Applications of Path Integral Monte Carlo methods for Bosons

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Applications of Path Integral Monte Carlo methods for Bosons

- Helium droplets
- Solid helium and supersolids

Liquid helium
the prototypic quantum fluid

- A helium atom is an elementary particle. A weakly interacting hard sphere. First electronic excitation is 230,000 K.
- Interatomic potential is known more accurately than any other atom because electronic excitations are so high.

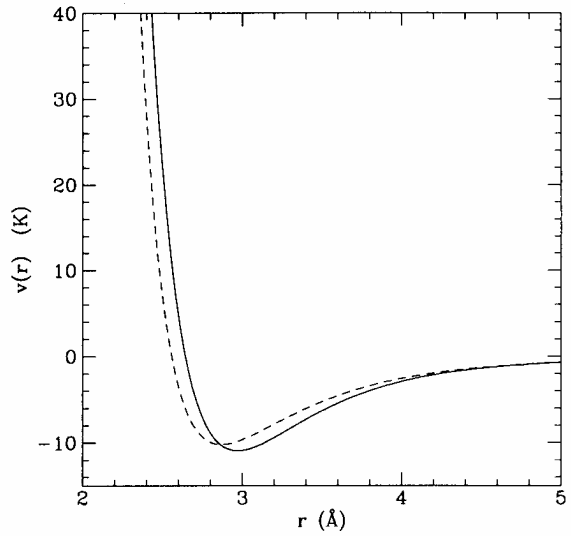


FIG. 1. The semiempirical pair potential between two helium atoms: solid line, Aziz *et al.* (1992); dashed line, Lennard-Jones 6-12 potential with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å.

- Two isotopes:
  - ^{3}He (fermion: antisymmetric trial function, spin 1/2)
  - ^{4}He (boson: symmetric trial function, spin zero)

Helium phase diagram

- Because interaction is so weak helium does not crystallize at low temperatures. Quantum exchange effects are important
- Both isotopes are quantum fluids and become superfluids below a critical temperature.
- One of the goals of computer simulation is to understand these states, and see how they differ from classical liquids starting from non-relativistic Hamiltonian:

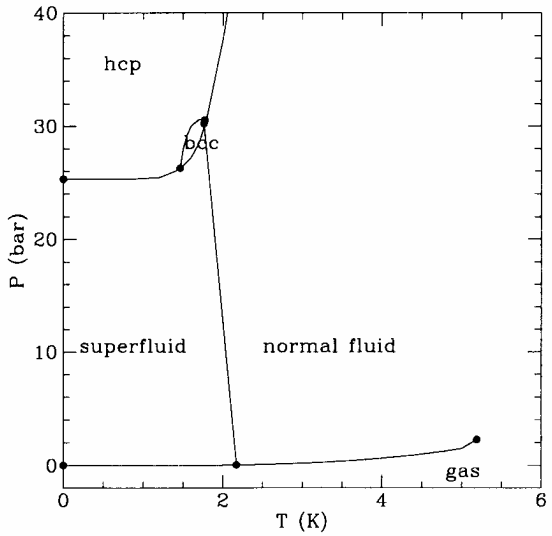


FIG. 2. The phase diagram of ^{4}He.

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 + V(R)$$

$$\lambda \equiv \frac{\hbar^2}{2m_i}$$

Droplets and PIMC

E. Draeger (LLNL) D. Ceperley(UIUC)

- Provide precise microscopic probes for phenomenon such as superfluidity and vortices.
- Provide a nearly ideal “spectroscopic matrix” for studying molecular species which may be unstable or weakly interacting in the gas phase.
- PIMC can be used to simulate ^{4}He droplets of up to 1000 atoms, at finite temperatures containing impurities, calculating the density distributions, shape deformations and superfluid density.
- Droplets are well-suited to take advantage of the strengths of PIMC:
  - Finite temperature (T=0.38 K)
  - Bose statistics (no sign problem)
  - Finite size effects are interesting.

Superfluidity in pure Droplets

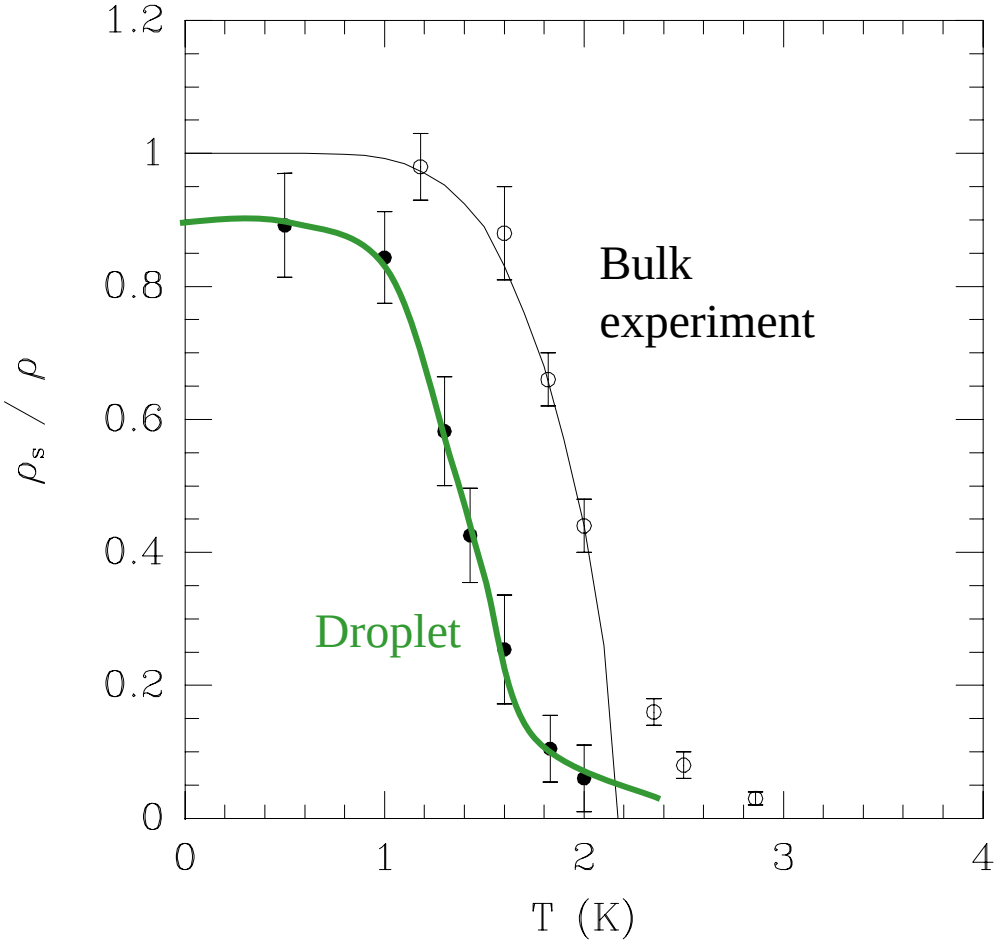
- 64 atom droplet goes into the superfluid state in temperature range 1K <T <2K.

  NOT A PHASE TRANSITION!

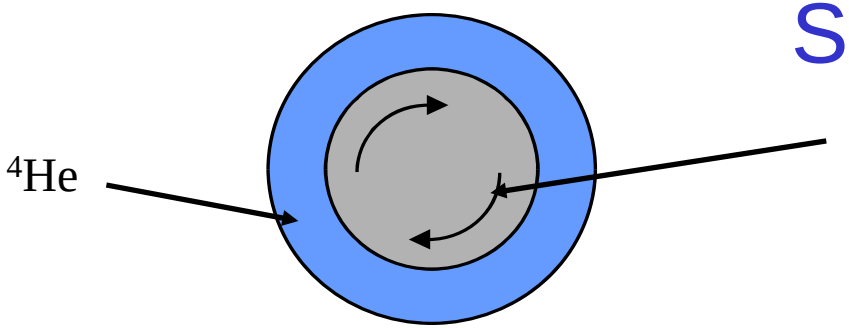
- But almost completely superfluid at 0.4K (according to response criteria.)

Sindzingre et al 1990

$$\frac{\rho_s}{\rho} = \frac{2m \left\langle A_z^2 \right\rangle}{\beta \lambda I_c}$$



Superfluidity and PIMC



rotating disks:

Andronikashvili's expt (1946)

$$(\rho_s + \rho_N \equiv \rho)$$

- We define superfluidity as a linear response to a velocity perturbation (the energy needed to rotate the system) "NCRI = nonclassical rotational inertia"

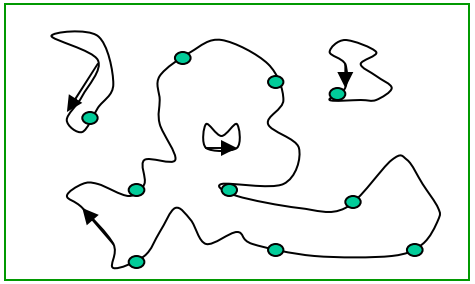
$$\frac{\rho_s}{\rho} = 1 - \frac{I}{I_c} = \left. \frac{dF}{d\omega^2} \right|_{\omega=0}$$

- To evaluate with Path Integrals, we use the Hamiltonian in rotating frame:

$$\hat{H}_\omega = \hat{H}_0 - \omega \hat{L}_z$$

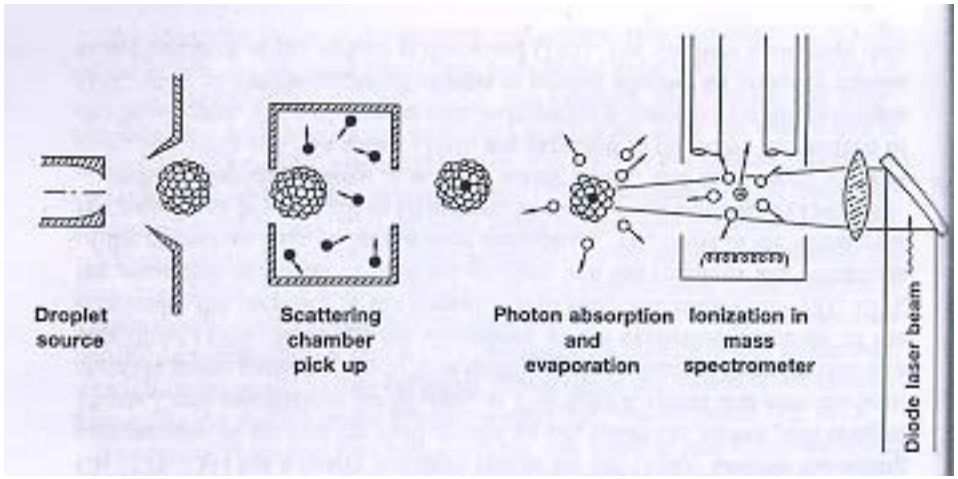
$$\frac{\rho_s}{\rho} = 1 - \frac{1}{I_c} \left\langle \int_0^\beta dt \, \hat{L}_z \, e^{-(\beta - t)\hat{H}_0} \, \hat{L}_z \, e^{-t\hat{H}_0} \right\rangle$$

$$\frac{\rho_s}{\rho} = \frac{2m \left\langle A_z^2 \right\rangle}{\beta \lambda I_c}$$



A = signed area of imaginary-time paths

Experimental Setup for He droplets



Toennies and Vilesov,
Ann. Rev. Phys. Chem. 49, 1 (1998)

- Adiabatic expansion cools helium to below the critical point, forming droplets.
- Droplets then cool by evaporation to:

  T=0.38 K, $N \approx 10^4$ (^{4}He)

  T=0.15 K, $N \approx 10^3$ (^{3}He)
- The droplets are sent through a scattering chamber to pick up impurities, and are detected either with a mass spectrometer with electron-impact ionizer or a bolometer.
- Spectroscopy yields the rotational-vibrational spectrum for the impurity to accuracy of 0.01/cm. Almost free rotation in superfluid helium but increase of MOI of rotating impurities.

Demonstration of droplet superfluidity

Grebenev, Toennies, Vilesov: *Science 279, 2083 (1998)*

- An OCS molecule in a ^{4}He droplet shows rotational bands corresponding to free rotation, with an increased moment of inertia (2.7 times higher)

  → ^{4}He are "coat" the impurity allowing it to freely rotate in the superfluid

- They replaced boson ^{4}He with fermion ^{3}He. If Bose statistics are important, then rotational bands should disappear. → they didn't!

- However, commercial ^{3}He has ^{4}He impurities, which would be more strongly attracted to an impurity.

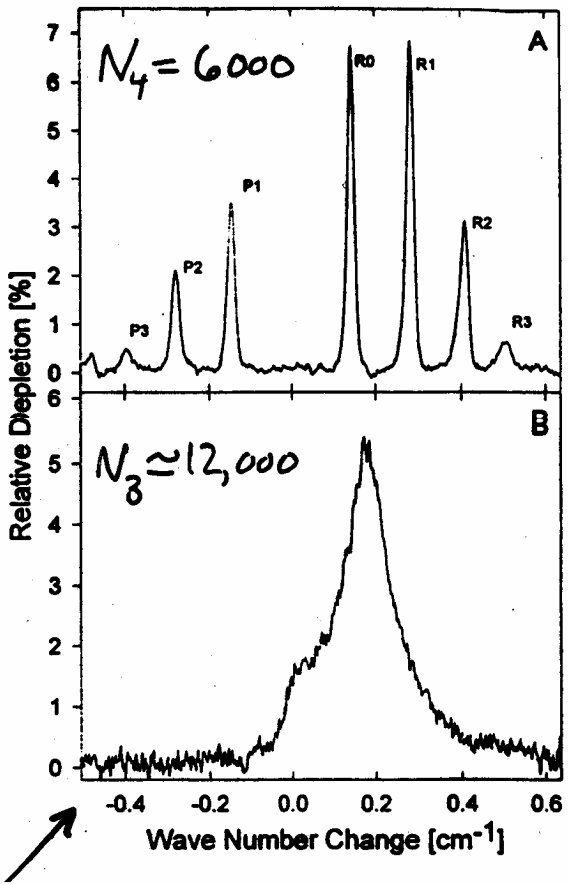
  → How much ^{4}He does it take to "coat" the impurity and get free rotation?

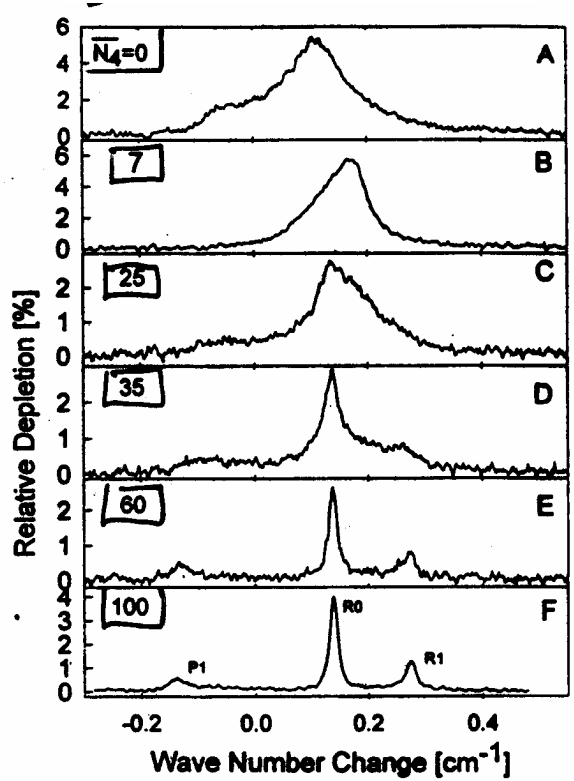
- They found that it takes around 60 ^{4}He atoms.

Small impurities of ^{4}He in ^{3}He

^{4}He

^{3}He

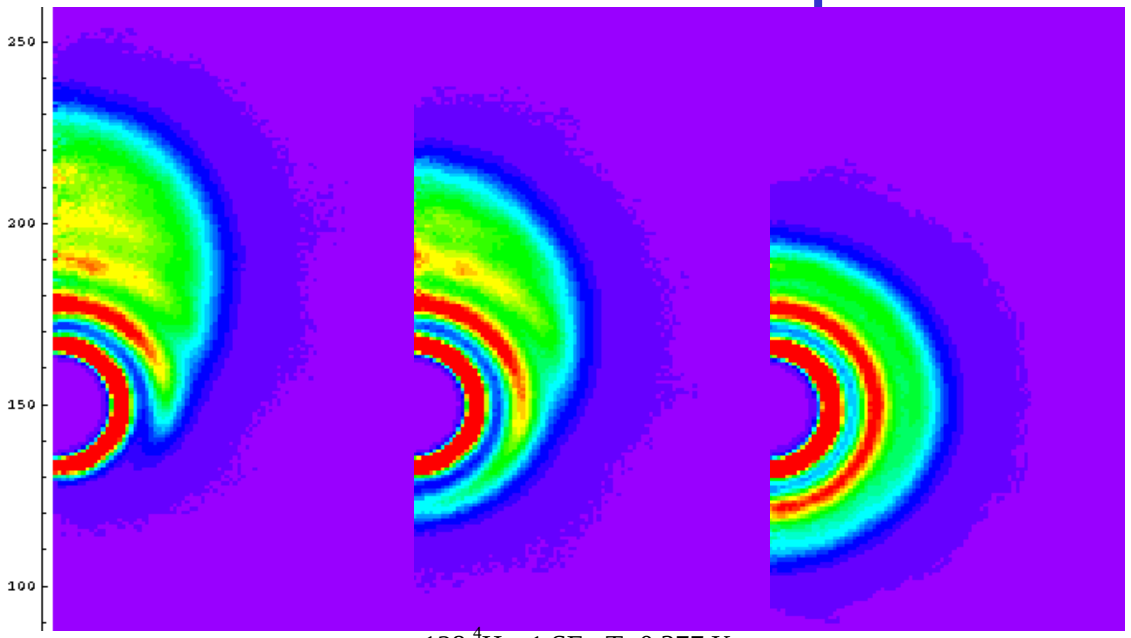




^{4}He is more strongly attracted to impurity because of zero point effects, so it coats the impurity, insulating it from the ^{3}He.

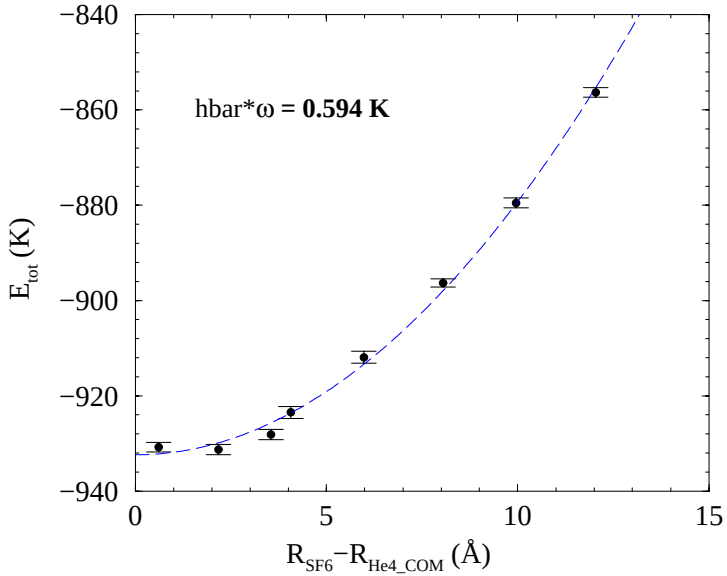
Density distribution within a droplet

- Helium forms shells around impurity (SF_6)
- During addition of molecule, it travels from the surface to the interior boiling off 10-20 atoms.



128 ^{4}He, 1 SF_6, T=0.377 K

- How localized is it at the center?
- We get good agreement with experiment using the energy vs. separation from center of mass.



Local Superfluid Density Estimator

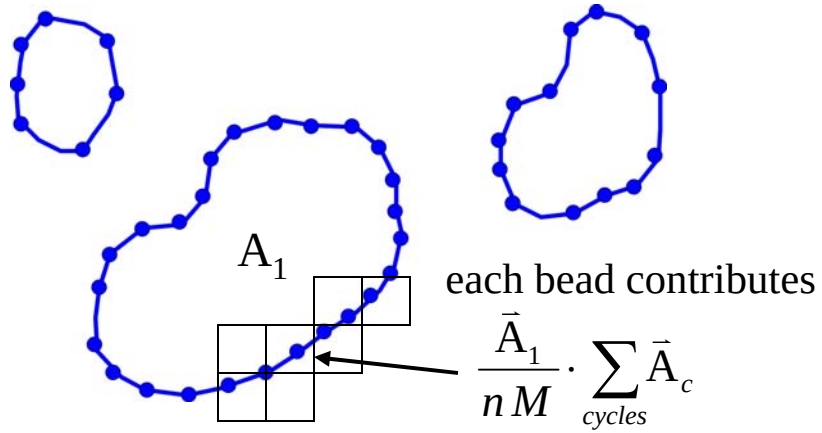
Although superfluid response is a non-local property, we can calculate the local contribution to the total response.

$$\rho_s = \frac{4m^2\rho}{3\hbar^2\beta I_c \Omega^2}\int d\vec{r}\, d\vec{r}\,' \vec{A}(\vec{r})\cdot\vec{A}(\vec{r}\,') = \frac{1}{\Omega}\int d\vec{r}\,\rho_s(\vec{r})$$

Where A is the area.

$$\vec{A}(\vec{r}) \equiv \int_0^\beta dt \sum_i (\vec{r}_{it}\times\vec{v}_{it})\,\delta(\vec{r}_{it}-\vec{r})$$

$$\Rightarrow \quad \rho_s(\vec{r}) = \frac{4m^2 N}{3\hbar^2\beta I_c}\int d\vec{r}\,' \vec{A}(\vec{r})\cdot\vec{A}(\vec{r}\,')$$



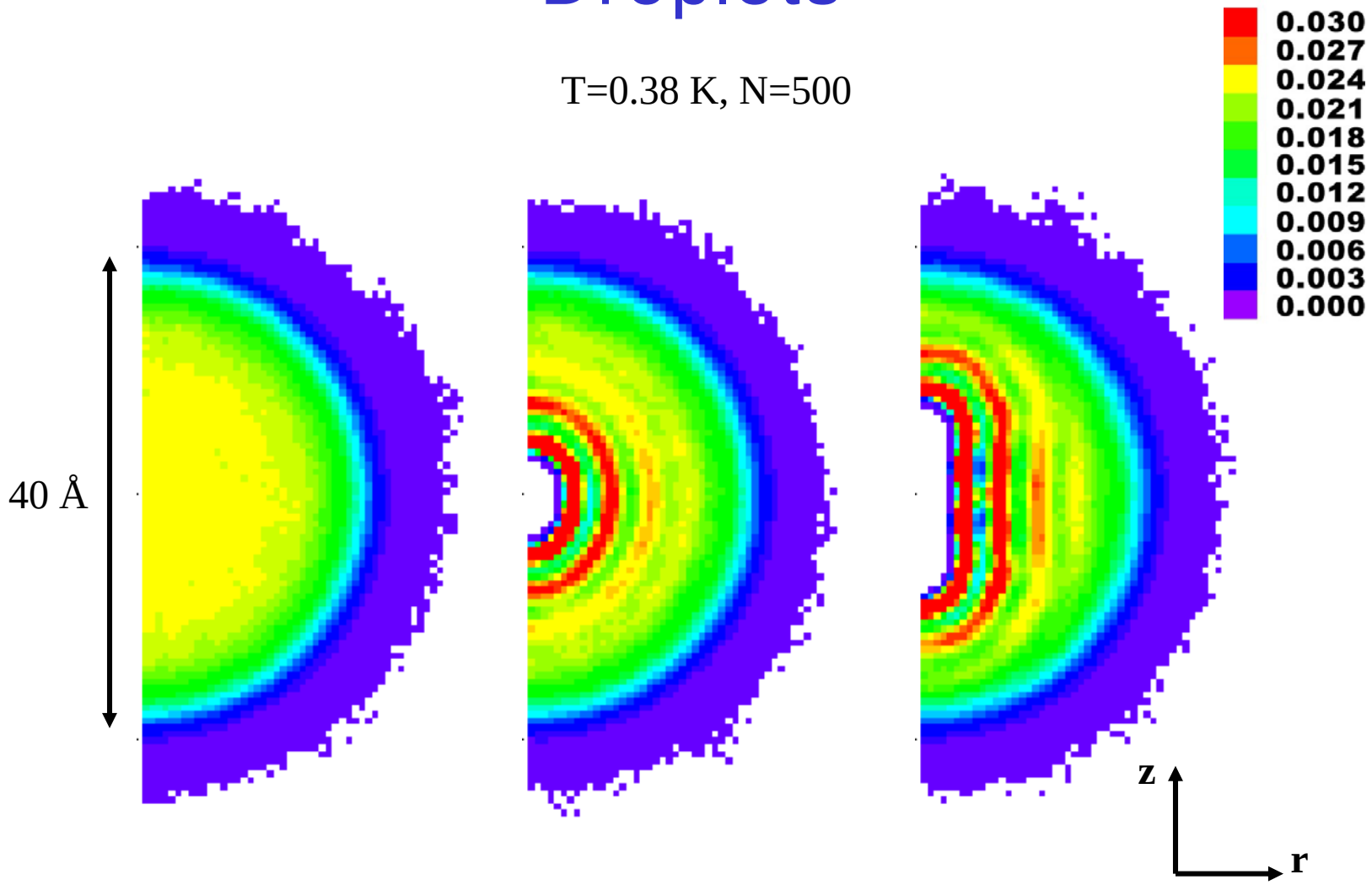
$$\rho_s(\vec{r}) \propto \frac{\vec{A}_1}{n\ M}\cdot\sum_{cycles}\vec{A}_c = \frac{A_1^2}{n\ M} + \frac{\vec{A}_1}{n\ M}\cdot\sum_{c\neq 1}\vec{A}_c$$

approximation: use only diagonal terms

not positive definite could be noisy

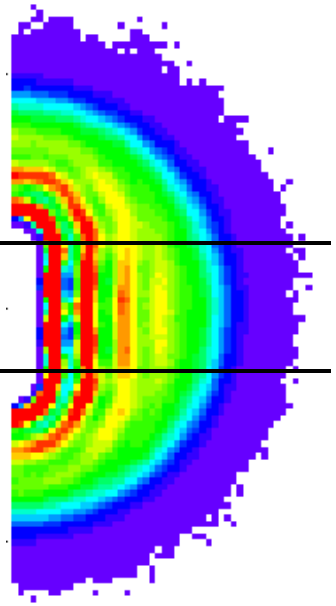
Density Distribution of $^4He+(HCN)_x$ Droplets

T=0.38 K, N=500

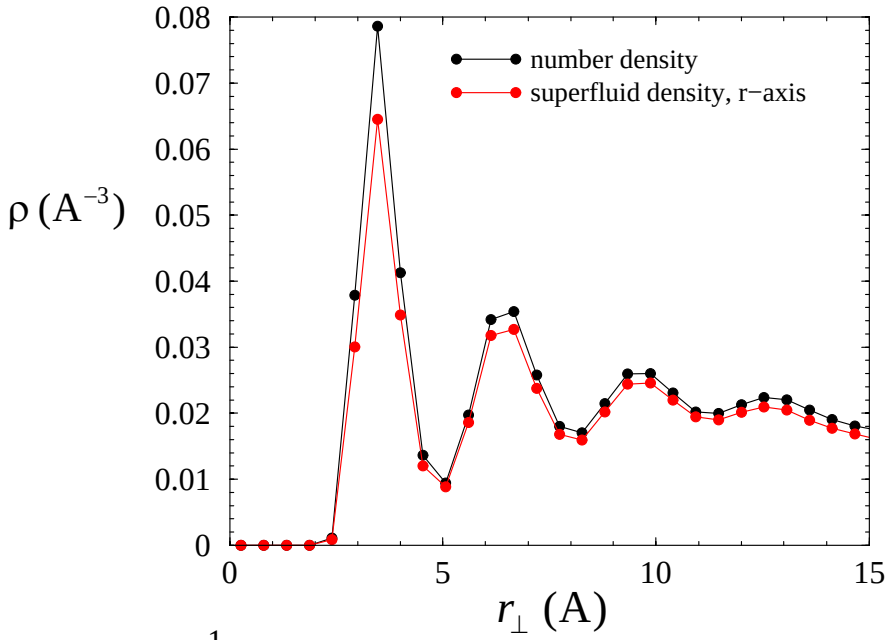


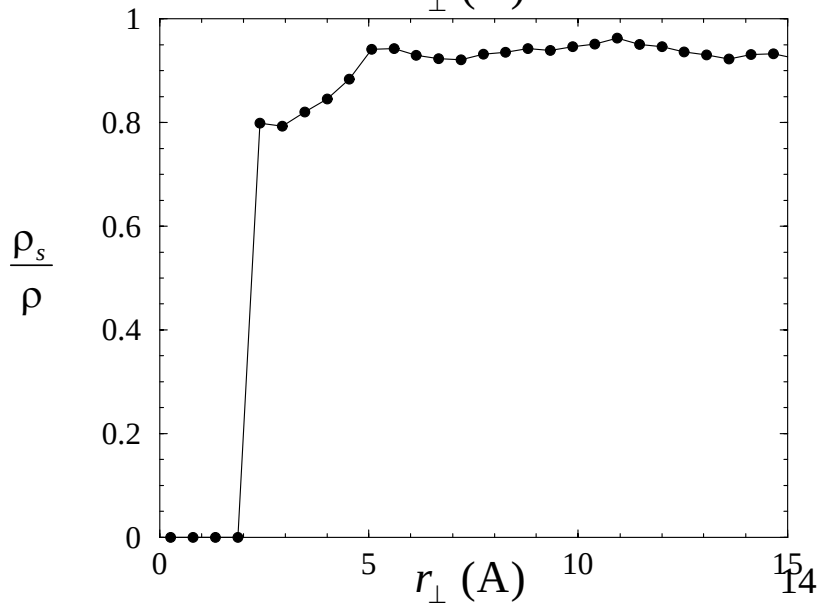
Local Superfluid Reduction

Average over region with cylindrical symmetry



T=0.38 K, N=500
$(HCN)_3$





The local superfluid estimator shows a decrease in the superfluid response throughout the first solvation layer.

Bose condensation

- BEC is the macroscopic occupation of a single quantum state (e.g. momentum distribution in the bulk liquid).

$$n_k = \int \frac{d^3 r d^3 s}{(2\pi)^3 V} \exp(-ik(r-s)) n(r,s)$$

- The one particle density matrix is defined in terms of open paths:

$$n(r,s) = \frac{V}{Q} \int dr_2 ... dr_N \left\langle r, r_2 ... r_N \left| e^{-\beta H} \right| s, r_2 ... r_N \right\rangle$$

- We cannot calculate n(r,s) on the diagonal. We need one open path, which can then exchange with others.
- Condensate fraction is probability of the ends being widely separated versus localized. **ODLRO** (off-diagonal long range order) (*The FT of a constant is a delta function.)*
- The condensate fraction gives the linear response of the system to another superfluid.

Derivation of momentum formula

- Suppose we want the probability n_k that a given atom has momentum hk.
- Find wavefunction in momentum space by FT wrt all the coordinates and integrating out all but one atom

$$\Pr(k_1,..k_N) = \left| \int dR\ e^{-i(k_1 r_1 + ... + k_N r_N)} \Psi(R) \right|^2$$

$$n_k = \int dk_2 .... dk_N \Pr(k, k_2, ... k_N)$$

- Expanding out the square and performing the integrals we get.

$$n_k = \int \frac{d^3 r d^3 s}{(2\pi)^3 V} \exp(-ik(r-s)) n(r,s)$$

Where: $$n(r,s) = \frac{V}{Q} \int dr_2 ... dr_N \left\langle r, r_2 ... r_N \left| e^{-\beta H} \right| s, r_2 ... r_N \right\rangle$$

occupy the states with the Boltzmann distribution.

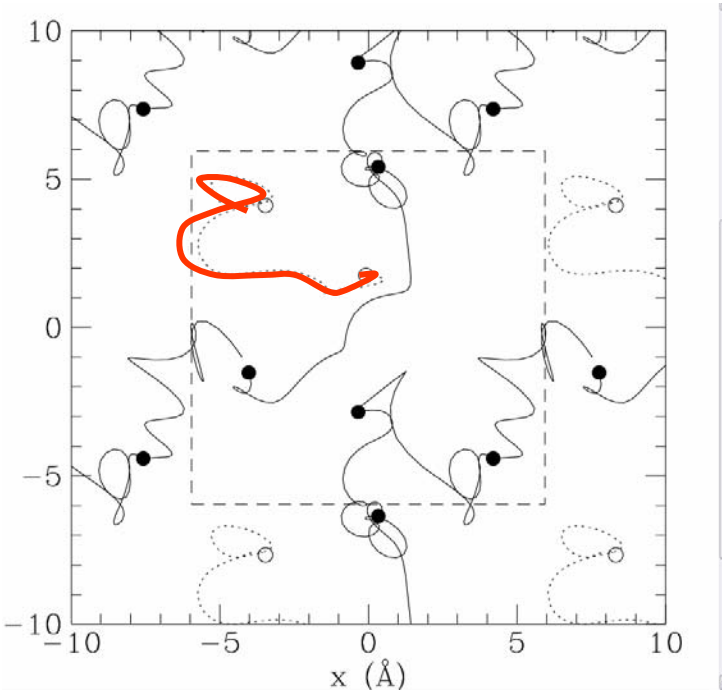
How to calculate n(r)

1. Take diagonal paths and find probability of displacing one end.

- advantage:
  - simultaneous with other averages,
  - all time slices and particle contribute.
- disadvantage: unreliable for $r>\Lambda$.

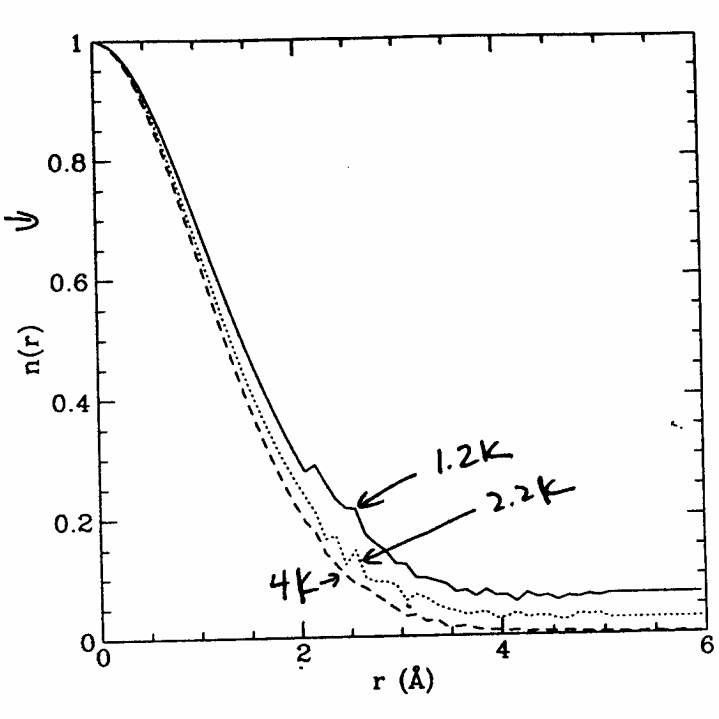
2. Do simulation off the diagonal and measure end-end distribution. Will get condensate when free end hooks onto a long exchange.

- advantage: works for any r
- Disadvantage:
  - Offdiagonal simulation not good for other properties
  - Normalization problem.

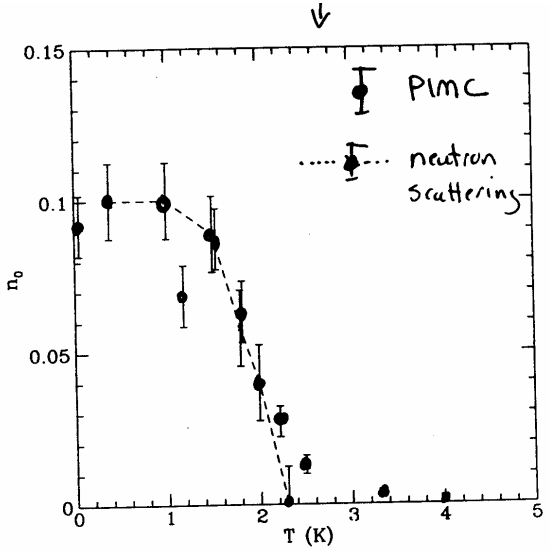


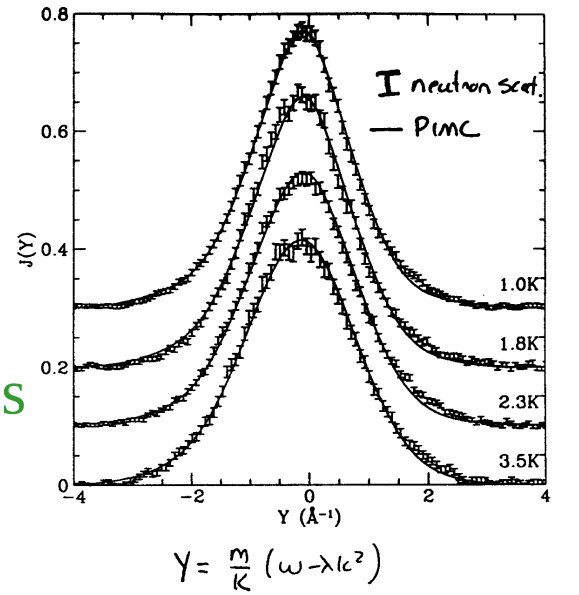
Comparison with experiment for bulk helium

Single particle density matrix



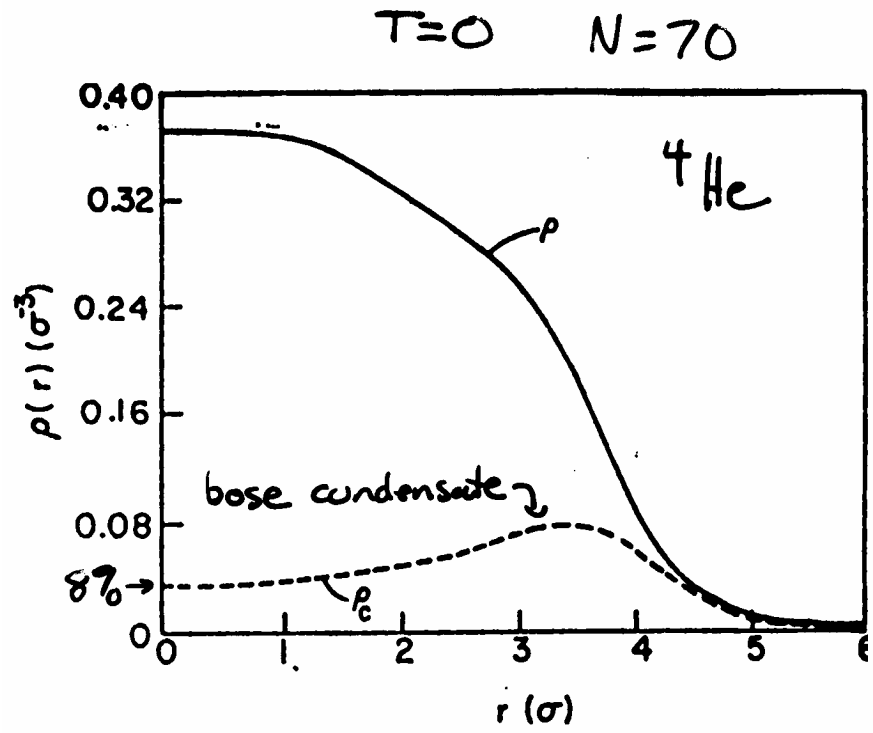
Condensate fraction





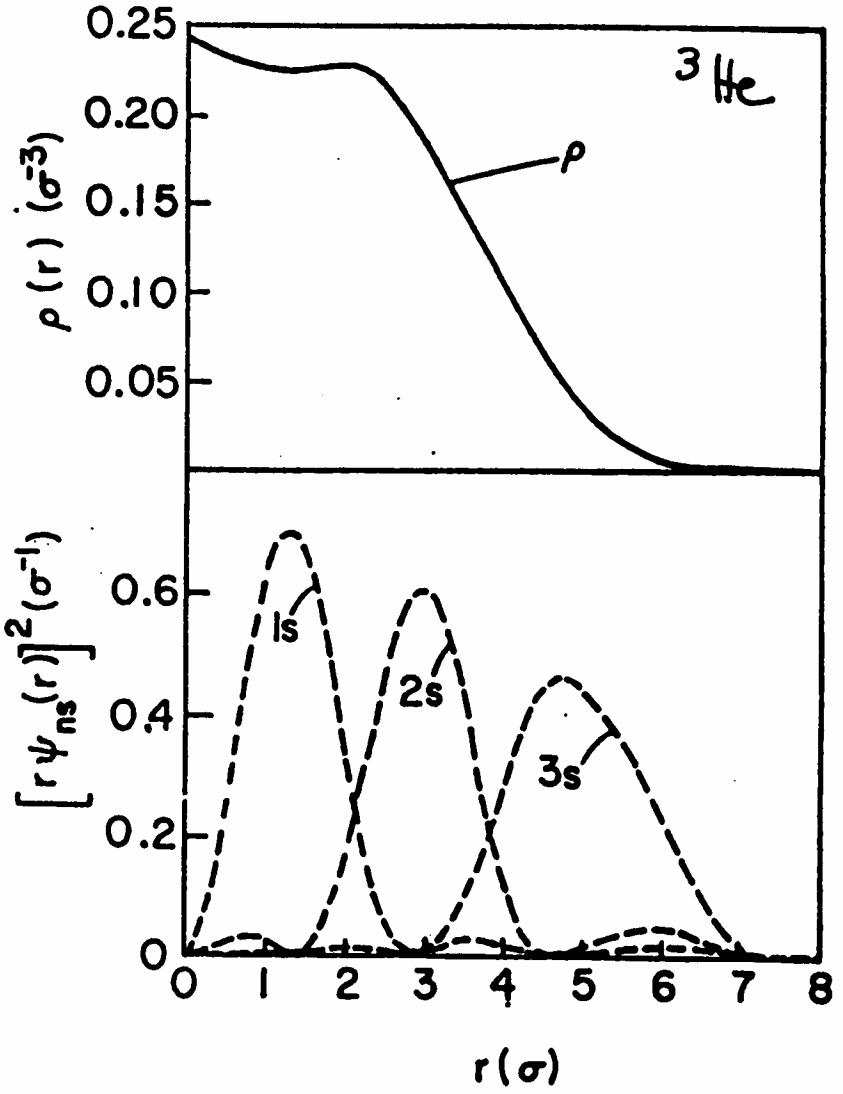
Neutron scattering cross section

Condensate in a ^{4}He droplet is enhanced at the surface



Lewart et al., PRB 37,4950 (1988).

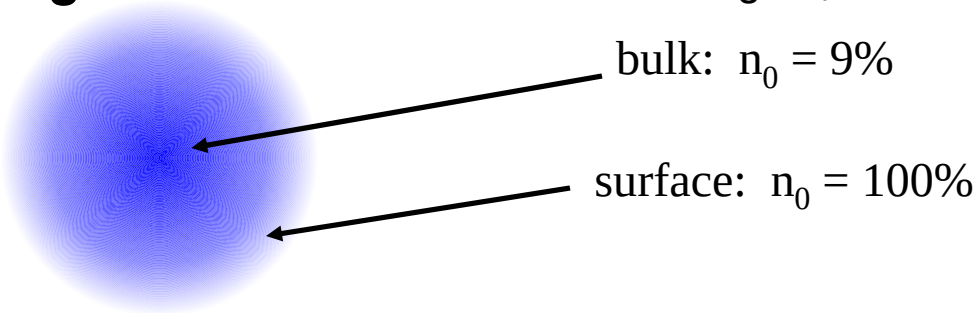
Shell effects in ^{3}He



Surface of Liquid Helium

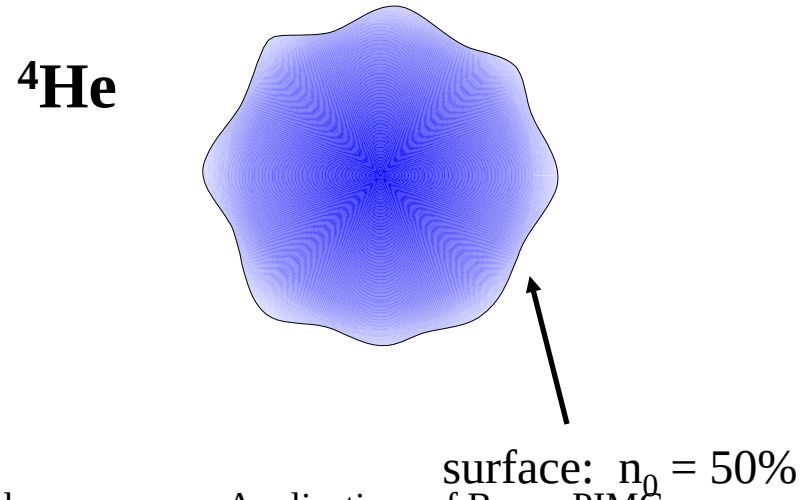
2 possible pictures of the surface

- **Dilute Bose gas model:** Griffin and Stringari, PRL 76, 259 (1996).

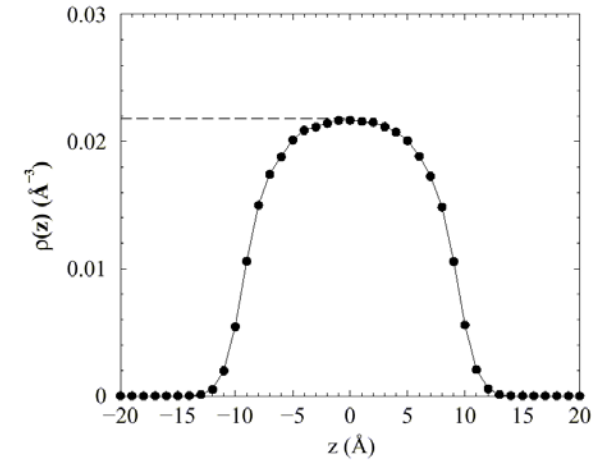


- **Ripplon model:** Galli and Reatto, J. Phys. CM 12,6009 (2000).

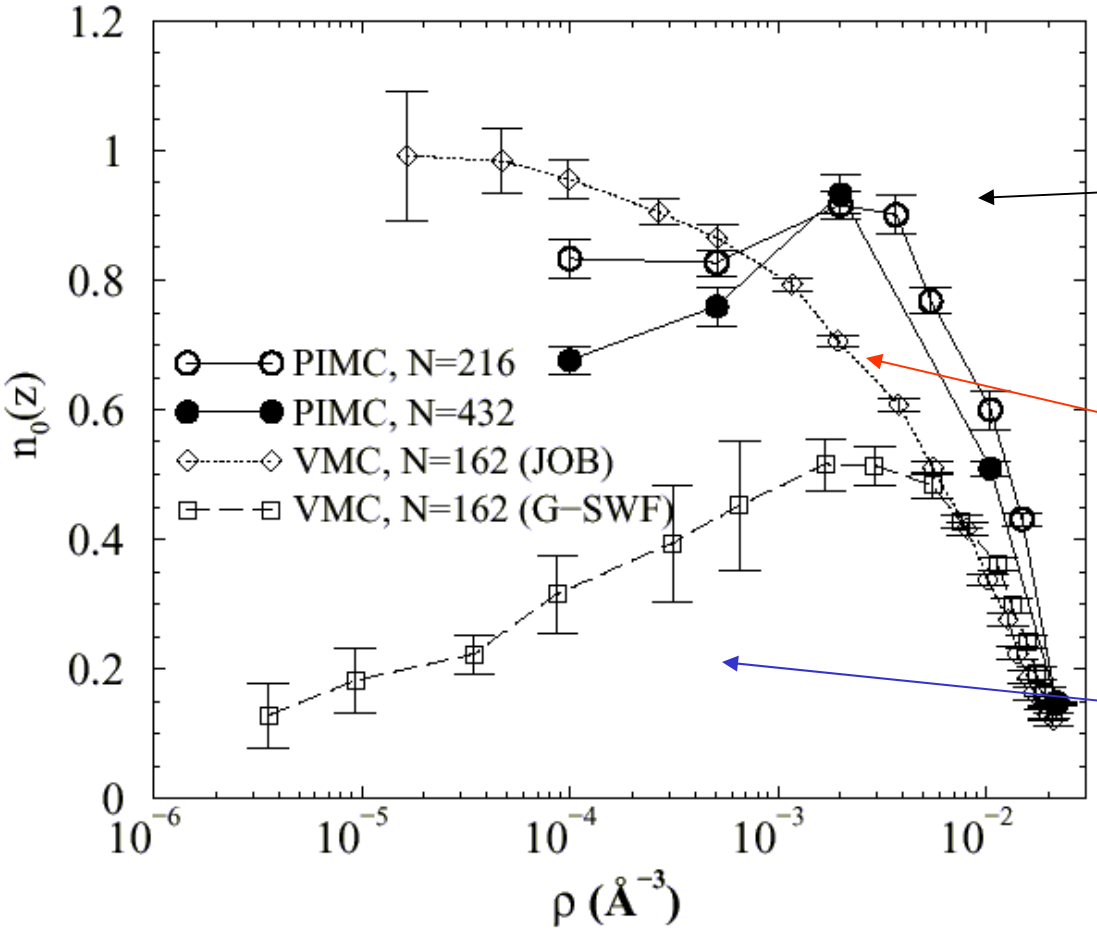
Can smeared density profile be caused by ripplons alone?



Density profile does not distinguish



Condensate Fraction at the Surface of ^{4}He



- PIMC supports dilute gas model.
- Jastrow wavefunction
- Shadow wavefunction

Is Solid ^{4}He a Supersolid?

- Some background on superfluid and supersolids
- Kim-Chan experiments
- Calculations with Path Integral Monte Carlo
- How can we explain supersolidity?

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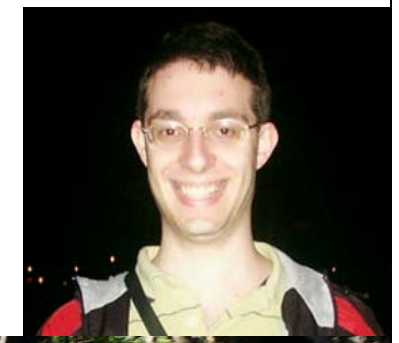

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Observation of Superflow in Solid Helium

E. Kim and M. H. W. Chan*

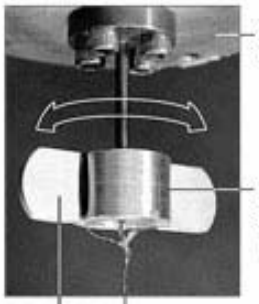
Science, September 2004

NewYorkTimes

Some Surprising Moves

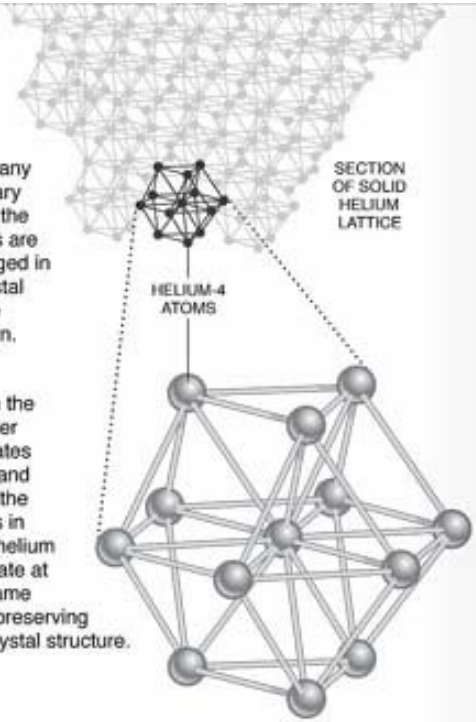
Helium may turn into a new state of matter called a supersolid — when rotated, it does not quite act solid.

1. Helium gas inside a cylinder (below, actual size) is chilled and squeezed until it turns into a solid. The cylinder then oscillates.



2. As in any ordinary solid, the atoms are arranged in a crystal lattice pattern.

When the cylinder oscillates back and forth, the atoms in solid helium all rotate at the same rate, preserving the crystal structure.

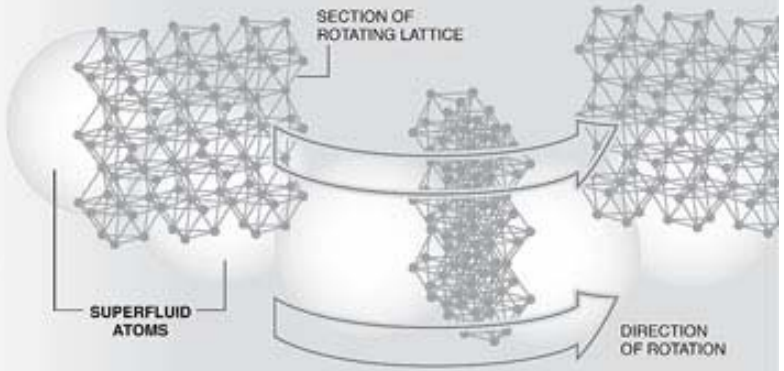


Sources: Dr. Moses H. W. Chan and Dr. David S. Weiss, Penn State University; Dr. Wayne Saslow, Texas A&M University

A NEW STATE OF MATTER, BOTH SOLID AND SUPERFLUID

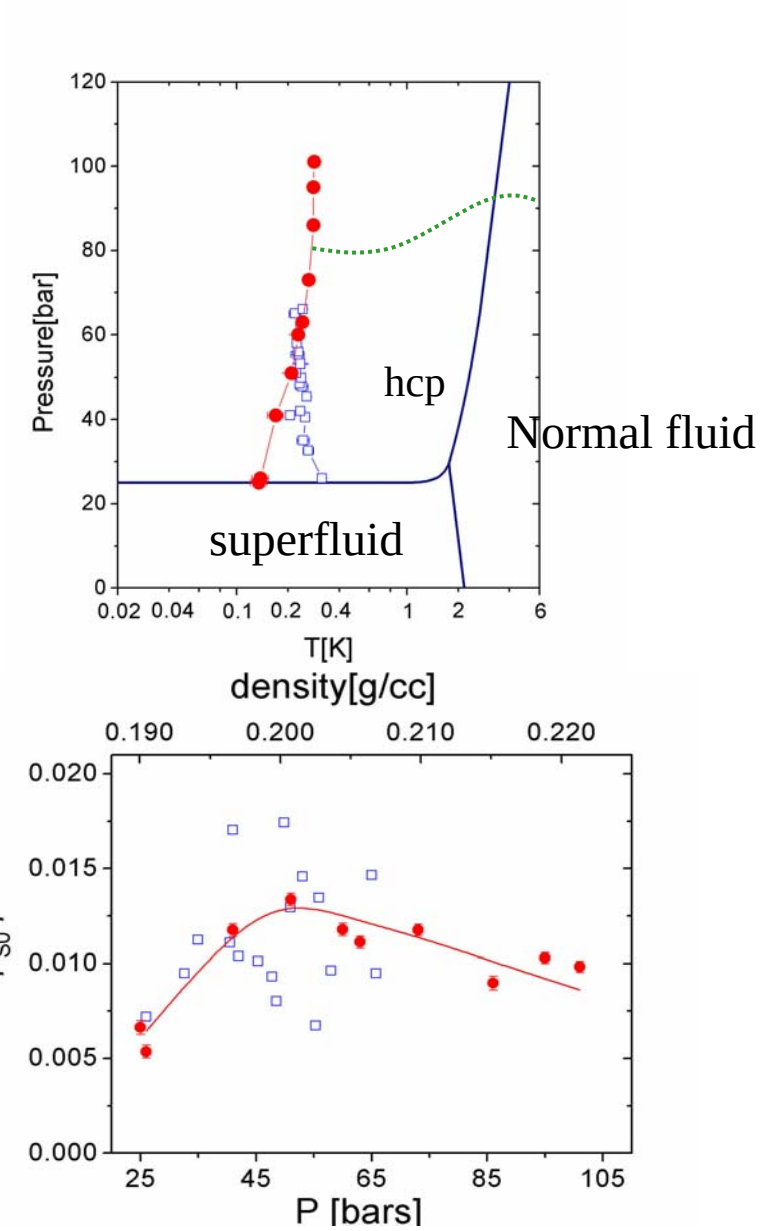
3. To turn solid into a supersolid, the temperature is lowered further, to almost absolute zero.

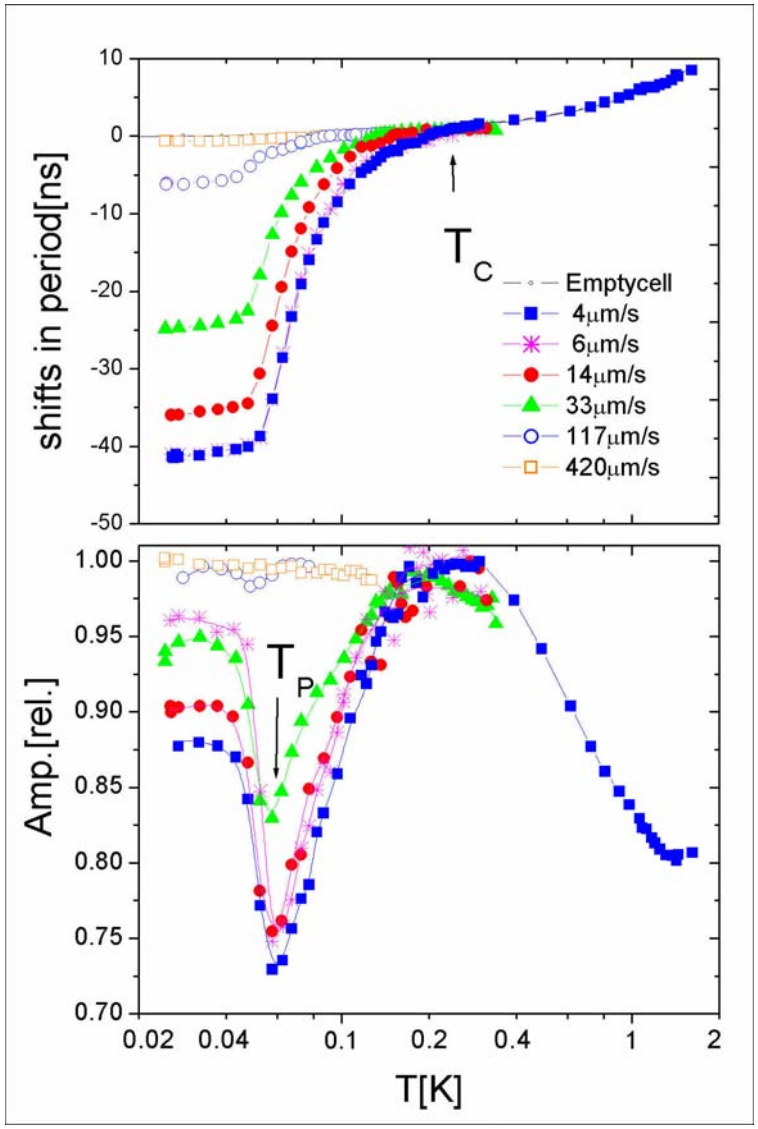
4. A small portion (1.5 percent) of the atoms are free to move away from their lattice sites, becoming superfluid. Their positions are blurred; they coalesce and suffuse the entire solid.



During rotation, as the lattice flows by, the blurry superfluid atoms stay in place. There is no friction between moving and stationary atoms.

Kim-Chan experiments on bulk ^{4}He





What is a super-solid?

Crystal has long range spatial order. Proof: Bragg scattering peaks?

Translational symmetry is spontaneously broken- no underlying lattice.

Superfluid has a non-classical response to rotation as in the torsional oscillator experiment at zero frequency. Related to persistent currents, vortices,…

BEC is macroscopic occupation of a single state or ODLRO.

Can both exist at the same time or does solidity preclude superfluidity?

- Penrose & Onsager, Phys. Rev. **104**, 576(1956): no supersolid possible.
- C. N. Yang, Rev. Mod. Phys. 34, 694 (1962): Solids could be superfluid if atoms are mobile.

Supersolid mechanisms

- Ground state vacancies are sufficient for BEC. Andreev-Lifshitz: Zh.Eksp.Teor.Fiz. 56, 205 (1969).
- Reatto-Chester: there exist supersolids: Phys. Rev. A 2, 256 (1970)
  - Take a classical crystal (e.g. neon) interpret the distribution quantum mechanically. Implies BEC
- Leggett: NCRI related to connnectivity of wavefunction: Phys. Rev. Lett. 25, 1543 (1970)
  - if you drag a particle around a torus, does the wavefunction remain non-zero?

Chester: Vacancies $\Rightarrow$ BEC

Prokof'ev: Vacancies $\Leftarrow$ BEC or NCRI

Solid He

Solid helium is a very quantum solid

Lindemann's rule: solids melt when:

$$\left\langle r^2 \right\rangle^{1/2} = 0.14 r_{NN}$$

Helium melts when:

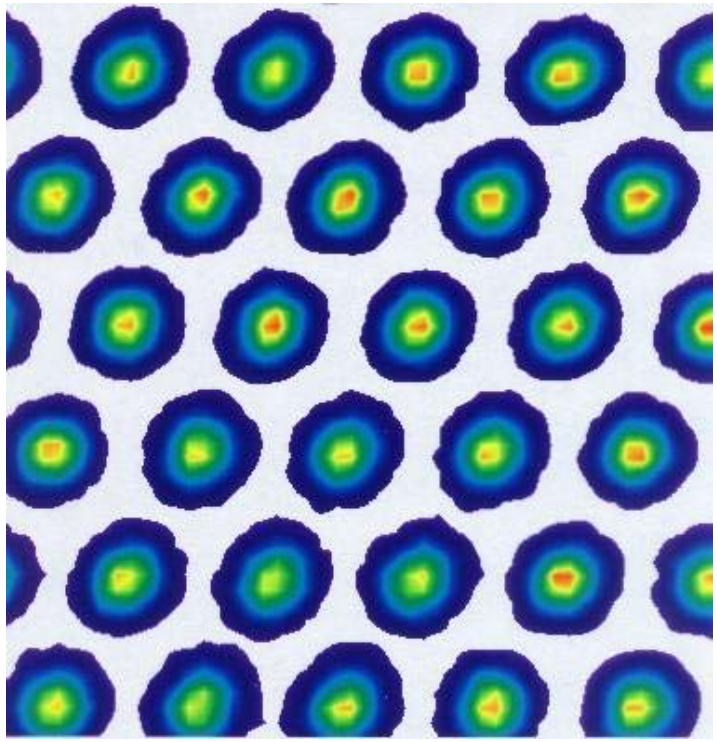
$$\left\langle r^2 \right\rangle^{1/2} = 0.3 r_{NN}$$

In solid He there are lots of vacancy-interstitial fluctuations.

How do we define defects in such a disordered system?

Commensurate means:

atoms = # lattice sites



Conditions for BEC

- BEC occurs when thermal wavelength is greater than interatomic spacing.

$$k_B T_c \approx h^2 \rho^{2/3} / m$$

Mass and density are of the delocalized quasiparticles

- If T_c= 0.2K what is the density of defects?

relative concentration of defects ~ $0.012\left(\frac{m}{m_4}\right)^{3/2} \sim 2\times10^{-3}$

- Even for a relatively light defect, such a large concentration could be detected by X-ray scattering. Simmons has established an upper limit of roughly $3\text{x}10^{-3}$
- What does simulation tell us about vacancies?

Two types of quantum bose solids

"Metal"

- Zero point vacancies
- V-I pairs unbound
- Condensate fraction >0
- Superfluid density >0
- Lindemann's ratio < 1/7

$$\Psi = \prod_{i<j} f(r_{ij})$$

"Mott insulator"

- No vacancies at T=0
- V-I pairs bound
- Condensate fraction = 0
- Superfluid density = 0
- Lindemann's ratio > 1/7
- Explicit lattice symmetry breaking

$$\Psi = \left[\prod_{i<j} f(r_{ij})\right] \sum_{P} \prod_{i} \phi\left(r_i - Z_{Pi}\right)$$

Either trial function is a possible quantum solid, but which is correct for ^{4}He?

Point defects in a quantum crystal

- Calculate total energy using QMC in hcp lattice Add or subtract an atom keeping density fixed.

$$E_D = [e(N \pm 1, \rho) - e(N, \rho)](N \pm 1)$$

- Vacancy energy at melting is ~15K and increases rapidly with density: *Pederiva, Chester, Fantoni, Reatto, PRB 5909 (1997).*
- Consistent with experimental measurements.
- Interstitial energy is even higher ~30K
- But measured NCRI is independent of density.

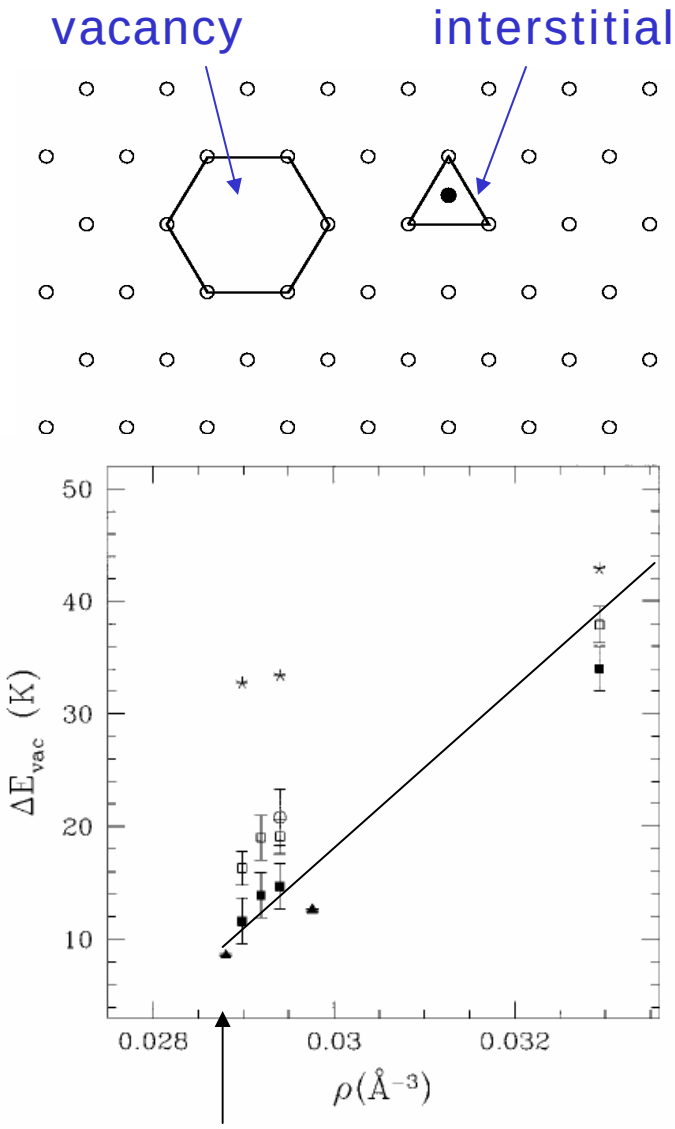
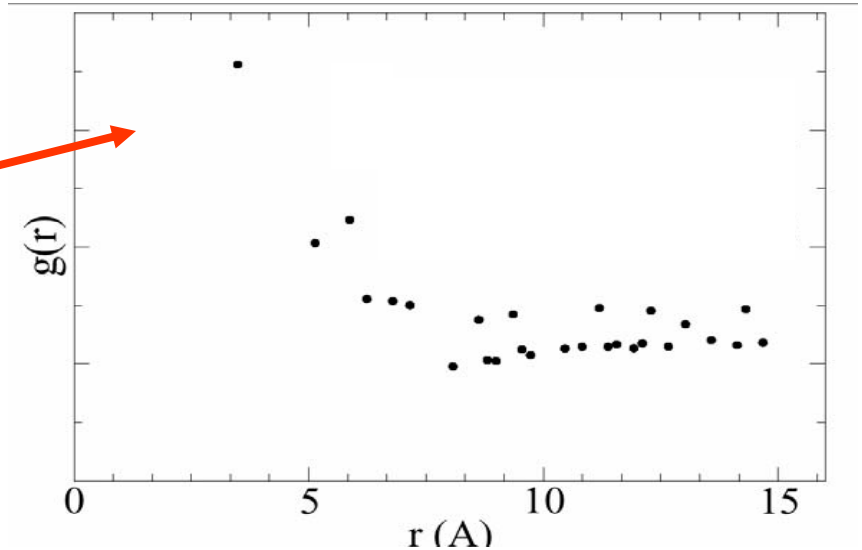
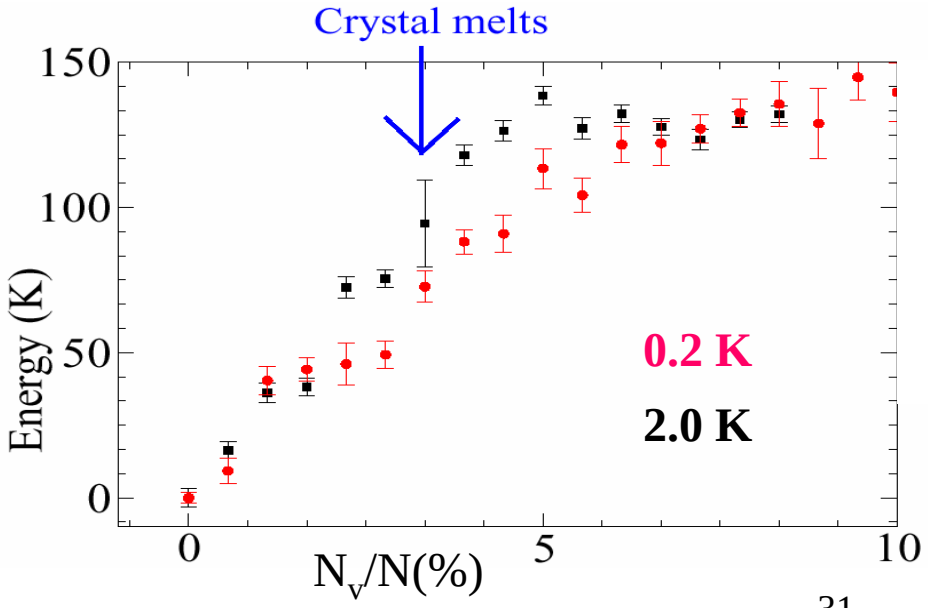


FIG. 1. Vacancy formation energy ΔE_{vac} vs reduced density. Solid triangles: data from Ref. 3, open squares: variational estimates for the fcc phase; filled squares: for the hcp phase; open circle: for the bcc phase. Stars: formation energy of a static vacancy [see Eq. (10) in text].

Multiple vacancies

- Simulation of system with 2 vacancies
- Vacancies are pairwise attractive!
- As in “Tetris,” if enough vacancis accumulate in one region, they disappear.
- Crystal can sustain about 3% vacancies before it becomes unstable to liquid



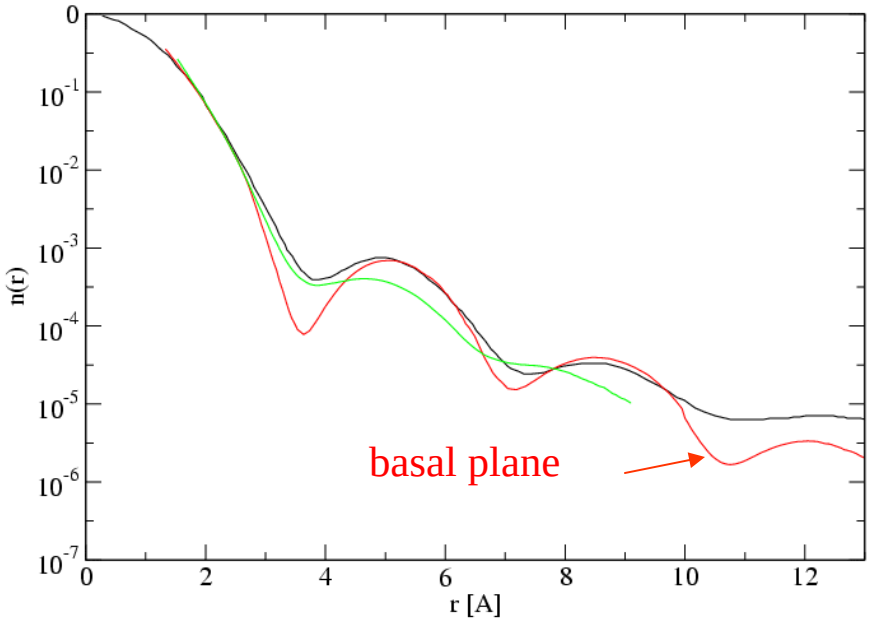


BEC in solid Helium?

Clark & DMC cond-mat/0512547

Boninsegni, Prokof'ev & Svistunov cond-mat/0512103

- BEC: Single particle density matrix goes to a finite value at large r
- n(r) from PIMC gets very small. No BEC
- Separating 2 ends costs a constant "energy" unit length.
- Oscillations are due to lattice effects
- 2 independent PIMC calculations agree



Thouless theory of exchange in quantum crystals

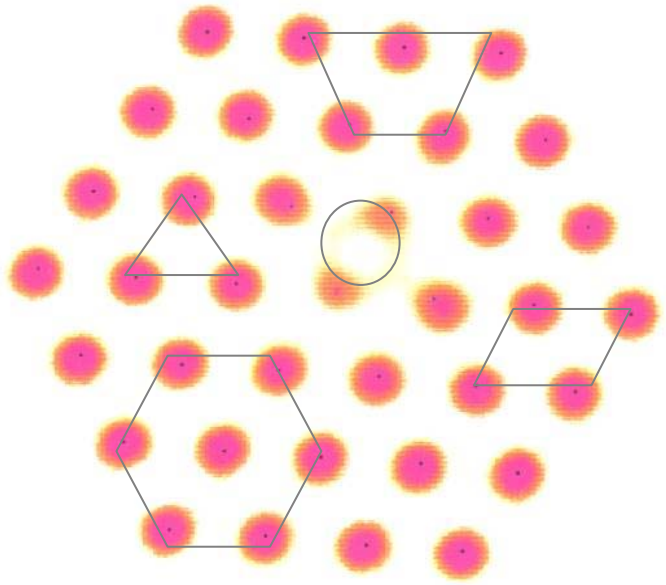
- At low temperature there are **very** few defects, phonons, etc.
- The many body wavefunction has N! peaks, corresponding to possible atom relabelings.
- We can write the partition function in terms of permutation of lattice sites:

$$Q(\beta) = \sum_{p=1}^{N!} Q_p(\beta)$$

Break permutation into "cycles"

$$Q_P(\beta) = Q_o(\beta) \prod_{k=1}^{c} f_{p_k}(\beta)$$

$$f_p(\beta) = \beta J_p$$



Q_0 unimportant at low temperatures

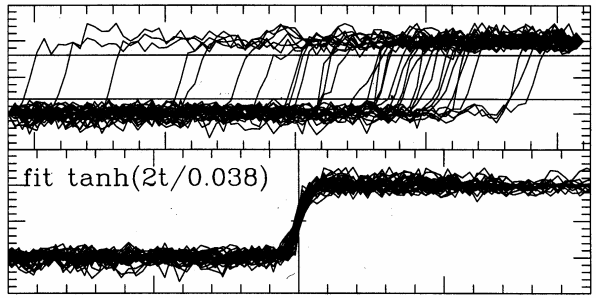
- Related to magnetism in solid ^{3}He.

Path Integral Method to determine exchange frequency

- We make a path with a permutation and evaluate the cost to the free energy.

$$f_P(\beta) = \frac{Q_P(\beta)}{Q_0(\beta)} = \tanh(J_P\,\beta) \sim J_P\,\beta$$

$$Q_P(\beta) = Tr\left(R\left|e^{-\beta\hat{H}}\right|PR\right)$$



- X is the "reaction coordinate" for the exchange.
- J_P is the imaginary time tunneling rate.
- $Q_P \sim \beta$ because it is an "instanton", localized in "time." *How many ways to place the exchange?*
- How do we calculate a "free energy difference?": map paths from exchange to non-exchange & record the average change in action

Solid ^{3}He

- We have calculated *(Ceperley & Jacucci PRL 58, 1648, 1987)* exchange frequencies in bcc and hcp ^{3}He for 2 thru 6 particle exchanges.
- PIMC gives convincing support for the empirical multiple exchange model. *(Roger, Delrieu and Hetherington)*
- Main problem with MEM: there are too many parameters! But if they are determined with PIMC, they are no longer parameters!
- Exchanges of 2,3,4,5 and 6 particles are important because of Metro effect.
- Large cancellation of effects of various exchanges leads to a frustrated broken symmetry ground state (u2d2).
- Agrees with experiment measurements on magnetic susceptibility, specific heat, magnetic field effects, ….

Tests wrt ^{3}He experiment

- RHD have shown that MEM gives qualitative agreement with experiment.
- θ is Curie temperature
- e_2 coef of C.
- more than 3 exchanges!

Property	Three frequencies	All frequencies	Experiment[a]
θ (mK)	0.1 ± 1.0	-2.2 ± 1.0	-1.7 ± 0.1
e_2 (mK^2)	5.0 ± 0.8	5.9 ± 1.6	5.9
e_3 (mK^3)	2.0 ± 4.0		<2.4
B (mK^2)	0.7 ± 0.8		0.0 ± 1
H_{c2} (T)	9.7 ± 2.1	19.0 ± 2.2	...

- Experimentally all exchanges scale as [density]^{18}
- At B~20T the system goes to a ferromagnetic phase
  - The mean field value of $H_{c2}=\Sigma\ h_P J_P$ is exact
  - Using PIMC $H_{c2}=19T\ \pm 2T$
  - With only 3 freq. One gets 9T
- *See also Godfrin & Osheroff Phys. Rev. B 38, 4492 (1988)*

nn	19
nnn	22.5
t	19.5
4f	23
4p	18

Ring exchange frequencies in hcp ^{4}He.

•Exchange frequencies for localized exchanges are about 10^{-6} K. They are very small! (Note: these are old results ~1990)

p	Name	J (μK)	% error
2	nn	3.2	13%
	nn'	3.4	13%
3	T	2.3	12%
	$T*$	0.5	13%
	T'	2.3	12%
4	K'	1.4	20%

•Could they cause a supersolid at 0.2K? We have:

$$\frac{\rho_s}{\rho} = \lim_{N\to\infty} \frac{m}{\hbar^2 N} \sum_P J_P W_P^2 > 0$$

•Localized exchanges have no winding, do not transport mass, and are not related to supersolidity.

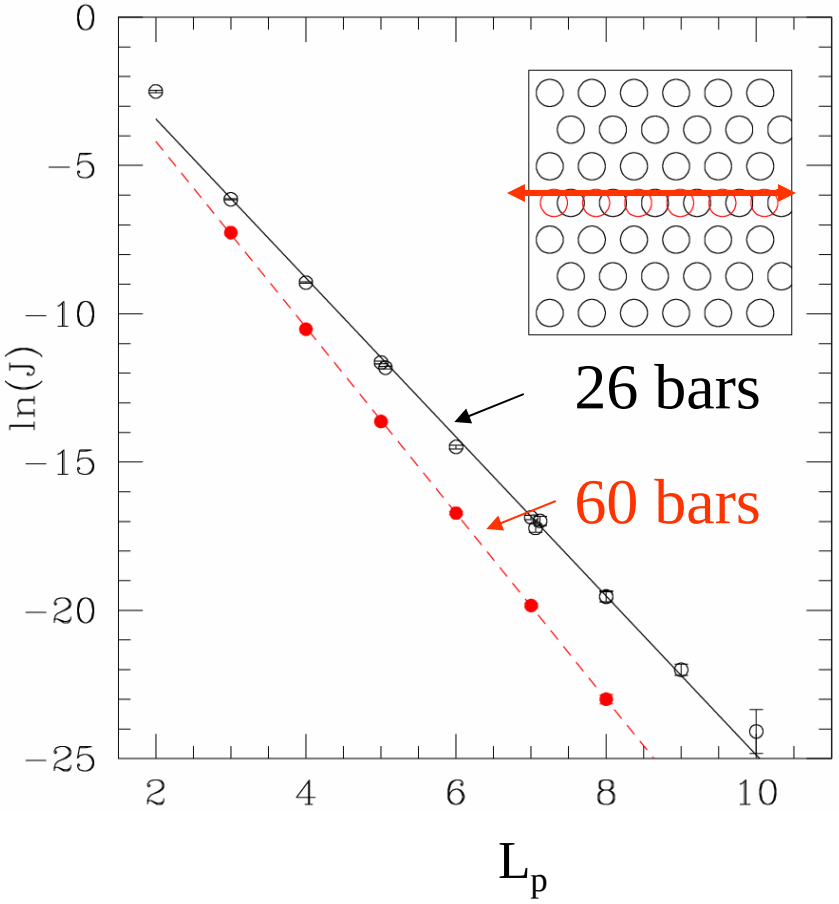
•Need frequent, macroscopic exchanges for supersolidity.

Winding exchanges

- Winding exchanges are much more probable because they are straight.
- PIMC exchange frequencies in the basal plane are found to decrease exponentially

$$J = J_0 \exp\left[-\alpha L_p\right] \quad \alpha = 2.7$$

- If we consider exchanges with various angles, we increase the entropy.
- Coordination number in hcp lattice is 12; 11=exp(2.4)
- Can this compensate for the exponential drop?
- To find out, we did calculations of 50 different exchanges in solid ^{4}He with 4<L<9.



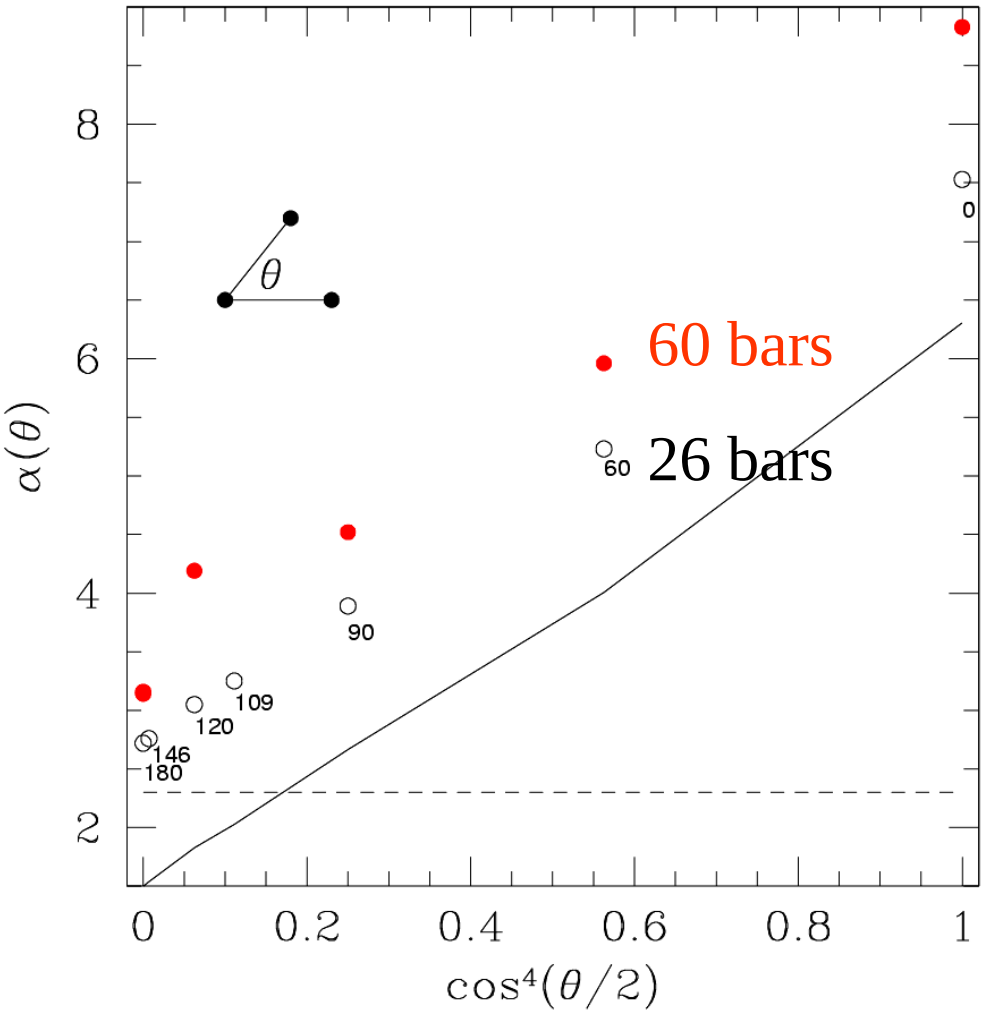
Angular dependence

- Exchange frequencies depend strongly on direction because of collisions between incoming and outgoing atom.
- Fit J_p to

$$J = J_0 \exp\left[-\sum_{k=1}^{L_p} \alpha(\theta_k)\right]$$

- We find a good 2 parameter model

$$\alpha(\theta) = \alpha + \alpha' \cos^4(\theta/2)$$

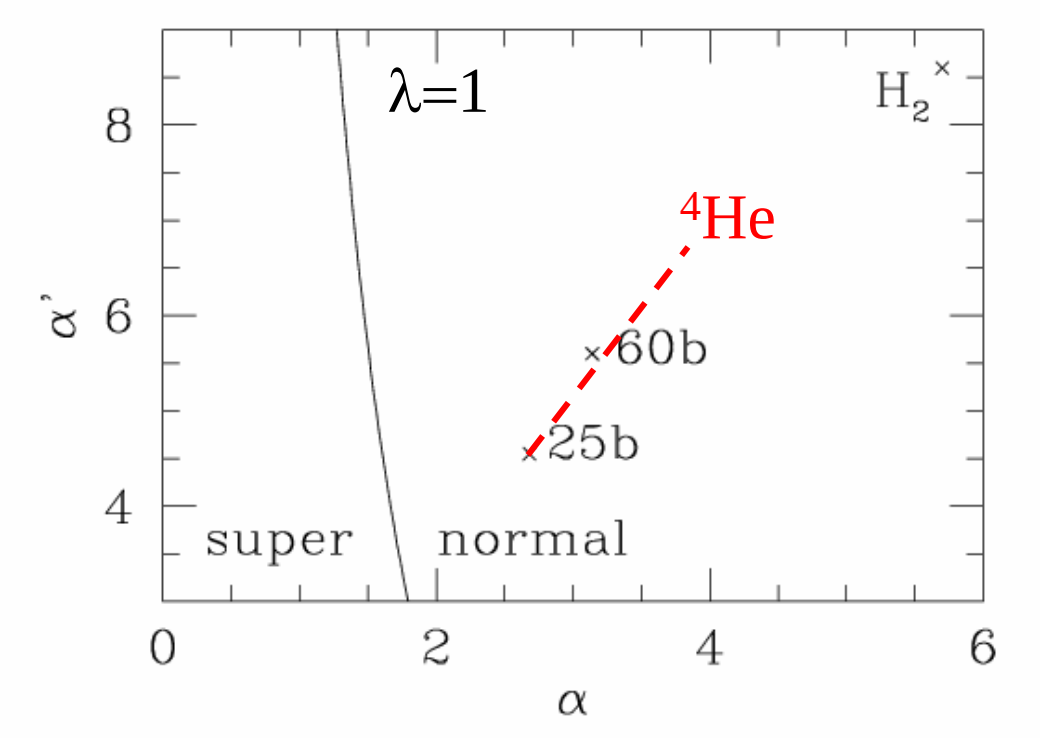


Phase diagram of lattice model

*DMC & Bernu PRL **93**, 155303 (2004): cond mat/0409336*

- Ring exchange model with parameters from fit, is not a supersolid
- Probability of long exchanges *decreases* faster than number of polygons increases
- Increasing the density makes it worse!

$$J_p = J_0 e^{-\alpha L_p - \alpha' \sum_{k=1}^{L_p} \cos^4(\theta_k/2)}$$



At least 2 types of quantum bose solids theoretically exist

"metallic" supersolid

- Jastrow (Chester) wf

$$\Psi = \prod_{i<j} f(r_{ij})$$

- Zero point vacancies
- V-I pairs unbound
- Condensate fraction >0
- Superfluid density >0
- Lindemann's ratio < 1/7

"insulator" normal solid

- Hartree (Jastrow-Nosanow)

$$\Psi = \left[\prod_{i<j} f(r_{ij})\right] \sum_{P} \prod_{i} \phi(r_i - Z_{Pi})$$

- No vacancies at T=0
- V-I pairs bound
- Condensate fraction = 0
- Superfluid density = 0
- Lindemann's ratio > 1/7

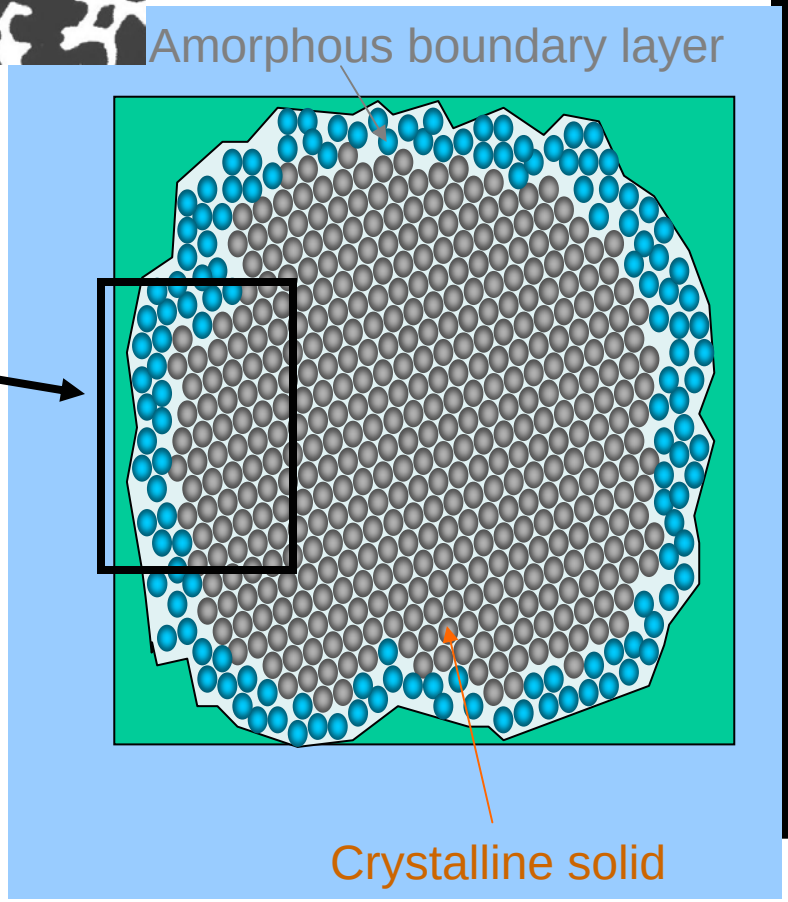
PIMC strongly favors the insulator picture for ^{4}He:

The low temperature state of ^{4}He crystal is not supersolid

Solidification in Vycor

Kim and Chan, Science 305,1941 (2004).

They find NCRI exists in porous glass and porous gold under the same conditions.



PIMC model

Vycor is glass with very small (7nm pores that absorb helium)

Solidification proceeds in two different directions:

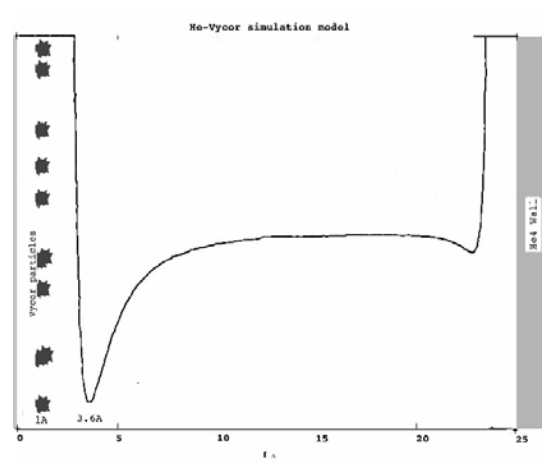
1) In the center of the pore a solid cluster has crystalline order identical to bulk ^{4}He
2) On the wall of a pore amorphous solid layers are found due to the large van der Waals force of the substrate
3) Liquid layer in between?

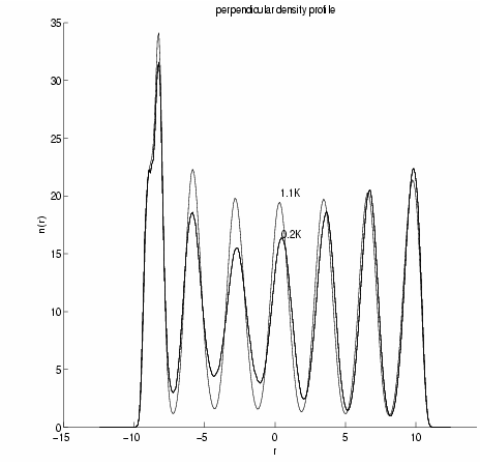
Vycor model

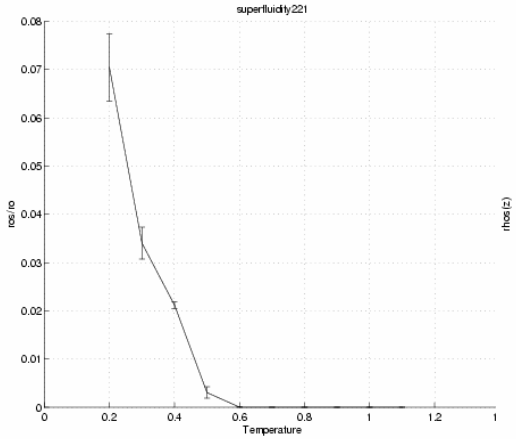
*Khairallah & DMC, PRL **95**, 185301 (2005); physics/0502039*

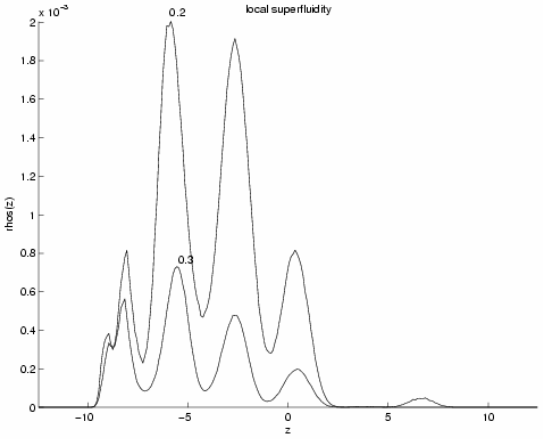
- Model a single pore, assuming a rough Vycor surface on left and a smooth helium surface on the right.

- Helium forms a layered system.
- Superfluidity is in the layers 2-5 above the vycor
- Transition temperature and superfluid density is within a factor of 2 of experiment
- Superfluid is about 30% of one layer
- Is this a solid?

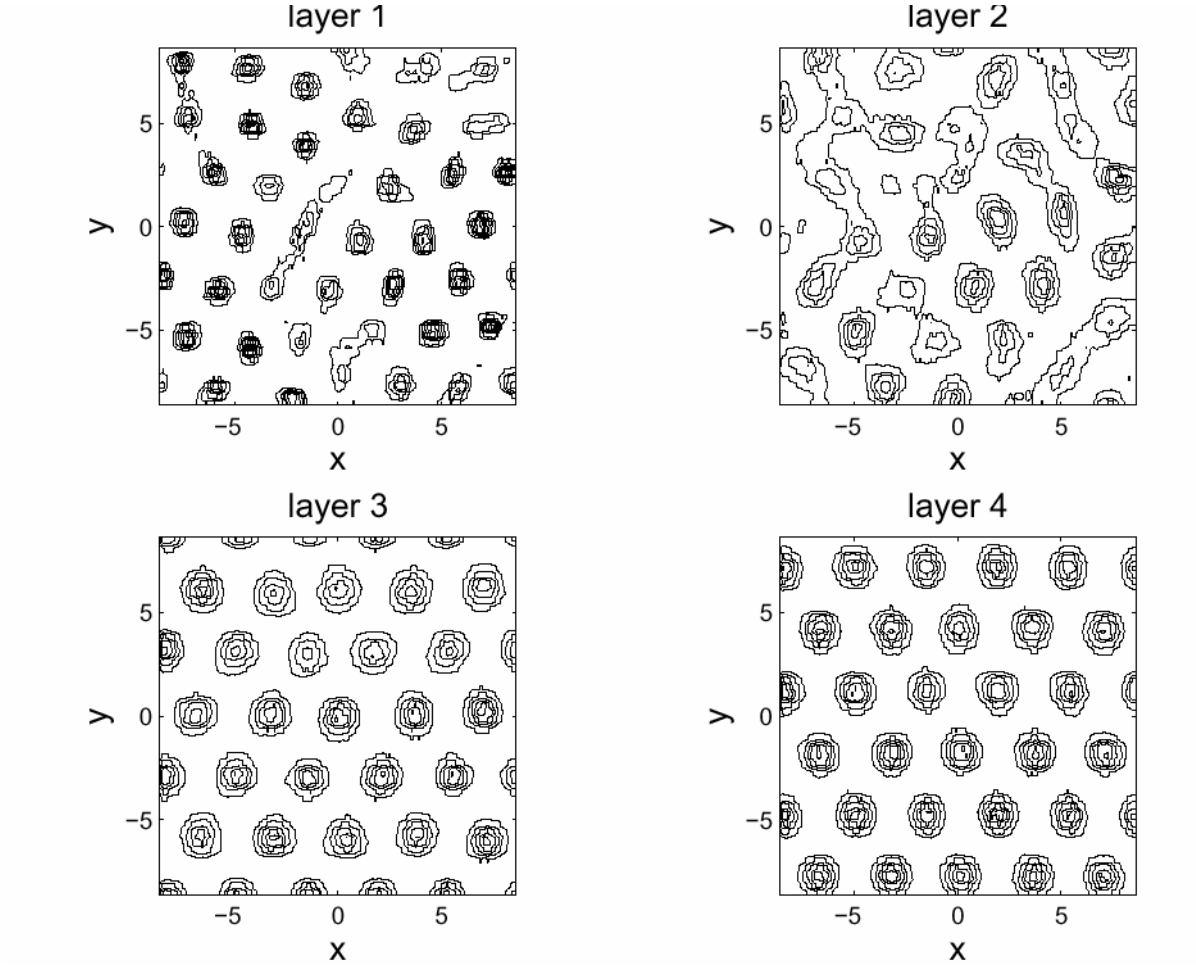






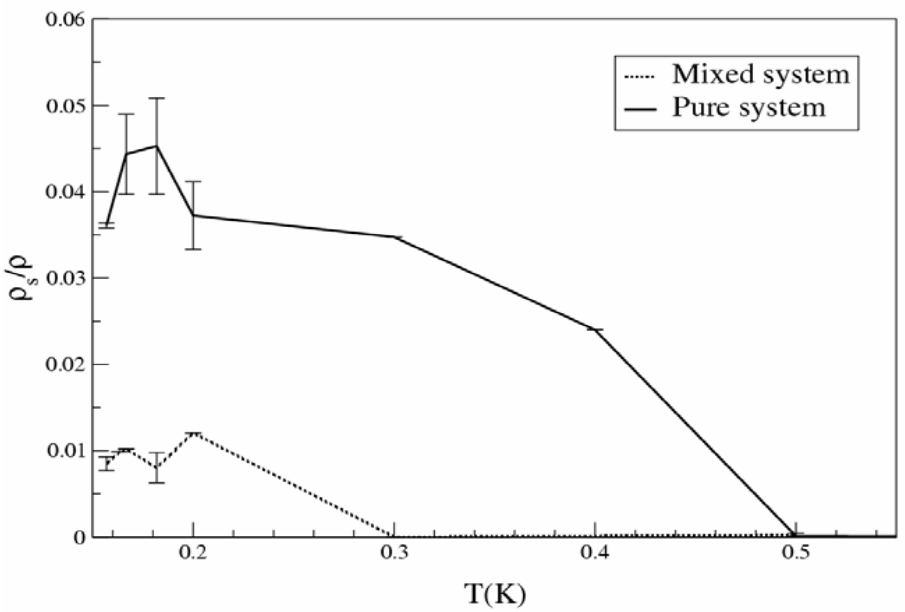


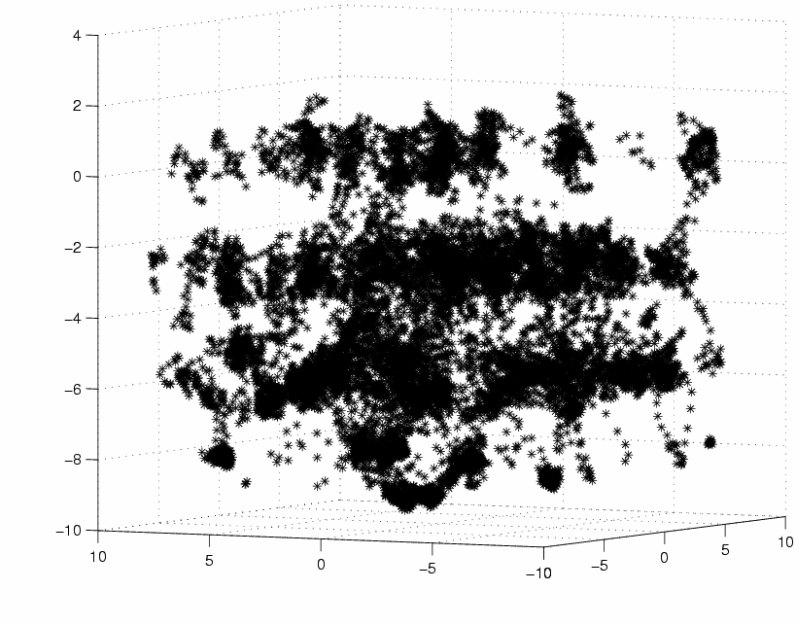
Helium density layer by layer

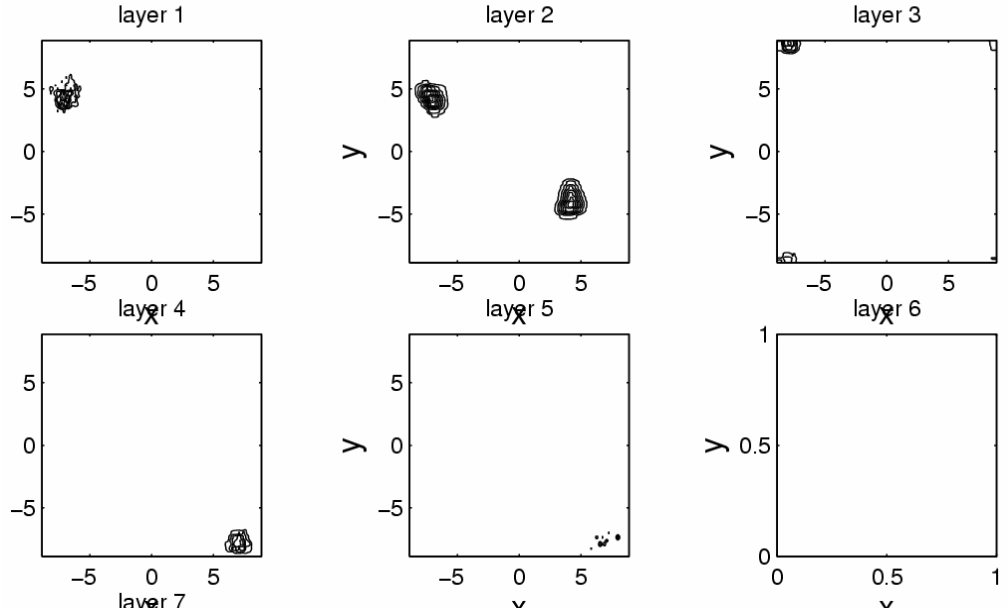


Effect of ^{3}He

- ^{3}He goes to regions where ^{4}He superfluidity is
- Since it cannot exchange, it poisons the windings as in experiment





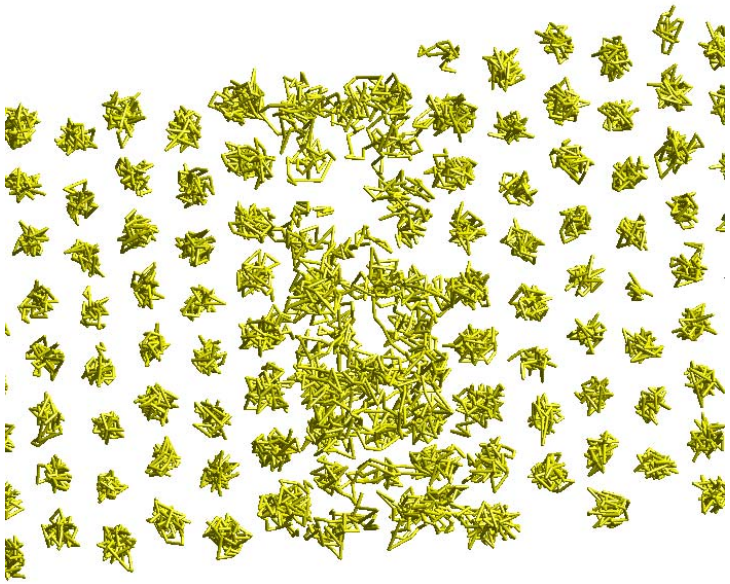


Vycor model

- Reasonable agreement wrt to experiment
- Most superfluid response is in the first few layers.
- Superfluid response is about 2 times larger than experiment (but our cell only has short range disorder)
- ^{3}He poisons superfluid by going to high exchange positions. But 1 atom in our cell is equivalent to 1000ppm.
- How to relate to bulk helium?

Surface model of superfluidity

- Could the effect be due to surface superfluidity?
- With 2% of the sample showing NCRI, then the spacing between the layers would be 500nm
- Grain boundaries: (Burovski et al. PRL 2005) Are there enough grain boundaries?
- Why would the same effect be in vycor, porous gold and bulk helium and be preparation independent and pressure independent?



SUMMARY

- For single-crystal, pure ^{4}He; vacancies, superfluidity, BEC and solidity are in conflict.
- **Contradiction wrt bulk experiment implies at least one approximation must be invalid!**
- **What could it be?**
  - More complicated defects?
    - Grain boundaries or dislocations
    - Large scale quantum defects which oscillate in such a way as to appear to have mass
    - ^{3}He complexes
  - Non-equilibrium/finite frequency effects

The Kim-Chan experiments are not understood from microscopic theory and simulations!

Perhaps study of helium will lead to a deeper understanding of quantum defects!