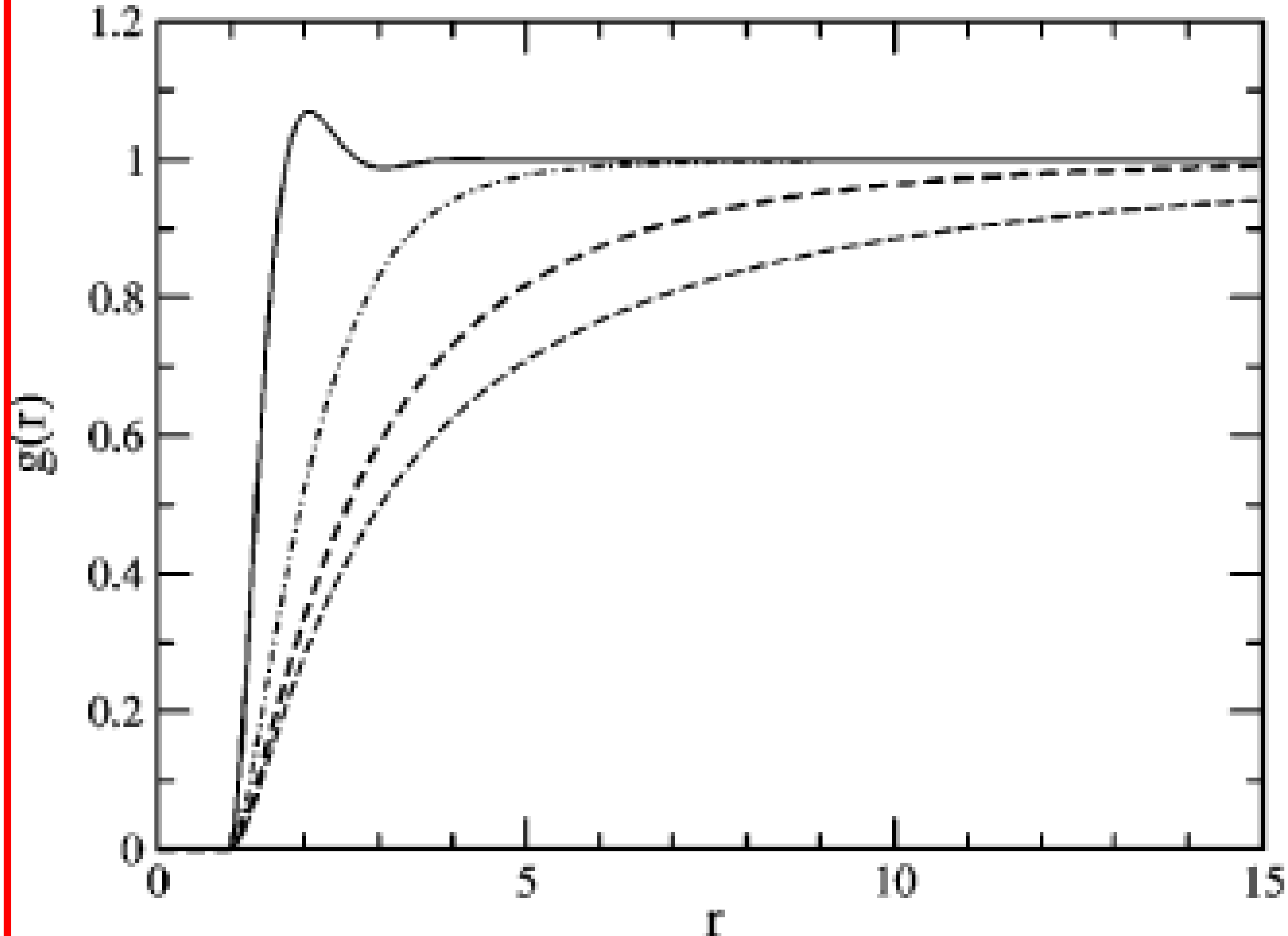
Scaled energy per particle of the HS gas as a function of the gas parameter

Open squares: DMC
Solid circles: HNC-op
Stars: HNC-f
Dashed line: Low density expansion.

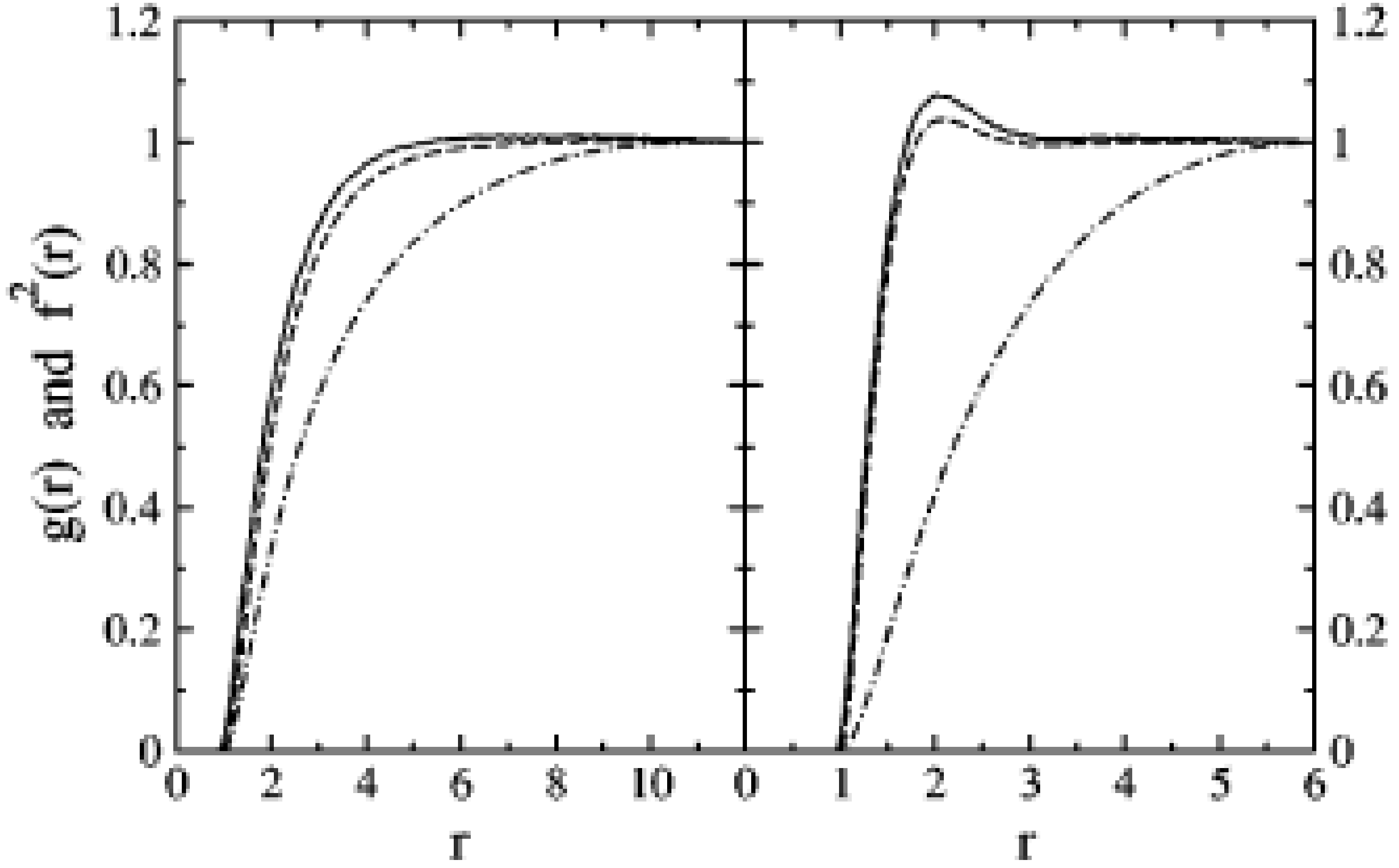
Two-body radial distribution function for several gas parameters.

$$g(r) - 1 \sim 1/r^4; r \to \infty$$

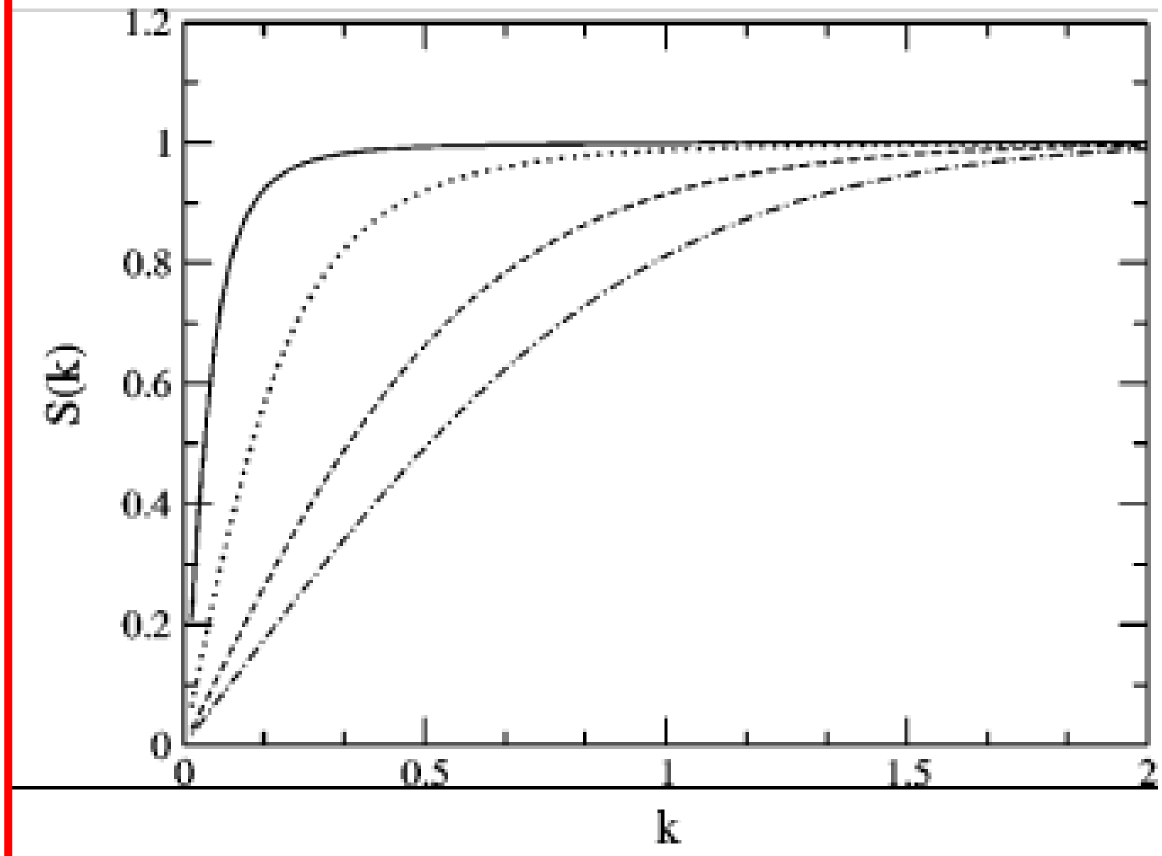
X=0.1 (solid line), 0.01 (dot-dashed), 0.001 (long-dashed), 0.0001 (short-dashed)



VMC g(r) (solid line) and HNC g(r) (dashed line) for x=0.01 (left panel) and x=0.1 (right panel). f(r) (dot-dashed line) is the short-range analytical one.



Static structure function for x=0.0001 (solid line), x=0.001 (dotted line) x=0.005 (dashed line) and x=0.01 (dot-dashed line)

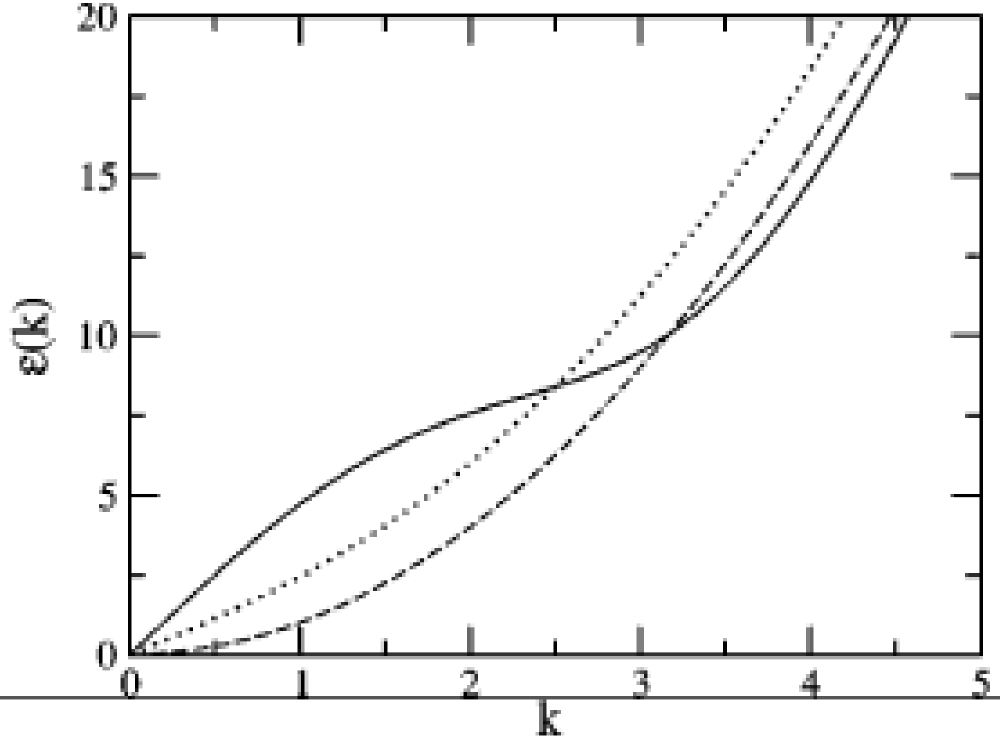


$S(k\rightarrow 0) \rightarrow k/c$

The slope of S(k) becomes smaller when x increases because the speed of sound increases with density. The linear low-k behavior guarantees the correct low-energy spectrum.

Excitation spectrum at x=0.1 (solid line) and x=0.001 (dashed line).
The dotted line corresponds to Bogoliubov spectrum for x=0.1

$e(k) = t(k)/S(k)$



Coincides with the energy of a Feynman phonon

Linear behavior at small k

The first oscillation of S(k) can be large enough to produce a maxon-roton.
At x=0.001, Bogoliubov and EL almost coincide

Momentum distribution and one-body density matrix

One-body density matrix for a homogeneous Bose gas

$$\rho_1(\mathbf{r}_1, \mathbf{r}_{1'}) = \rho_1(r_{11'}) = N \frac{\int d\mathbf{r}_2 d\mathbf{r}_3 \cdots d\mathbf{r}_N \Psi_0(1,2,\ldots,N)\Psi_0(1',2,\ldots,N)}{\int d\mathbf{r}_1 \cdots d\mathbf{r}_N |\Psi_0|^2}$$

Diagonal part = density of the homogeneous system.

The condensate fraction Is related to the long-range behavior:

$$n_0 = \rho_1(r \to \infty)/\rho$$

n(k) is obtained through the Fourier transform of the one-body density matrix

$$n(k) = (2\pi)^3 \rho n_0 \delta(\mathbf{k}) + \int d\mathbf{r} \exp(i\mathbf{k}\cdot\mathbf{r})[\rho_1(r) - \rho n_0].$$

Normalization of n(k)

$$1 = \frac{1}{(2\pi)^3 \rho} \int d\mathbf{k}\, n(k),$$

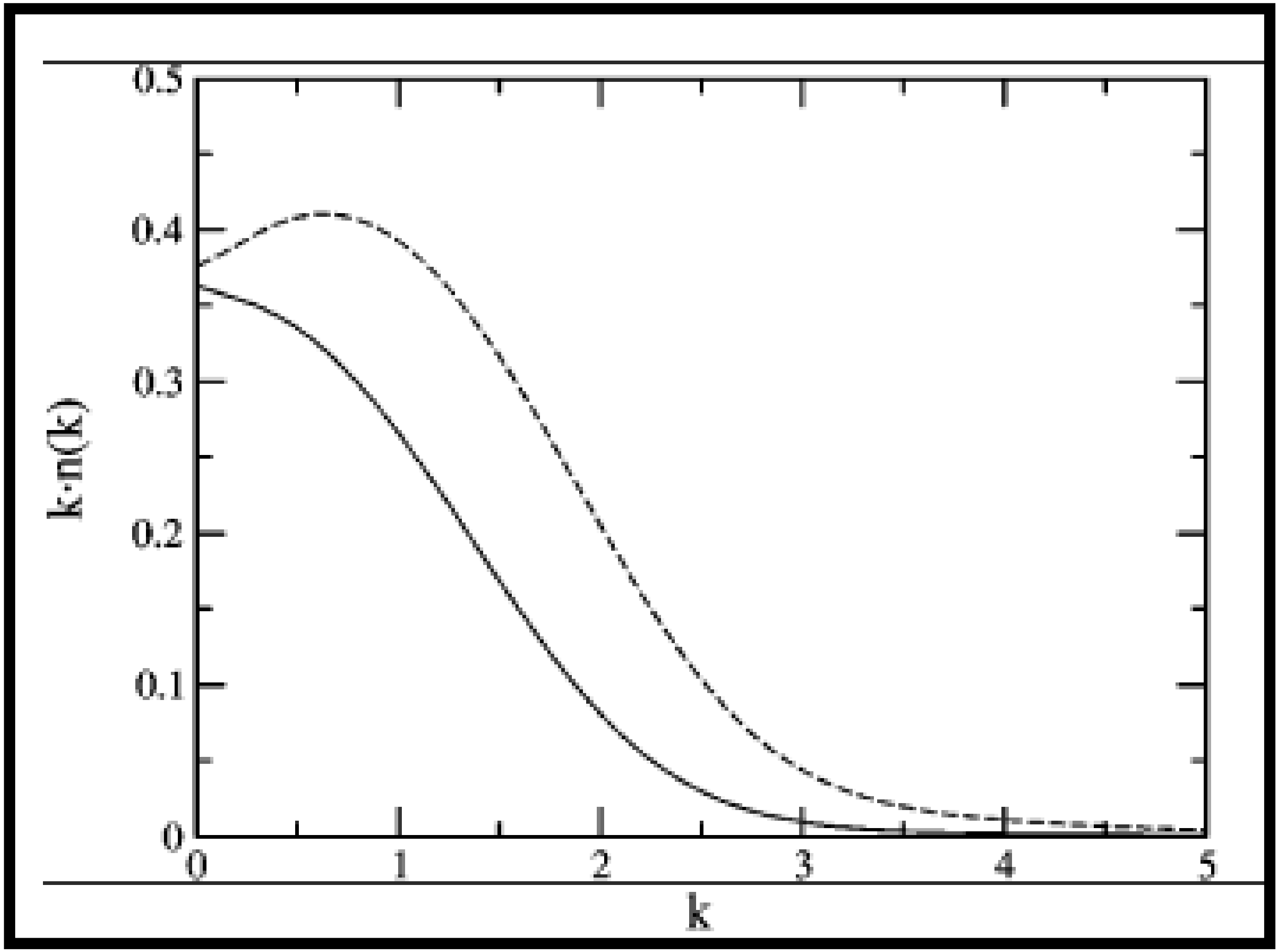
Kinetic energy from n(k)

$$\frac{T}{N} = \frac{1}{(2\pi)^3 \rho} \int d\mathbf{k} \frac{\hbar^2 k^2}{2m} n(k).$$

That for HS should coincide with the total energy.

k*n(k) for x=0.05 (solid line) and x=0.08 (dashed line)

The n(k) for the optimal correlation has the correct long-wavelength limit



$$\lim_{k \to 0} kn(k) = \frac{n_0 c}{4},$$

Competition between n0 and c.

K*n(k) develops a peak when x increases due to short range effects

Soft spheres

A simple estimate of the energy is provided by the first-order perturbation theory

$$\frac{E_1(\rho)}{N} = \frac{\langle \Phi_0 | H | \Phi_0 \rangle}{N} = \frac{1}{2}\rho V_0 \frac{4}{3}\pi R^3 = \frac{1}{2}\tilde{V}(0),$$

Where $\tilde{V}$ **Is the Fourier transform of the potential and** $\phi_0 = 1/\Omega^{N/2}$

is the wave function of the free system, with all particles occupying the zero momentum state.

The second-order perturbative correction :

$$\frac{E_2(\rho)}{N} = -\frac{1}{2\rho}\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{|\tilde{V}(q)|^2}{\hbar^2 q^2/m}$$

$E(\rho) = E_1(\rho) + E_2(\rho)$ **Is no longer an upper-bound to the energy.**

Uniform limit approximation

$$\frac{E_{UL}(\rho)}{N} = \frac{1}{2}\tilde{V}(0) + \frac{1}{2}\int \frac{d\mathbf{k}}{(2\pi)^3\rho}\left[(S(k)-1)\tilde{V}(k) + \frac{\hbar^2 k^2}{4m}\frac{[S(k)-1]^2}{S(k)}\right],$$

$$g(r) \sim 1$$

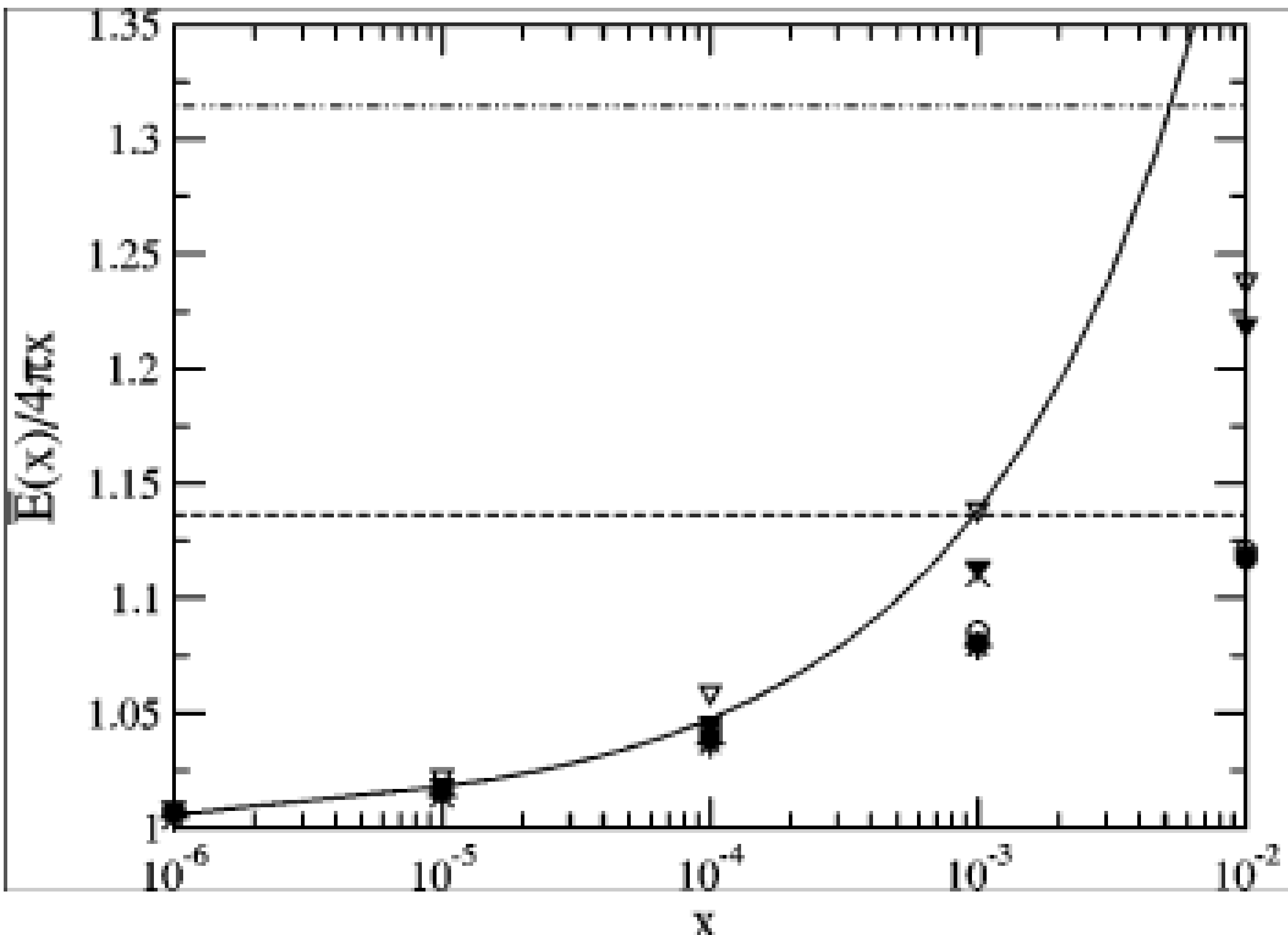
$$\ln g(r) \approx g(r) - 1$$

Minimization with respect to S(k) provides the Euler-Lagrange equation

$$\tilde{V}(k) + \frac{\hbar^2 k^2}{4m}\frac{[S^2(k)-1]}{S^2(k)} = 0,$$

$$S_{UL}(k) = \frac{t(k)}{\sqrt{t^2(k) + 2t(k)\tilde{V}(k)}}.$$

Scaled energy per particle for the SS5 (triangles) and SS10 (circles) potentials in the EL (filled triangles and circles) and UL (empty triangles and circles).
The stars and crosses are DMC results for SS10 and SS5 respectively.
The solid line corresponds to the EL energies for the HS potential.
The horizontal lines gives the upper bounds for the SS5 (dash-double dotted) and SS10 (dashed) potentials.

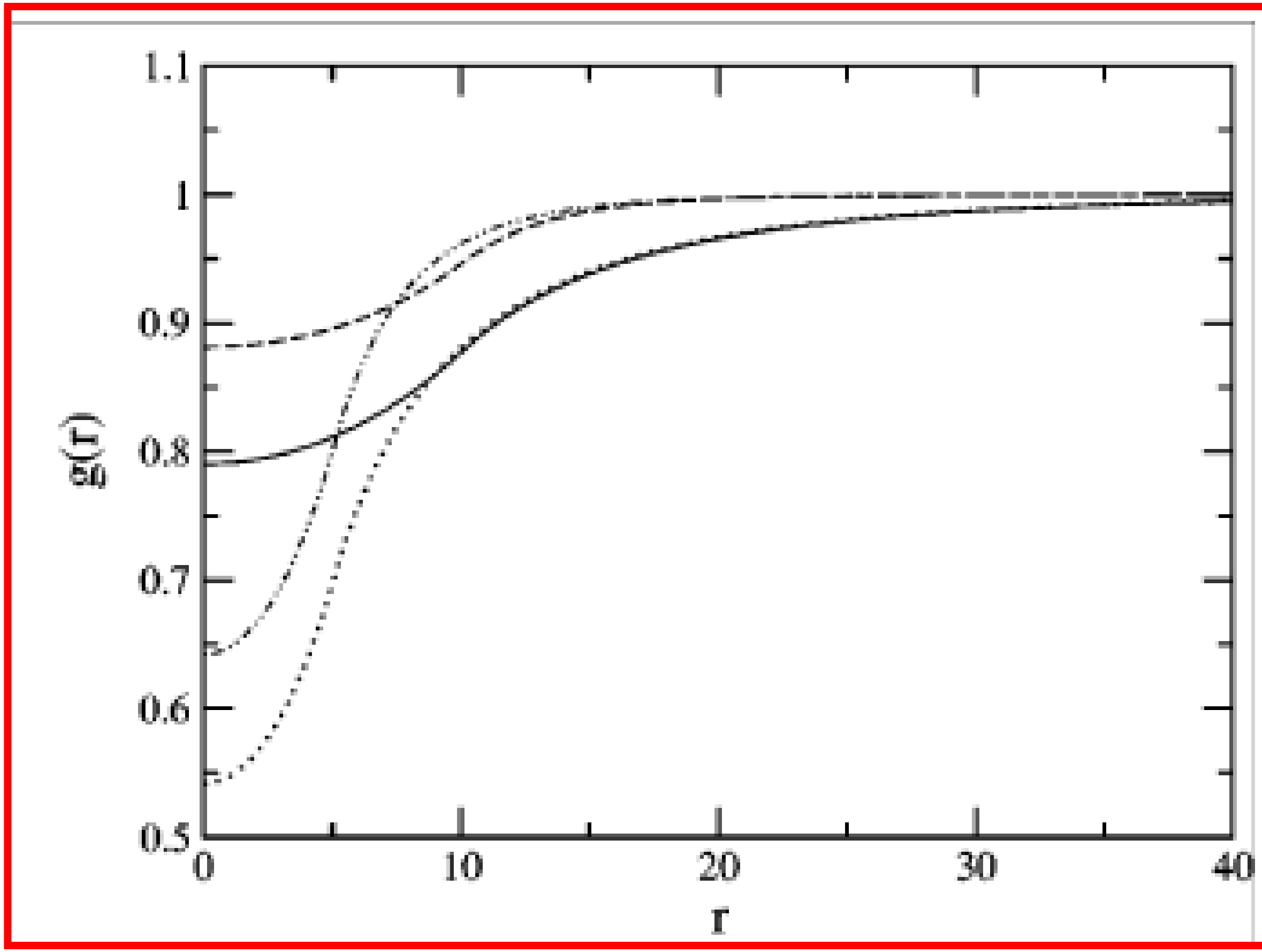


$$f_{SR}(r) = 1 - b e^{-cr^2}$$

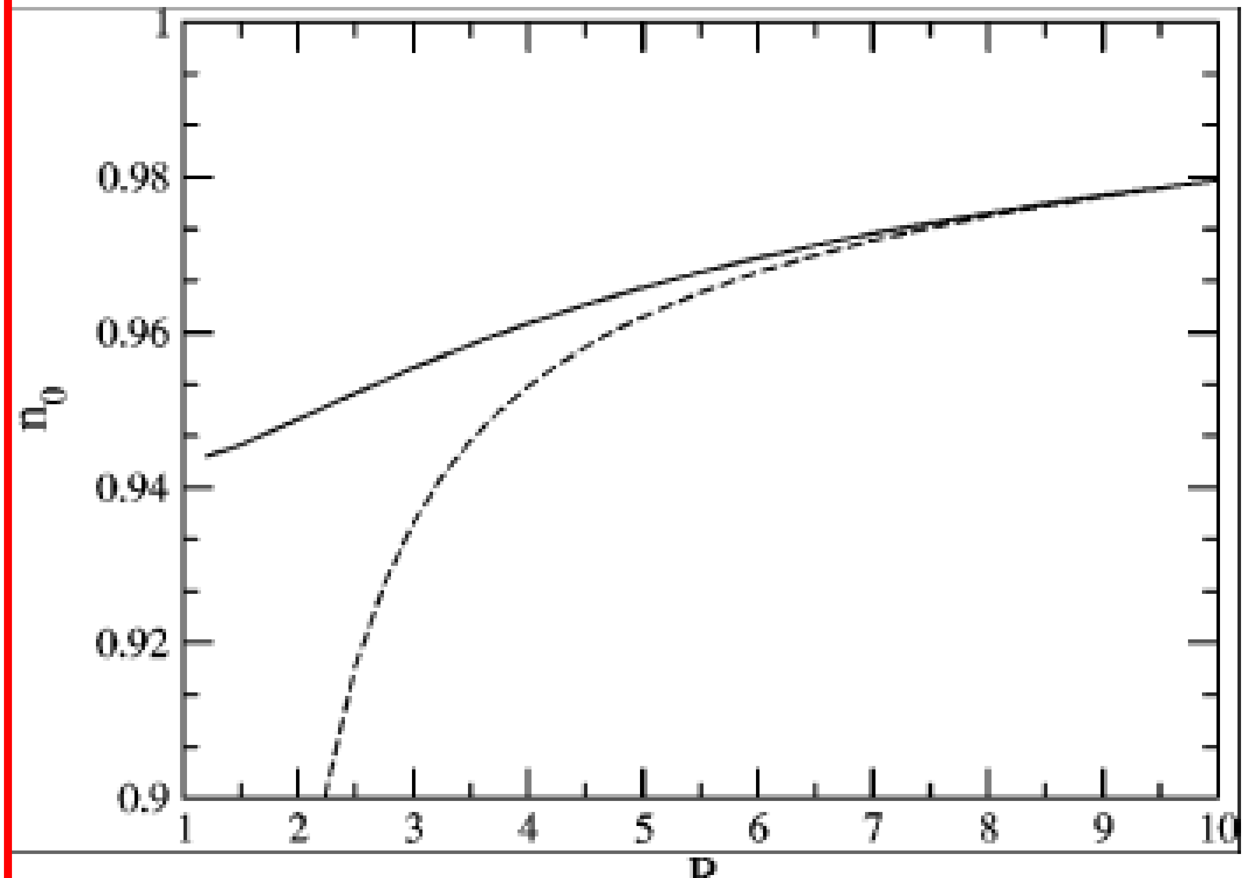
Scaled energies and condensate fractions for the soft-sphere gas for two Potentials having the same scattering length

	x	R	$\bar{E}/N$	$\bar{V}/N$	$\bar{T}_g/N$	$\bar{T}_n/N$	n_0
EL	10^{-4}	10	1.305×10^{-3}	1.202×10^{-3}	1.038×10^{-4}	1.000×10^{-4}	0.988
SR	10^{-4}	10	1.317×10^{-3}	1.241×10^{-3}	0.765×10^{-4}	0.765×10^{-4}	0.997
UL	10^{-4}	10	1.295×10^{-3}	1.184×10^{-4}		1.110×10^{-4}	0.992
IPC	10^{-4}	10	1.311×10^{-3}				
DMC	10^{-4}	10	1.303×10^{-3}				0.989
EL	10^{-4}	5	1.314×10^{-3}	1.044×10^{-3}	2.708×10^{-4}	2.630×10^{-4}	0.985
SR	10^{-4}	5	1.361×10^{-3}	1.138×10^{-3}	2.231×10^{-4}	2.231×10^{-4}	0.996
UL	10^{-4}	5	1.231×10^{-3}	0.853×10^{-3}		3.780×10^{-4}	0.982
IPC	10^{-4}	5	1.331×10^{-3}				0.987
DMC	10^{-4}	5	1.309×10^{-3}				0.989
EL	10^{-2}	10	1.404×10^{-1}	1.394×10^{-1}	0.990×10^{-3}	0.981×10^{-3}	0.980
SR	10^{-2}	10	1.405×10^{-1}	1.395×10^{-1}	0.960×10^{-3}	0.960×10^{-3}	0.977
UL	10^{-2}	10	1.404×10^{-1}	1.395×10^{-1}		0.963×10^{-3}	0.980
IPC	10^{-2}	10	1.408×10^{-1}				
EL	10^{-2}	5	1.532×10^{-1}	1.468×10^{-1}	6.445×10^{-3}	6.480×10^{-3}	0.951
SR	10^{-2}	5	1.535×10^{-1}	1.481×10^{-1}	5.350×10^{-3}	5.350×10^{-3}	0.960
UL	10^{-2}	5	1.528×10^{-1}	1.464×10^{-1}		6.375×10^{-3}	0.950
IPC	10^{-2}	5	1.556×10^{-1}				0.953

Radial distribution functions for SS10 and SS5 at x=0.0001 (solid line for SS10 and dotted for SS5) and x=0.001 (dashed line for SS10) and dashed-dot-dot for SS5).



Dependence of the condensate fraction on the shape of the potential at x=0.001 as a function of the radius of the SS potential at fixed scattering length. The condensate fraction grows with R, since the interaction softens.



The dashed line is for UL that becomes accurate for large R as the interaction softens.

Summary

* HNC with a Jastrow wave function and a optimal two-body correlation function provides a good description of both hard- and soft-spheres.

* The dependence of the energy on the shape of the potential appears around x=0.001.

• For smaller x, the universality applies only to the total energy, but not to the potential and kinetic energy. We have found a shape dependence of the condensate fraction for soft-spheres at x=0.001.

•The UL approach becomes reliable when the potentail is soft.

•Appearance of structure in g(r) and in the excitation spectrum when x increases.

Other applications: mainly related to cold gases. Remember that in cold gases one can control the geometry and the interaction.

- **Consider different dimensionalities.**

- **Trapped hard- and soft-spheres. Model for BEC in cold atoms.**

- **Fermi-hard spheres: Ground-state, single-particle spectrum, effective mass, n(k), spectral functions (PhD Angela Mecca)**

- **Ferromagnetic transition.**

- **Multicomponent systems: Mixtures of Bose and Fermi hard- and soft-spheres**

Summer 2004 in Costa Brava, close to Barcelona