Supersolid ^{4}He ?

- Some background on superfluid and supersolids
- Path Integral methods for bosons
- Other mechanisms for supersolids?

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What is a super-solid?

Crystal has long range spatial order.

Is translational symmetry spontaneously broken or does it have an external potential such as disordered vycor?

No underlying lattice!

Superfluid has a non-classical response to rotation.

Implies 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.

Solid He

Solid helium is a very quantum solid

Lindemann's rule: solids melt when: $\langle r^2 \rangle^{1/2} = 0.14 r_{NN}$

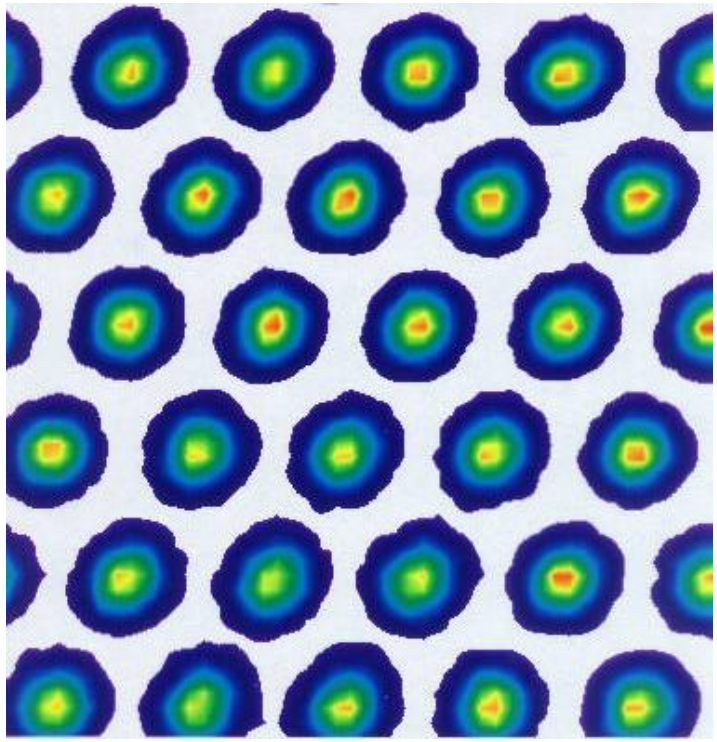
Helium melts when:

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

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

How do we define defects in such a disordered system?

Whether helium is commensurate is a well-defined both theoretically and experimentally.



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?
  - Inhomogenous density gives upper bound to superfluid density

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

Defects and BEC

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

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

Mass and density are of the delocalized quasiparticles

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

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

- Even for a relatively light defect, such a large concentration would have been detected by X-ray scattering. upper limit of roughly 10^{-3} (Simmons)
- Is solid Helium commensurate or not? At T=0, does
  # of lattice sites = # of atoms?

Point defects in a quantum crystal

- Add or subtract an atom keeping density fixed. $E_D = [e(N \pm 1, \rho) - e(N, \rho)](N \pm 1)$
- Calculate total energy using QMC in hcp lattice
- Vacancy energy at melting is ~10K and increases rapidly with density: *Pederiva, Chester, Fantoni, Reatto, PRB 5909 (1997).*
- Consistent with experimental measurements: c<<0.001
- Interstitial energy is even higher ~50K
- Hard to reconcile with ss density dependence.
- Anderson, Brinkman, Huse: Specific heat anomaly suggests incommensurate solid.

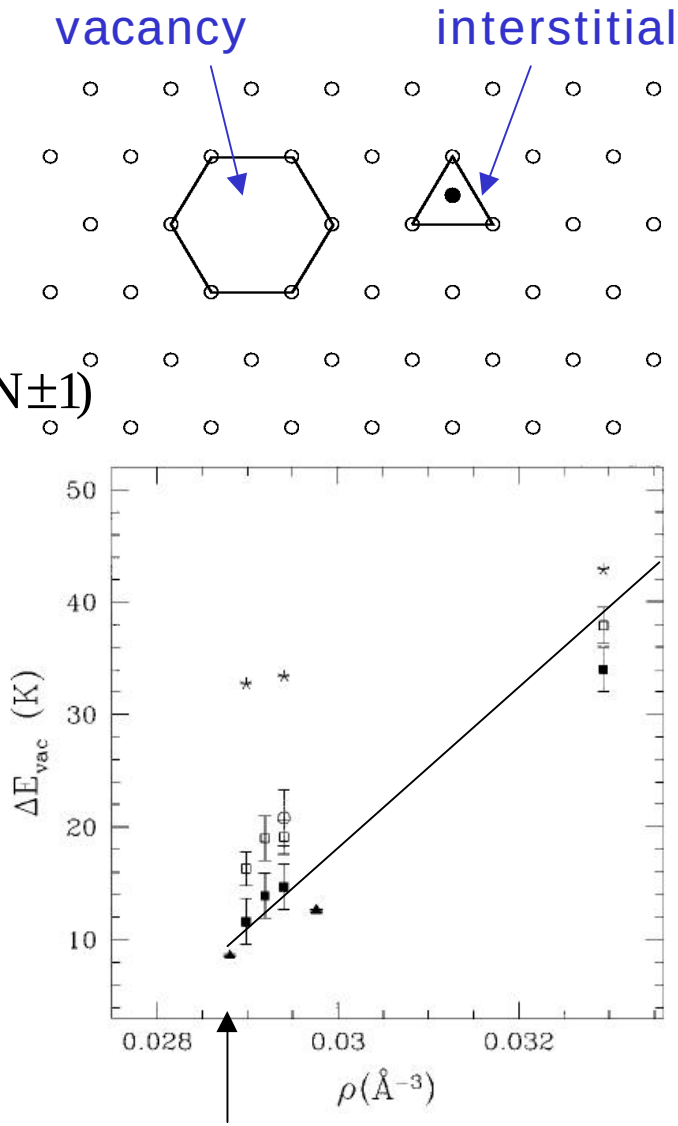


FIG. 1. Vacancy formation energy ΔE_{vac} vs reduced density. Solid triangles: data from Ref. 3, open squares: variational estimates for the fcc phase; filled squares: for the hcp phase; open circle: for the bcc phase. Stars: formation energy of a static vacancy [see Eq. (10) in text].

Assuming no defects, what can theory say what is the trial function for solid helium?

- Wave function (variational) based theories are unreliable because helium is strongly correlated
- Superfluidity and BEC depend on properties of wavefunction tails: when it is small and far off-diagonal. These are very different than energy, structure,… which are all diagonal.
- Path integral Monte Carlo is an exact numerical method, no trial wavefunction, no parameters, except the Hamiltonian
- PIMC has successfully calculated thermodynamics, Lindemann's ratio, correlations, momentum distributions, exchange frequencies,… for liquid and solid helium 3 & 4

Helium: the prototypic quantum system

- A helium atom is an elementary particle. A hard sphere with a weak attraction.
- Interatomic potential is known more accurately than any other atom because electronic excitations are so high.
- Strong correlations in the liquid state caused by the repulsion.

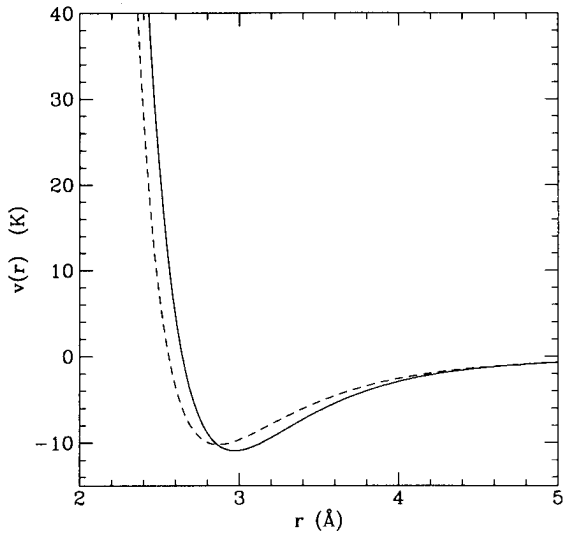


FIG. 1. The semiempirical pair potential between two helium atoms: solid line, Aziz *et al.* (1992); dashed line, Lennard-Jones 6-12 potential with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å.

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

Trotter's theorem

The density matrix is: $\hat{r} = e^{-b(\hat{T}+\hat{V})}$

- Trotter's theorem (1959): $\hat{r} = \lim_{M\to\infty}\left[e^{-t\hat{T}}e^{-t\hat{V}}\right]^M$
- n is number of time slices. $t = b/M$
- Then:

$$Z = \int dR_1 \ldots dR_M \, e^{-\sum_{i=1}^{M} S(R_i, R_{i+1}; t)}$$

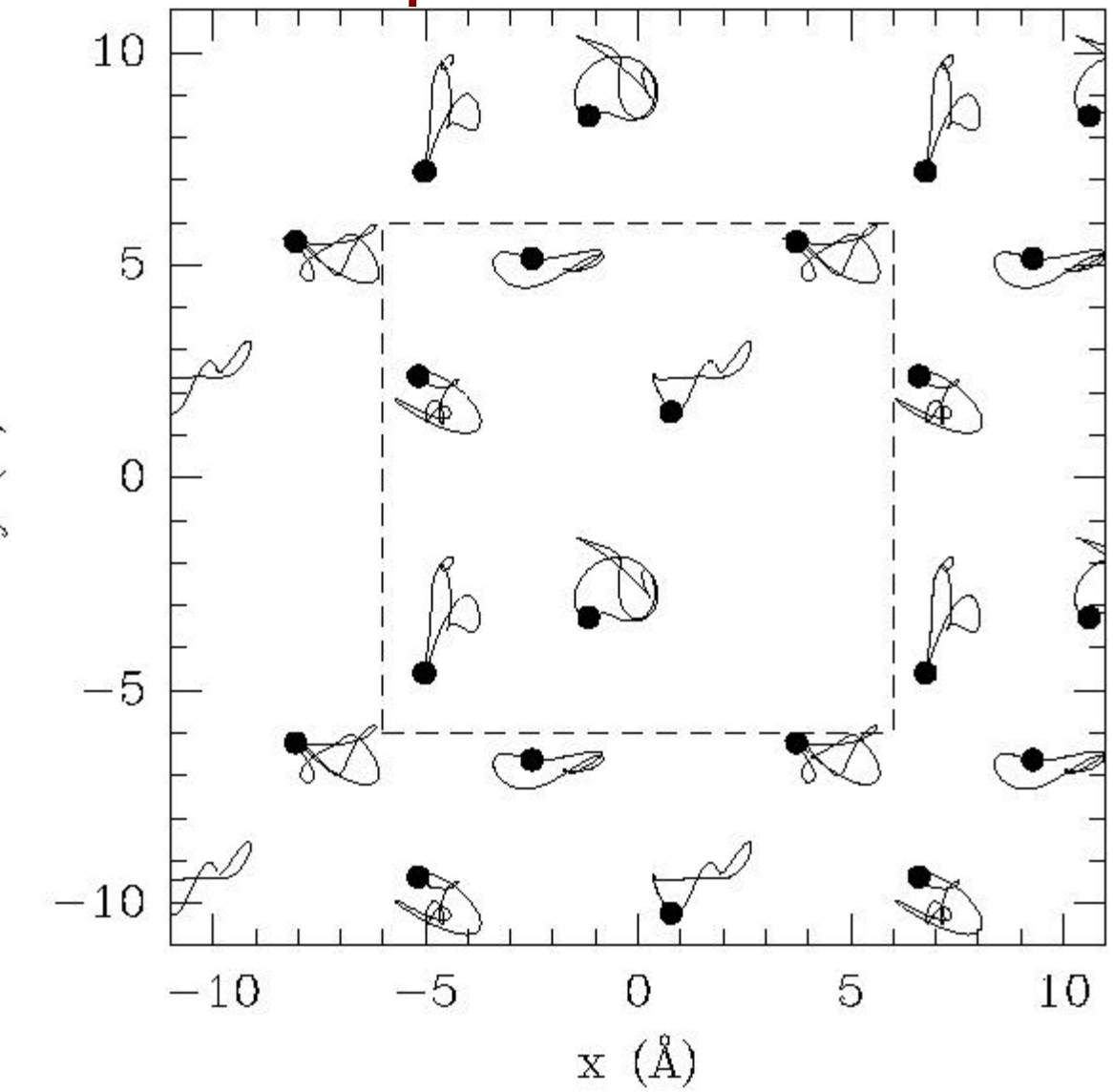
Where the primitive link action is:

$$S(R_0, R_1; t) = -\frac{3N}{2}\ln(4plt) + \frac{(R_0 - R_1)^2}{4?t} + \frac{t}{2}\left[V(R_0) + V(R_1)\right]$$

- Analogous to a classical problem where each particle turns into a "polymer."
- Trace implies $R_0 = R_M$ ⇨ closed or ring polymers

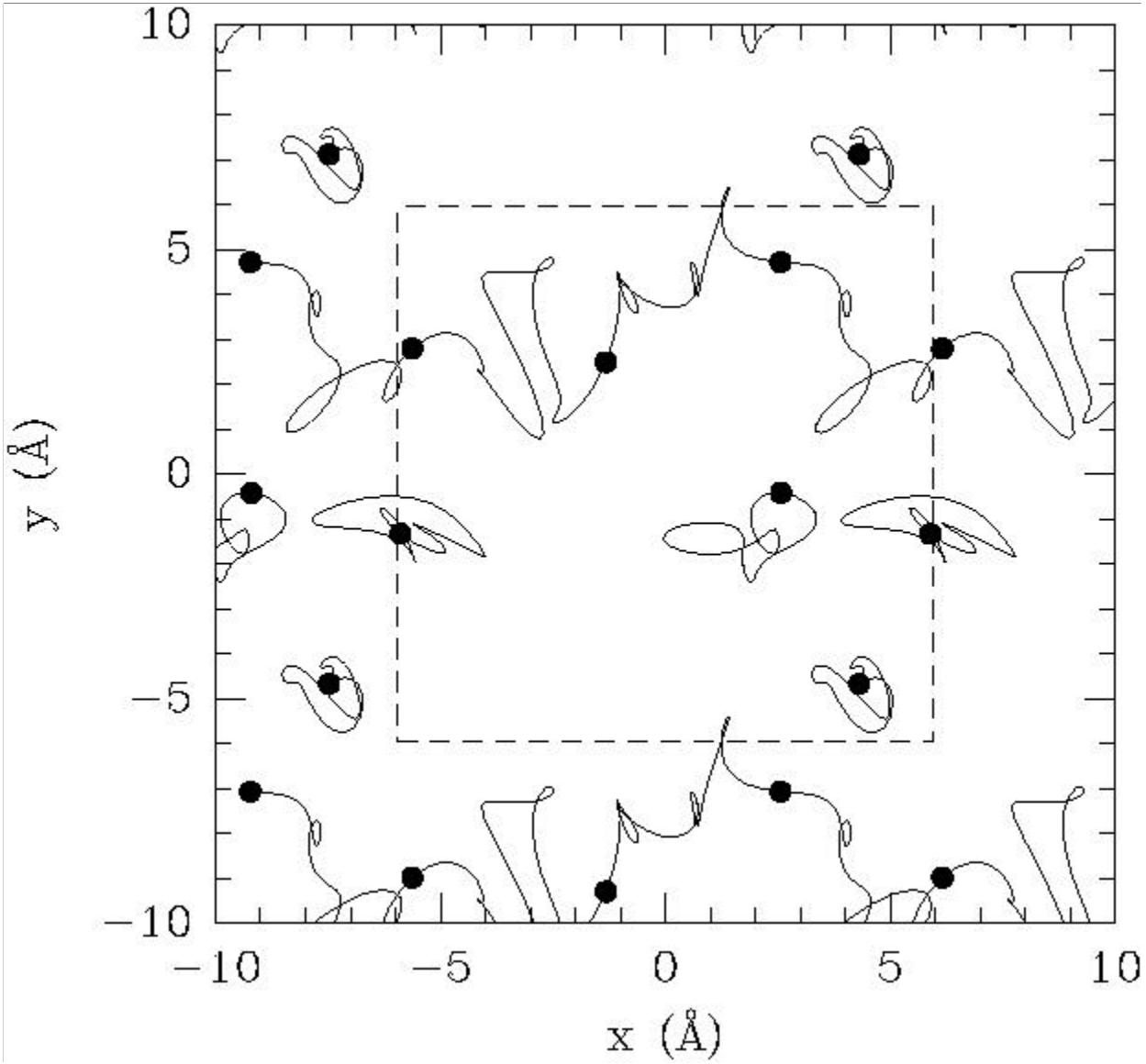
“Distinguishable” particles

- Each atom is a ring polymer; an exact representation of a quantum wavepacket in imaginary time.
- Integrate over all paths
- Trace picture of 2D helium. The dots represent the “start” of the path. (but all points are equivalent)
- The lower the real temperature, the longer the “string” and the more spread out the wavepacket.

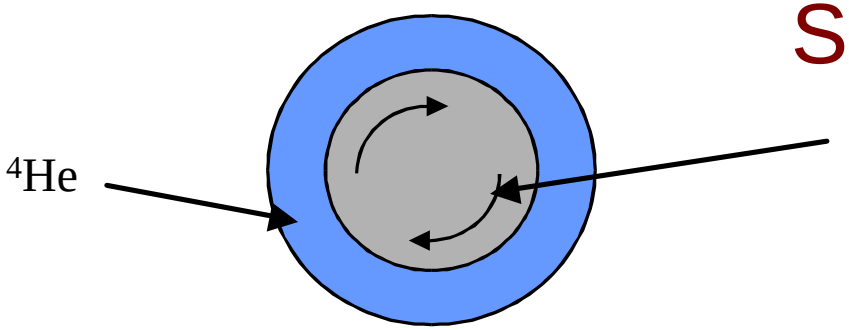


Exchange picture

- Sum over all paths and over connections.
- Trial moves involve changing the connections
- At the superfluid transition a “macroscopic” permutation appears.
- This is reflection of bose condensation within PIMC.



Superfluidity and PIMC



rotating disks:

Andronikashvili's expt (1946)

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

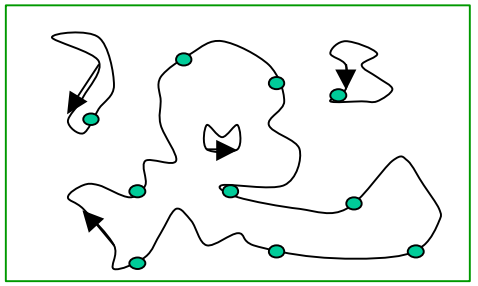
- We define superfluidity as a linear response to a velocity perturbation (the energy needed to rotate the system) "NCRI = nonclassical rotational inertia"

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

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

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

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

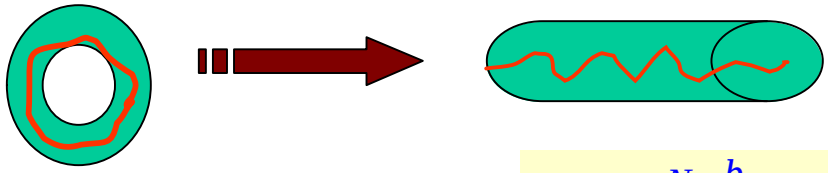


$$\frac{r_s}{r} = \frac{2m}{b\ l\ I_c}\left\langle A_z^2 \right\rangle$$

A = signed area of imaginary-time paths

Winding numbers in periodic boundary conditions

- Distort annulus



- The area becomes the **winding** (average center of mass velocity)

$$W = \sum_{i=1}^{N} \int_{0}^{b} dt \, \frac{dr_i(t)}{dt}$$

- The superfluid density is now estimated as:

$$\frac{r_s}{r} = \frac{\langle W^2 \rangle}{2lbN}$$

- Exact linear response formula. (analogous to relation between $\chi \sim \langle M^2 \rangle$ for Ising model.
- Relates **topological** property of paths to dynamical response. Explains why superfluid is "protected."
- Imaginary time dynamics is related to real time response.
- How the paths are connected is more important than static correlations.

Thouless theory of exchange in quantum crystals

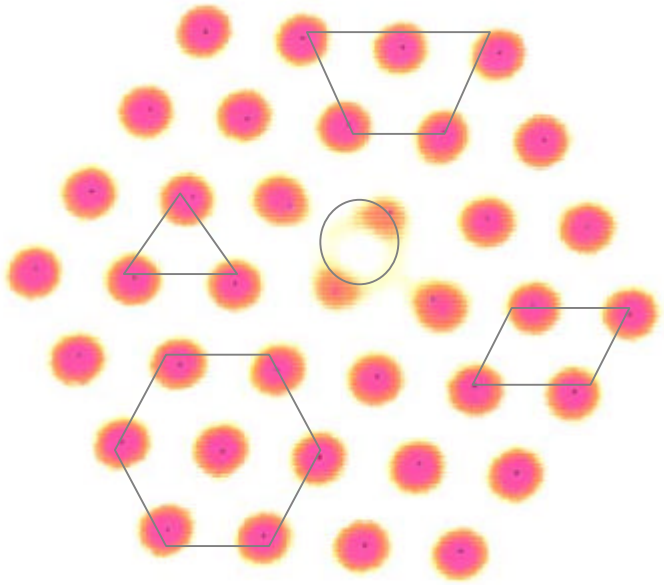
- At low temperature there are **very** few defects, phonons, etc.
- The many body wavefunction has N! peaks, corresponding to possible atom relabelings.
- We can write the partition function in terms of permutation of lattice sites:

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

Break permutation into "cycles"

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

$$f_p(b) = b\, J_p$$



Q_0 unimportant at low temperatures

- Related to the Feynman-Kikuchi model of lambda transition in liquid helium and to magnetism in solid ^{3}He.

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:

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

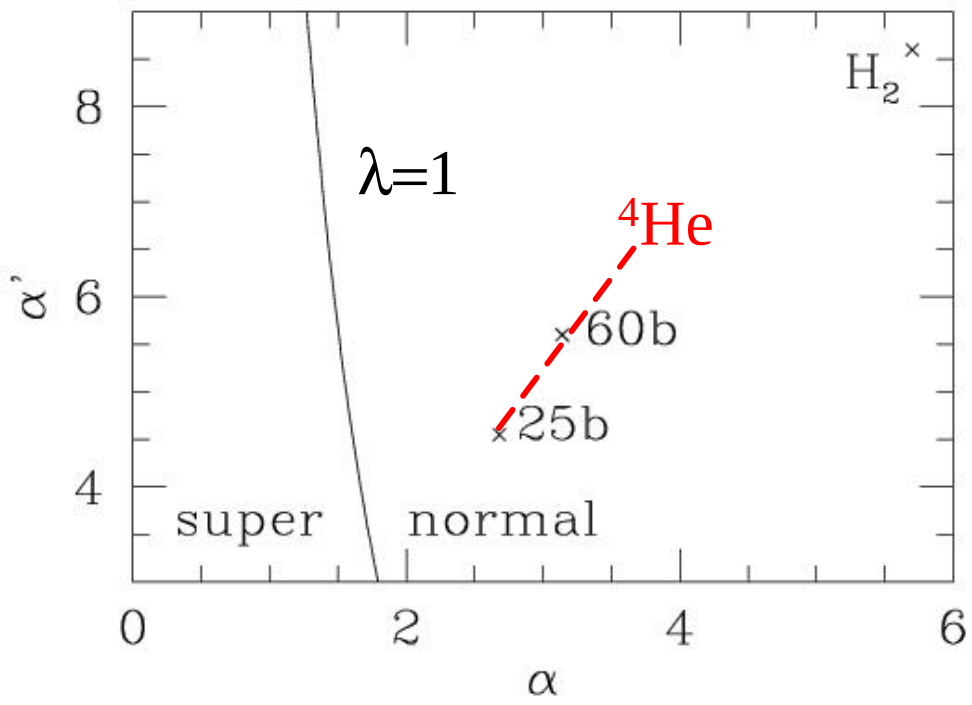
•Localized exchanges have no winding, do not transport mass, and are not related to supersolidity.

•Need frequent, macroscopic exchanges for supersolidity.

Phase diagram of lattice model

- 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!
- H_2 is even worse.

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



Bose condensation

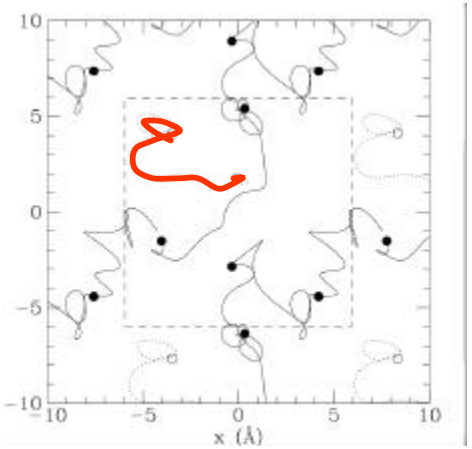
- BEC is the macroscopic occupation of a single quantum state (e.g. zero momentum state).

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

- The one particle density matrix is defined as:

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

- For n(r,s) we need one open path:



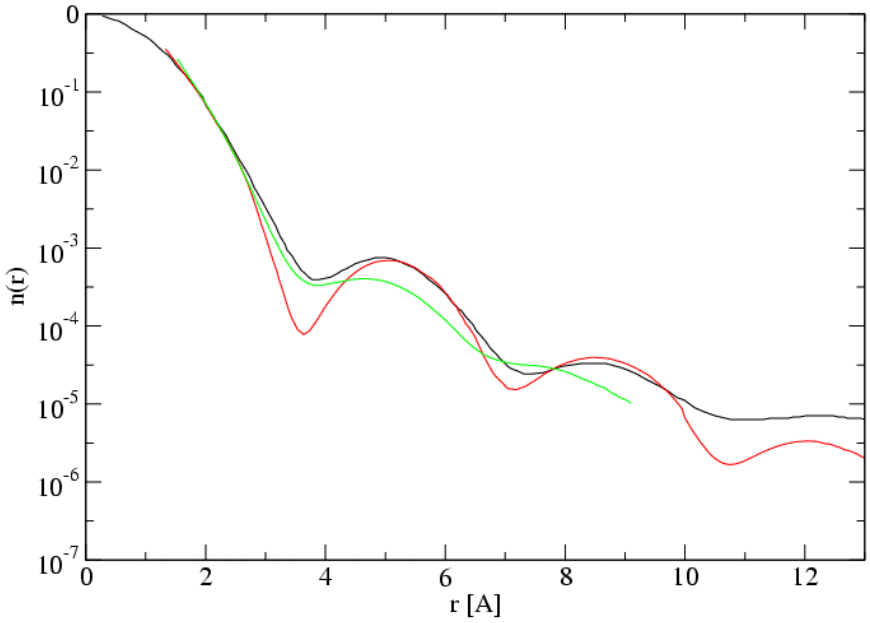
- It can then exchange & separate

- Condensate fraction is probability of the ends being widely separated versus localized. **ODLRO** (off-diagonal long range order)

BEC in solid Helium?

- 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

- Galli & Reatto use “shadow wave functions” find a very small (10^{-5}) but non-zero condensate, probably because of trial function bias.



Two types of quantum bose solids

"metallic"

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

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

"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

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

PIMC strongly favors the insulator picture:

a perfect ^{4}He crystal is not superfluid

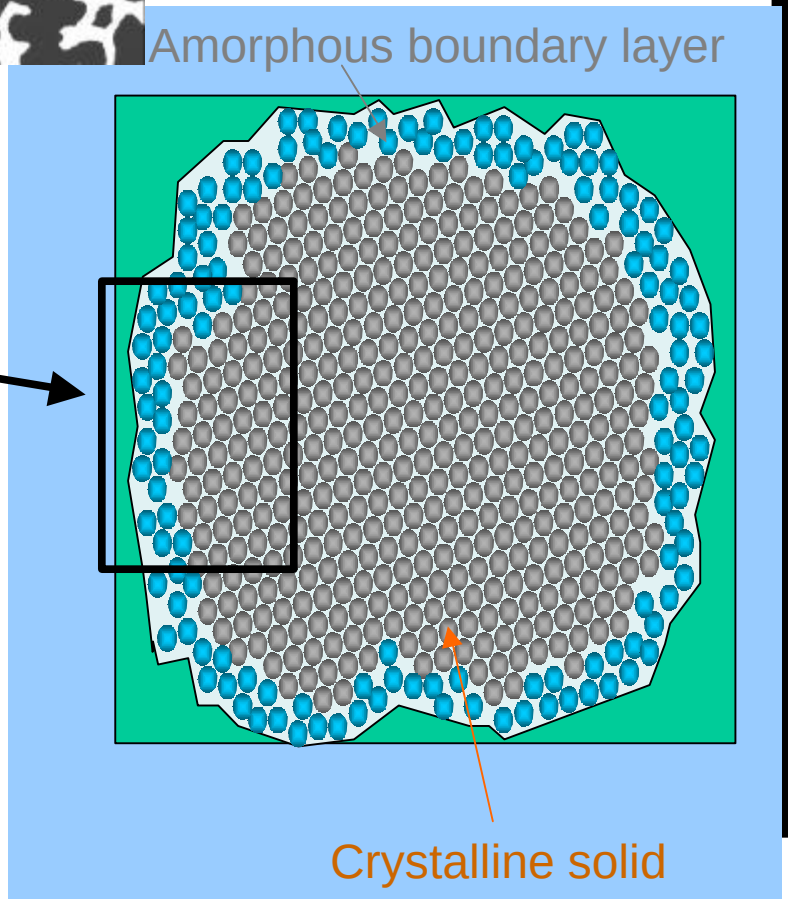
Surface model of superfluidity

- Could the effect be due to surface superfluidity?
- With 2% of the sample superfluid, then the spacing between the layers would by 500nm. (Need to know the width of the superfluid layer; width cannot depend on pressure)
- grain boundaries: (Burovski et al. PRL 2005) Are there enough grain boundaries? How many superfluid layers at a grain boundary?
- Why would the same effect be in vycor, porous gold and bulk helium and be preparation independent and pressure independent?

Solidification in Vycor

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

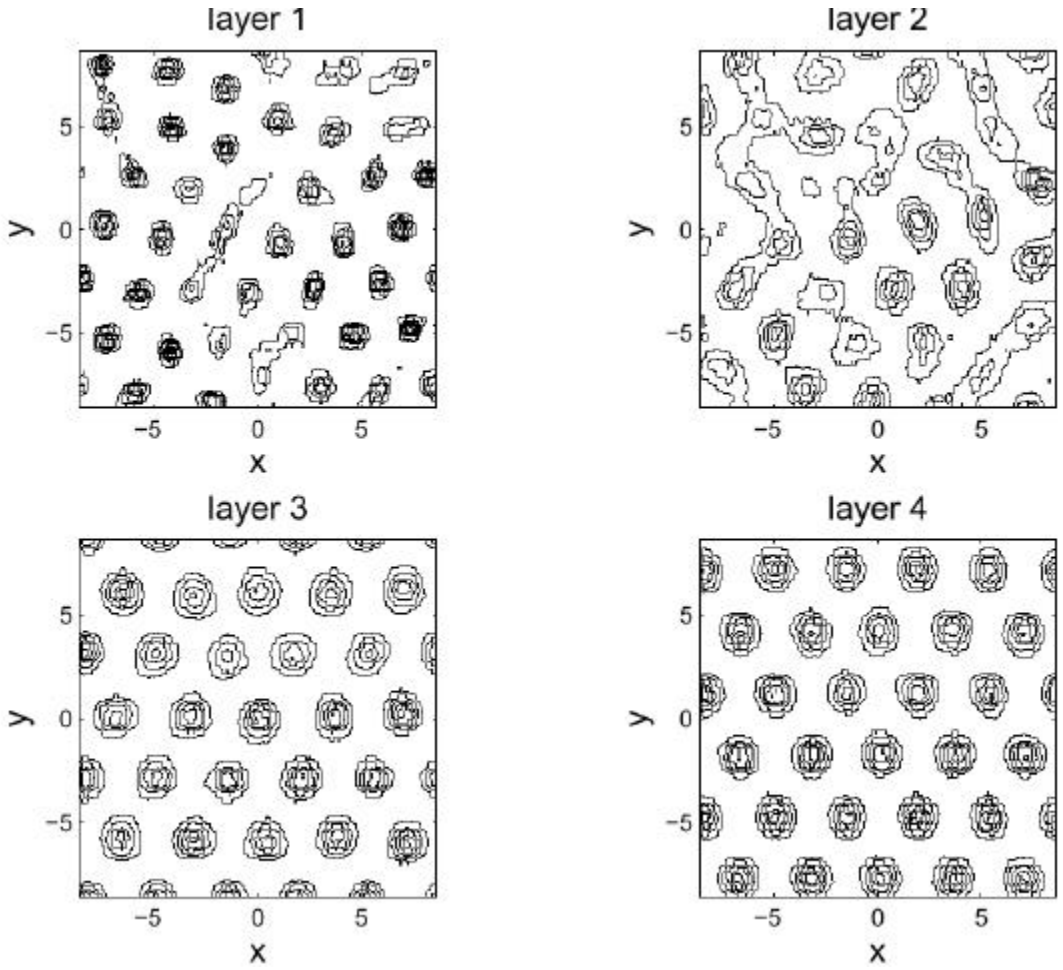
PIMC model



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?

Configuration of Helium



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?

Dislocation model

- Perhaps dislocations undergo a transition below 0.2K (open a gap, move freely, kinky-BEC….)

- Could explain the sensitive dependence on ^{3}He. (They are known localize on dislocations below 1K and to pin their motion)
- Are dislocation properties weakly dependant on pressure?

- Could explain Day-Beamish experiment if the dislocations cannot move very far because of pinning.

Questions

- What mechanism would be independent of pressure, confining medium and even of quantum solid
- How sensitive is the effect to crystal growth?
- What is the frequency dependence?
- Why no feature in the specific heat?
- Is the ground state commensurate?(anything more sensitive than scattering?)
- What is the ^{3}He dependence?