^{4}He supersòlid o la compatiblitat entre l'ordre sòlid i la superfluïdesa

Jordi Boronat

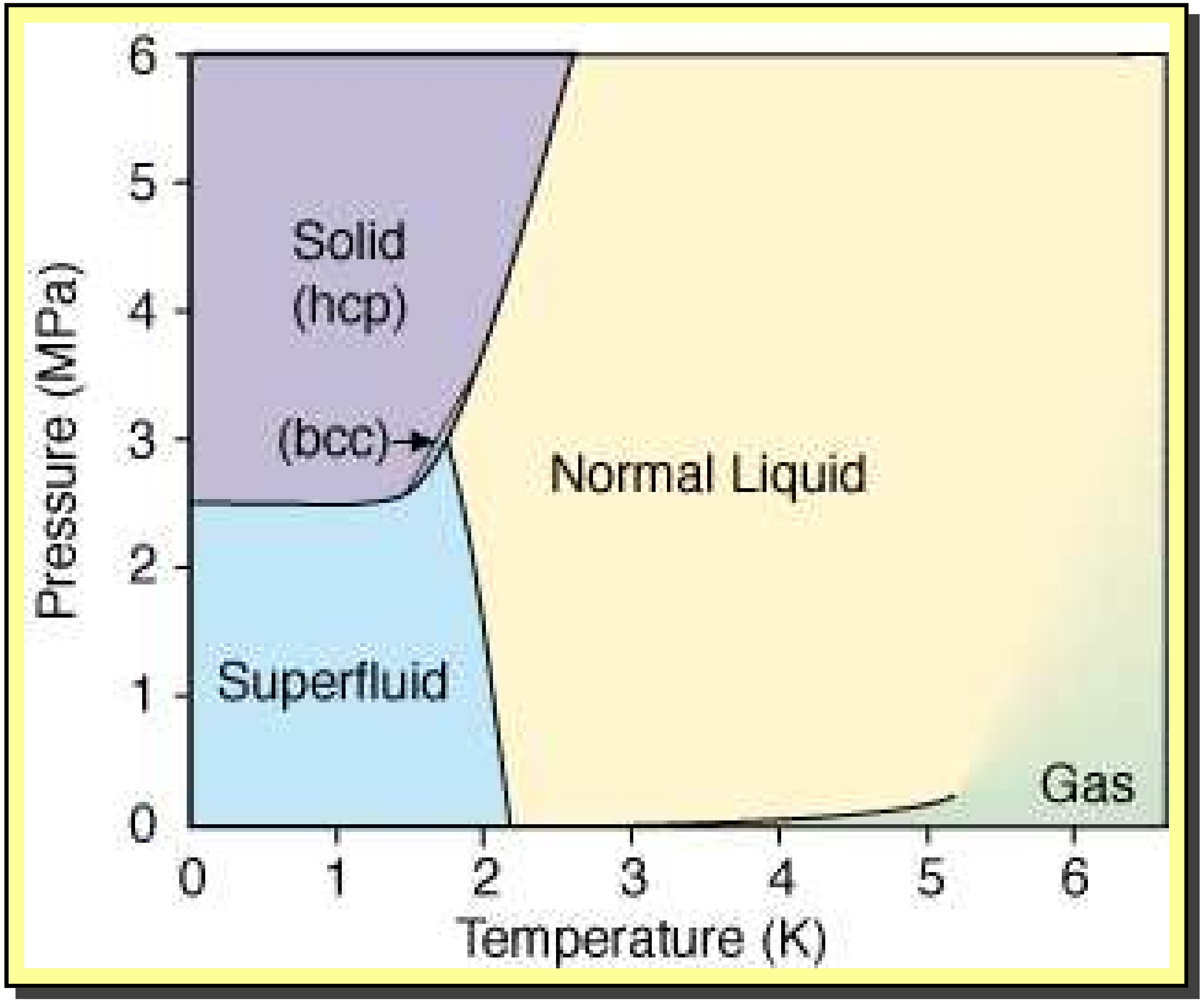
Departament de Física i Enginyeria Nuclear
Universitat Politècnica de Catalunya
E-08034 Barcelona, Spain
jordi.boronat@upc.edu

En col·laboració amb Claudi Cazorla, Gregory Astrakharchik i Joaquim Casulleras

Liquid helium: the quantum liquid

- Going down in temperature quantum effects are expected to be more and more relevant.
- This is specially true for the lighter elements like H or He since quantum mechanical zero-point energy is inversely proportional to the mass.
- Quantum gases (H), liquids (He), and solids (H_2) present macroscopic quantum behavior: the most evident its phase in the $T = 0$ limit.
- We will focus our attention to liquid helium, the paradigm of a quantum liquid. In particular, to boson ^{4}He (^{3}He is a fermion).

Equation of state (standard)



P/T equation of state.

Superfluid properties

- At svp, ^{4}He presents a superfluid transition when $T = T_\lambda = 2.17$ K.
- In the superfluid state the viscosity becomes zero and peculiar manifestations appear (Keesom, Allen, Misener, Kapitza, Andronikashvili,... (1930-1940)).

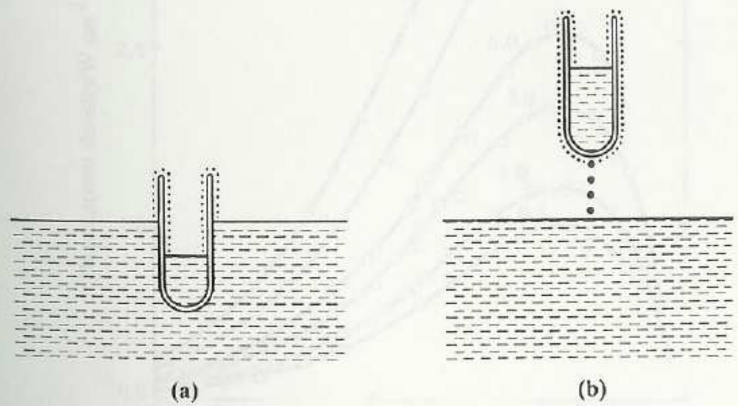


Fig. 4.2. (a) If an empty beaker is lowered into a bath of helium II, the liquid flows over the surface of the beaker until the levels are equalized. (b) If the beaker is then lifted above the bath, the helium flows out over the rim, drops off the bottom of the beaker, and returns to the bath (after Daunt and Mendelssohn [37]).

Andronikashvili’s experiment

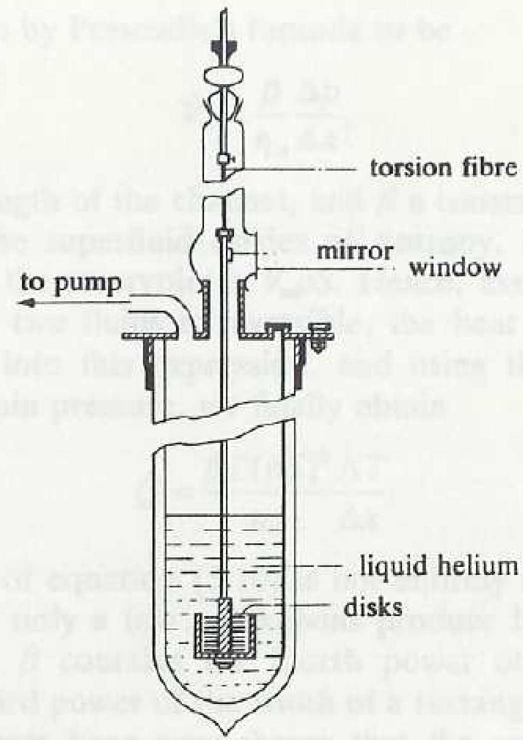


Fig. 5.3. Schematic diagram to illustrate Andronikashvili’s experiment. Note that the discs are not drawn to scale; see text (Andronikashvili [46]).

Andronikashvili's experiment

§5.4

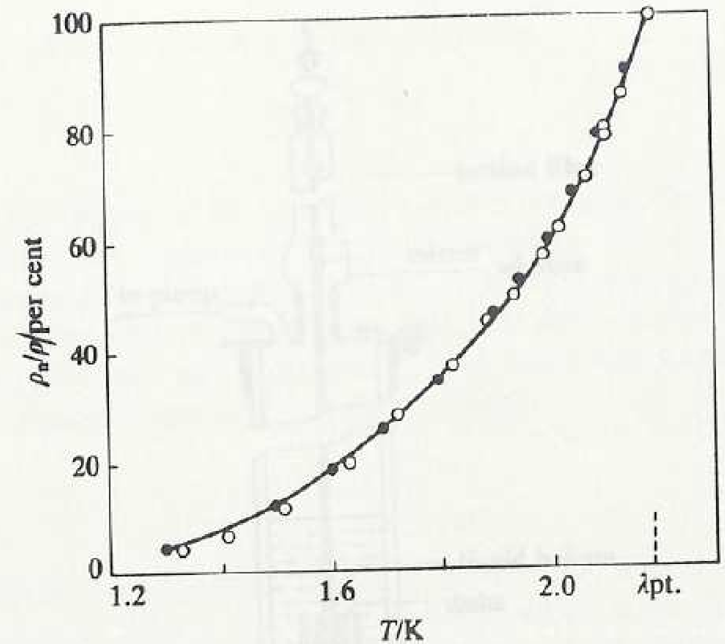


Fig. 5.2. The density of the normal fluid ρ_n as a function of temperature: ○ derived from oscllating disc experiments, ● from the velocity of second sound (Andronikashvili [46]).

Superfluidity and Bose-Einstein condensation

- What's behind this strikingly peculiar behavior ?

Superfluidity and Bose-Einstein condensation

- What's behind this strikingly peculiar behavior ?
- London (1938) was the first to suggest that the transition is similar to the one of a non-interacting Bose gas. He predicted a temperature 3.1 K, not far from the experimental value.

Superfluidity and Bose-Einstein condensation

- What's behind this strikingly peculiar behavior ?
- London (1938) was the first to suggest that the transition is similar to the one of a non-interacting Bose gas. He predicted a temperature 3.1 K, not far from the experimental value.

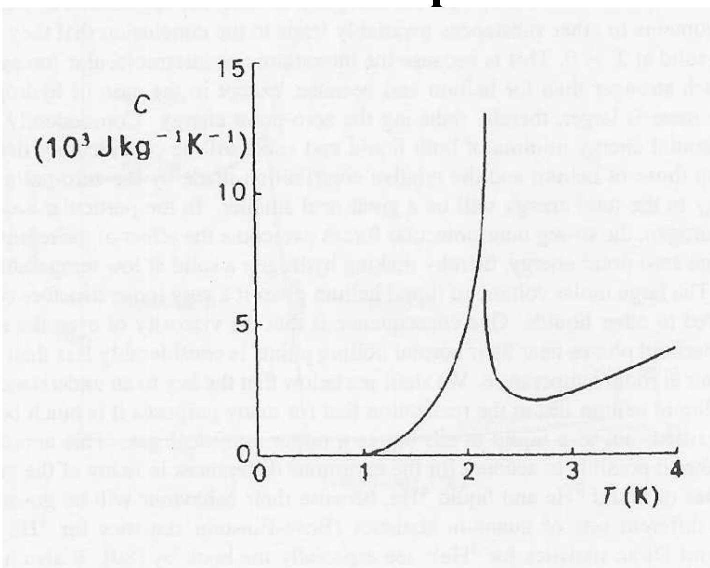
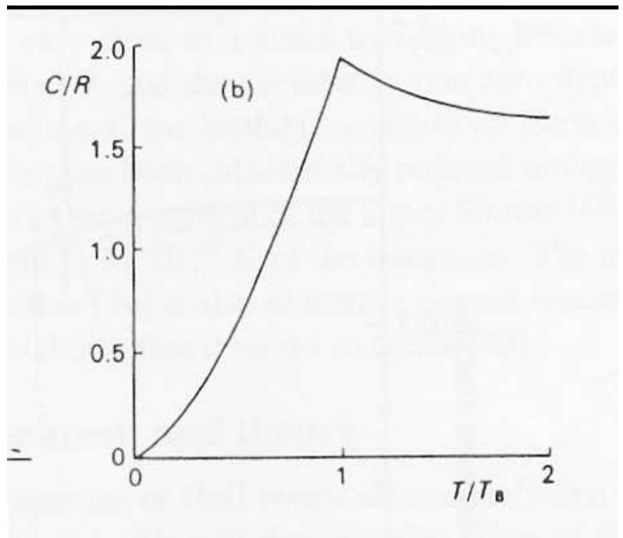


Figure 2. The specific heat of liquid ^{4}He at low temperatures



Liquid ^{4}He | Bose gas

Superfluidity and Bose-Einstein condensation

♦ Nowadays we know from experiment (neutron scattering) and theory that there is a fraction of particles occupying the zero-momentum state ($n_0 = 8 - 10\ \%$).

♦ But a rigorous connection between superfluidity and Bose-Einstein condensation is still lacking after 80 years !

Is a supersolid possible?: an old topic

- Supersolid: a quantum solid with superfluid signal; experimentally, a solid with non-classical rotational inertia (NCRI).

Is a supersolid possible?: an old topic

- Supersolid: a quantum solid with superfluid signal; experimentally, a solid with non-classical rotational inertia (NCRI).
- The natural candidate: solid ^{4}He, with displacements of atoms around lattice sites very large ($\gamma = 0.26$, classic solids at melting $\gamma = 0.14$).

Is a supersolid possible?: an old topic

- Supersolid: a quantum solid with superfluid signal; experimentally, a solid with non-classical rotational inertia (NCRI).
- The natural candidate: solid ^{4}He, with displacements of atoms around lattice sites very large ($\gamma = 0.26$, classic solids at melting $\gamma = 0.14$).
- The possibility of a supersolid phase is an old proposal: Wolfke (1939), Andreev & Lifshitz (1969), Chester (1970). They suggested that a BEC of vacancies or interstitials could be possible in ^{4}He.

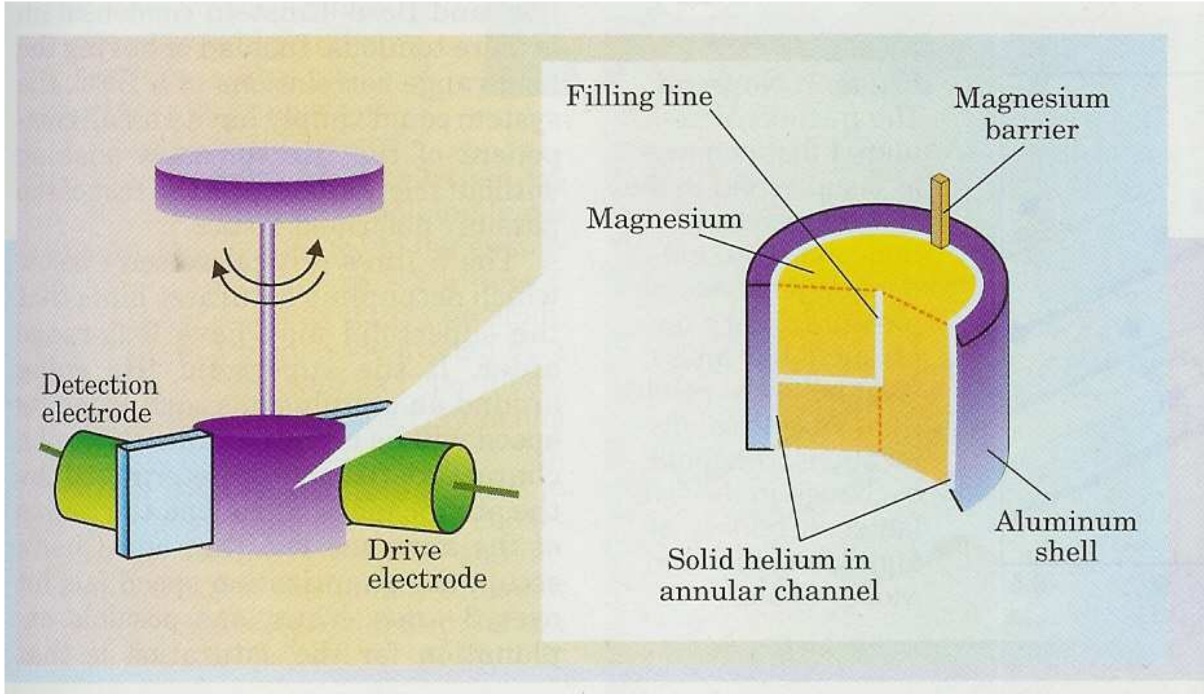
Is a supersolid possible?: an old topic

- Supersolid: a quantum solid with superfluid signal; experimentally, a solid with non-classical rotational inertia (NCRI).
- The natural candidate: solid ^{4}He, with displacements of atoms around lattice sites very large ($\gamma = 0.26$, classic solids at melting $\gamma = 0.14$).
- The possibility of a supersolid phase is an old proposal: Wolfke (1939), Andreev & Lifshitz (1969), Chester (1970). They suggested that a BEC of vacancies or interstitials could be possible in ^{4}He.
- But experimental data show absolutely negligible concentration of vacancies in the limit $T \to 0$.

News from experiments

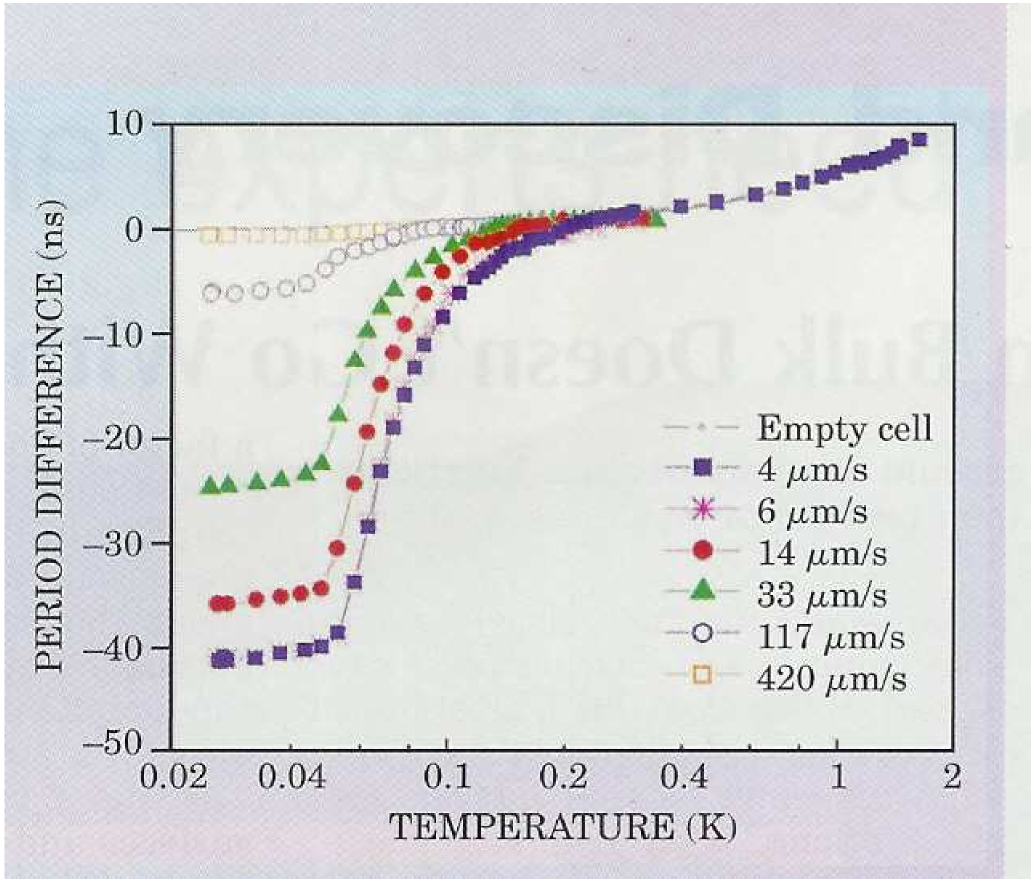
- The search for superfluid behavior in solid ^{4}He always showed negative results (see, for example, the review of Meisel (1992))
- The breakthrough in the field is produced by Kim and Chan in 2004. They reported NCRI in solid ^{4}He confined in Vycor and also in the bulk. The transition temperature is $T_c \simeq 230$ mK. The superfluid densities are very small ! $\rho_s/\rho = 0.7 - 1.5\%$ with a slight dependence on the pressure.
- Chan argues that the success of the new experiments is mainly due to the extremely high purity of the sample. They checked that ^{3}He impurities always reduce the signal.

News from experiments



Torsional oscillator used by Kim and Chan

News from experiments



Determination of the transition temperature from the torsional oscillator measures

News from experiments

tively), must be less than 1.5×10^{-11} Pa·s.

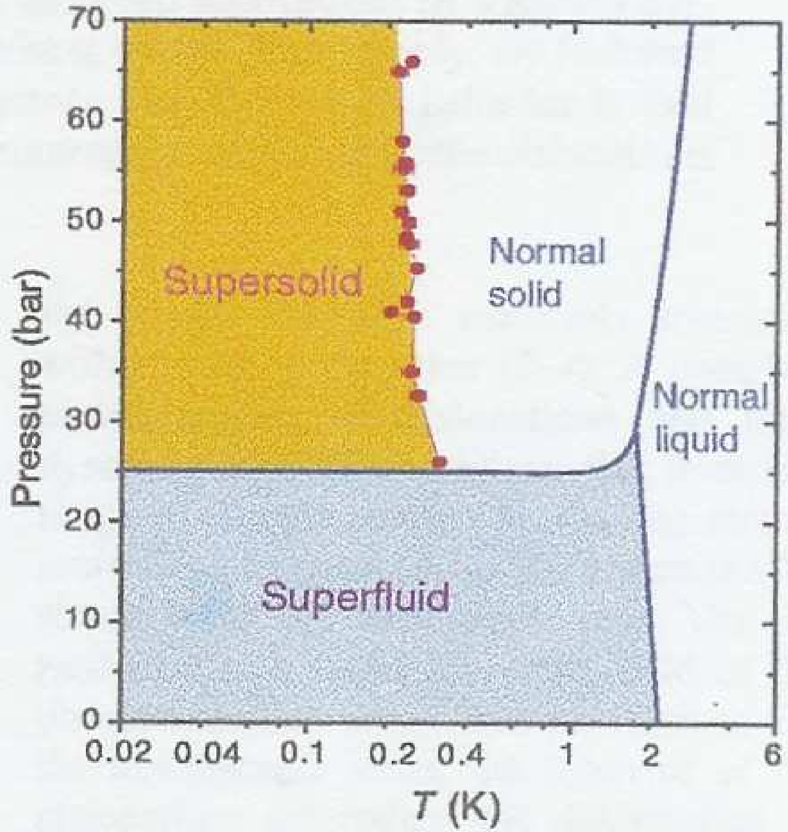


Fig. 4. Phase diagram of liquid and solid helium

From E. Kim and M. H. W. Chan, Science **305**, *1941 (2004).*

Intense experimental research

- No sign of the superfluid transition in the specific heat (Clark and Chan (2005))
- Rittner and Reppy (2006) reproduce Chan's results but they loose the superfluid signal after annealing.
- Kim and Chan (2006) repeat the experiments going at higher pressures. They observe that superfluidity disappears for $P > 170$ bar. And the signal remains after annealing !
- Supersolid is also observed by Shirahama group (Keio University) and Kubota group (University of Tokyo). But with ρ_s smaller.
- Recently, Clark, Lin, and Chan (2006) have reported negative results for superfluidity in solid H_2.

Intense experimental research

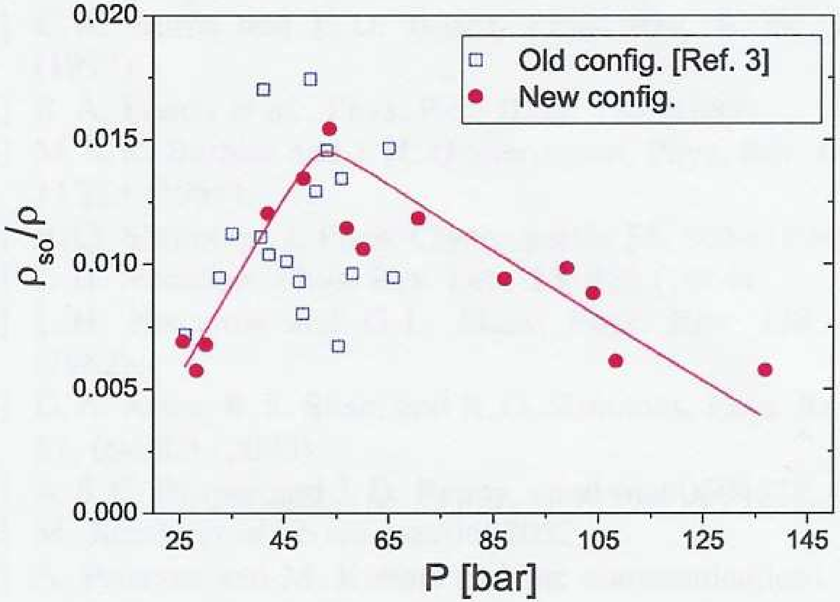


FIG. 4 (color online). Supersolid fraction in the low temperature limit, ρ_{so}/ρ, as a function of pressure. Solid samples prepared with heat switch (new configuration) yield data with less scatter. The solid line is a guide to the eyes.

From E. Kim and M. H. W. Chan, Physical Review Letters **97***, 115302 (2006).*

Recent theoretical work: supersolid, yes or not?

After Chan's results, several theoretical works have appeared. Most of them based on Quantum Monte Carlo methods: VMC and DMC at zero temperature; PIMC at finite temperature

- Ceperley and Bernu (2004); Clark and Ceperley (2005) carried out PIMC simulations of solid ^{4}He with negative results for both ρ_s and n_0.
- Prokof'ev and Svistunov (2005) argue the necessary presence of zero-point vacancies or interstitial atoms $\Longrightarrow$ Incommensurate solid.
- Galli, Rossi, and Reatto (2005) Using VMC-SDW obtain finite condensate fraction for the commensurate solid $n_0 = 5 \times 10^{-6}$; Galli and Reatto (2006) the same theory but with vacancies $n_0 = 2 \times 10^{-3}$.

Finite versus zero temperature

PIMC is an exact method but its application to this problem presents several drawbacks:

$\Longrightarrow$ Transition temperature extremely low
$\Longrightarrow$ Signal at the level of the typical noise (low efficiency of permutation sampling)

Finite versus zero temperature

PIMC is an exact method but its application to this problem presents several drawbacks:

$\Longrightarrow$ Transition temperature extremely low
$\Longrightarrow$ Signal at the level of the typical noise (low efficiency of permutation sampling)

Why not a simulation at $T = 0$ with DMC?

Finite versus zero temperature

PIMC is an exact method but its application to this problem presents several drawbacks:

$\Longrightarrow$ Transition temperature extremely low
$\Longrightarrow$ Signal at the level of the typical noise (low efficiency of permutation sampling)

Why not a simulation at $T = 0$ with DMC?

(+): No sampling problems with DMC
(−): A trial wave function for the supersolid is required … not trivial

In our first approach we used a very simple model where localization was introduced in the Hamiltonian (PRB **73**, 224515 (2006))

Trial wave functions for a quantum solid

- Standard approach: Nosanow-Jastrow

$$\Psi_{\mathrm{NJ}}(\mathbf{R}) = \prod_{i<j}^{N} f(r_{ij}) \prod_{i,I}^{N} g(r_{iI})$$

with $g(r_{iI}) = \exp(-\alpha r_{iI}^2)$. Good model for the energy, structure,…but it is not symmetric under particle exchange.

Trial wave functions for a quantum solid

- Standard approach: Nosanow-Jastrow

$$\Psi_{\rm NJ}(\mathbf{R}) = \prod_{i<j}^{N} f(r_{ij}) \prod_{i,I}^{N} g(r_{iI})$$

with $g(r_{iI}) = \exp(-\alpha r_{iI}^2)$. Good model for the energy, structure,...but it is not symmetric under particle exchange.

- Formally, one can symmetrize summing over all the permutations (*permanent*)

$$\Psi_{\rm NJS}(\mathbf{R}) = \prod_{i<j}^{N} f(r_{ij}) \frac{1}{N!} \sum_{P} \prod_{i}^{N} g(r_{iPI})$$

but with very small efficiency due to the extremely low permutations acceptance rate.

Trial wave functions for a quantum solid (II)

- Bloch-like wave functions. Tested at the variational level with poor results (Ceperley, Chester, and Kalos (1978)).

Trial wave functions for a quantum solid (II)

- Bloch-like wave functions. Tested at the variational level with poor results (Ceperley, Chester, and Kalos (1978)).

- Shadow wave functions: symmetric model but of difficult use in DMC. *Alternative: PIGS*

Trial wave functions for a quantum solid (II)

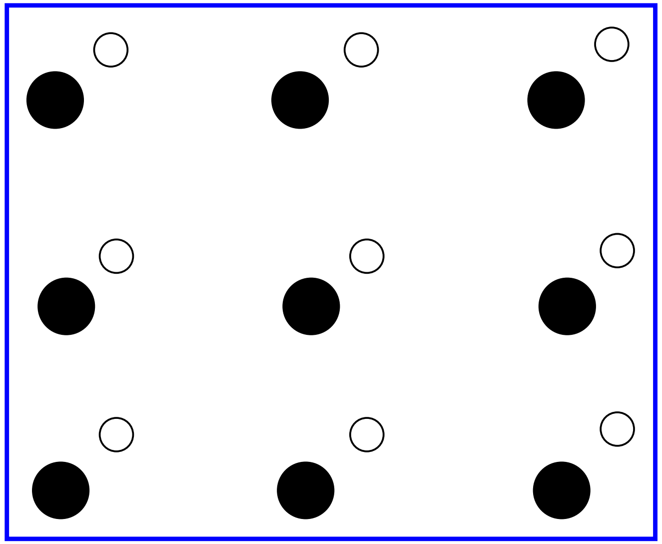
- Bloch-like wave functions. Tested at the variational level with poor results (Ceperley, Chester, and Kalos (1978)).
- Shadow wave functions: symmetric model but of difficult use in DMC. *Alternative: PIGS*
- Symmetrization of NJ in a different way:

  (a) Kalos (1978), $\Psi_{\mathrm{S1}} = \Psi_{\mathrm{J}} \prod_i (\sum_I g(r_{iI}))$

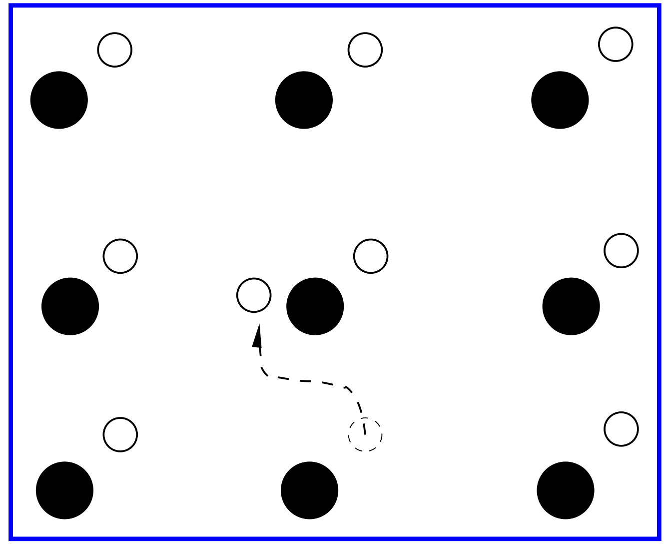
  (b) Our proposal, $\Psi_{\mathrm{S2}} = \Psi_{\mathrm{J}} \prod_I (\sum_i g(r_{iI}))$

  They look very similar, but only S2 can describe in a proper way the degree of localization required in a solid.

S1 versus S2



(I)



(II)

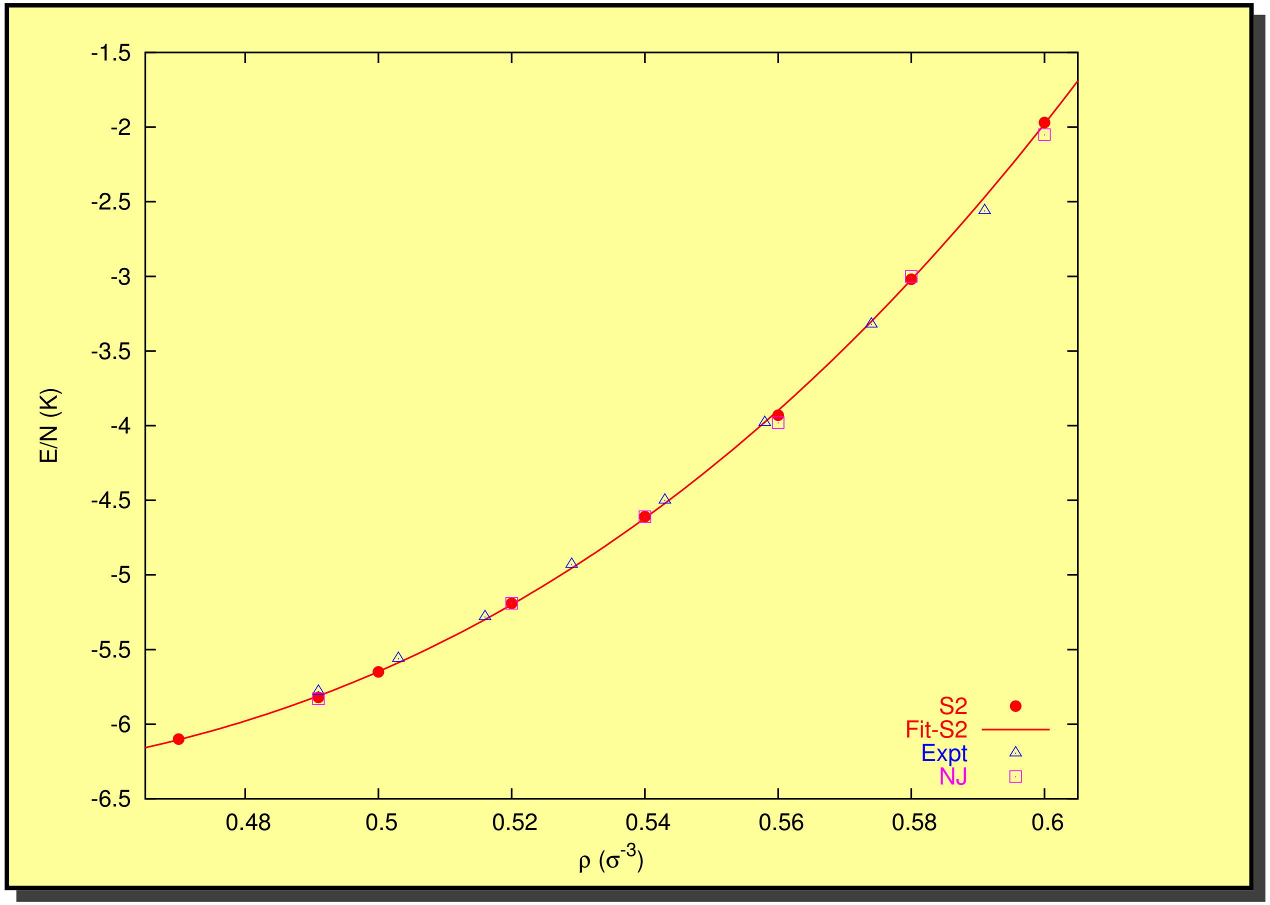
$$\Psi_{S1}(I) \simeq \Psi_{S1}(II)$$
$$\Psi_{S2}(I) \gg \Psi_{S2}(II)$$

S2 penalizes double occupancy; S1 not

$\downarrow$

only S2 can describe a supersolid !

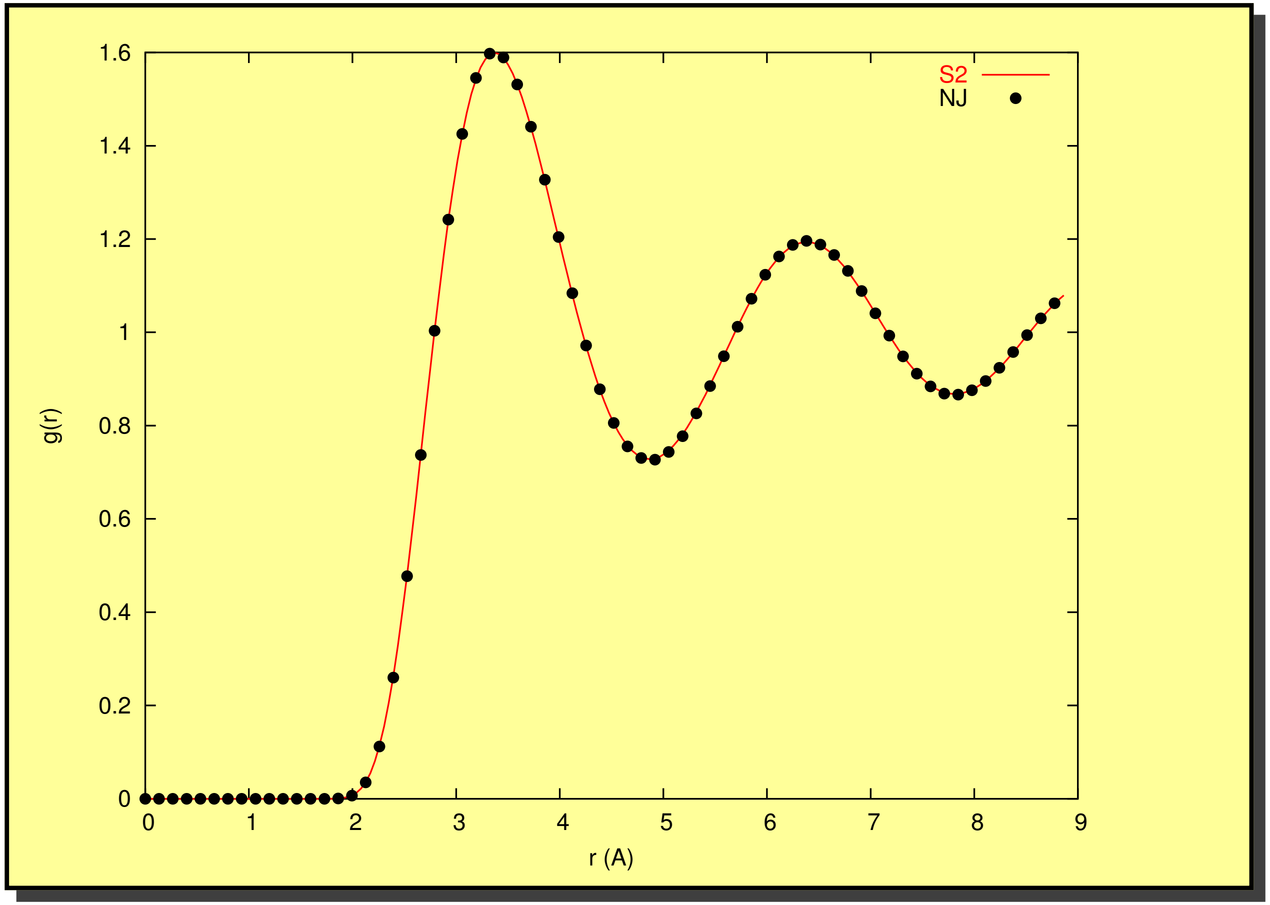
DMC results with the new function S2



Results for the energy of solid ^{4}He using the NJ and S2 models. Also compared with experimental data.

S2 REPRODUCES THE EXPERIMENTAL EOS !

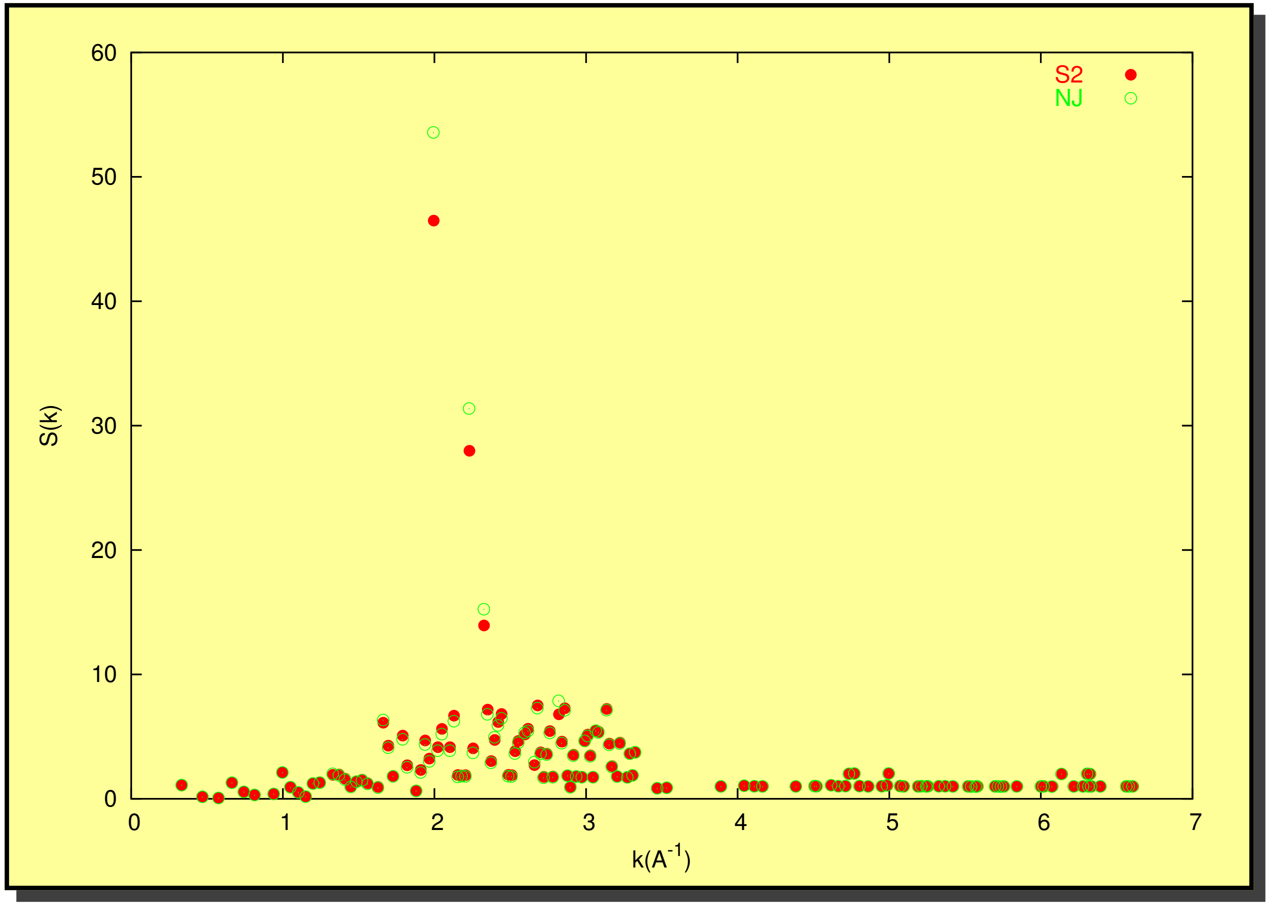
DMC results with the new function S2



Comparison between NJ and S2 results for g(r). The density is $\rho = 0.491\ \sigma^{-3}$ ($\sigma = 2.556$ Å) which corresponds to a pressure of ~ 34 bar, close to melting.

NO SIGNIFICANT DIFFERENCES

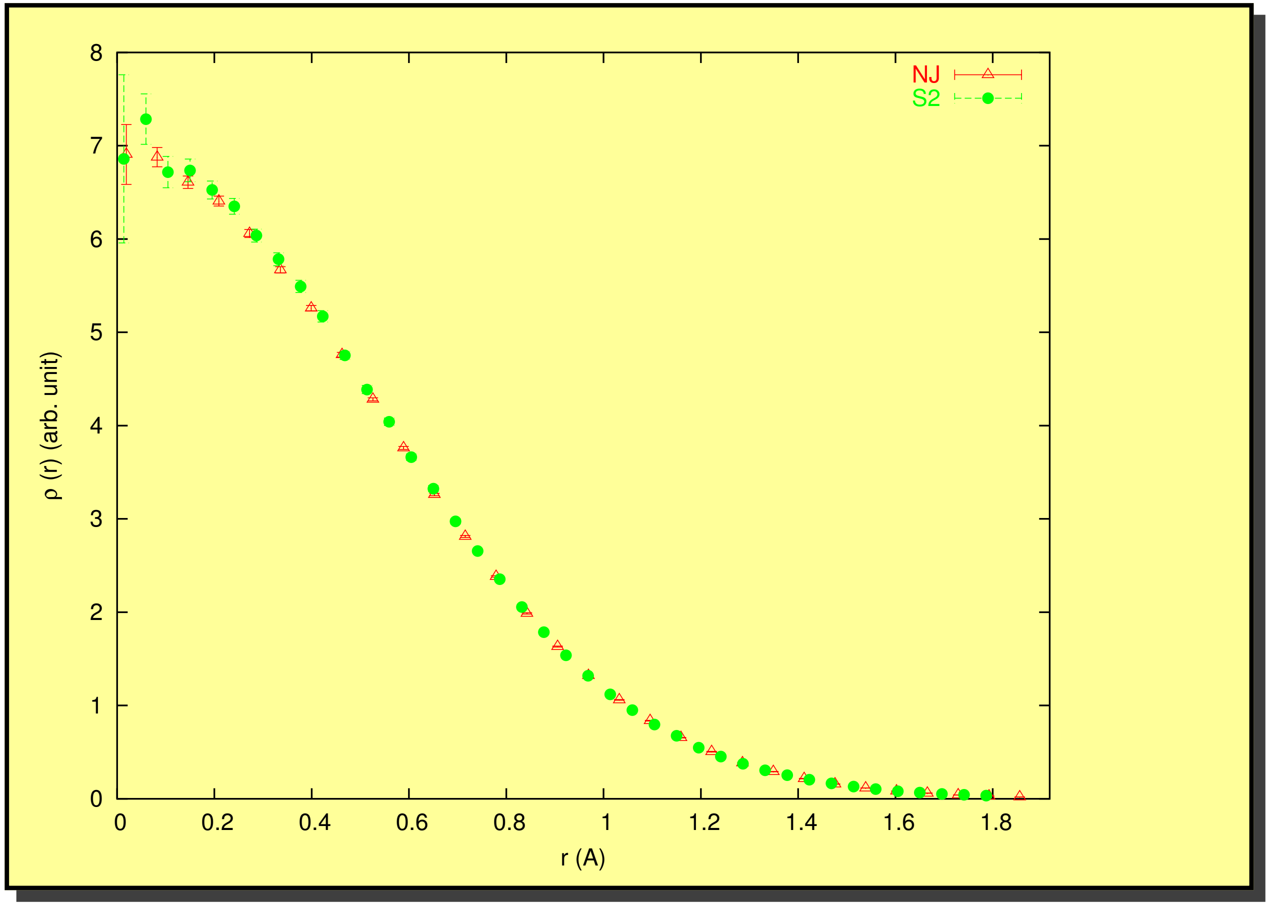
DMC results with the new function S2



Comparison between NJ and S2 results for S(k). Same thermodynamic point.

S2 LOOSES SOME STRENGTH ON THE MAIN PEAK

DMC results with the new function S2

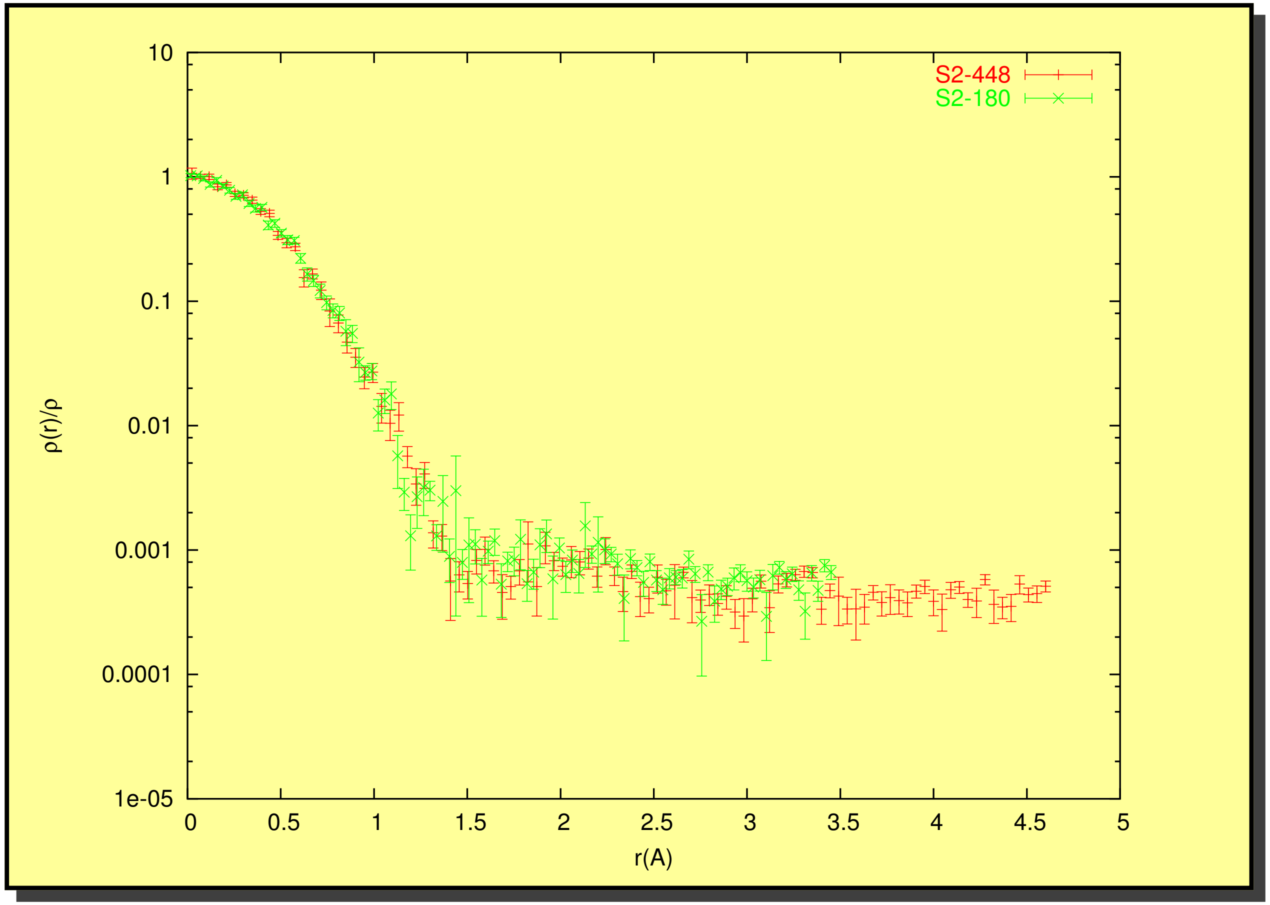


Comparison between NJ and S2 results for the density profile around a lattice point. Same thermodynamic point.

NO DIFFERENCES; SAME LINDEMANN'S RATIO

$(\gamma \simeq 0.26)$

DMC results with the new function S2



OBDM with the S2 trial wave function. Extrapolated estimator.

The condensate fraction (extrapolated estimator) is $n_0 = 0.00045(2)$ (0.045 %).

VERY SMALL BUT NOT ZERO !

DMC results with the new function S2

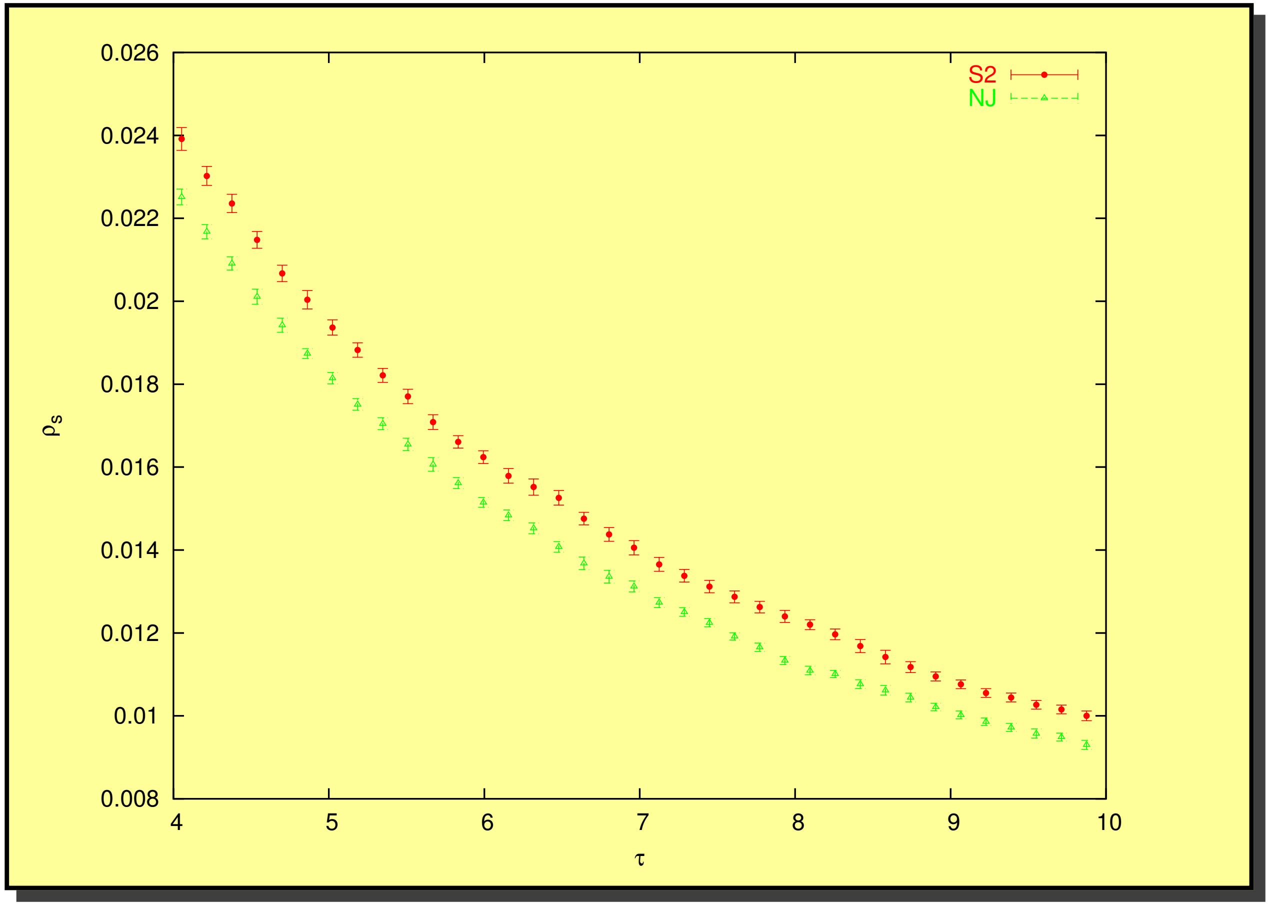
- The superfluid fraction can be calculated using an extension at $T = 0$ of the winding number estimator used in PIMC.

$$\frac{\rho_s}{\rho} = \lim_{\tau \to \infty} \frac{1}{6N\tau} \left(\frac{D_s(\tau)}{D_0} \right)$$

with $D_s(\tau) = \langle (\mathbf{R}_{\mathrm{CM}}(\tau) - \mathbf{R}_{\mathrm{CM}}(0))^2 \rangle$ and $D_0 = \hbar^2/2m$.

- Difficult estimation due to the expected very small value of the superfluid fraction, *if any*. The calculation is still running ...

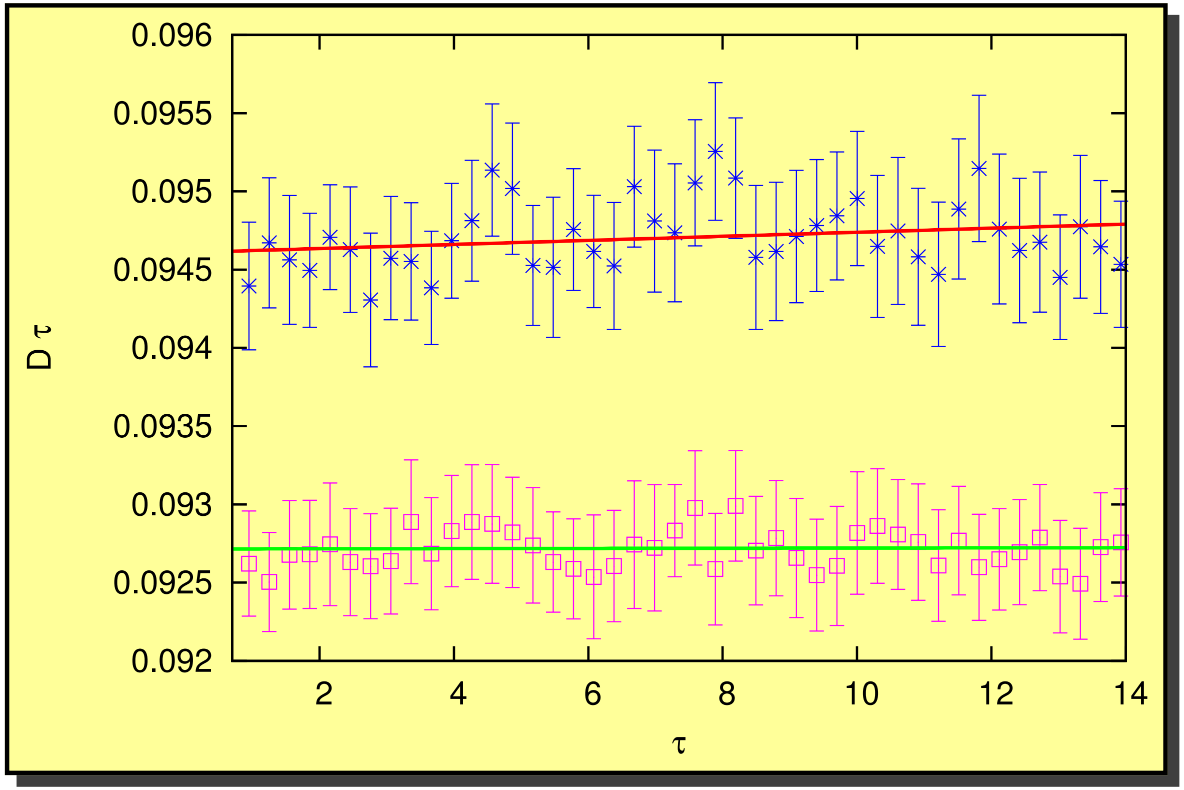
DMC results with the new function S2



Estimation of the superfluid fraction using NJ and S2.

VERY LARGE SIMULATION TIMES ARE REQUIRED, AT LEAST IN THIS REPRESENTATION

DMC results with the new function S2



Estimation of the superfluid fraction using NJ and S2. A different plot: multiplying the function by τ.

SIGNAL VERY SMALL BUT NOT ZERO

$\rho_s/\rho \simeq 1 - 2 \times 10^{-5}$ (0.001-0.002 %).

Remarks

- The new trial wave function S2 has the correct symmetry and reproduces accurately the equation of state of solid ^{4}He.
- We can now address questions related to the bosonic nature of ^{4}He using DMC: one-body density matrix, superfluid fraction, vacancies, …
- The condensate fraction is small (0.045 %) but not zero, contrarily to PIMC results.
- The superfluid fraction is extremely small. According to our present results $\rho_s/\rho \simeq 10^{-5}$.

Remarks

- The experimental results of Kim and Chan about ρ_s are much larger than our present estimation. Other effects have to be considered: glassy phase ?, dislocations and/or vacancies ?
- Also a relevant concern from the theoretical side: is it possible in an homogeneous boson system to have a finite value for the condensate fraction and simultaneously zero superfluid density ?
- Work in progress is at present carried out to explore supersolid behavior in 2D solids and in a 3D ^{4}He glassy phase.

Remarks

"All in all, at the time of writing I think the only statement which we can make with any confidence about solid ^{4}He is that we do not understand it nearly as well as we thought we did three years ago".

Anthony Leggett (2006)

Remarks

“All in all, at the time of writing I think the only statement which we can make with any confidence about solid ^{4}He is that we do not understand it nearly as well as we thought we did three years ago".

Anthony Leggett (2006)

GRÀCIES PER LA VOSTRA ATENCIÓ !