



Higher-order actions and their applications in
many-body, few-body, classical problems

Quantum Monte Carlo simulation of spin-polarized tritium

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Outline

- Introduction
- Method
- Interatomic potential
- Spin-polarized hydrogen ($\text{H}\downarrow$)
- Liquid spin-polarized tritium ($\text{T}\downarrow$)
- Solid $\text{T}\downarrow$
- Liquid-Solid Transition in $\text{T}\downarrow$
- Pure and mixed $\text{T}\downarrow$ clusters
- Summary

Introduction

- Spin-polarized hydrogen has 3 isotopes: $^1\text{H}\downarrow = \text{H}\downarrow$ - boson, $^2\text{H}\downarrow = \text{D}\downarrow$ - fermion and $^3\text{H}\downarrow = \text{T}\downarrow$ - boson
- BEC for $\text{H}\downarrow$ suggested by Stwaley and Nosanow in 1976, realized by Fried *et al.* in 1998
- In 2002. Blume *et al.* suggested using $\text{T}\downarrow$ to achieve BEC with the advantage of nearly exact knowledge of interatomic potential
- bulk $\text{H}\downarrow$ has been studied from 1975. – shown to be gas (Etters, Miller and Nosanow, Lanto and Nieminen, Entel and Anlauf,..)

Introduction

- $D\downarrow$ have three versions involving one ($D\downarrow_1$), two ($D\downarrow_2$) and three ($D\downarrow_3$) nuclear spin states
- studied in 80ties by Kortscheck et al., Panoff and Clark, Flynn et al.: ($D\downarrow_2$) and ($D\downarrow_3$) are both liquids at zero pressure; confirmed in '99 by Skjetne and Ostgaard
- $T\downarrow$ is predicted to be liquid
- Blume et al. did DMC calculations of $T\downarrow$ clusters; ($T\downarrow$)₃ is Borromean or halo state with energy of only -4.2(7)mK (confirmed by Salci et al.)

Introduction

- there where no studies of the mixed clusters
- similary to ^3He it is expected that it'll take more than 30 atoms to form a bound state of $(\text{D}\downarrow)_N$ cluster
- best candidates for small mixed clusters are $\text{T}\downarrow$ - $\text{D}\downarrow$ and $\text{T}\downarrow$ - $\text{H}\downarrow$ clusters
- new experimental development: Magnetic trapping of hydrogen after multistage Zeeman deceleration
- Hogan et al. PRL **101**, 143001 (2008).
 - starting from a supersonic beam $\text{H}\downarrow$ cooled to about 100mK
 - expected to work well with $\text{D}\downarrow$ and $\text{T}\downarrow$ atoms

Method

- Variational and diffusion Monte Carlo
- Imaginary-time Schrödinger equation

$$-\frac{\partial \Psi(\mathbf{R}, t)}{\partial t} = (H - E_t) \Psi(\mathbf{R}, t) \quad (*)$$

- N-particle Hamiltonian

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

- E_t is a constant acting as a reference energy,
 $\mathbf{R} \equiv (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is a walker in MC terminology
 $V(r)$ is the interaction potential
- DMC solves stochastically the equation (*)

- use of importance sampling;

$$\Psi(\mathbf{R}, t) \rightarrow \Phi(\mathbf{R}, t) = \Psi(\mathbf{R}, t) \psi(\mathbf{R})$$

↙ importance sampling
wave function

- in the limit $t \rightarrow \infty$ only the lowest energy state, not orthogonal to $\psi(\mathbf{R})$ survives
- for liquid ground state and clusters— Jastrow approximation

$$\psi_J(R) = \prod_{i < j}^N f(r_{ij})$$

$$\text{liquid: } f(r_{ij}) = \exp(-b_1 \cdot \exp(-b_2 \cdot r_{ij}))$$

Method

for clusters

$$N < 70, \quad f(r_{ij}) = \exp\left(-\left(\frac{b}{r_{ij}}\right)^5 - s \cdot r_{ij}\right)$$

$$N \geq 70, \quad f(r_{ij}) = \exp\left(-\left(\frac{b}{r_{ij}}\right)^5 - s \cdot r_{ij}^2\right)$$

for solid, simulations of crystalline hcp, fcc and bcc
phase Nosanow-Jastrow model for trial wave function

$$\psi_{NJ}(\mathbf{R}) = \psi_J(\mathbf{R}) \times \prod_{i=1}^N h(r_{iI})$$

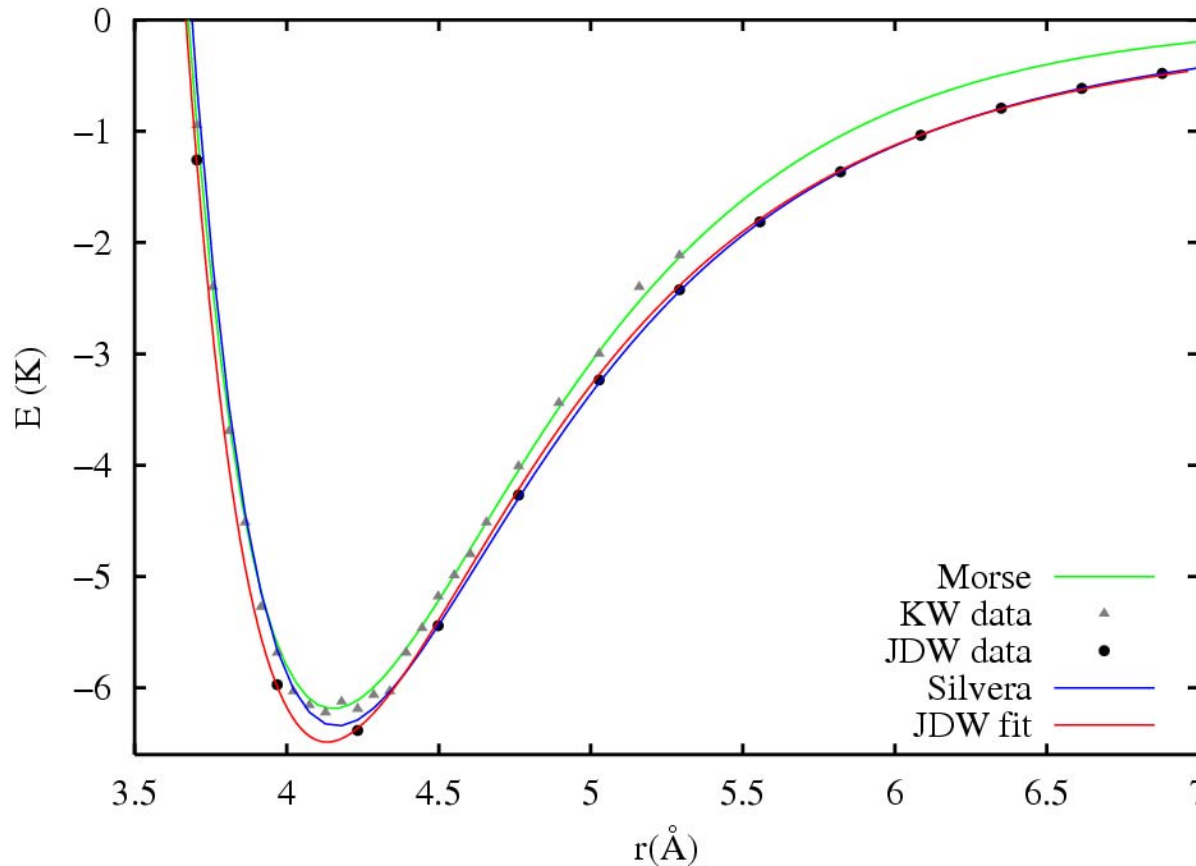
$h(r)$ is a Gaussian function linking every particle i to a
fixed point $\mathbf{r}_I$ of the lattice

periodic boundary conditions

Method

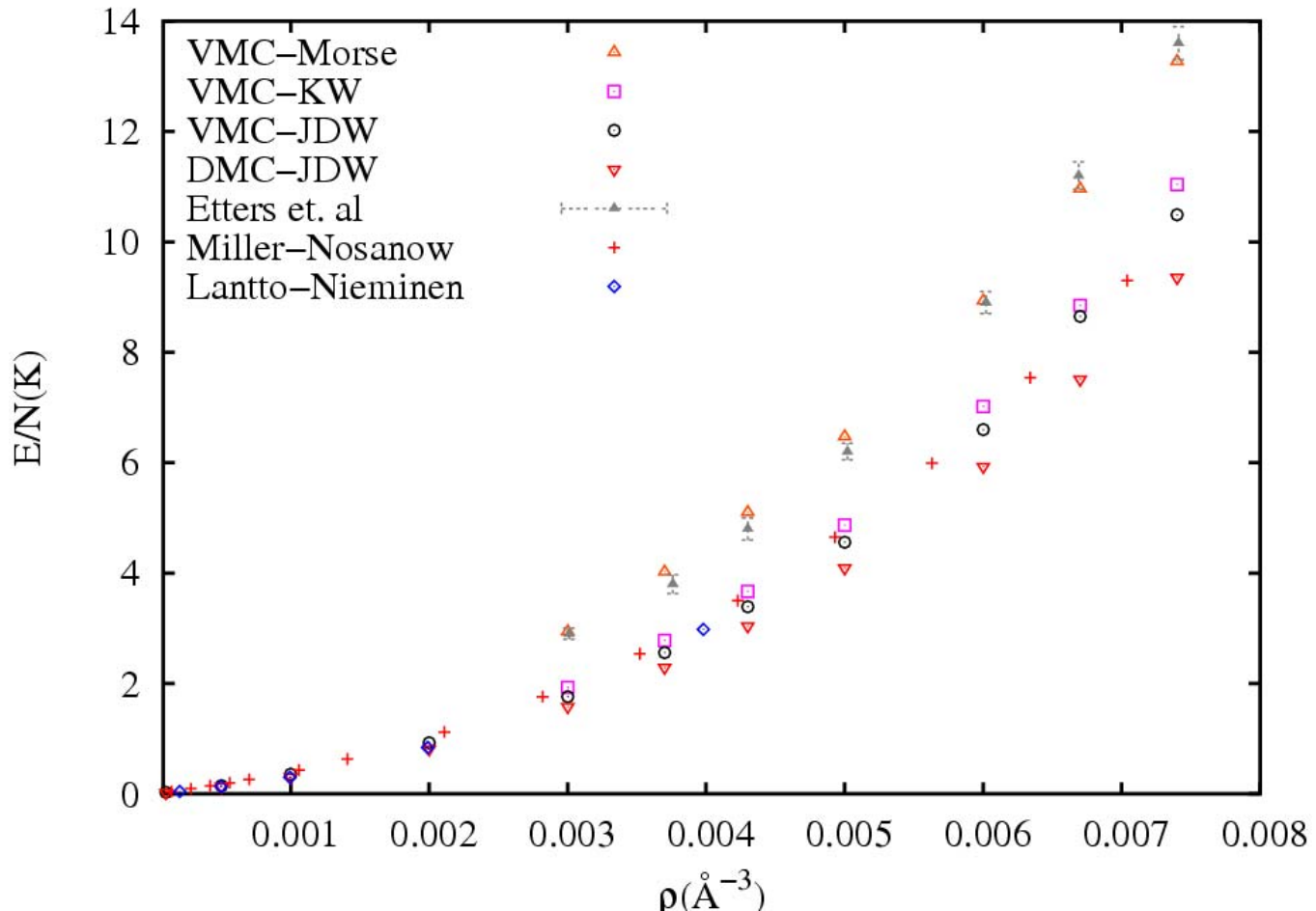
- possible bias reduced to the level of statistical noise by:
 - summing proper tail corrections to the potential and kinetic energy
 - calculating the energies using different number of particles (from $N=180$ -250)
 - checking the dependence with mean population of walkers and with the time step in the second order method

Interatomic potential

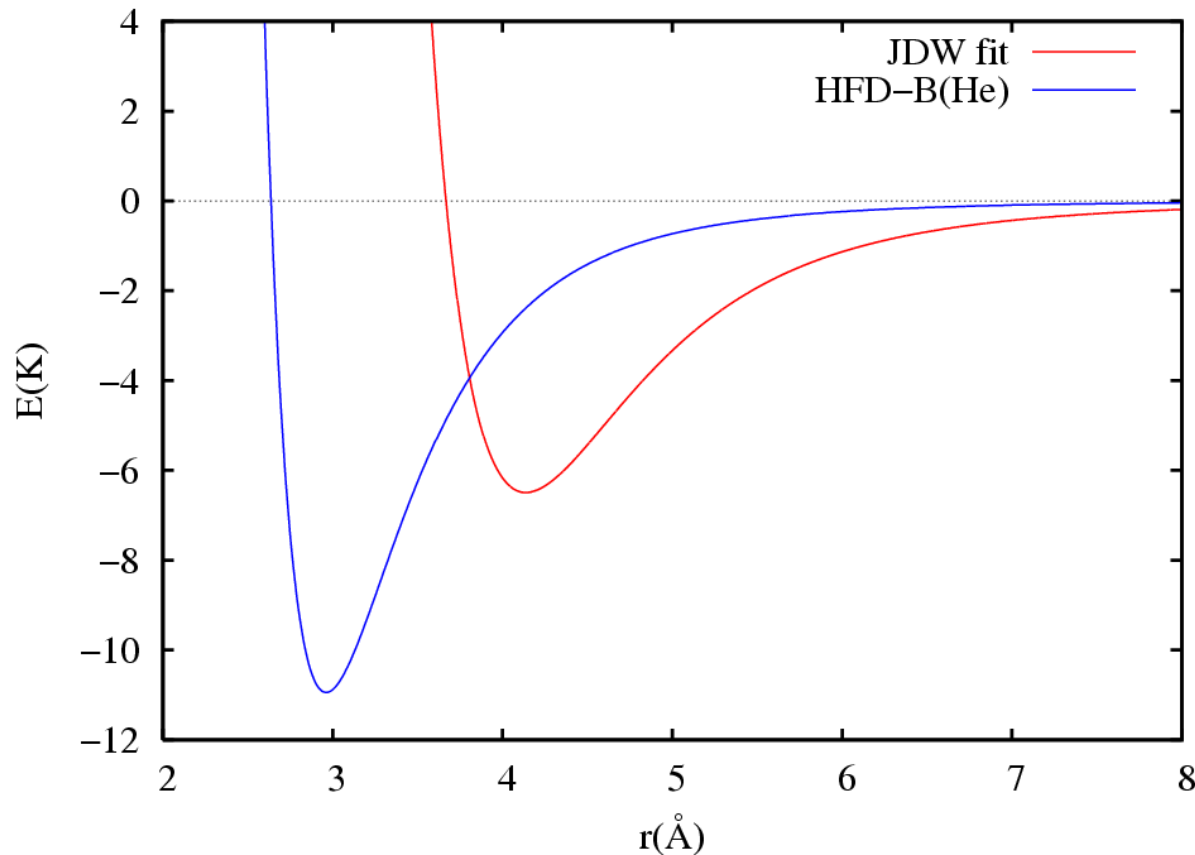


triplet potential $b^3\Sigma_u^+$ (W. Kolos and L. Wolniewicz, Chem. Phys. Lett. **24**, 457 (1974).
recalculated to larger distances by Jamieson, Dalgarno, and Wolniewicz, PRA **61**, 042705 (2000).
We use spline fit to JDW data and connect to long-range behavior Phys. Rev A **54**, 2824(1996).

Interatomic potential



Interatomic potential



$$\sigma = 3.67 \text{\AA}$$

$$\text{Minimum: } \varepsilon = -6.49 \text{ K}$$

$$r_m = 4.14 \text{\AA}$$

$$\sigma = 2.556 \text{\AA} \text{ in } {}^4\text{He}$$

Spin-polarized H, equation of state

solid points: equation of state of H↓
 (PRB **75**, 064506)
 triangles HS gas
 (PRA **60**, 5129)

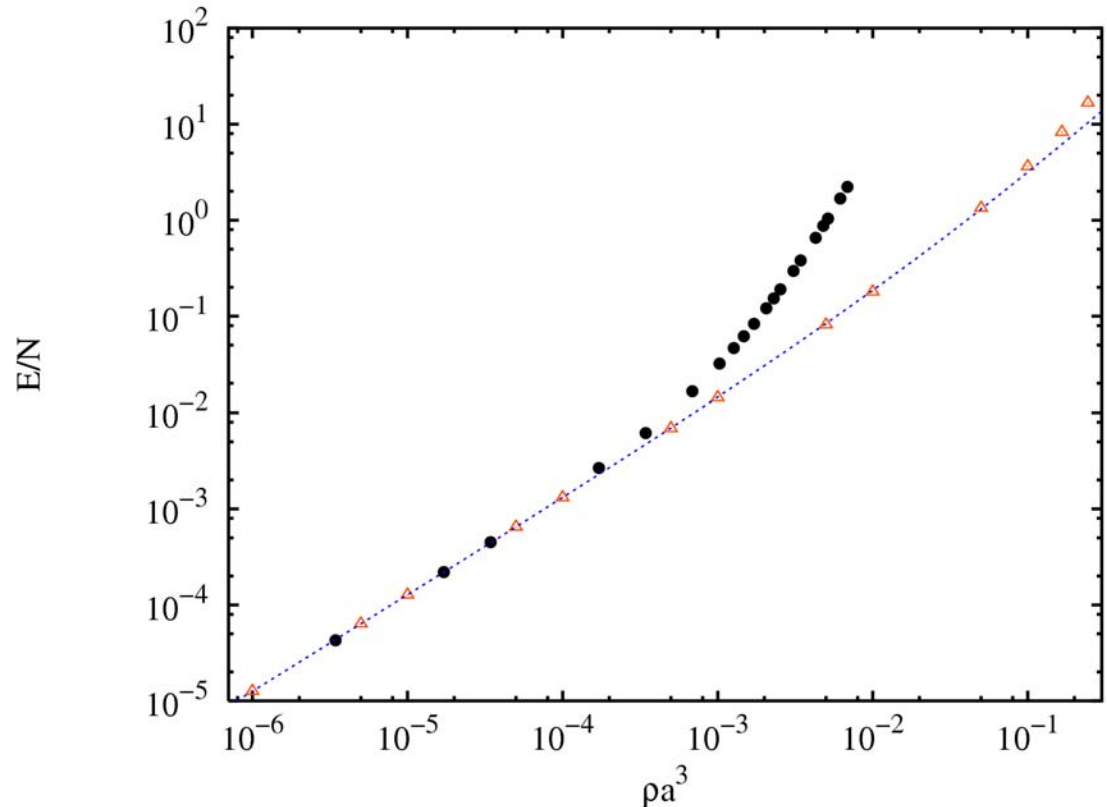
ne:

$$\left(\frac{E}{N}\right) = 4\pi x \left(1 + \frac{128}{15\sqrt{\pi}} x^{1/2}\right)$$

$$x = \rho a^3$$

mean-field
 result

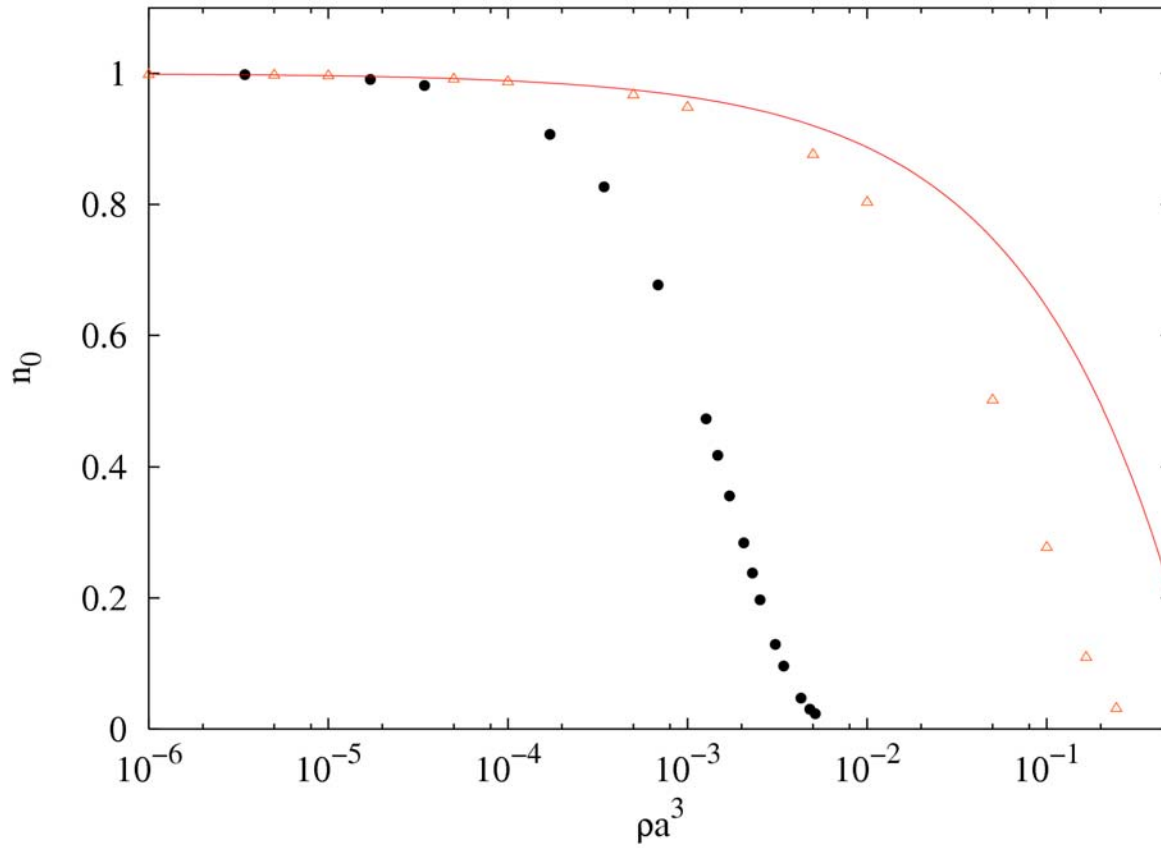
Lee-Huang
 correction



$$E/N \text{ in units } \frac{\hbar^2}{2ma^2}$$

$$a=0.697\text{\AA}$$

Spin-polarized H – condensate fraction



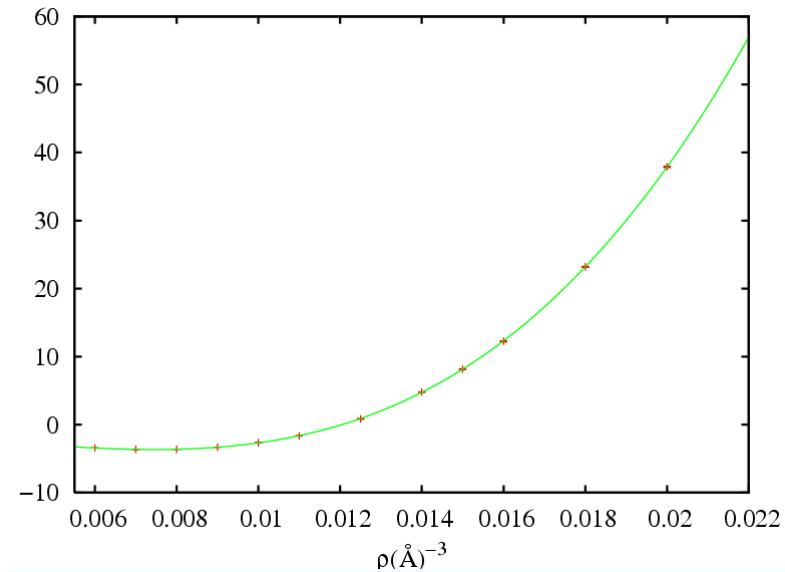
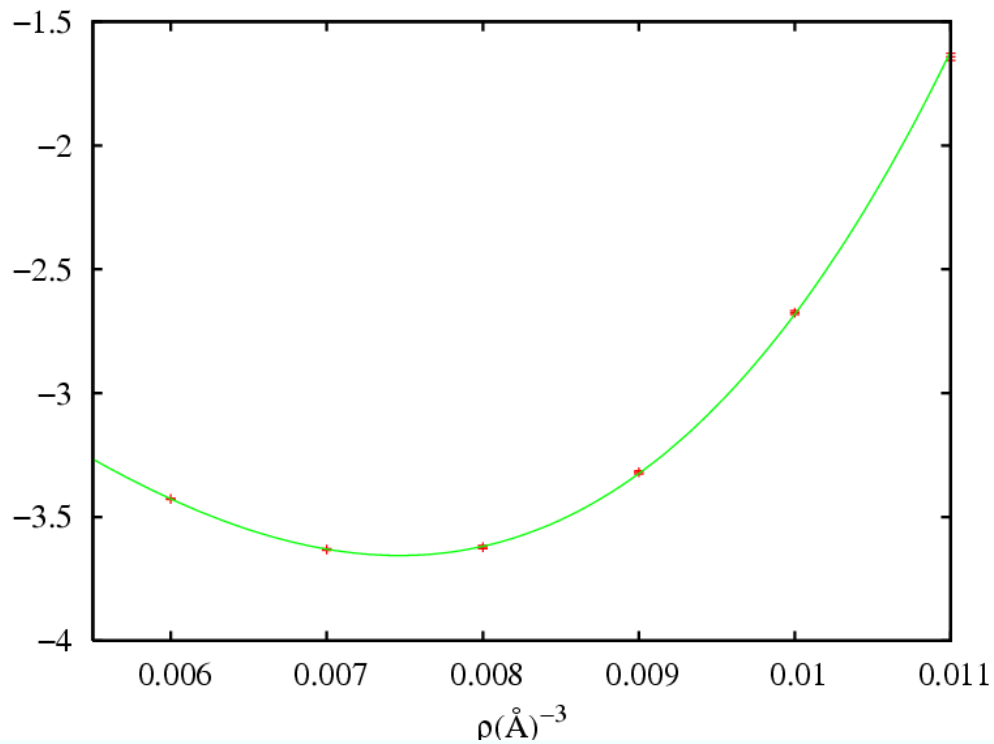
-solid points $H\downarrow$

-triangles HS gas
(PRA **60**,5129)

-line: Bogoliubov
approximation

$$n_0 = 1 - \frac{8}{3\sqrt{\pi}} x^{1/2}$$

Liquid $T \downarrow$ - equation of state



Liquid $T \downarrow$ - equation of state

the analytical form

$$e(\rho) = e_0 + e_1 \left(\frac{\rho}{\rho_0} - 1 \right)^2 + e_2 \left(\frac{\rho}{\rho_0} - 1 \right)^3$$

fits DMC data from the spinodal point to the highest density calculated, high in the overpressurized regime

$$e = E/N$$

$\rho_0 = 0.007466(7) \text{ \AA}^{-3}$ is the equilibrium density ($0.369\sigma^{-3}$),

$$e_0 = -3.656(4) \text{ K},$$

$$e_1 = 6.86(7) \text{ K},$$

$$e_2 = 4.70(5) \text{ K}$$

(in ^4He $\rho_0 = 0.365\sigma^{-3}$, $e = -7.267(13) \text{ K}$)

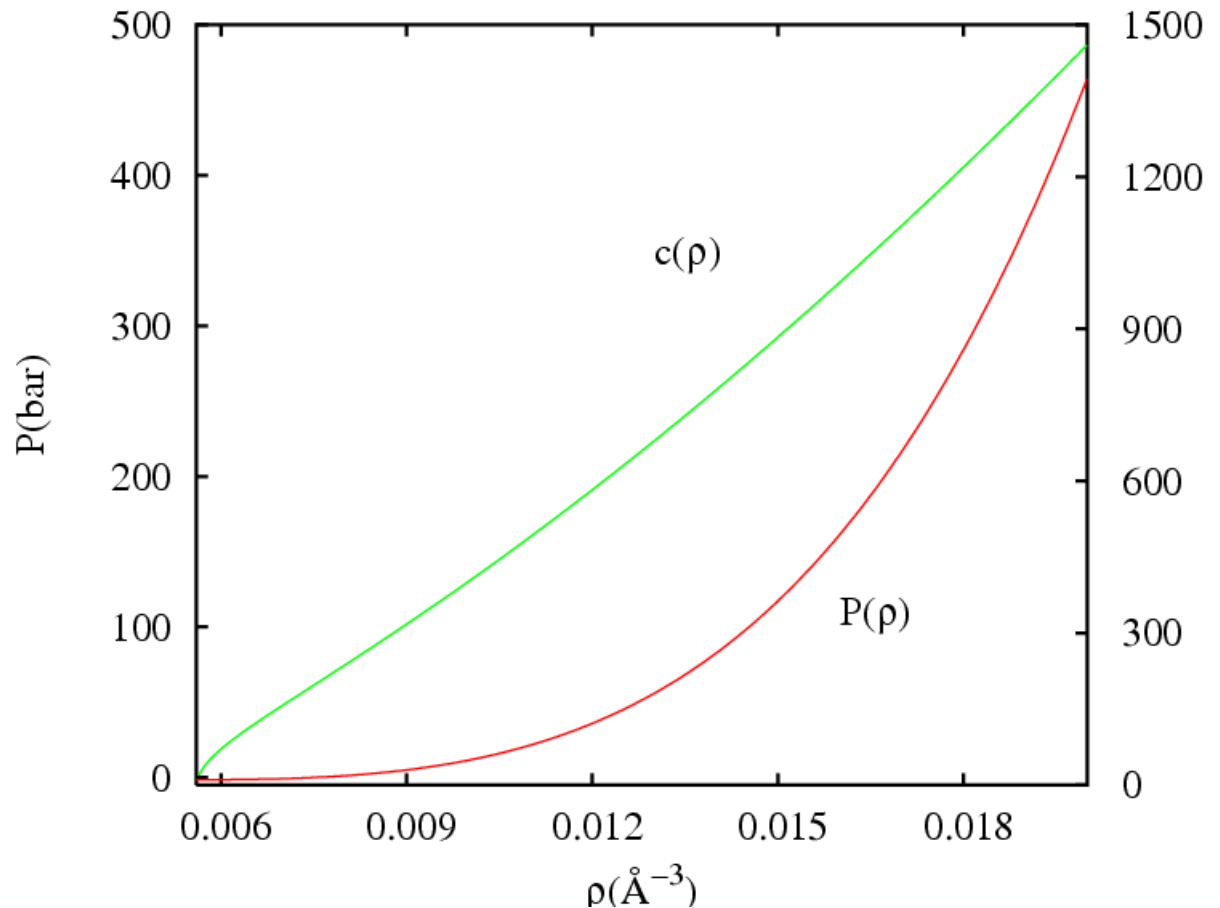
Liquid $T\downarrow$ - equation of state

$\rho(\text{\AA}^{-3})$	E/N	T/N	P (bar)	c(m/s)
0.006	-3.427(1)	5.578(15)	-1.43(2)	71(3)
0.007	-3.632 (2)	7.120(12)	-0.73(1)	158(3)
0.008	-3.622(4)	8.85(2)	1.25(2)	237(3)
0.01	-2.675(4)	13.06(3)	11.6(1)	402(4)
0.015	8.147 (13)	27.05(7)	117.3(1.0)	884(7)

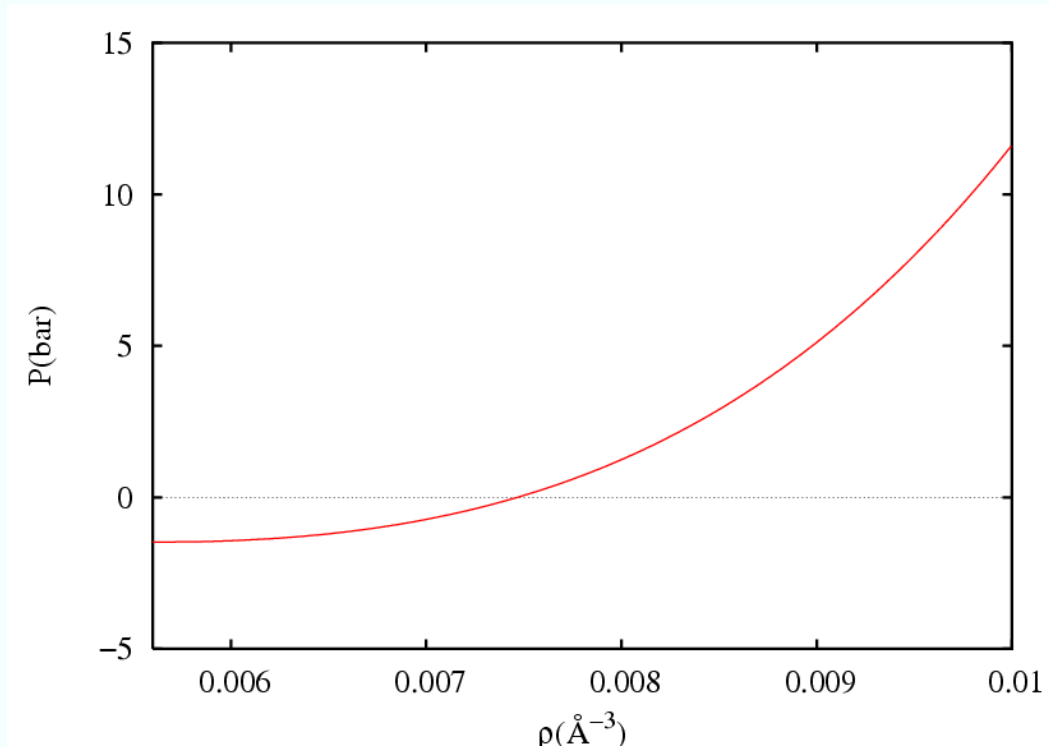
Liquid T↓ - pressure and speed of sound

$$P(\rho) = \rho^2 \frac{\partial e}{\partial \rho}$$

$$c^2(\rho) = \frac{1}{m} \frac{\partial P}{\partial \rho}$$



Liquid $T\downarrow$ - pressure

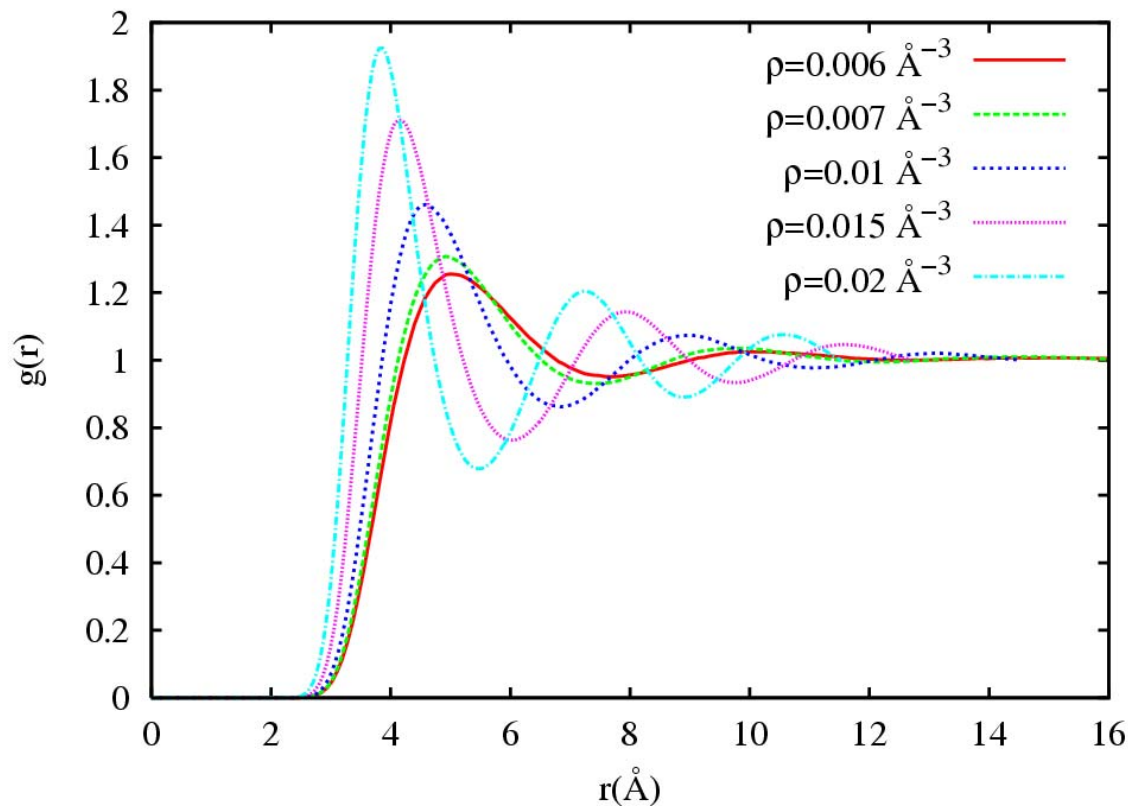


- spinodal density in $T\downarrow$: $\rho=0.0056\text{\AA}^{-3}=0.277\sigma^{-3}$, $P=-1.48(2)$ bar
- spinodal density in ^4He $\rho=0.264 \sigma^{-3}$, $P=-9.30(15)\text{bar}$

Liquid T↓

two-body radial distribution function

$$g(r) = \frac{N(N-1)}{\rho^2} \frac{\int |\Psi(r_1, r_2, \dots, r_N)|^2 dr_3 \dots r_N}{\int |\Psi(r_1, r_2, \dots, r_N)|^2 dr_1 \dots r_N}$$



obtained using
unbiased (pure)
estimators

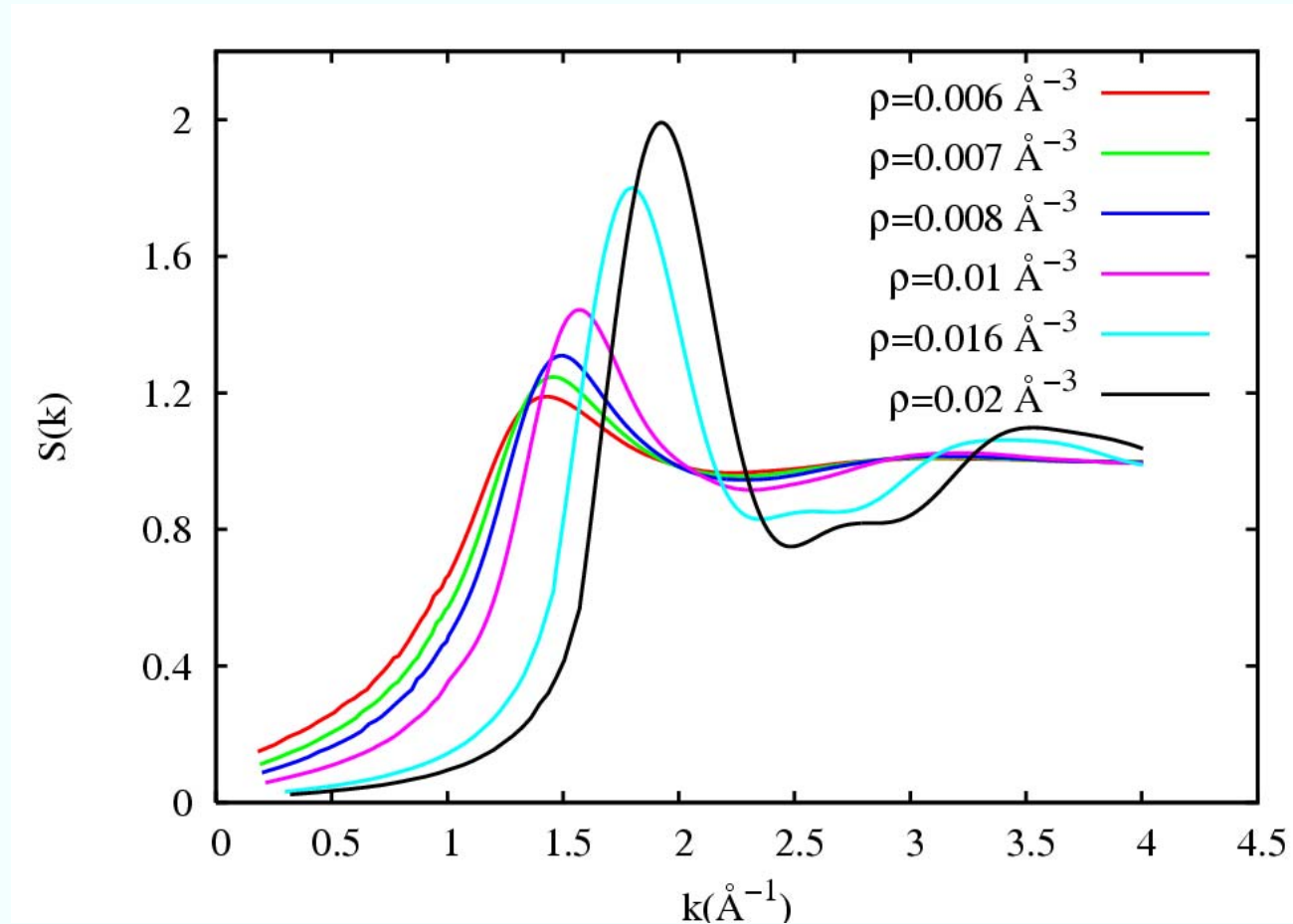
Casulleras, Boronat
(1995)

Liquid $T \downarrow$ - static structure function

$$S(q) = \langle \rho_q \rho_{-q} \rangle / N$$

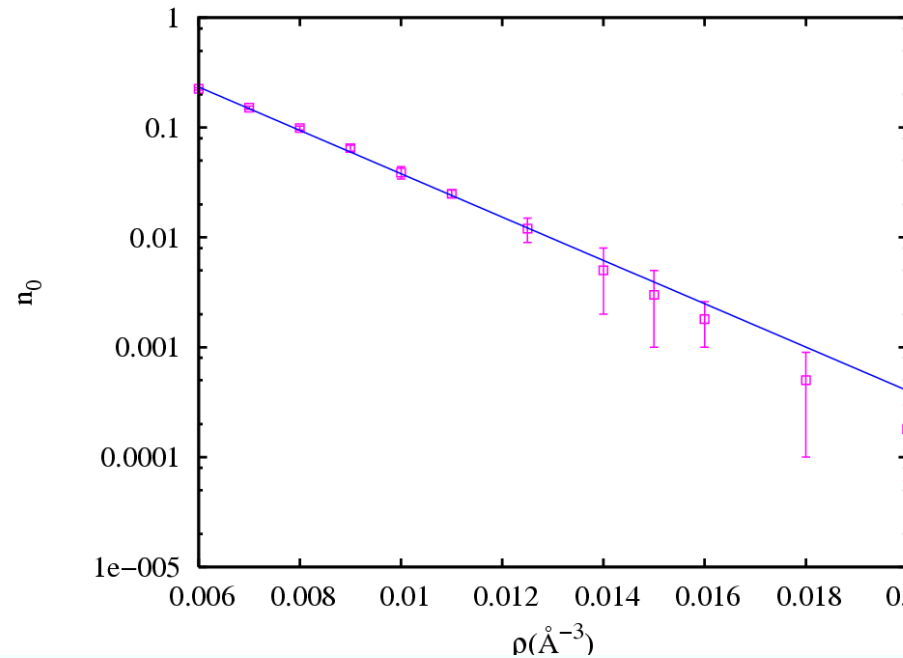
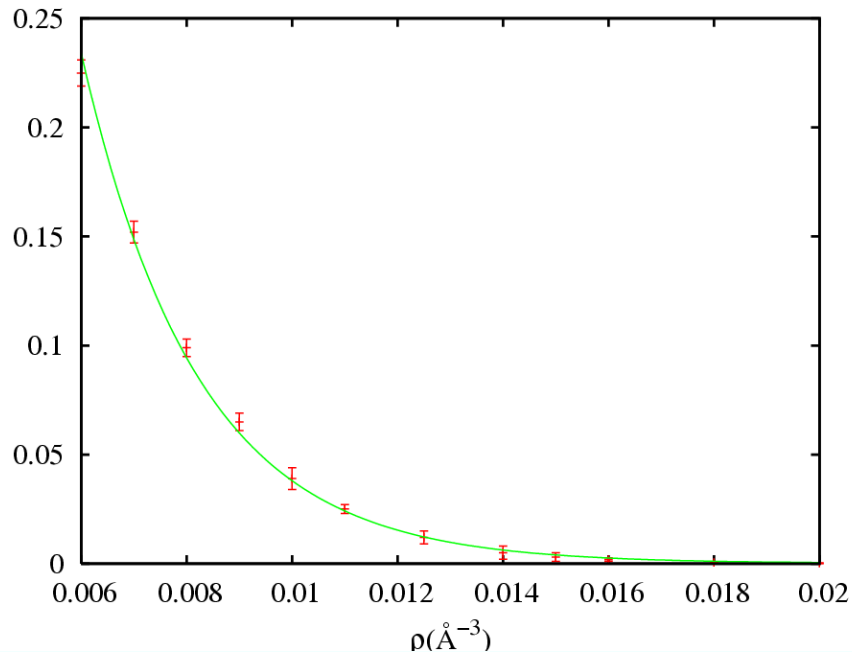
$$\rho_q = \sum_{i=1}^N e^{iq \cdot r_i}$$

$$\lim_{q \rightarrow 0} S(q) = \hbar q / 2mc$$



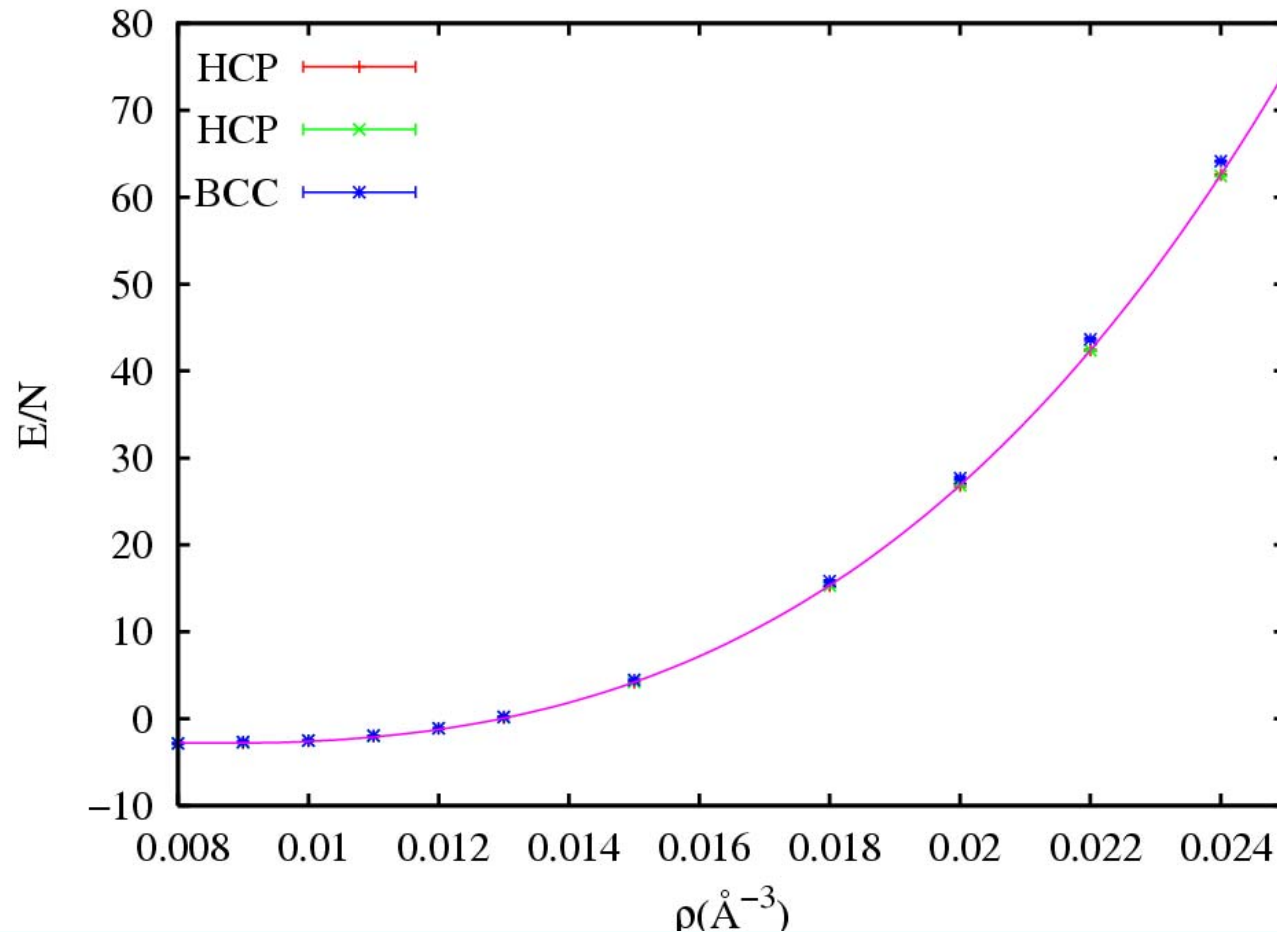
Liquid $T \downarrow$ - condensate fraction

$$n_0 = \lim_{r \rightarrow \infty} \rho(r)$$



$$f(x) = A \exp(-bx)$$

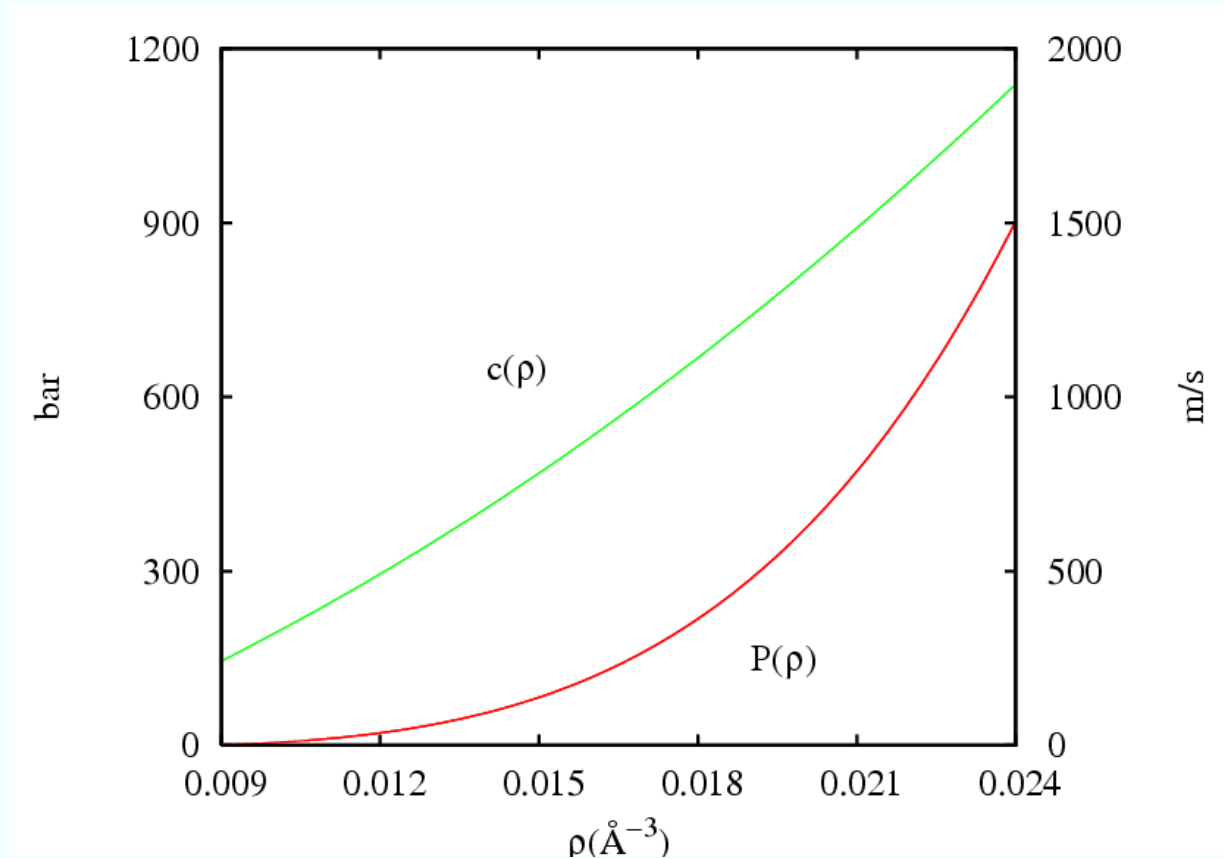
Solid T↓ - equation of state



$$f(x) = a_1x^2 + a_2x^3 + a_3x^4$$

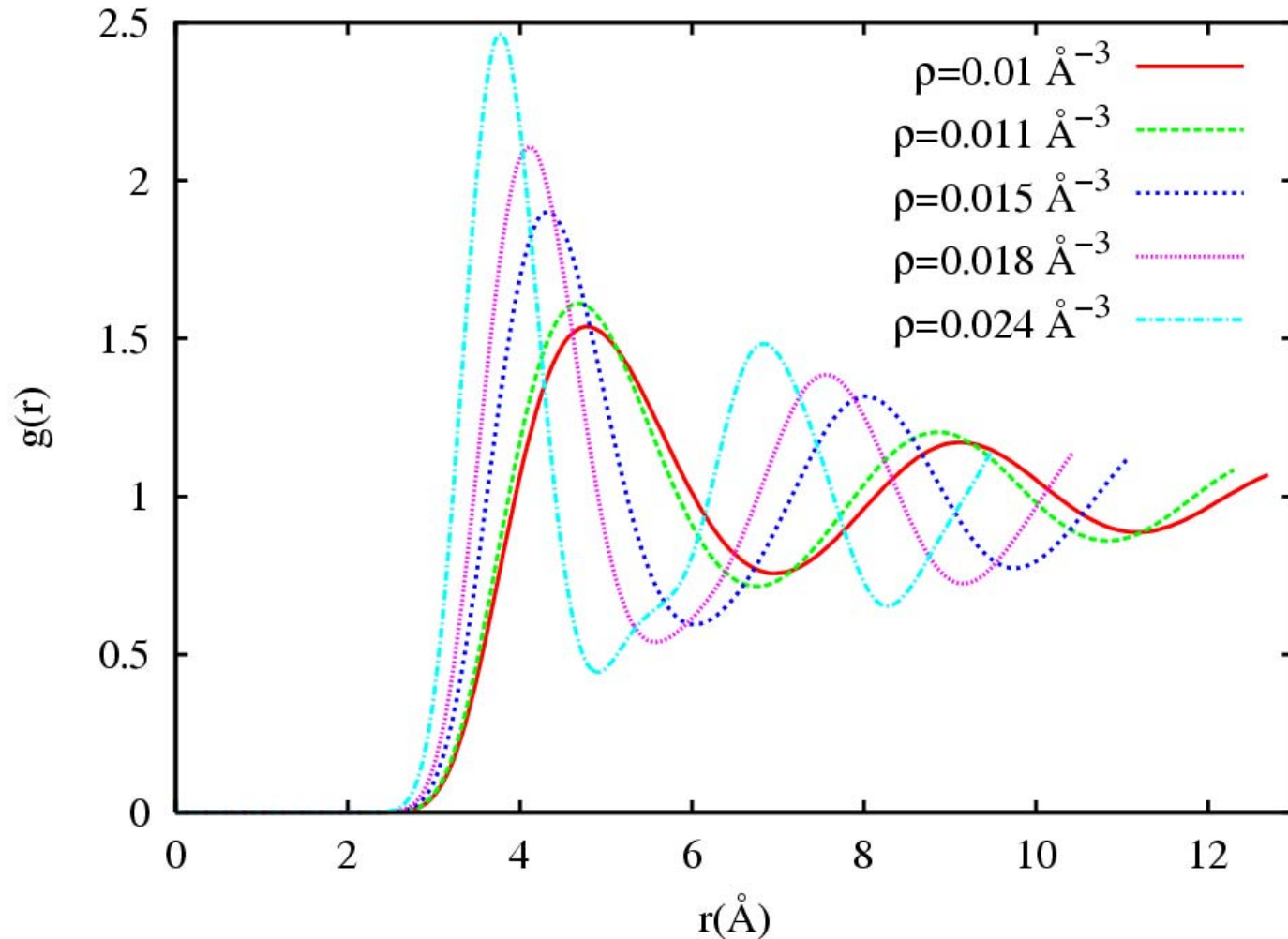
Solid T↓

-pressure and speed of sound



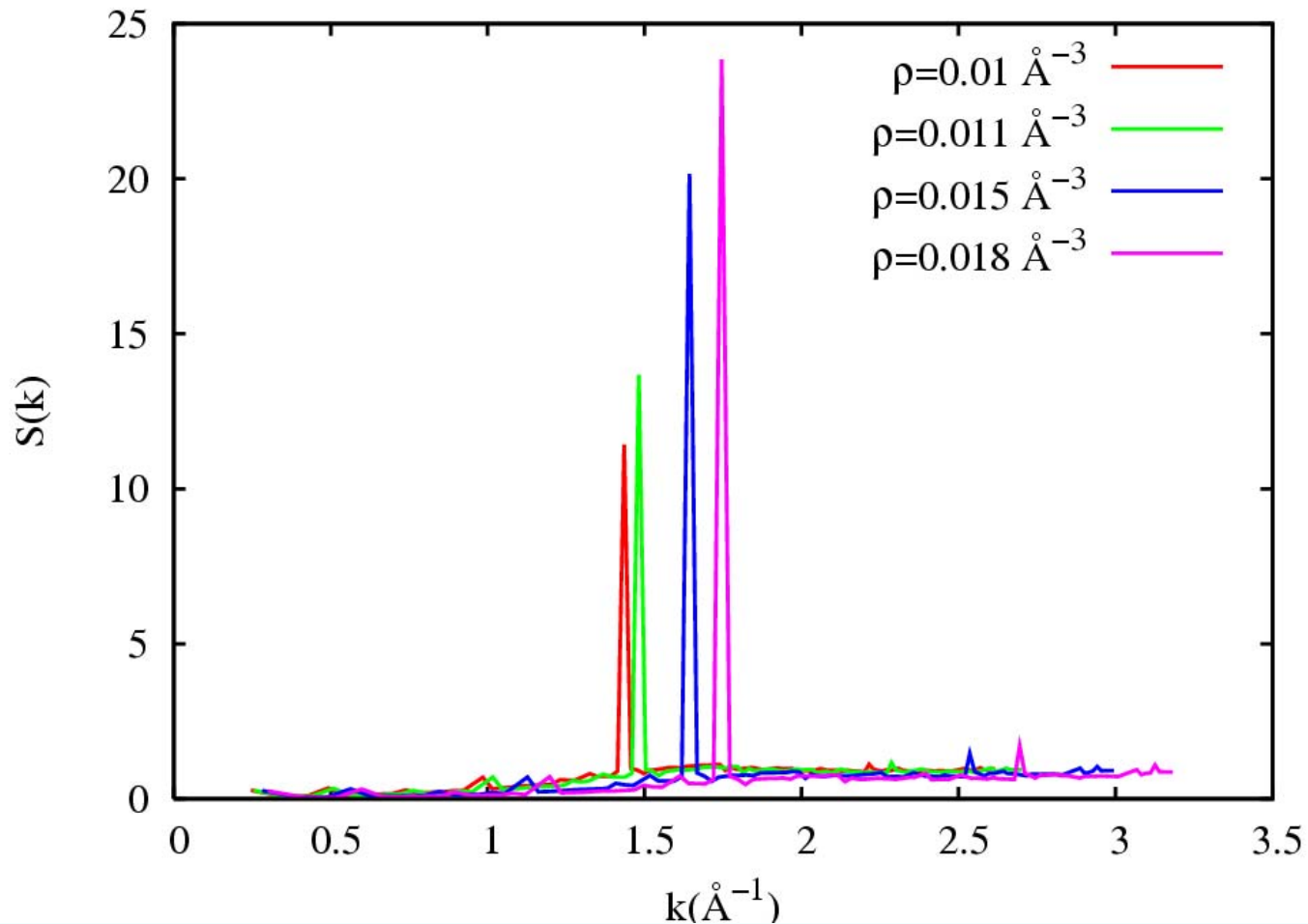
Solid T↓

two-body radial distribution function



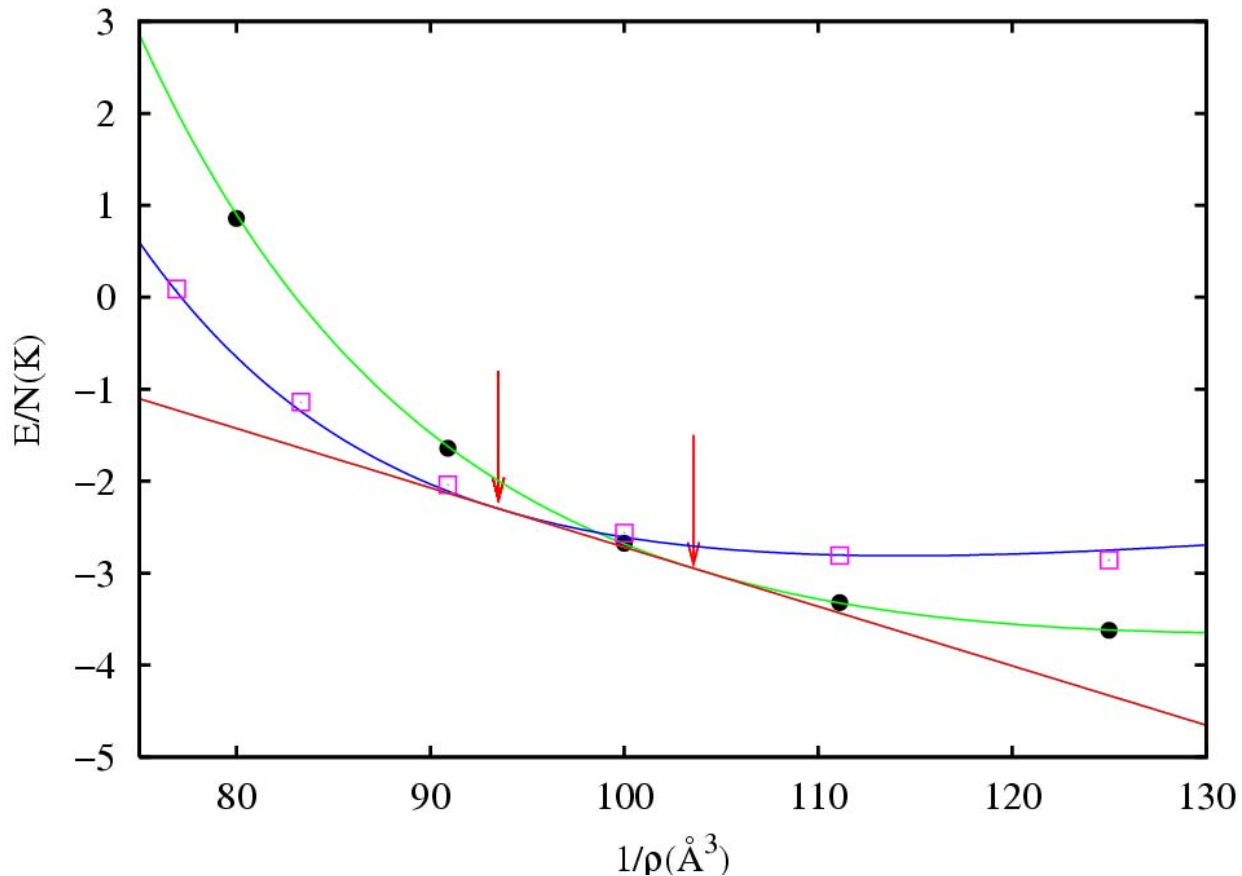
Solid T↓

static structure function



Liquid –solid transition in $T \downarrow$

-Maxwell double tangent construction



Liquid –solid transition in T↓

	BCC	FCC	HCP
ρ_f	$0.0977 \text{ \AA}^{-3}$	$0.00972 \text{ \AA}^{-3}$	$0.00964 \text{ \AA}^{-3}$ $=0.477 \sigma^{-3}$
ρ_m	$0.01075 \text{ \AA}^{-3}$	$0.01075 \text{ \AA}^{-3}$	$0.01069 \text{ \AA}^{-3}$ $=0.528 \sigma^{-3}$
P	9.9 (1.0) bar	9.5 (1.0) bar	8.9 (1.0) bar

Comparison:

-H↑ $P=173(15) \text{ bar}$ $\rho_f=0.01328 \text{ \AA}^{-3}$, $\rho_m=0.01379 \text{ \AA}^{-3}$

-He $P=25 \text{ atm}$ $\rho_f=0.430 \sigma^{-3}$, $\rho_m=0.468 \sigma^{-3}$

Liquid –solid transition in $T \downarrow$

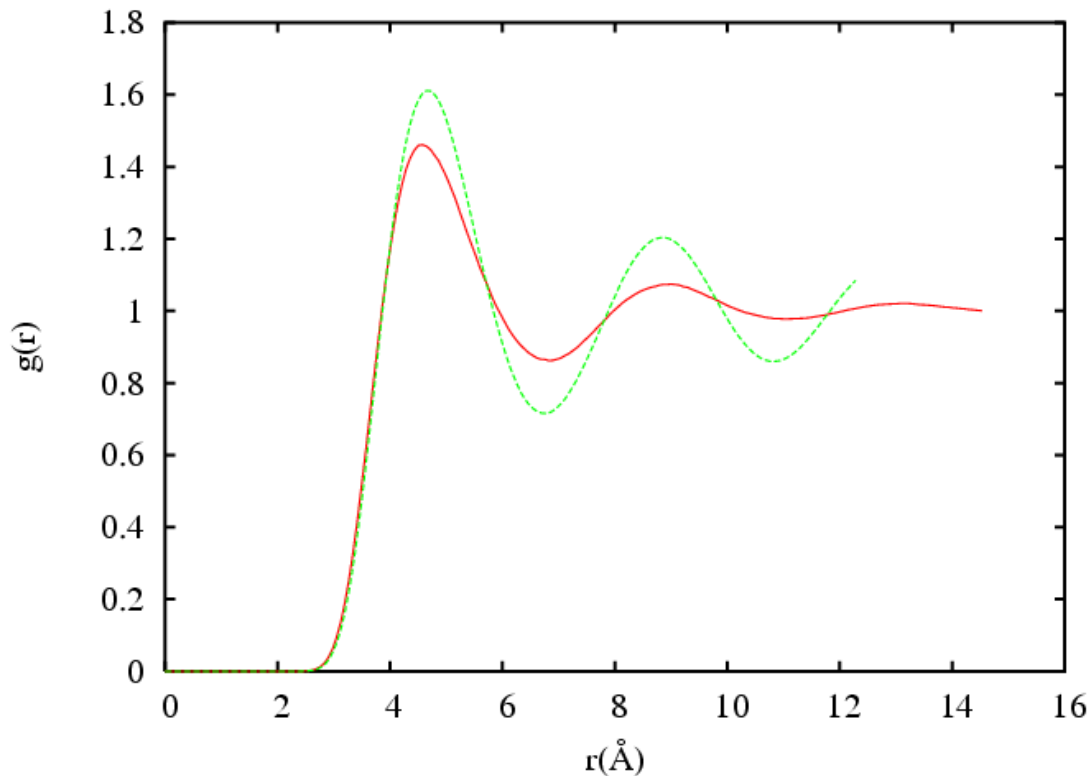
- Lindeman at the transition is 0.26

$$\gamma = \sqrt{\langle (\mathbf{r} - \mathbf{r}_I)^2 \rangle} / a_L$$

- For solid ^4He $\gamma=0.26$, $\text{H} \downarrow$ $\gamma=0.25$
- Discontinuity of the kinetic energy ~ 3.5 K
- At the freezing density condensate fraction $n_0 = 0.03$ (in $\text{H} \downarrow 0.04$)

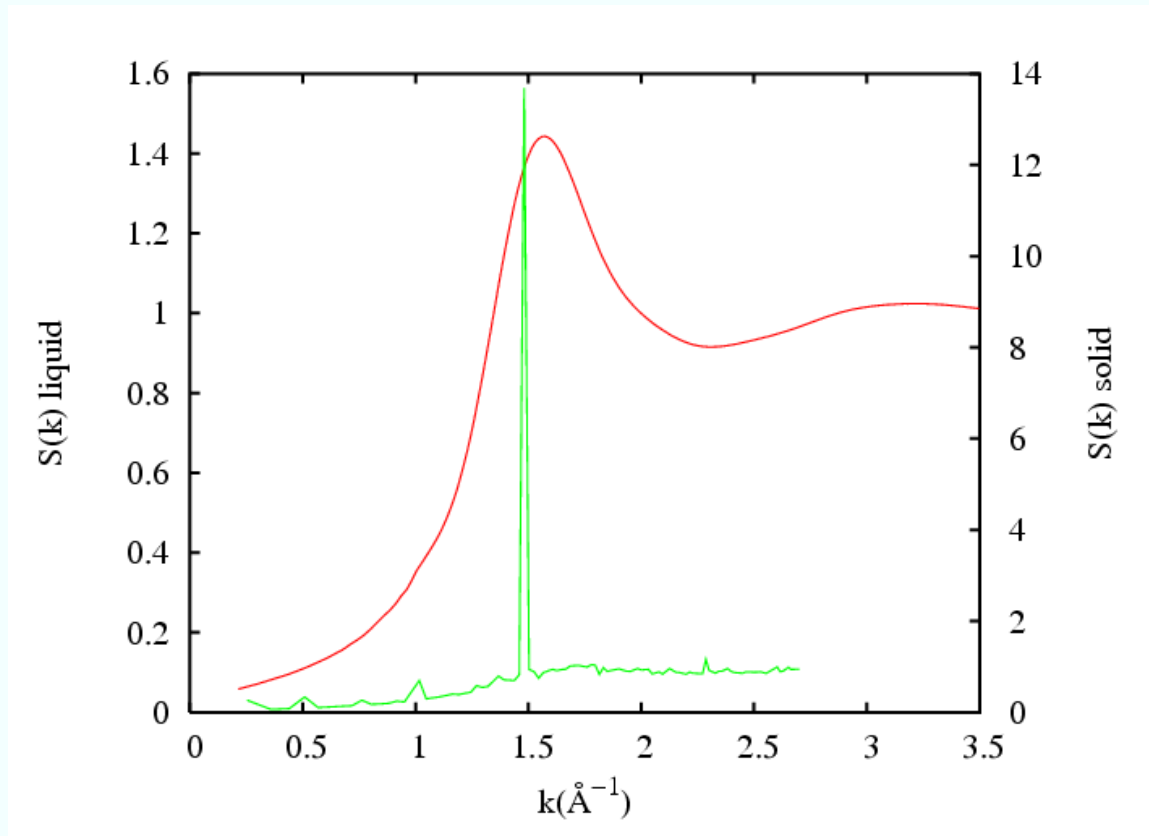
Liquid –solid transition in $T \downarrow$

- Two-body radial distribution function



Liquid –solid transition in $T \downarrow$

- Static structure factor



Pure $T \downarrow$ clusters

$$N = 20, \dots, 320$$

$$E(N)/N = E_0 + E_s x + E_c x^2,$$

$$x = N^{-1/3}$$

$$E_0 = -3.66(3)K$$

$$E_s = 10.2(2)K$$

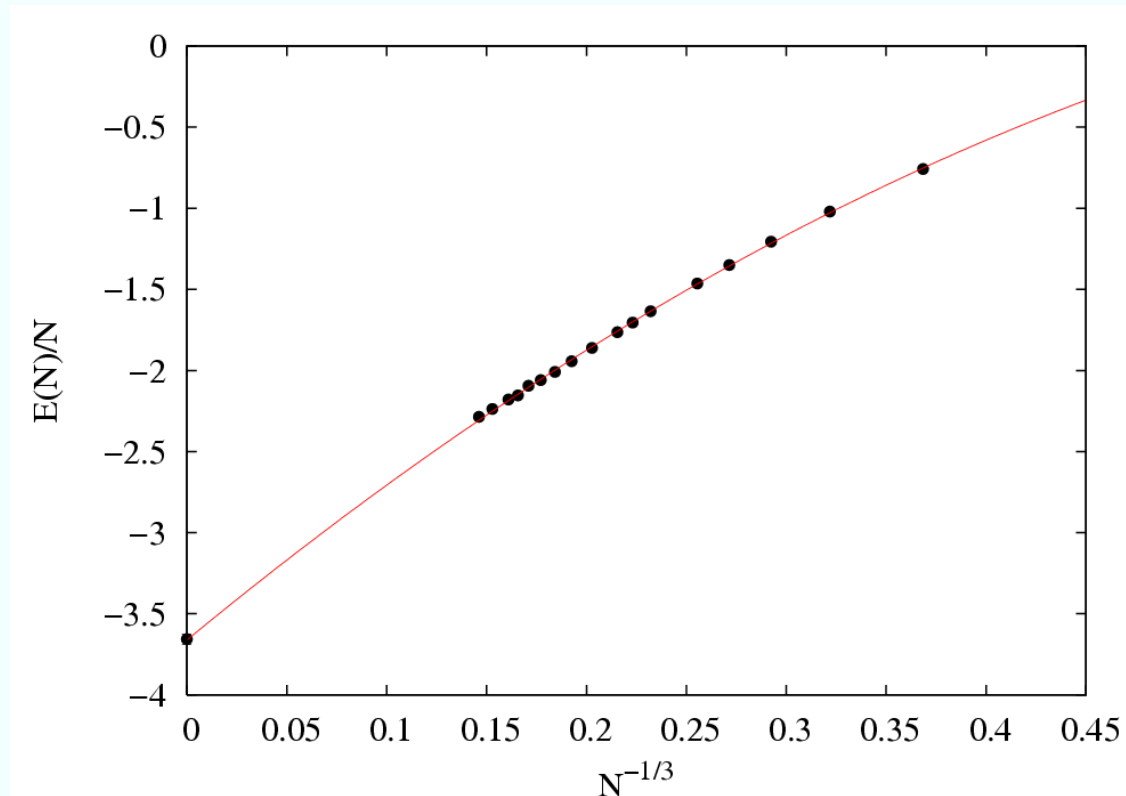
$$E_c = -6.1(4)K$$

surface tension t :

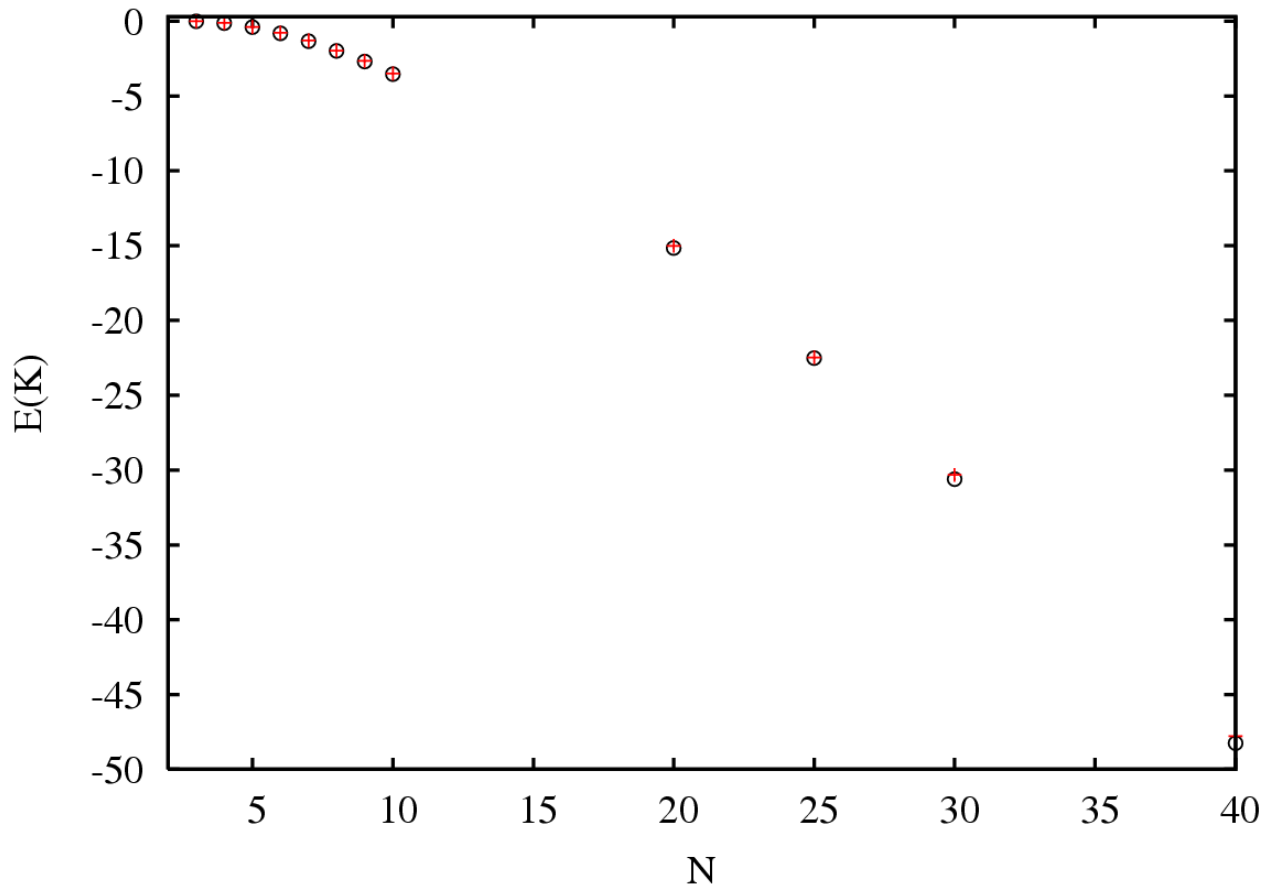
$$t = E_s / (4\pi r_0^2),$$

$$\frac{4\pi}{3} r_0^2 \rho_0 = 1$$

$$t = 0.08 \text{ K}\text{\AA}^{-2}$$

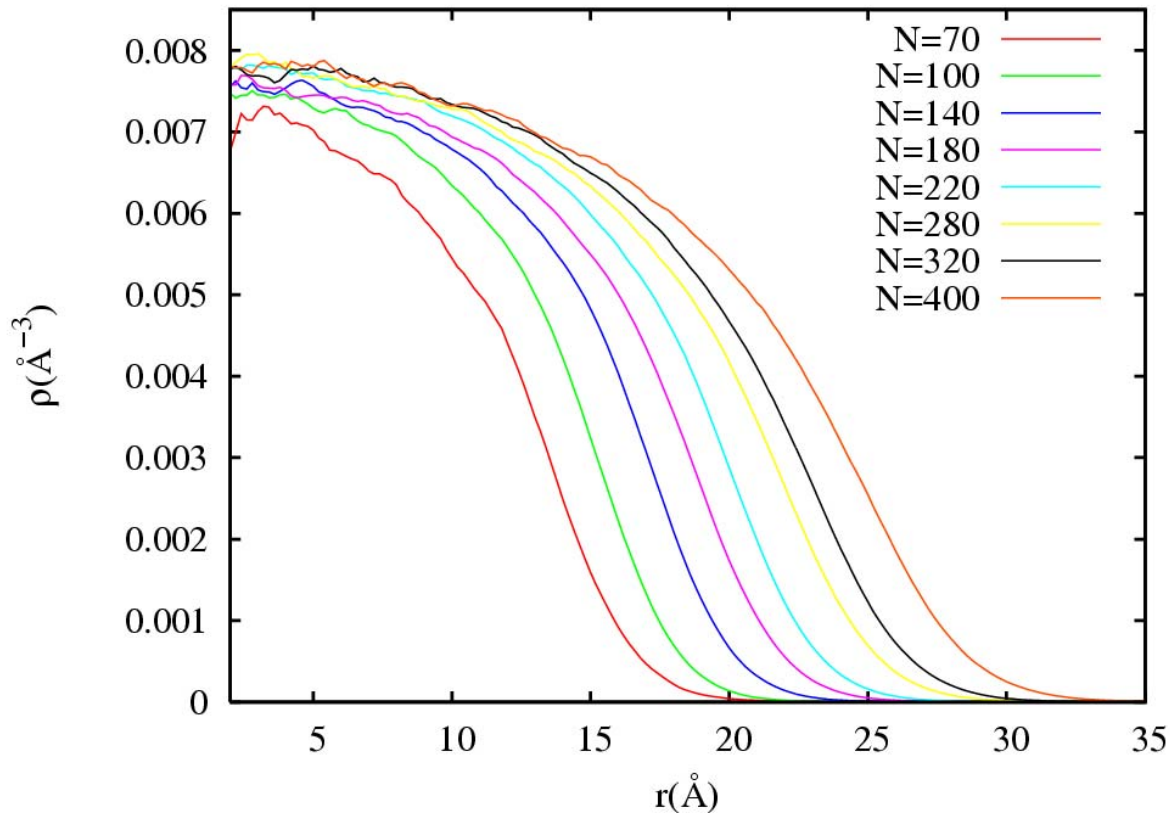


Pure $T\downarrow$ clusters



-red crosses
Blume et al.
PRL **89**, 163402

Pure T↓ clusters

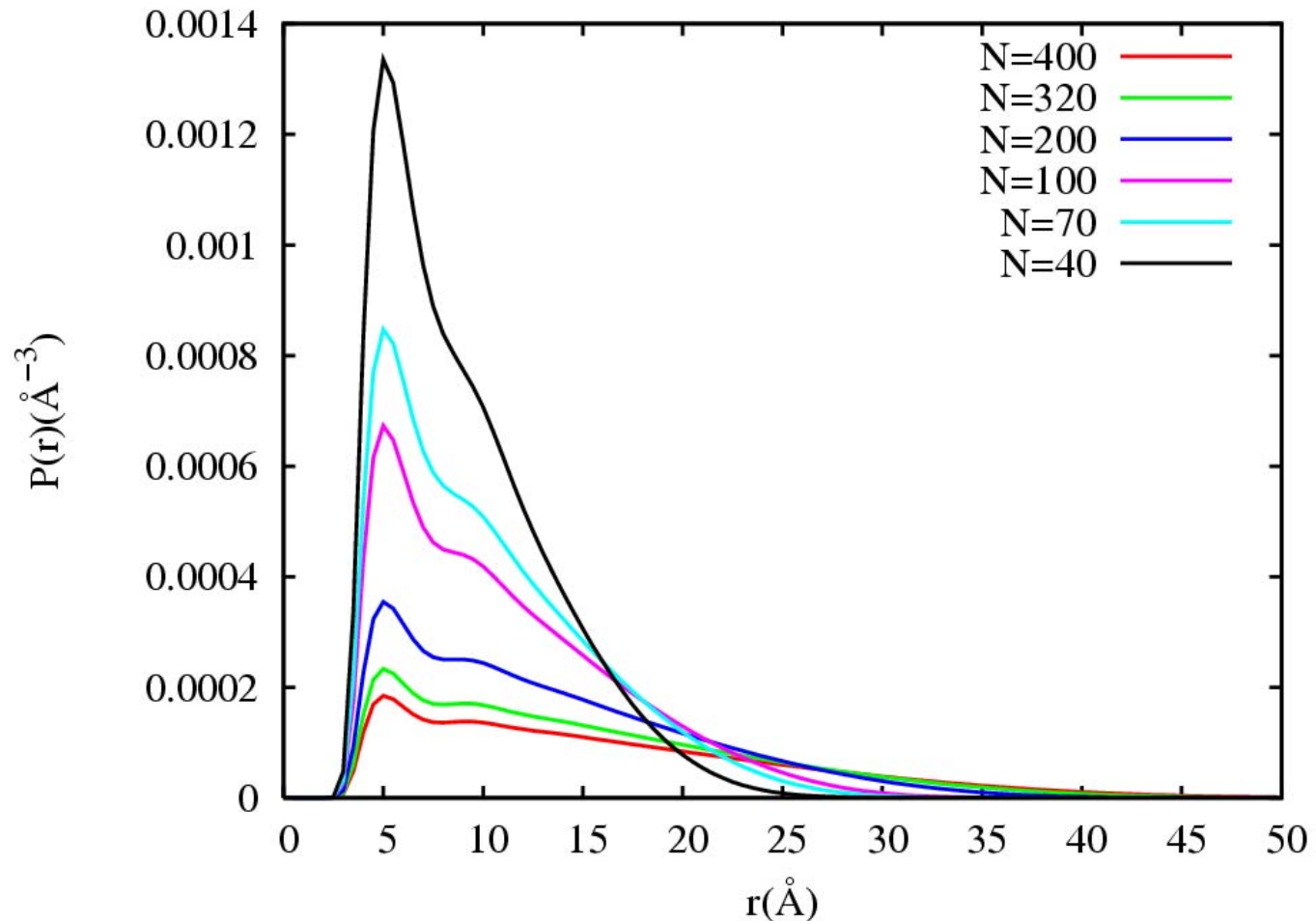


-surface tickness (difference between the radii where the density has decreased from central values by 10% and 90%)

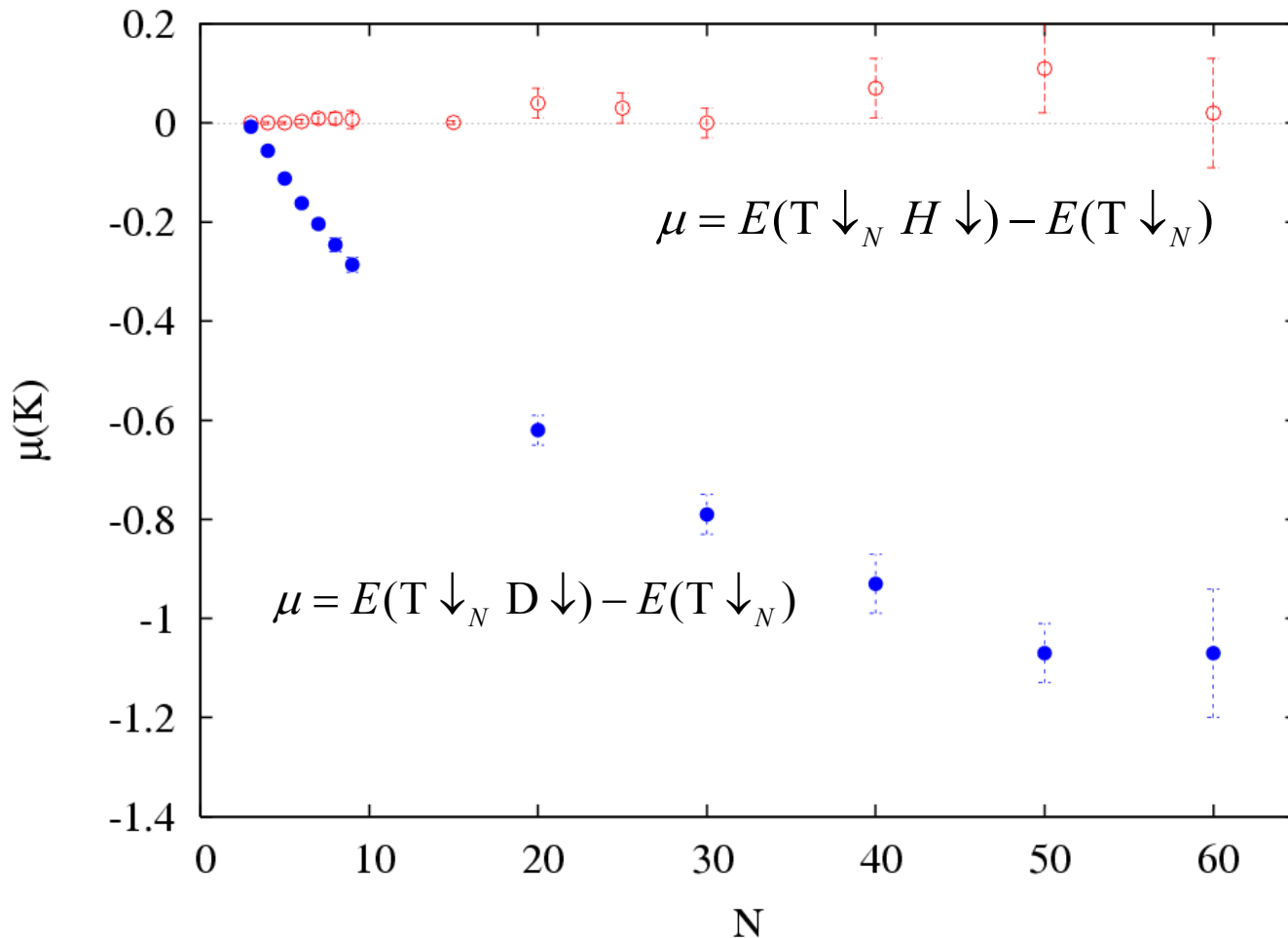
N=400 15.2 Å
N=320 14 Å
N=200 12 Å
N=100 9.2 Å
N=70 9.6 Å

-equilibrium density of the liquid $\rho = 0.007466(7) \text{ Å}^{-3}$

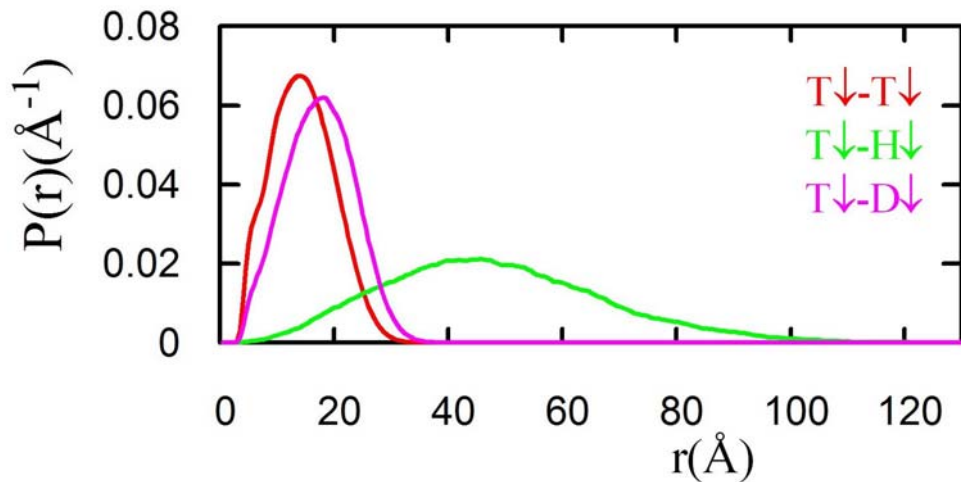
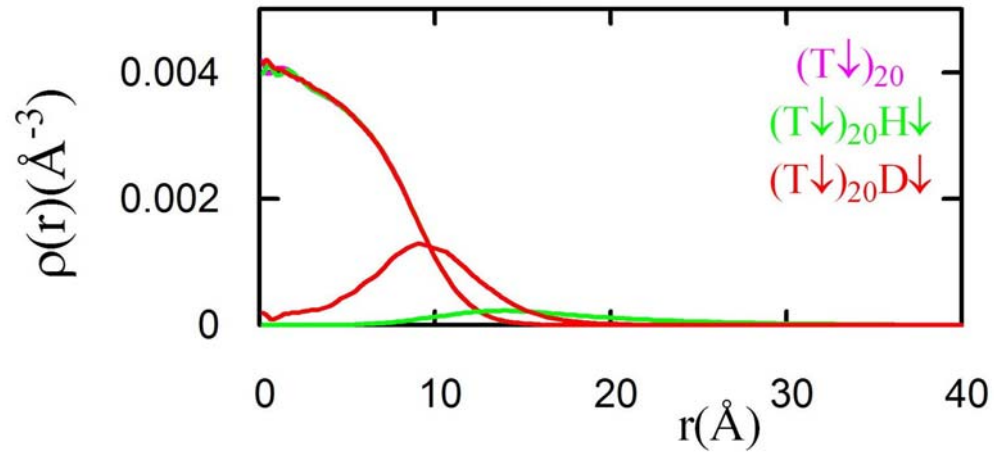
Pure $T\downarrow$ clusters



Mixed $T \downarrow$ clusters



Mixed $T\downarrow$ clusters



$(T\downarrow)_{60}D\downarrow$ and $(T\downarrow)_{60}H\downarrow$

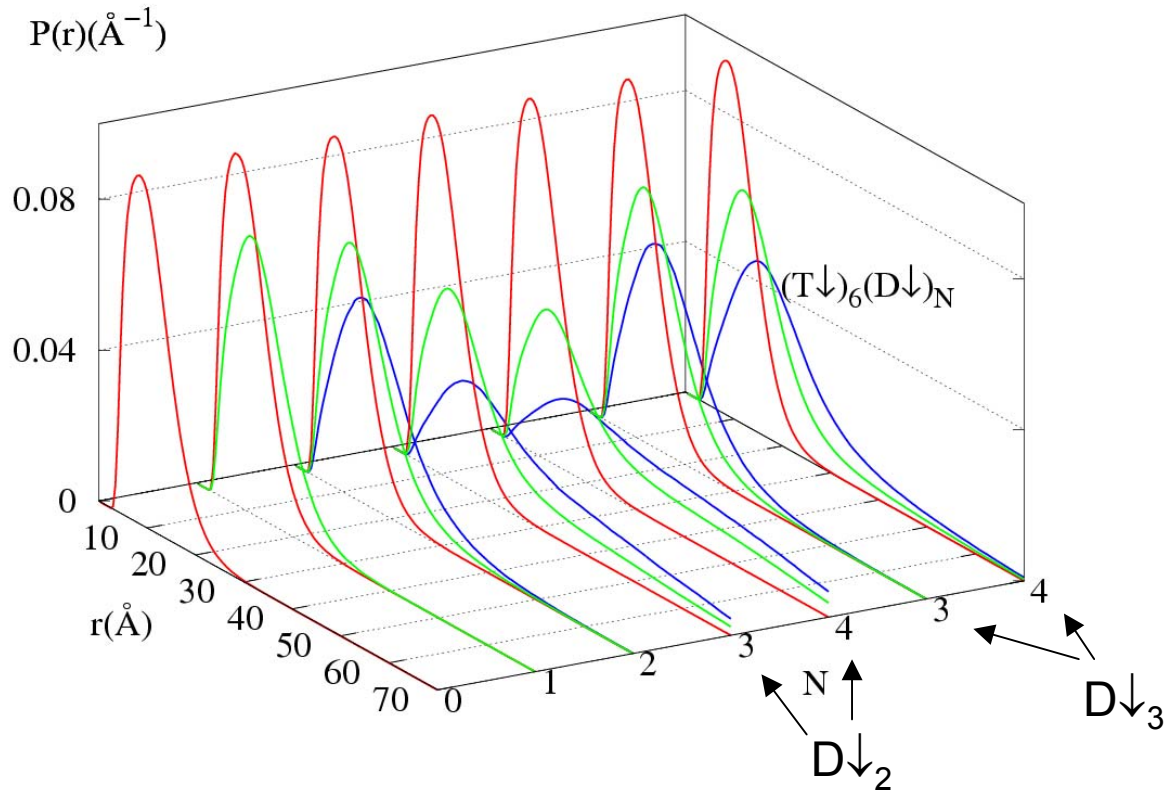
Small mixed T↓ clusters

T↓	D↓	D↓ ₂			D↓ ₃		
	1	2	3	4	3	4	5
3	-0.0122(9)	-0.031(3)	-0.027(3)	-0.021(2)	-0.056(2)	-0.058(5)	-0.046(6)
4	-0.182 (3)	-0.256(3)	-0.253(4)	-0.241(3)	-0.336(3)	-0.327(6)	-0.313(6)
5	-0.510 (4)	-0.629(4)	-0.633(6)	-0.610(6)	-0.769(4)	-0.755(7)	-0.732(6)
6	-0.972(4)	-1.139(3)	-1.145(9)	-1.135(5)	-1.322(5)	-1.326(10)	
7	-1.552(4)	-1.763(10)	-1.747(15)		-1.989(7)		
8	-2.237(6)	-2.492(12)	-2.554(15)		-2.755(8)		



Italic- clusters which appear to be unstable

Small mixed $T\downarrow$ clusters



Summary

- we have determined the ground state properties of bulk $\text{H}\downarrow$, bulk $\text{T}\downarrow$, pure and small mixed $\text{T}\downarrow$ clusters
- at low densities equation of state of gas $\text{H}\downarrow$ is well expressed in terms of the gas parameter ρa^3
- transition pressure in $\text{H}\downarrow$ is around 170 bar, in $\text{T}\downarrow$ around 9 bar
- mixed $\text{T}\downarrow$ - $\text{H}\downarrow$ clusters are unbound, binding of $\text{T}\downarrow$ - $\text{D}\downarrow$ depends on the number of atoms and nuclear spin states

Thank you for your attention!