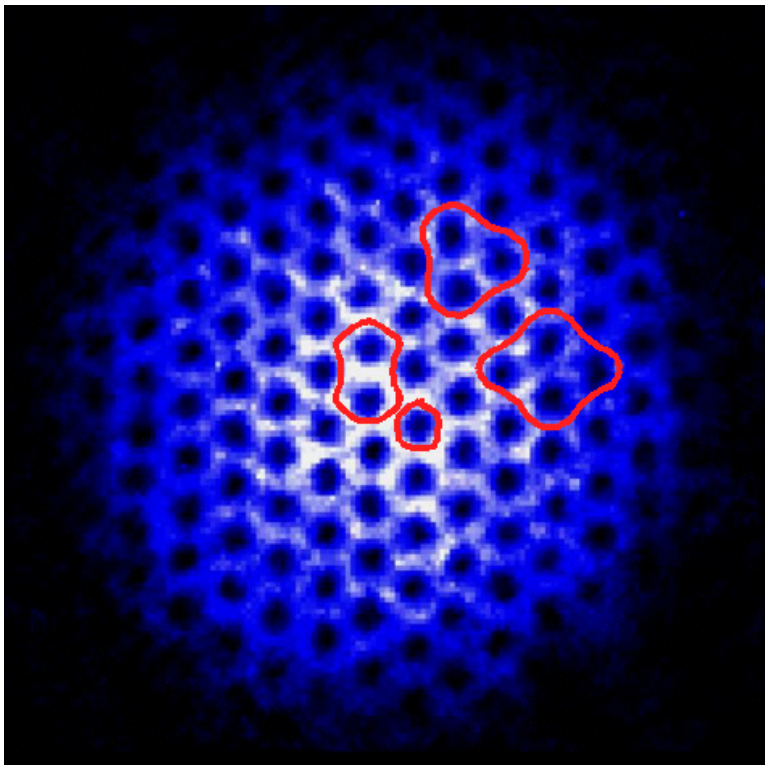


Path Integral Monte Carlo for Bosons

Summer school 2012 “QMC Theory and Fundamentals”



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Properties of Bosons and Fermions

	Bosons	Fermions
Spin	0, 1, 2, 3, ...	1/2, 3/2, ...
Elemental particles	Photons, W & Z bosons	Electrons, protons, neutrons, quarks
Compound particles	^4He atoms, phonons	^3He atoms
Statistics	Bose-Einstein	Fermi-Dirac
Wavefunction type	Symmetric	Antisymmetric
Effects	Bose condensation	Pauli exclusion

Bosonic and Fermionic Path Integrals

Bosonic density matrix:
Sum over all symmetric eigenstates.

$$\rho_B(R, R', \beta) = \sum_i e^{-\beta E_i} \Psi_S^{[i]*}(R) \Psi_S^{[i]}(R')$$

Fermionic density matrix:
Sum over all antisymmetric eigenstates.

$$\rho_F(R, R', \beta) = \sum_i e^{-\beta E_i} \Psi_{AS}^{[i]*}(R) \Psi_{AS}^{[i]}(R')$$

Project out symmetric and antisymmetric states:

$$\rho_{B/F}(R, R', \beta) = \sum_i e^{-\beta E_i} \sum_P (\pm 1)^P \Psi^{[i]*}(PR) \sum_{P'} (\pm 1)^{P'} \Psi^{[i]}(P'R')$$

Apply projection to the density matrix:

$$\rho_B(R, R', \beta) = \sum_P (+1)^P \rho_D(R, PR', \beta)$$

$$\rho_F(R, R', \beta) = \sum_P (-1)^P \rho_D(R, PR', \beta)$$

$$\langle R | \hat{\rho}_{F/B} | R' \rangle = \sum_P (\pm 1)^P \int dR_1 \dots \int dR_{M-1} \langle R | e^{-\tau \hat{H}} | R_1 \rangle \dots \langle R_{M-1} | e^{-\tau \hat{H}} | PR' \rangle$$

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Project out the symmetric states:

$$\rho_B(R, R', \beta) = \sum_P (+1)^P \rho_D(R, PR', \beta)$$

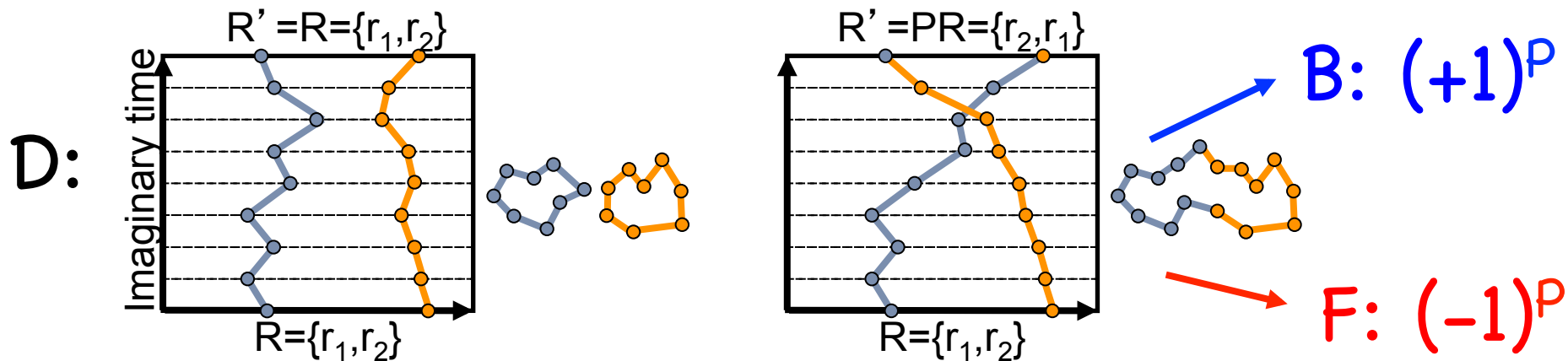
Fermionic density matrix:
Sum over all antisymmetric eigenstates.

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Project out the antisymmetric states:

$$\rho_F(R, R', \beta) = \sum_P (-1)^P \rho_D(R, PR', \beta)$$

$$\langle R | \hat{\rho}_{F/B} | R' \rangle = \sum_P (\pm 1)^P \int dR_1 \dots \int dR_{M-1} \langle R | e^{-\tau \hat{H}} | R_1 \rangle \dots \langle R_{M-1} | e^{-\tau \hat{H}} | PR' \rangle$$



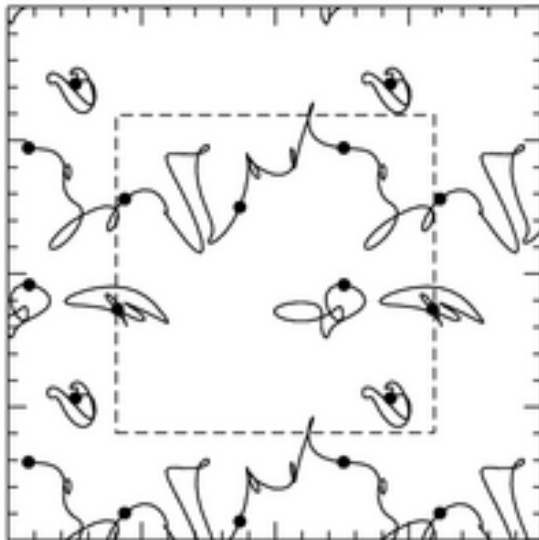
Particle Statistics

leads to exchange effects represented by permutations

Symmetry leads to bosonic and fermionic path integrals

$$\langle R | \hat{\rho}_{F/B} | R' \rangle = \sum_P (\pm 1)^P \int dR_1 \dots \int dR_{M-1} \langle R | e^{-\tau \hat{H}} | R_1 \rangle \dots \langle R_{M-1} | e^{-\tau \hat{H}} | PR' \rangle$$

Bosons: Long permutation cycles, only **positive** contributions
→ superfluidity in ^4He



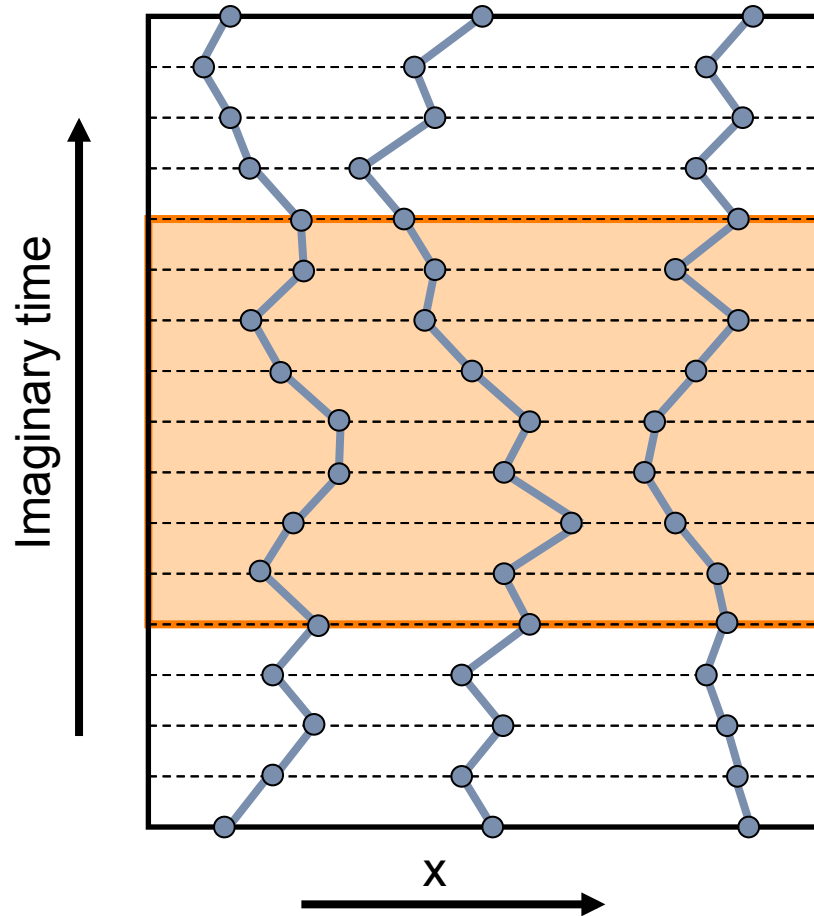
Fermions: Cancellation of **positive** and **negative** contributions
→ **Fermion sign problem**, efficiency $e^{-\beta N}$

Fixed node approximation

$$\langle R | \hat{\rho}_F | R' \rangle = \sum_P (-1)^P \oint_{\rho_T \geq 0} dR_t e^{-S[R_t]}$$

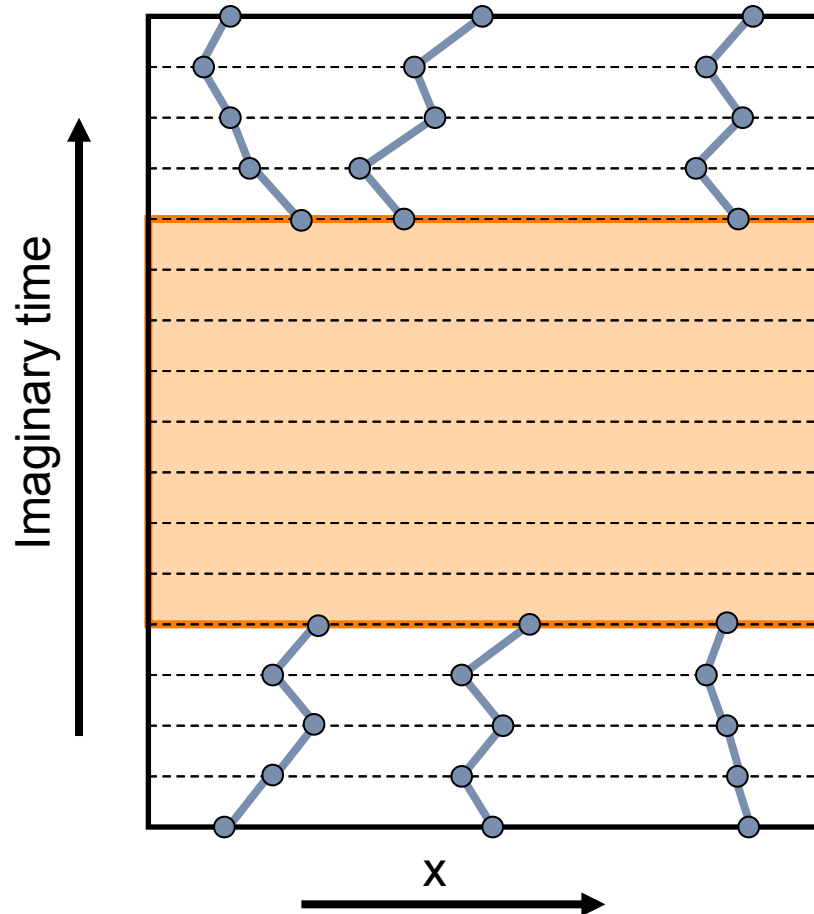
I. Permutation sampling

How do we sample the permutation space?



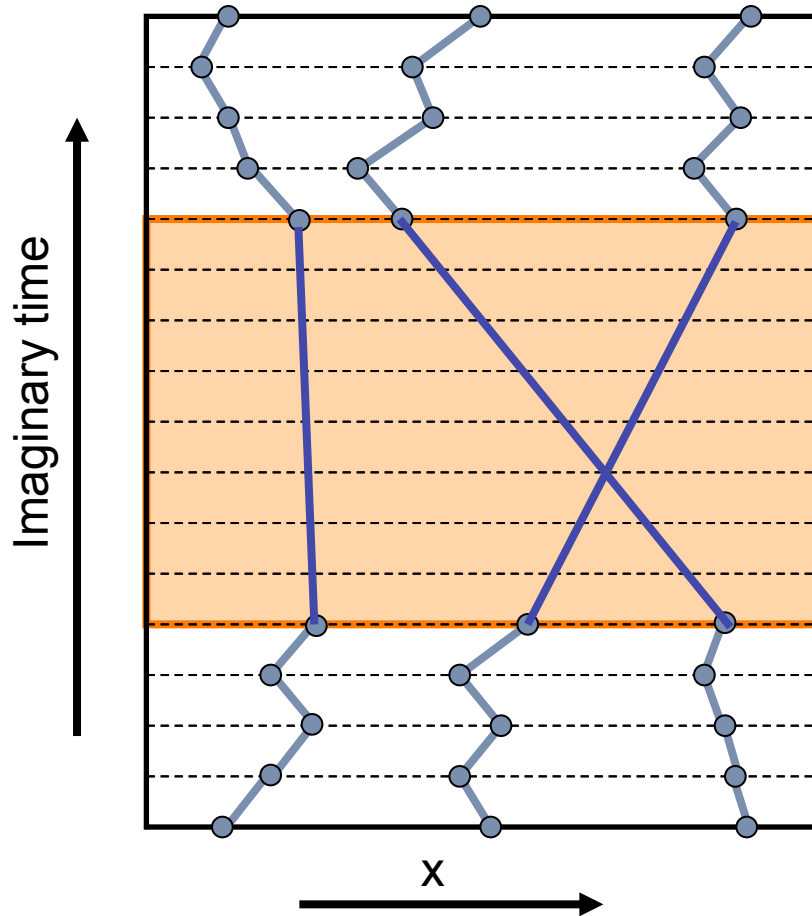
Step 0: Pick an imaginary time window

How do we sample the permutation space?



Step 0: Pick an imaginary time window
Step 1: Study all possible permutations
and determine their sign.

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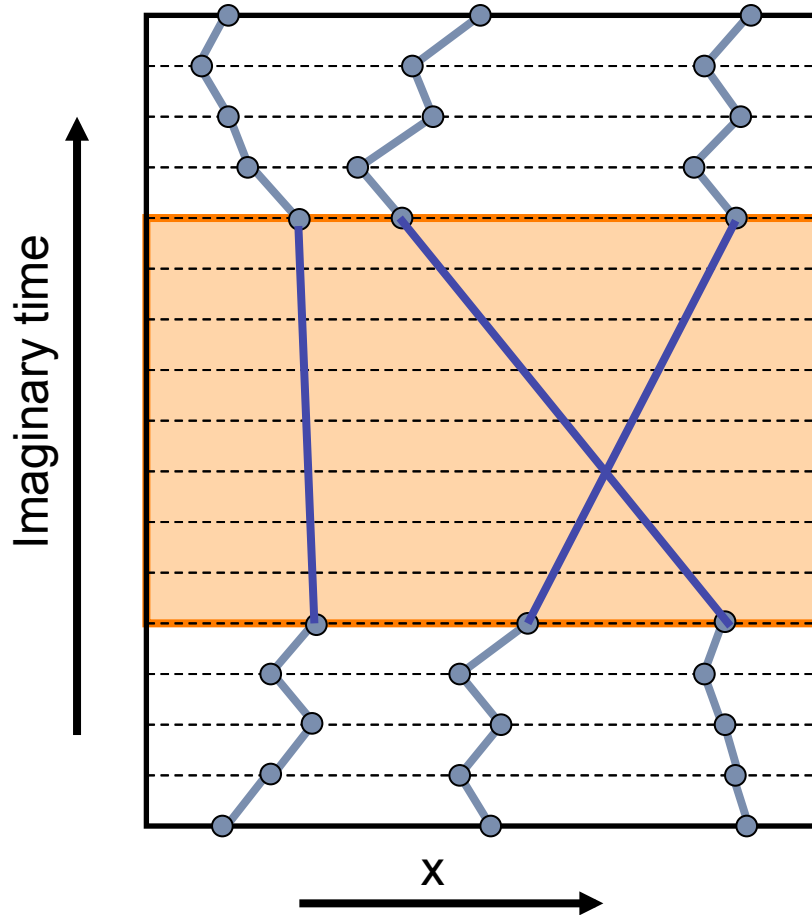
(1 2 3)
↓
(1 2 3)
P=+1

Identity permutation (1)

(1 2 3)
↓
(1 3 2)
P=-1

2-particle permutation (3)

How do we sample the permutation space?



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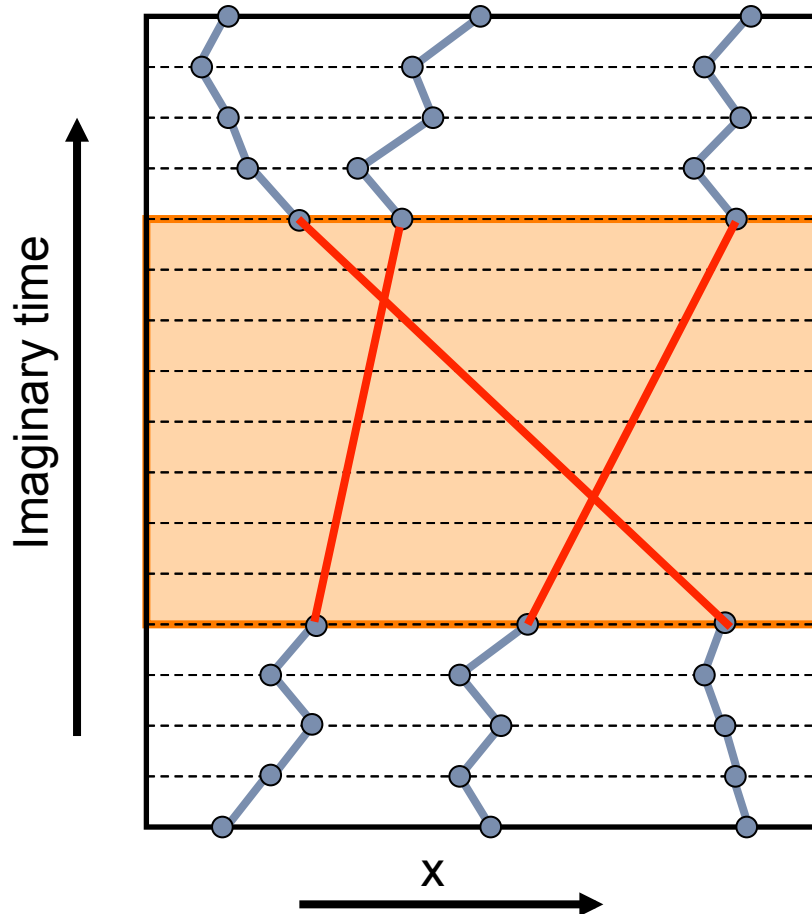
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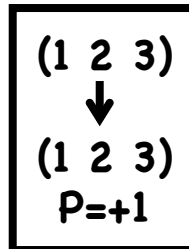
2-particle permutation

How many 2-particle permutations are there?

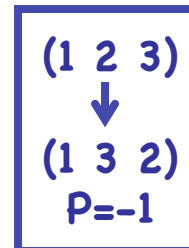
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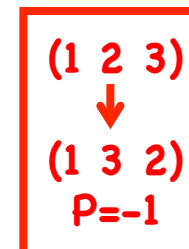
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Identity permutation (1)

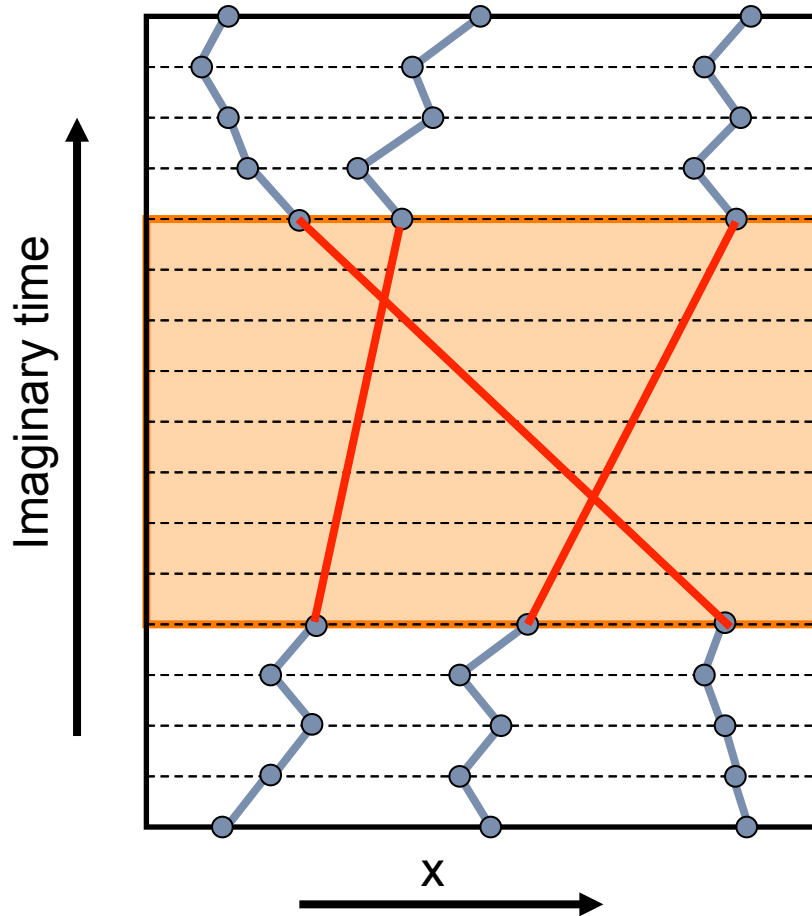


2-particle permutation (3)



3-particle cyclic permutation

How do we sample the permutation space?



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↓
(1 2 3)
 $P=+1$

Identity permutation (1)

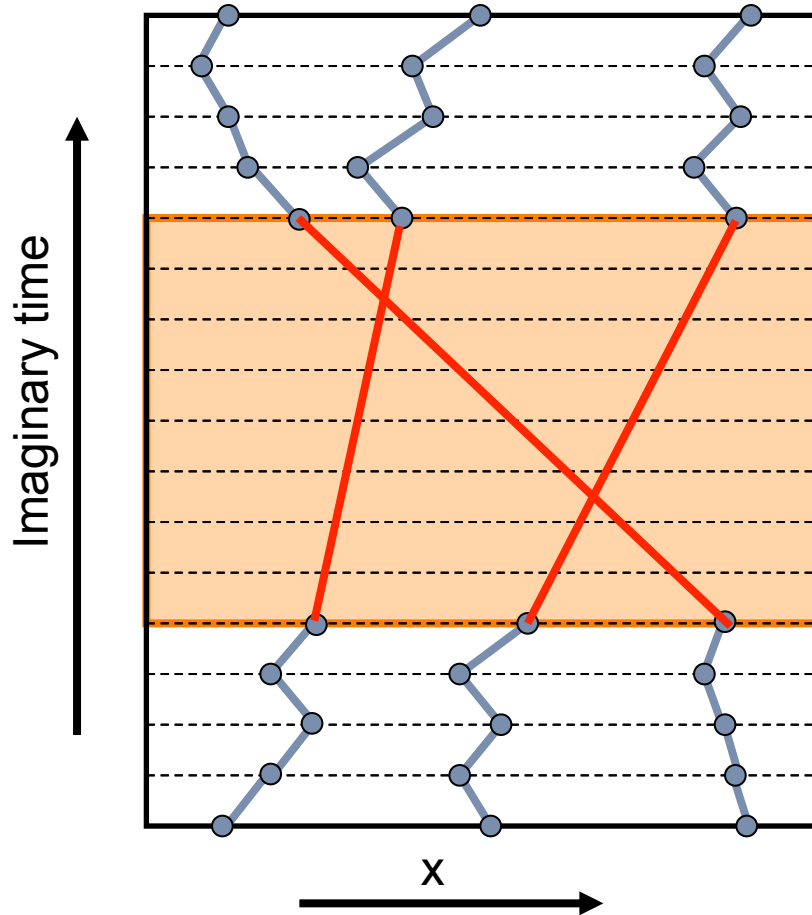
(1 2 3)
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(1 3 2)
 $P=-1$

2-particle permutation (3)

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↓
(1 3 2)
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3-particle cyclic permutation (2)

How do we sample the permutation space?



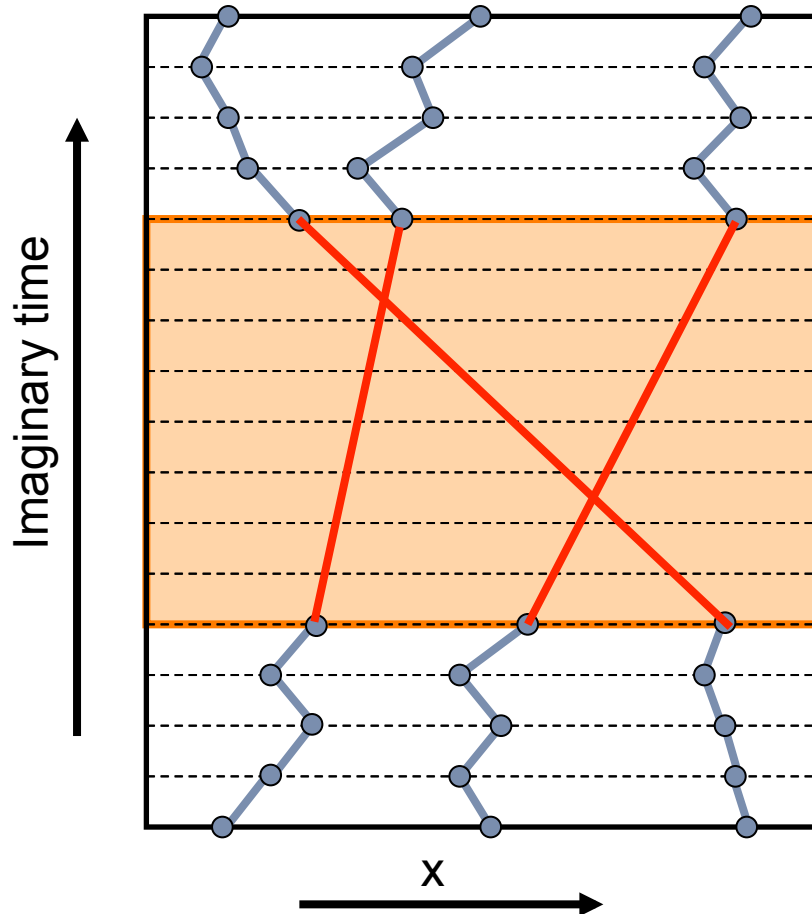
Step 0: Pick an imaginary time window

Step 1: Study all possible permutations and determine their sign.

Step 2: Build a table containing all possible permutations based on the free particle density matrix:

$$\pi(P) = \frac{\rho(R_0, PR_8, 8\tau)}{\sum_{P'} \rho(R_0, P'R_8, 8\tau)}$$

How do we sample the the **full** permutation space?



Step 0: Pick an imaginary time window

Step 1: Study all possible permutations and determine their sign.

Step 2: Build a table containing **all possible permutations** based on the free particle density matrix:

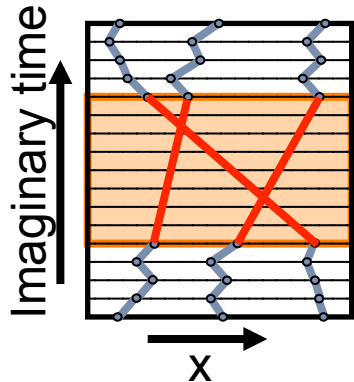
$$\pi(P) = \frac{\rho(R_0, PR_8, 8\tau)}{\sum_{P'} \rho(R_0, P'R_8, 8\tau)}$$

Step 3: Pick from permutation table

Step 4: Regrow the permuted path using the bisection or Levy method.

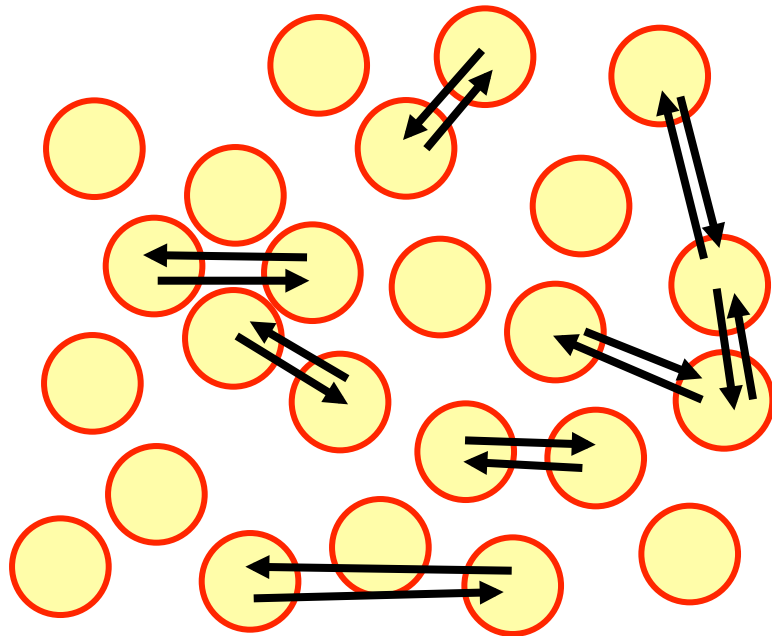
Step 5: Accept or Reject based on action.

How to construct a table containing all likely permutations?



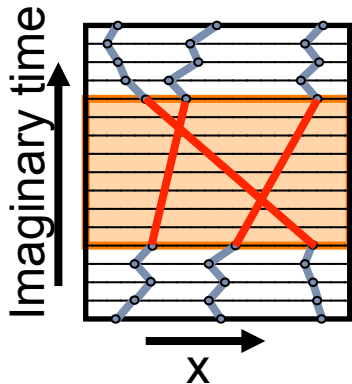
$$\pi(P) = \frac{\rho(R_0, PR_8, \delta\tau)}{\sum_{P'} \rho(R_0, P'R_8, \delta\tau)}$$

Step 0: Pick an imaginary time window
Step 1: Include all **two-particle permutations** that have a good chance of acceptance. Discriminate against distant pairs.



Step 3: Pick from permutation table
Step 4: Regrow the permuted path using the bisection or Levy method.
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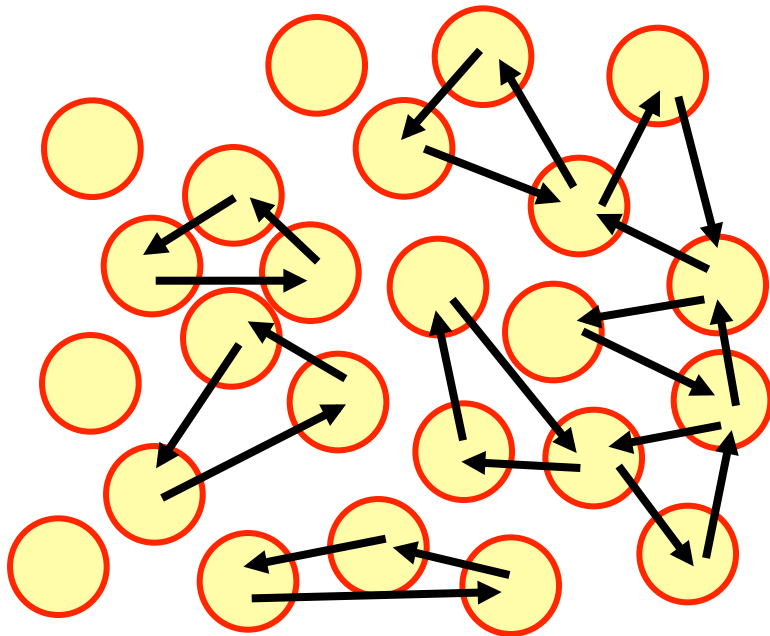
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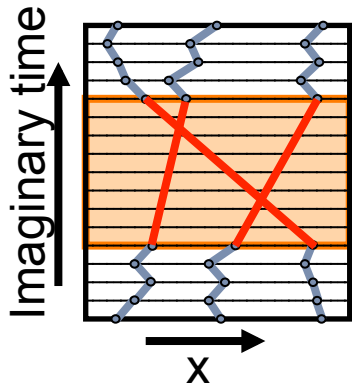
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Step 2: Include all likely **three-particle permutations**. Enter them with any increased probability to try to such move more often (to sample the superfluid state better). Detailed balanced remains satisfied.



How to construct a table containing all likely permutations?

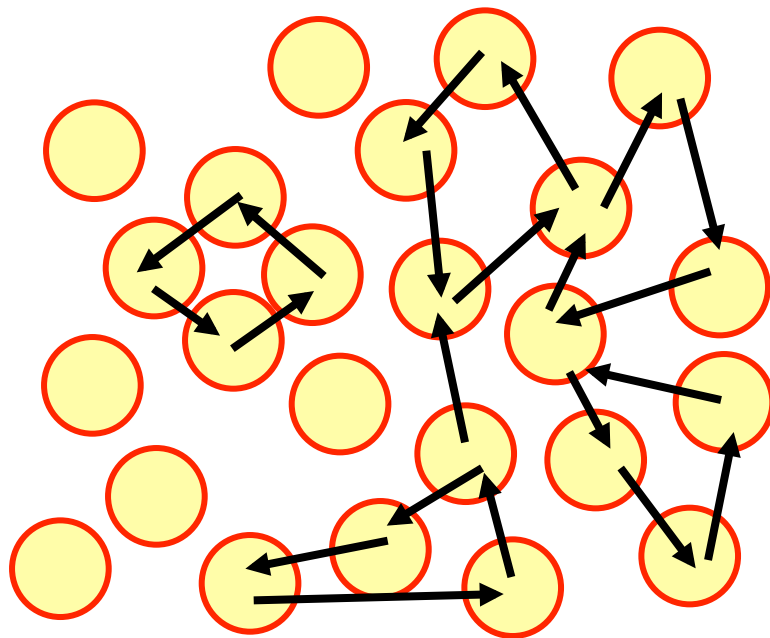


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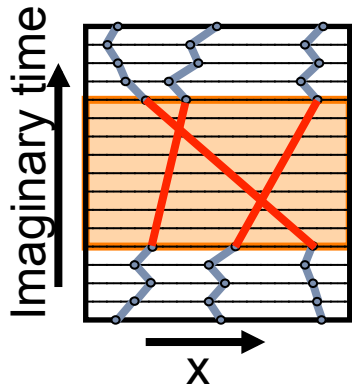
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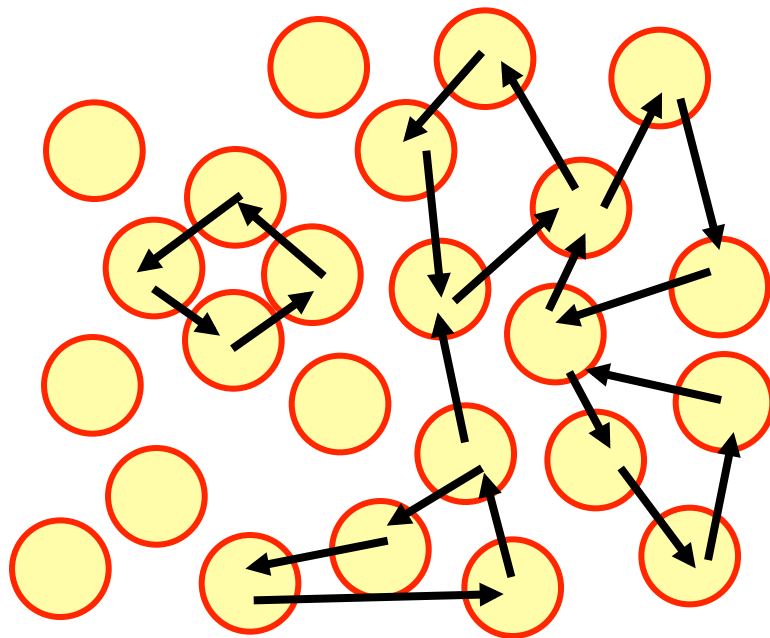
Step 3: **4 body-permutations**



How to construct a table containing all likely permutations?



$$\pi(P) = \frac{\rho(R_0, PR_8, \delta\tau)}{\sum_{P'} \rho(R_0, P'R_8, \delta\tau)}$$



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Step 3: **4 body-permutations**

Step 4: Regrow the permuted path using the bisection or Levy method.

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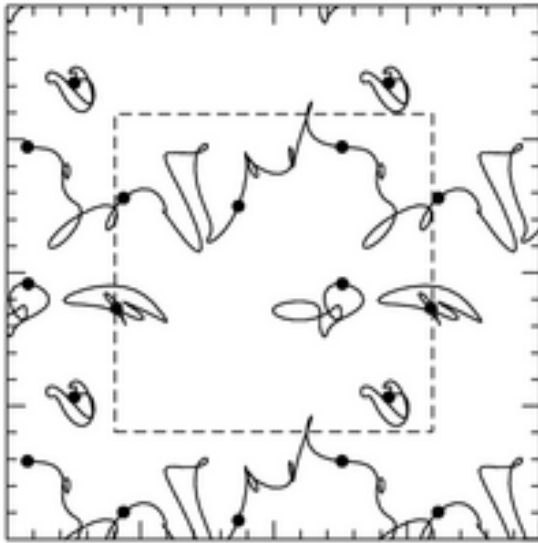
II. Superfluidity

Permutations in bosonic path integrals can explain superfluidity in ^4He

Symmetry leads to bosonic and fermionic path integrals

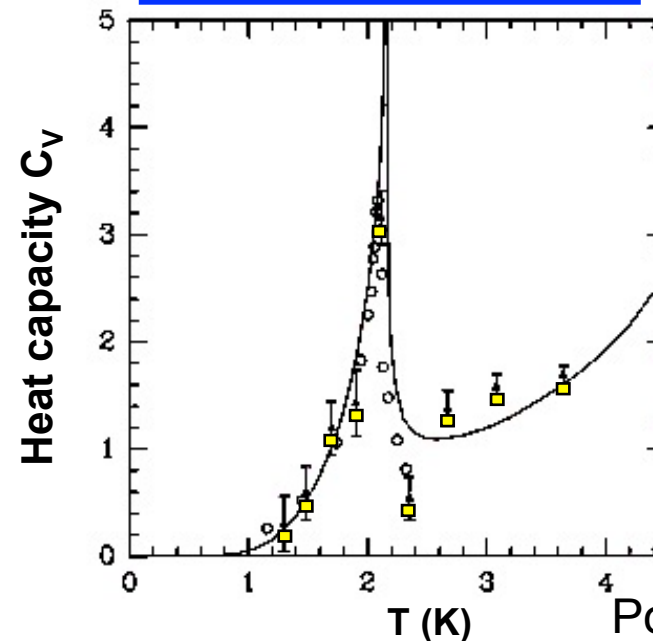
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Bosons: Long permutation cycles, only **positive** contributions
 \rightarrow superfluidity in ^4He



PIMC reproduces λ -transition in ^4He

$$\langle C_V \rangle = \frac{3}{2} - 2 \frac{T \langle x \rangle}{N} + \frac{T^2 \langle (x - \langle x \rangle)^2 \rangle}{N}$$



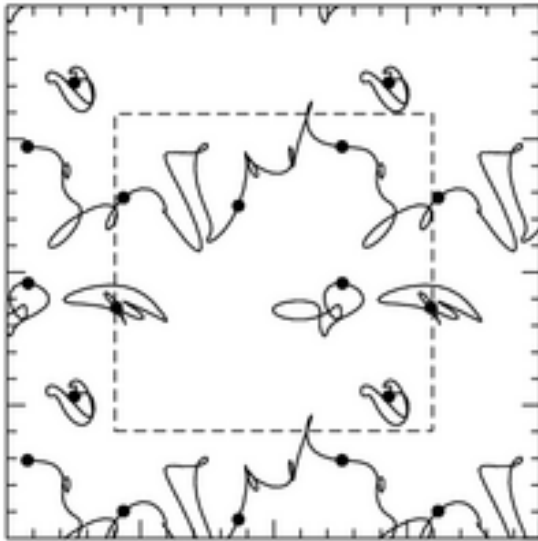
[Ceperley, Pollock (1986)]

Permutations in bosonic path integrals can explain superfluidity in ^4He

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Bosons: Long permutation cycles, only **positive** contributions
→ superfluidity in ^4He



Bose-Einstein condensation (BEC) occurs when the thermal de Broglie wavelength is of the interatomic spacing:

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

Most systems will **freeze** instead of becoming a superfluid, even light particles as H_2 molecules. In He^4 , the **zero-point energy** overcomes the lattice confinement.

What is superfluidity?

Pyotr Kapitza* discovered that liquid helium flows without friction when cooled below 2.17 K. This phenomenon is termed **superfluidity**. A superfluid shows several spectacular effects. For example, superfluid helium cannot be kept in an open vessel because then the fluid creeps as a thin film up the vessel wall and over the rim.

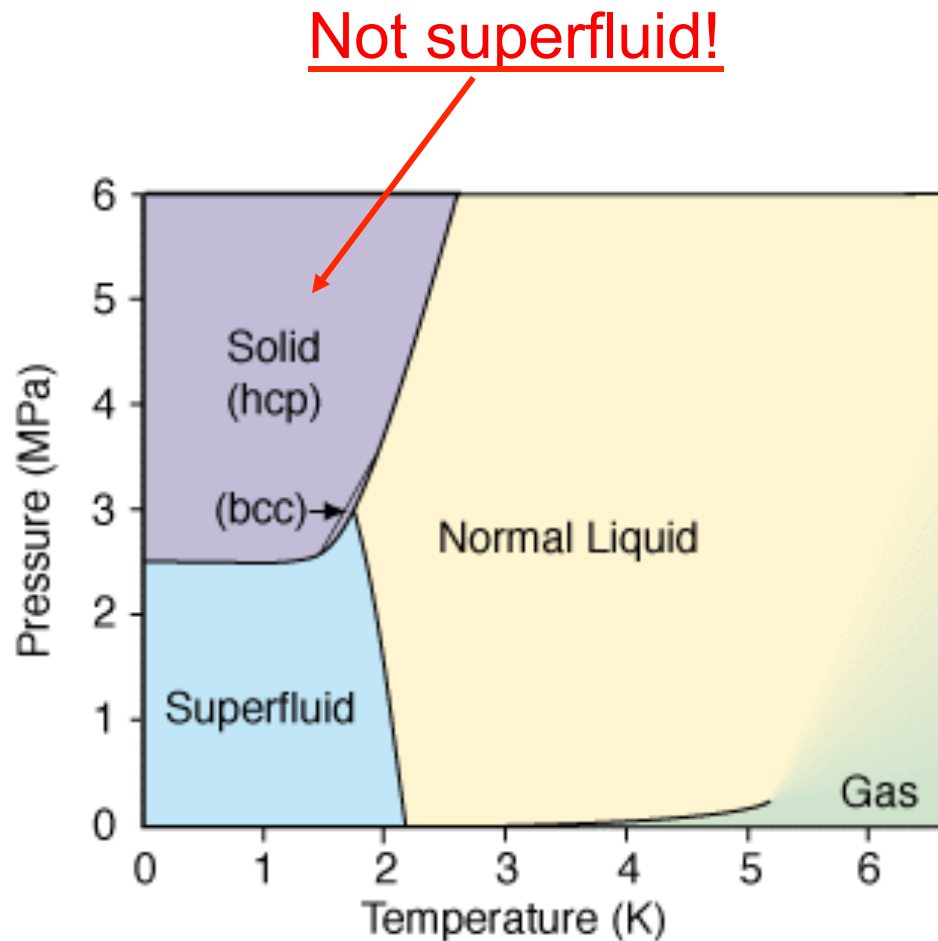


*Nobel Prize 1978

A superfluid has no surface tension.

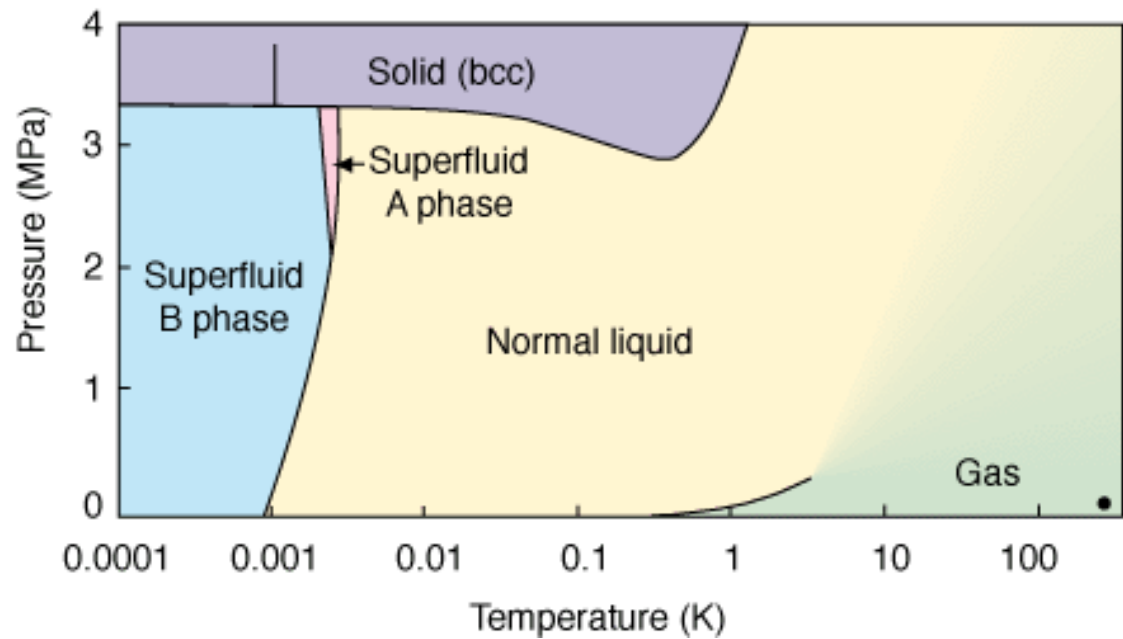
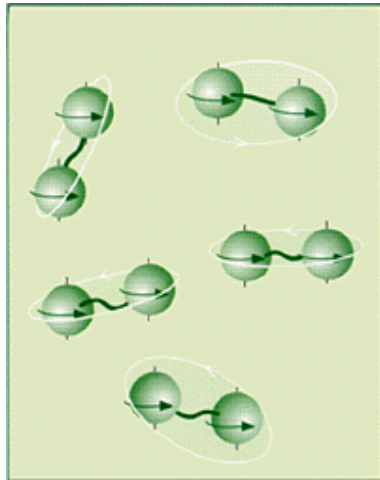
What materials exhibit superfluidity?

1. Fluid ^4He (boson)
- 2.
- 3.
- 4.
- 5.



What materials exhibit superfluidity?

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1. Fluid ^4He (boson)
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3. Lasercooled atoms magnet traps
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What materials exhibit superfluidity?

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2. Fluid ^3He (pairing)
3. Lasercooled atoms magnet traps
4. Molecules in magnetic traps.
5. Supersolid ^4He ?

Definition of the superfluid fraction Nonclassical rotational inertia (NCRI)

Experiment: spinning a bucket of fluid ^4He :
Below T_C , ^4He exhibits a **lowered moment of inertia**:

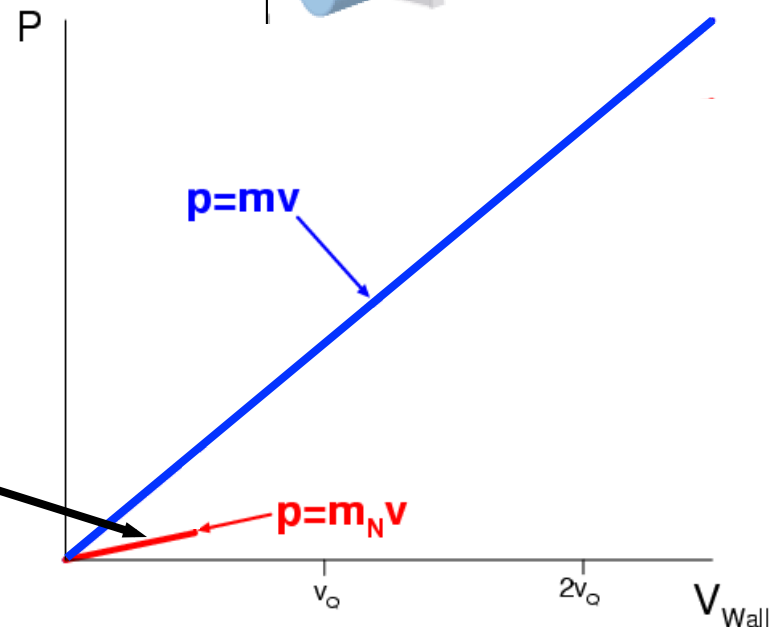
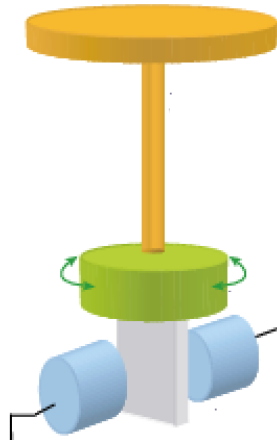
$$I = \left. \frac{dF}{d\omega^2} \right|_{\omega \rightarrow 0} = \left. \frac{d\langle \hat{L}_Z \rangle}{d\omega} \right|_{\omega \rightarrow 0}$$

$$m_N = \left. \frac{d\langle \hat{p} \rangle}{dv} \right|_{v \rightarrow 0}$$

Quantized circulations define v_0

$$2\pi n = \oint d\vec{l} \circ \vec{v}(\vec{l})$$

In the experiment, the slope (moment of inertia) deviates from classical value I_{cl} , called **nonclassical rotational inertia (NCRI)**. This is the definition of a superfluid.



Definition of the superfluid fraction Nonclassical rotational inertia (NCRI)

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This is “interpreted” as a fraction of the particle ρ that became superfluid and stopped spinning.

→ Two fluid model (Landau)

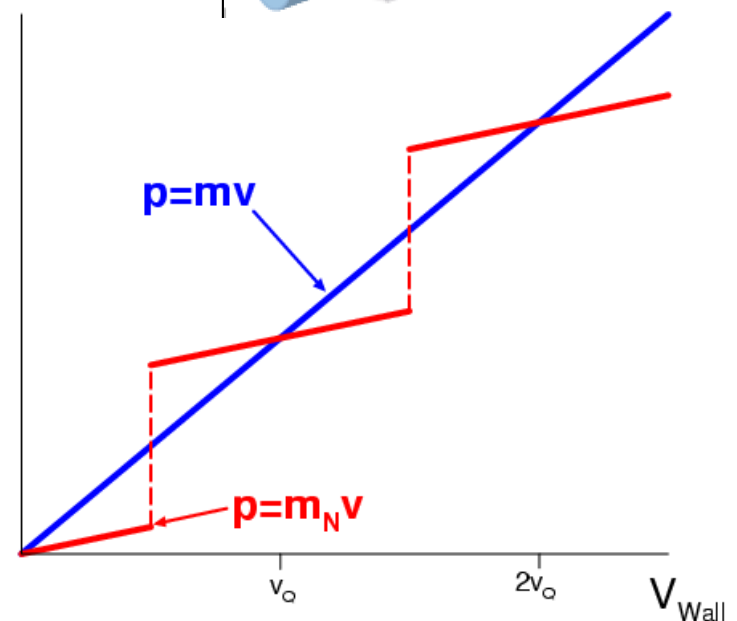
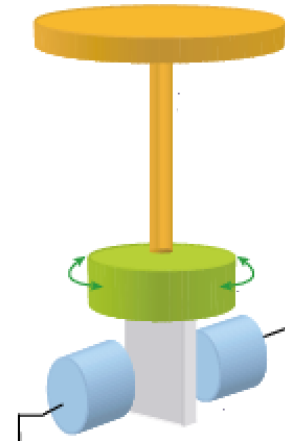
$$\rho = \rho_S + \rho_N$$

$$m = m_S + m_N$$

Normal fluid:

$$\vec{L}(T) = I(T) \vec{\omega}$$

$$\frac{\rho_N}{\rho} = \frac{I(T)}{I_{cl}}$$



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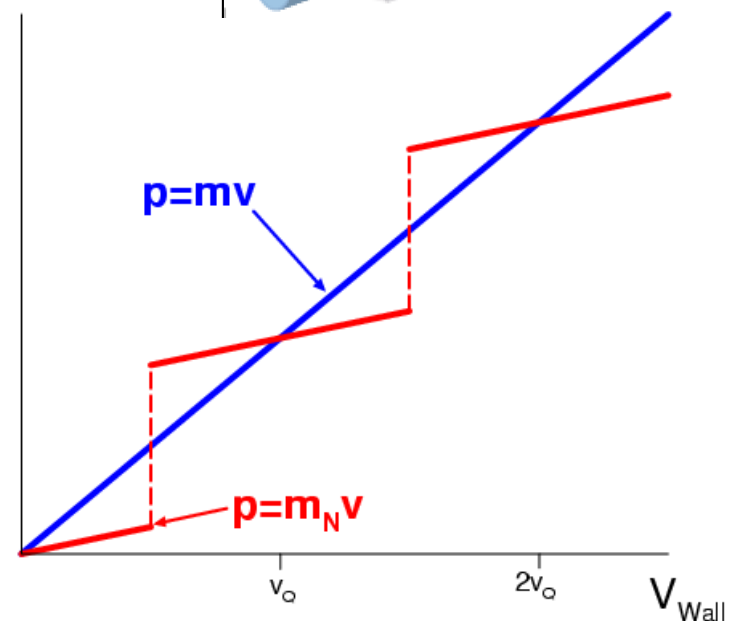
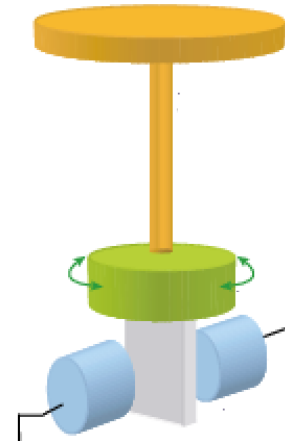
$$\vec{L}(T) = I(T) \vec{\omega}$$

$$\frac{\rho_N}{\rho} = \frac{I(T)}{I_{cl}}$$

Superfluid:

$$\frac{\rho_S}{\rho} = 1 - \frac{\rho_N}{\rho} = 1 - \frac{I}{I_C}$$

$$\frac{m_S}{m} = 1 - \frac{m_N}{m}$$



Superfluid moves frictionless, which leads to persistent currents

Experiment: spinning a bucket of fluid ^4He :
 Below T_C , ^4He exhibits a **lowered moment of inertia**:

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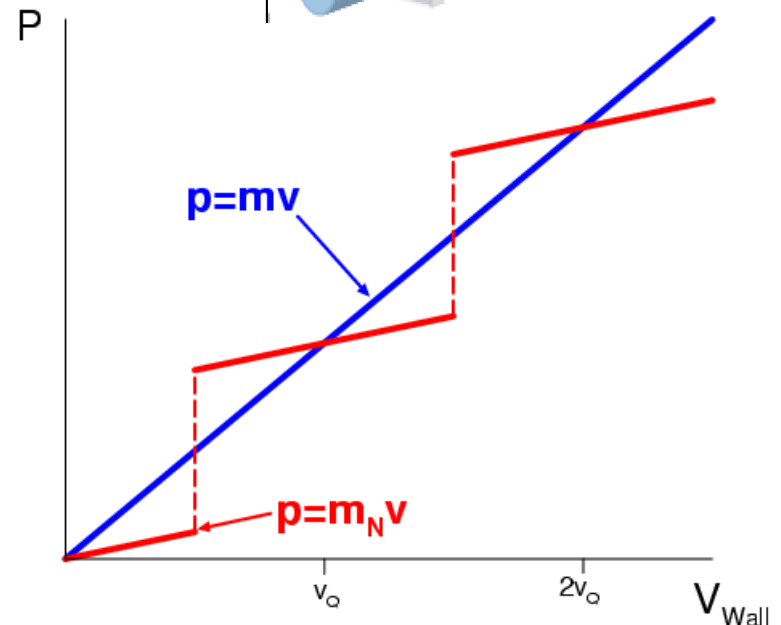
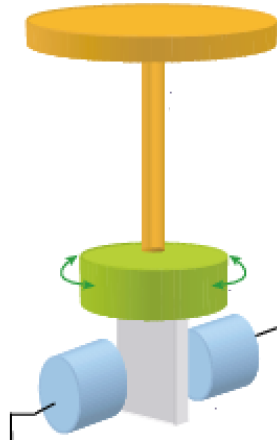
Different experiment: Spin the bucket and cool the system below transition temperature. Then stop the bucket.

$$\vec{L}(T) = \frac{\rho_s}{\rho} I_C \vec{\omega}$$

The superfluid keeps spinning.
 Normal component is at rest.

→ **Persistent currents.**

They disappear above the transition temp.



PIMC computation of the superfluid fraction

[Pollock, Ceperley, Phys. Rev. B 36 (1987) 8343]

Hamiltonian in a *system with moving walls*:

$$H_v = \sum_i \frac{(\vec{p}_i - m\vec{v})^2}{2m} + V$$

ρ_v satisfies periodic boundary conditions.

$$\rho_v(r_1, \dots, r_N ; r'_1, \dots, r'_j + L, \dots, r'_N) = \rho_v(r_1, \dots, r_N ; r'_1, \dots, r'_j, \dots, r'_N)$$

Derive the expectation value of momentum operator using the density matrix for a system with moving walls

$$\frac{\rho_N}{\rho} Nm \vec{v} = \langle \vec{P} \rangle_v = \frac{\text{Tr}[\vec{P} \hat{\rho}_v]}{\text{Tr}[\hat{\rho}_v]} = -\frac{\partial F_v}{\partial \vec{v}} + Nm \vec{v}$$

The s.f. fraction is related to the free energy change when the system is subject to rotation

Equivalent to system *with stationary walls*:

$$H = \sum_i \frac{(\vec{p}_i)^2}{2m} + V$$

with modified boundary conditions

$$\rho(r_1, \dots, r_N ; r'_1, \dots, r'_j + L, \dots, r'_N) = \exp\left[i m \vec{v} \circ \vec{L} / \hbar\right]^* \rho(r_1, \dots, r_N ; r'_1, \dots, r'_j, \dots, r'_N)$$

Free energy change a result of modified boundary conditions

$$e^{-\beta(F_v - F_{v=0})} = \frac{\int dR \rho_v(R, R; \beta)}{\int dR \rho_{v=0}(R, R; \beta)} = \left\langle e^{i\vec{W} \circ \vec{L}} \right\rangle$$

Only the winding path are affected:

$$\sum_i (\vec{r}_{P_i} - \vec{r}_i) = \vec{W}L$$

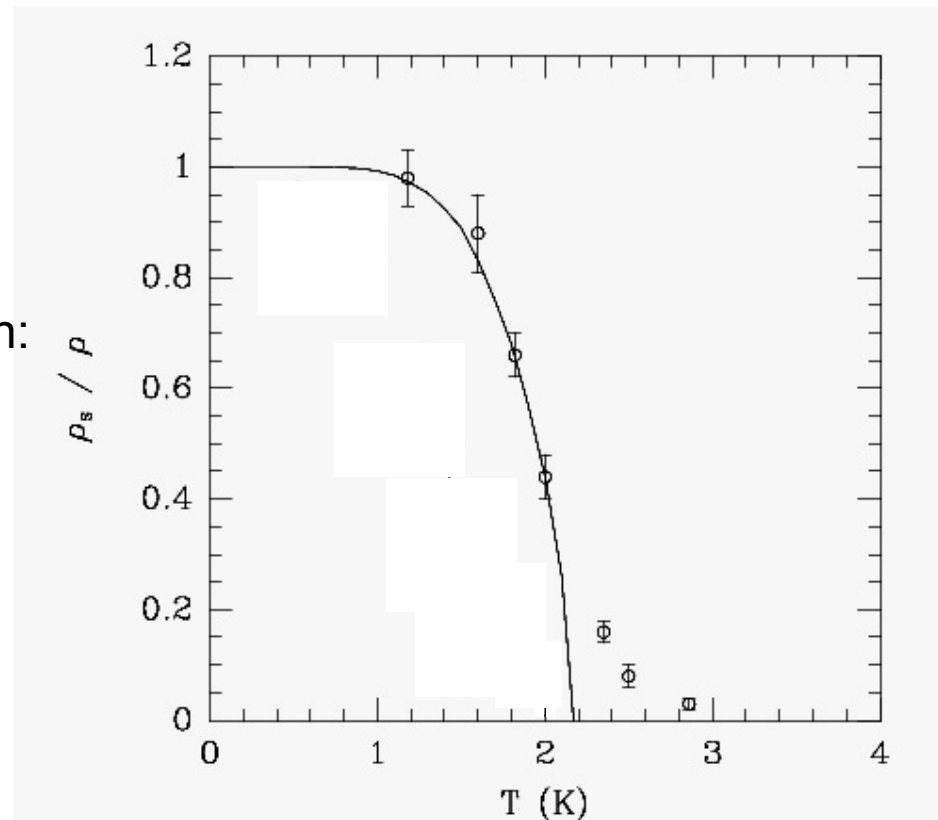
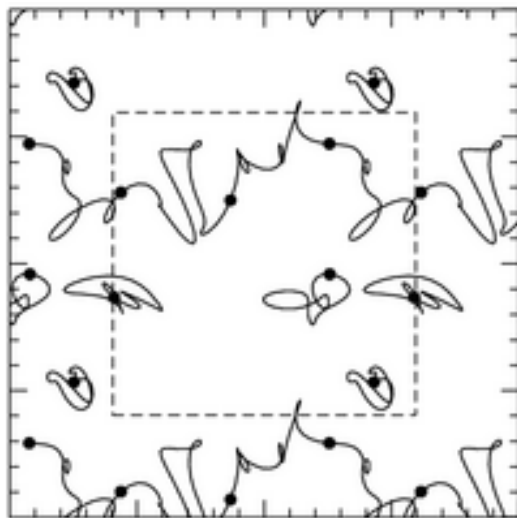
Computation of the **Superfluid Fraction** with PIMC in **periodic boundary conditions**

Definition of winding number:

$$\sum_i (\vec{r}_{P_i} - \vec{r}_i) = \vec{W}L$$

PIMC estimator for the superfluid fraction:

$$\frac{\rho_s}{\rho} = \frac{m}{\hbar^2} \frac{L^2}{3\beta N} \langle \vec{W}^2 \rangle$$



The superfluid fraction approaches 1 for low T, even for strongly interacting systems.

Challenge: Compute winding number for large system, especially in ^4He at higher pressures.

Computation of the Superfluid Fraction in Finite Systems with PIMC – Area Estimator

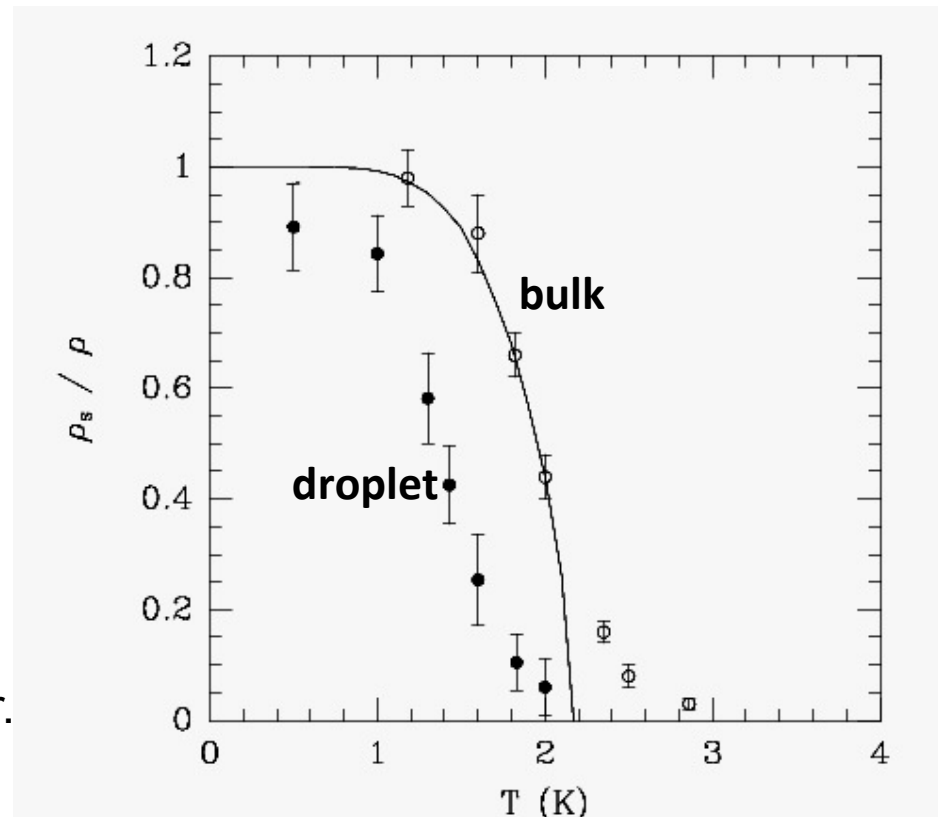
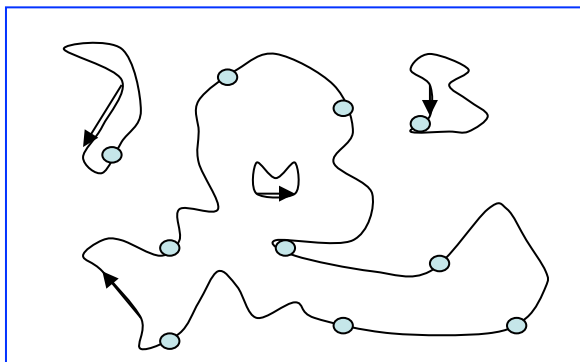
Hamiltonian in rotating frame:

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

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

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

A is the sign area of the loop polymer.



III. Condensate Fraction

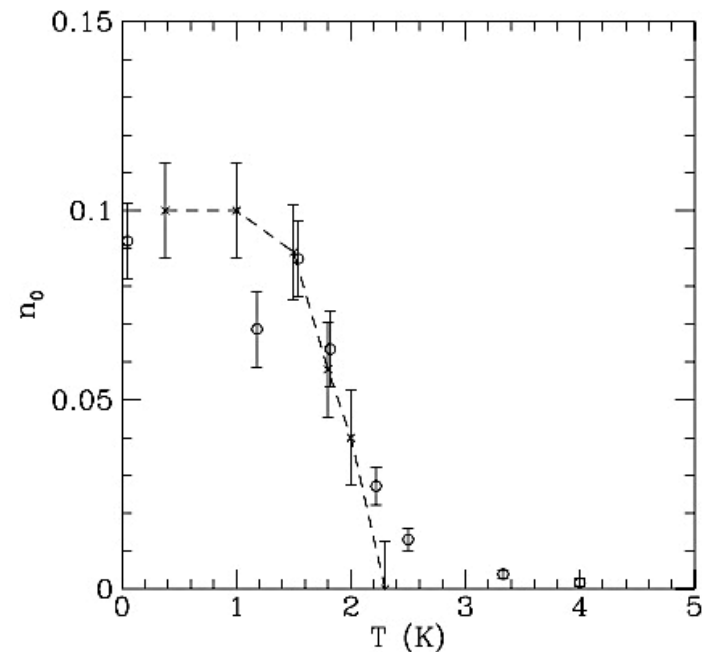
Definition of the condensate fraction

London (1938) suggested that superfluidity is Bose condensation. The question is whether this is a state of **zero momentum** as in the free particle system. One defines the “**condensate fraction**”

$$n_0 = \langle \delta(\hat{p} - 0) \rangle$$

as the number of particles with zero-momentum, which can be measured and computed.

Penrose and Onsager define Bose condensation as *macroscopic occupation of a single-particle state*.



For interacting systems, the T=0 limit of the condensate fraction is less than 1 (10% for ⁴He).

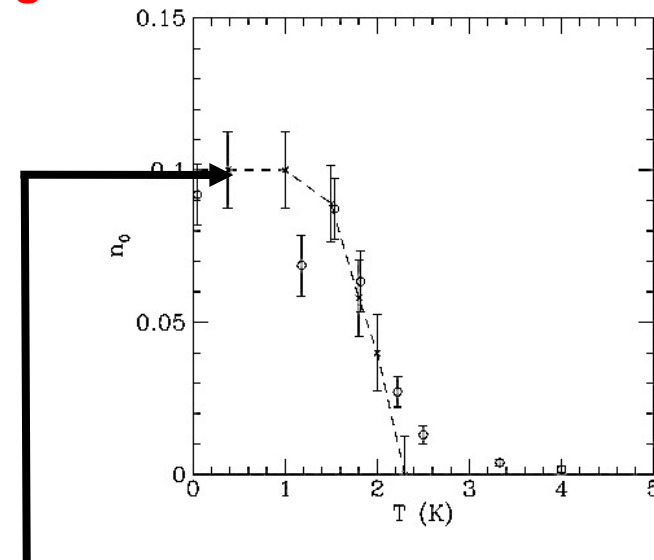
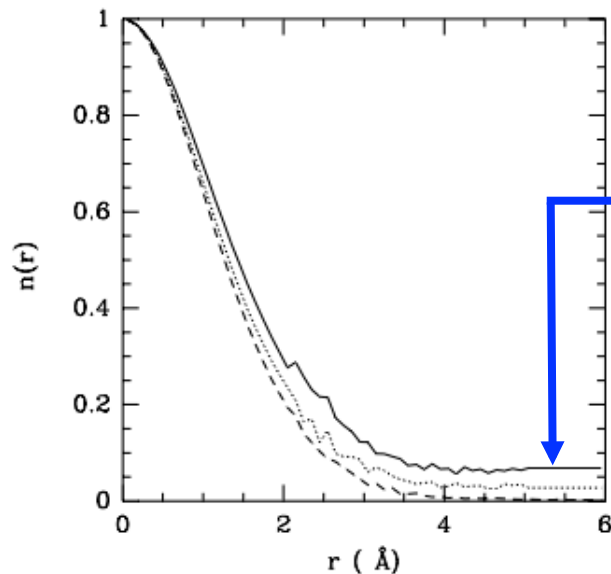
PIMC Computation of the momentum distribution

The momentum distribution can also be expressed in terms of the thermal density matrix. However, this requires **off-diagonal density matrix elements**

$$n(k) = \langle \delta(\hat{p} - \hbar k) \rangle$$

$$n(k) \sim \int dR dr'_1 e^{i(r_1 - r'_1) \cdot k} \rho(r_1 \dots r_N, r'_1 \dots r'_N)$$

which can only be computed with simulations with one open paths.



- $n(k=0) > 0$ implies **long tails** in the **single particle density matrix**.
- It decays algebraically instead of exponentially.
- This is called **off-diagonal long-range order**, one signature of superfluidity.

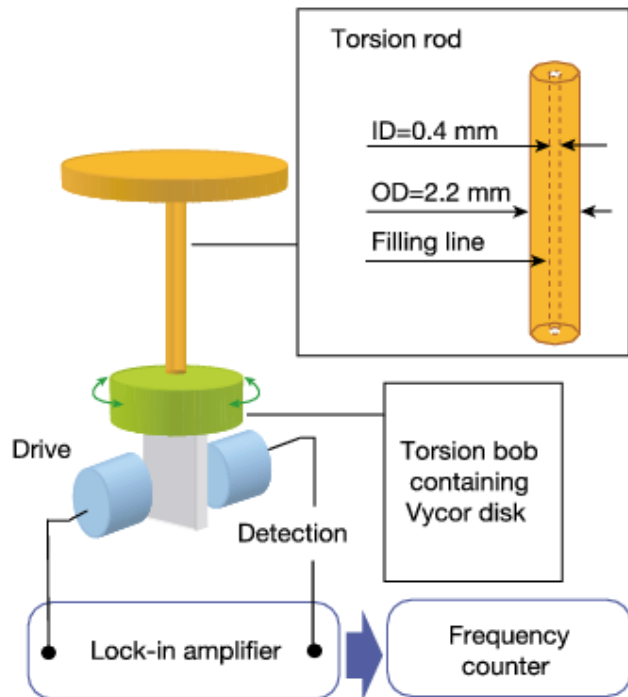
***IV. Does
Supersolid Helium
exist?***

Kim & Chan [Nature 427 (2004) 225] demonstrate that **solid ^4He** at pressures of 62 bar exhibits superfluidity.

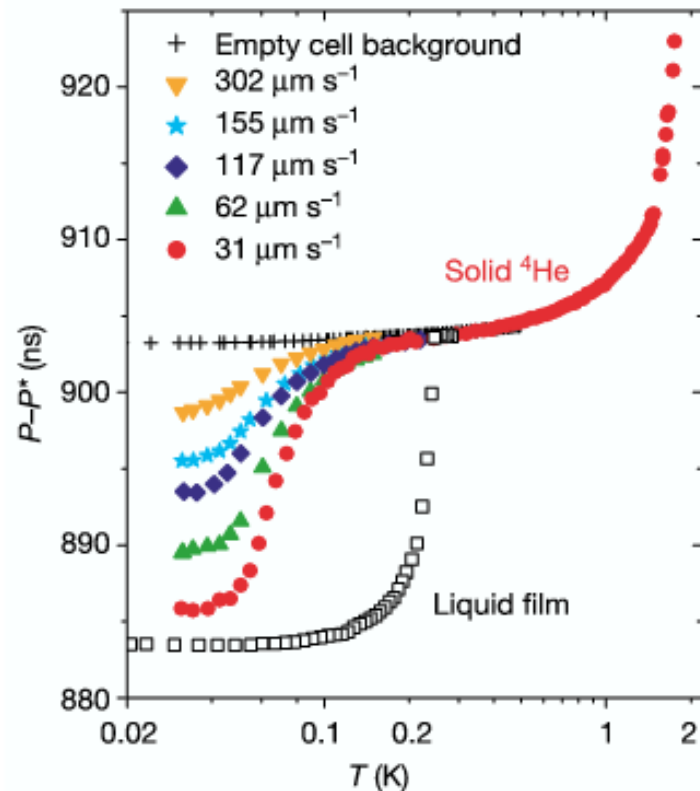
Probable observation of a supersolid helium phase

E. Kim & M. H. W. Chan

Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA



Below T_C , a fraction becomes superfluid. This lowers the moment of inertia I . This lowers the oscillation period P .



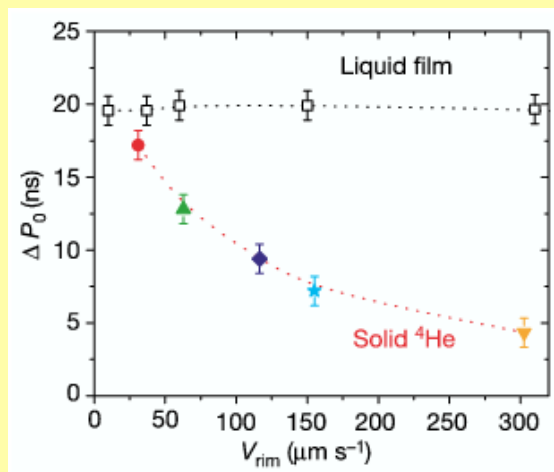
Possible interpretations of the experiment:

Superfluidity ok, but do we have a solid?

- At 62 bar is pure ^4He clearly is solid but if confined in Vycor?

Could Vycor be coated with a s.f. film?

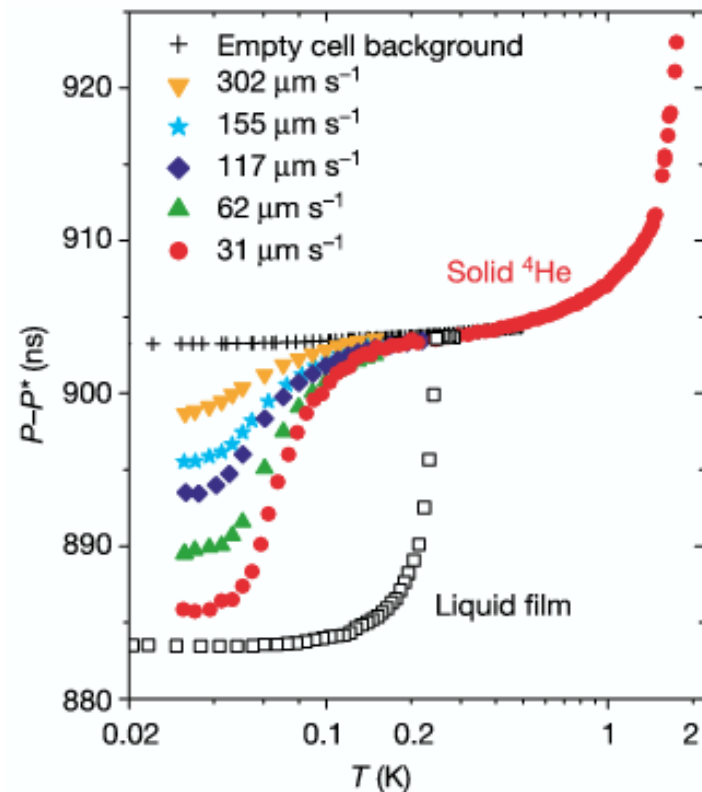
- Results are not consistent of picture of a film:



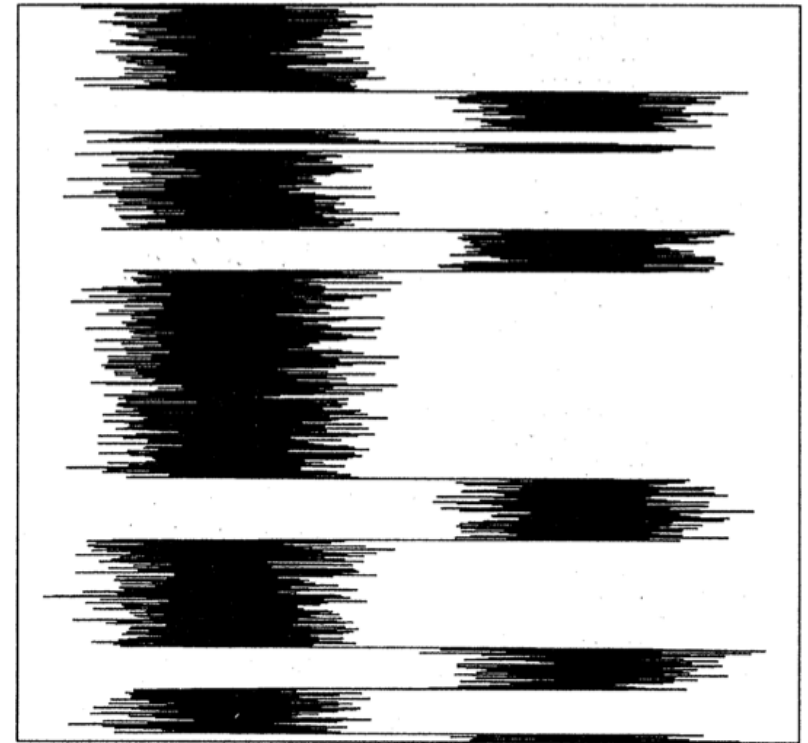
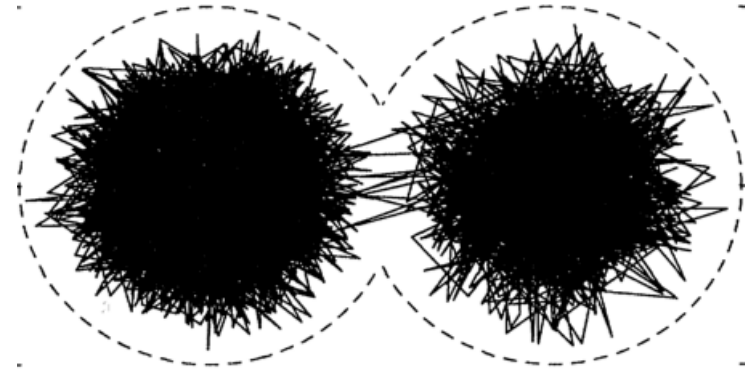
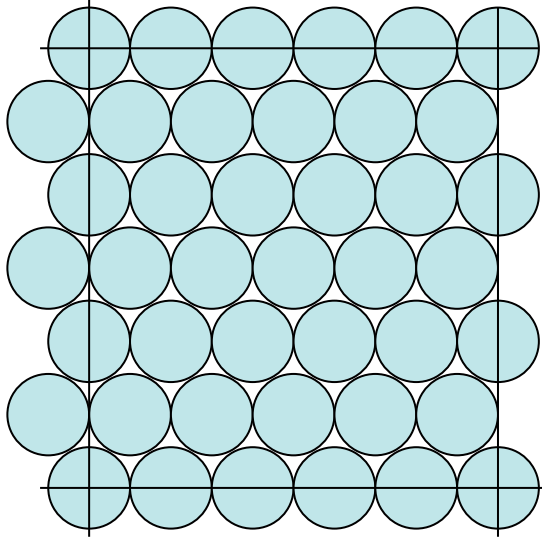
How can we explain the experiment:

- e.g. superfluid defects
- disorder could also introduce s.f.

Below T_C , a fraction becomes superfluid. This lowers the moment of inertia I . This lowers the oscillation period P .

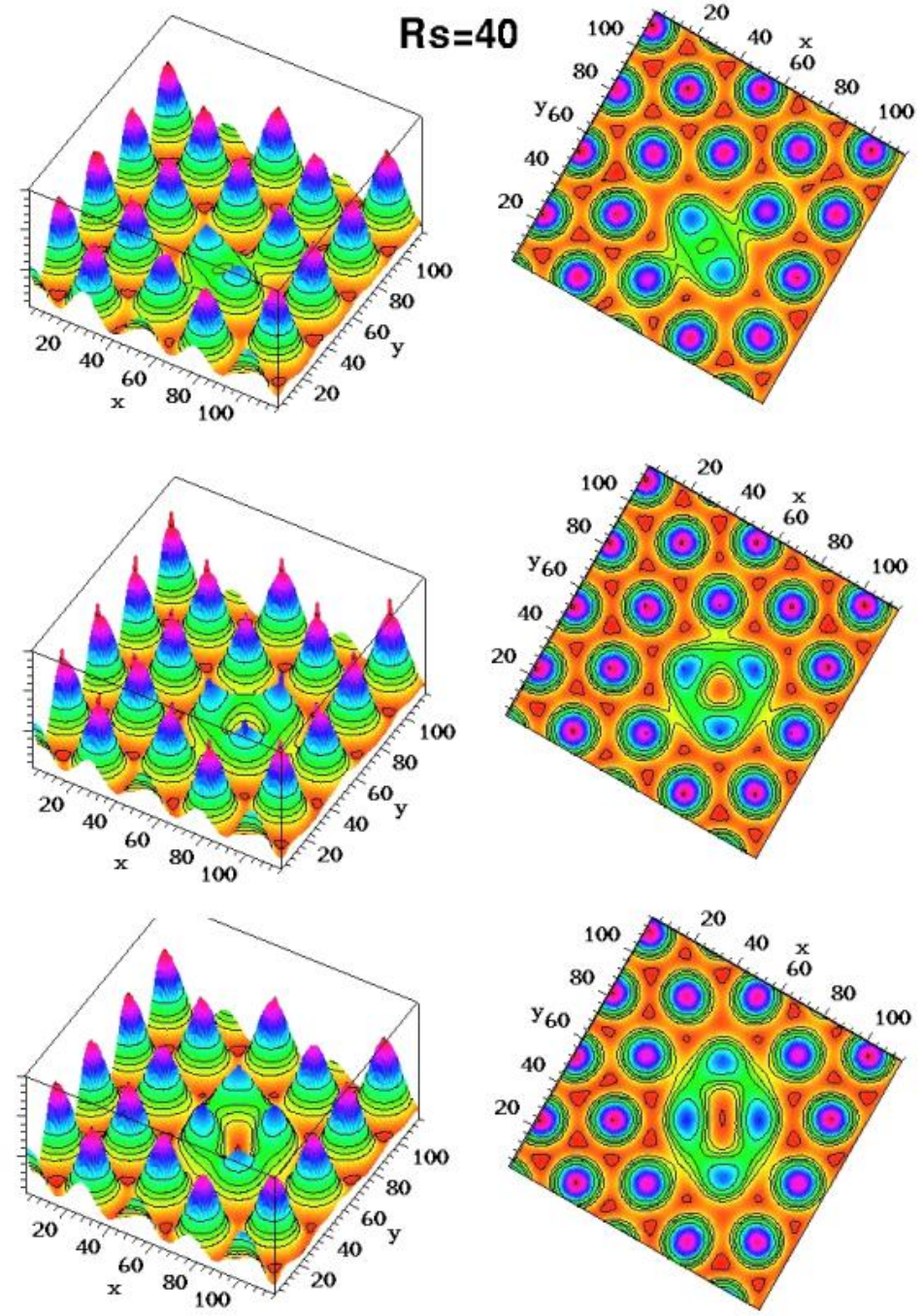
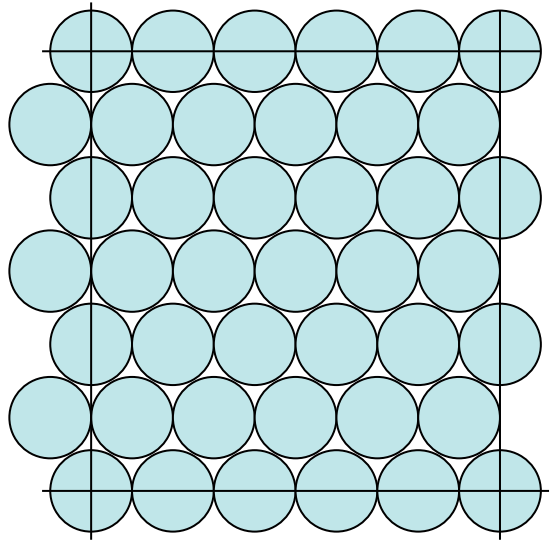


What permutation cycles do we expect for an hcp crystal?



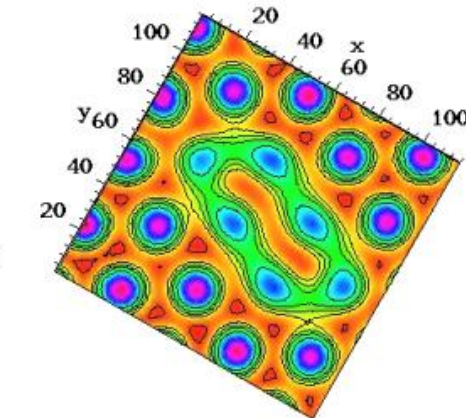
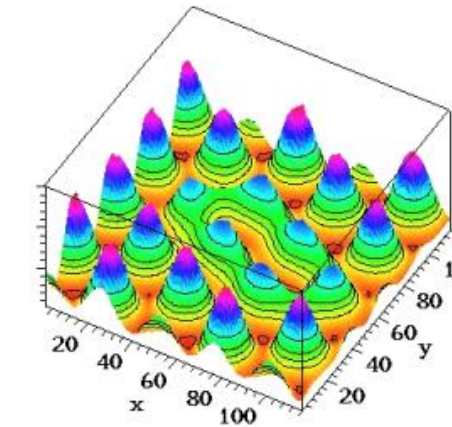
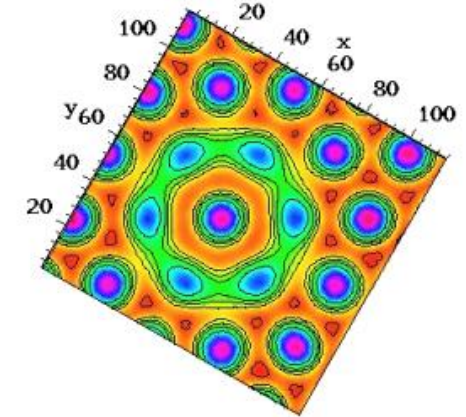
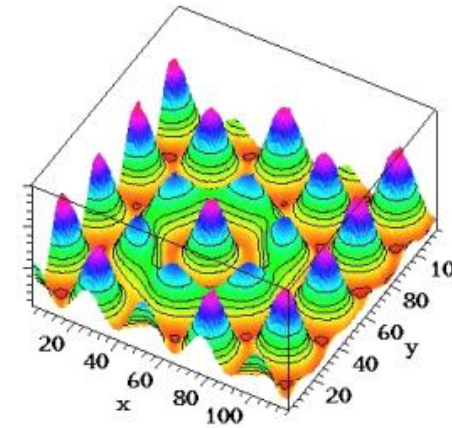
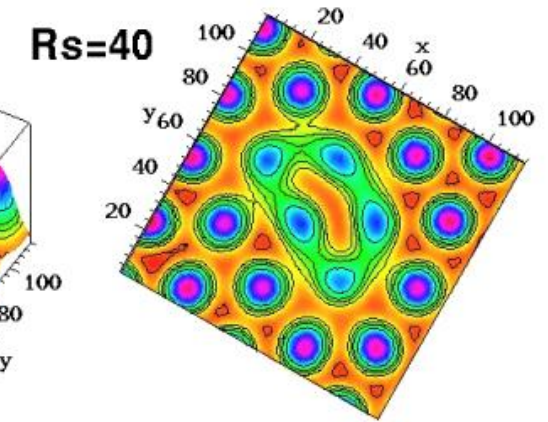
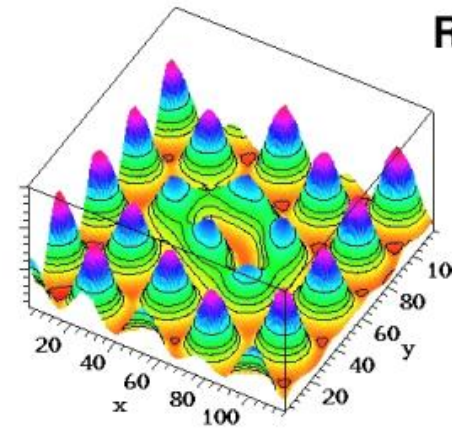
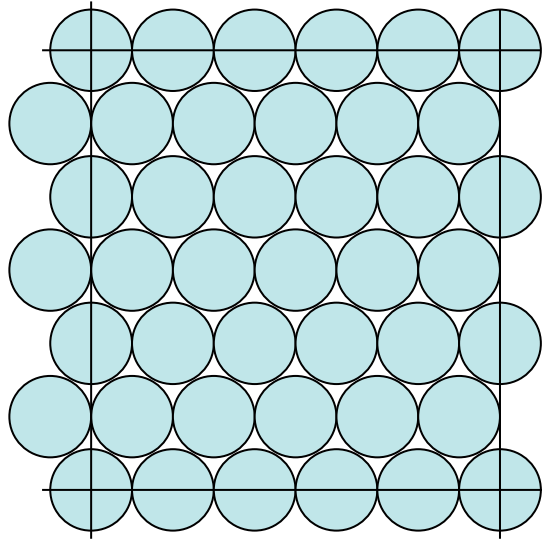
Two-particle exchange are unlikely because of the confinement. Others needs play along to make permutation cycles likely.

What permutation cycles do we expect for an hcp crystal?



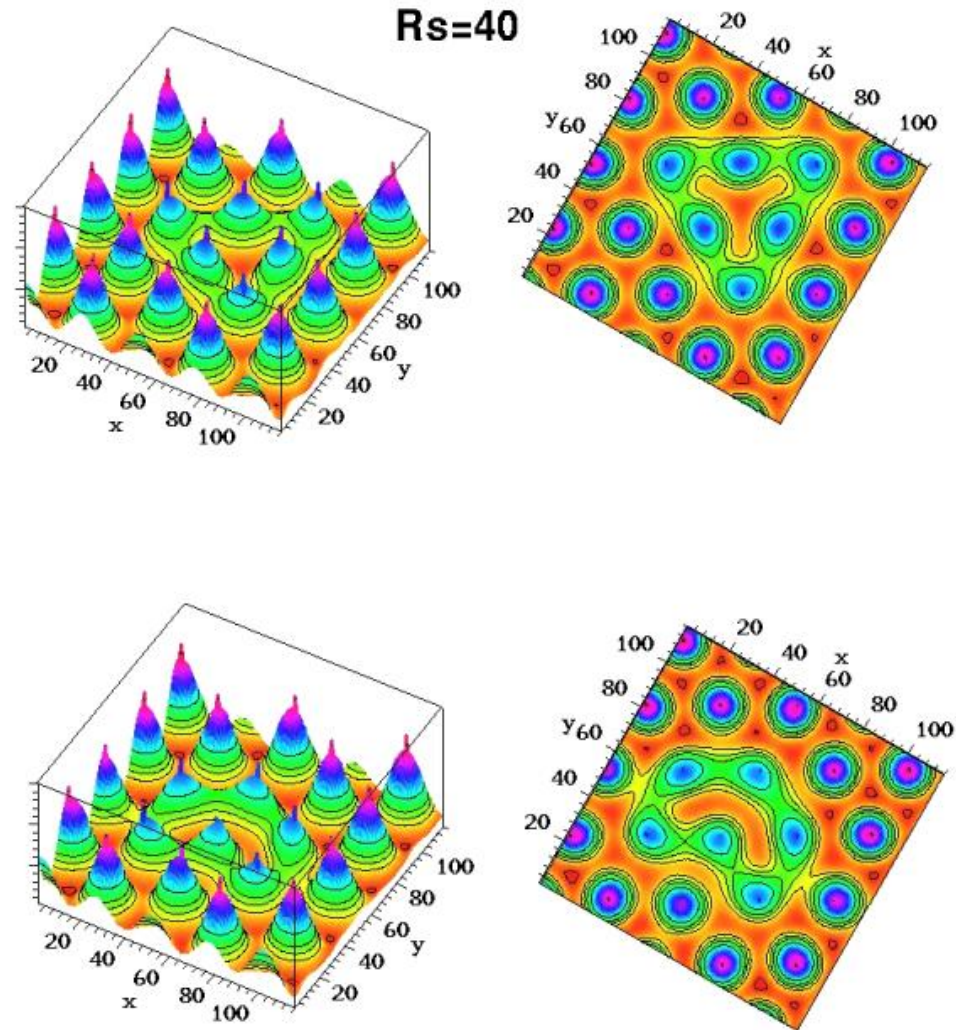
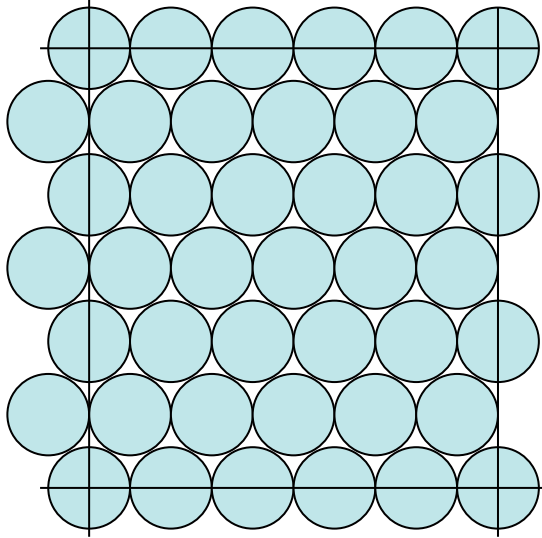
Let us look in 2D first:
2, 3, & 4 particle exchange
cycles (B. Bernu)

What permutation cycles do we expect for an hcp crystal?



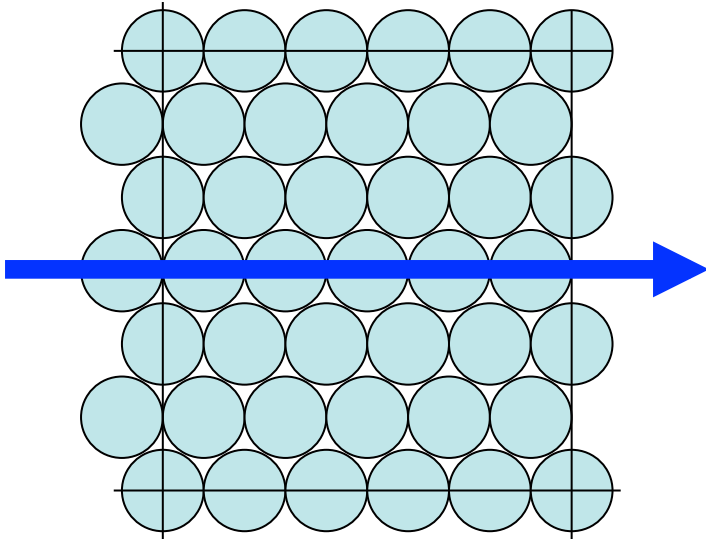
Let us look in 2D first:
6 particle exchange cycles
(B. Bernu)

What permutation cycles do we expect for an hcp crystal?

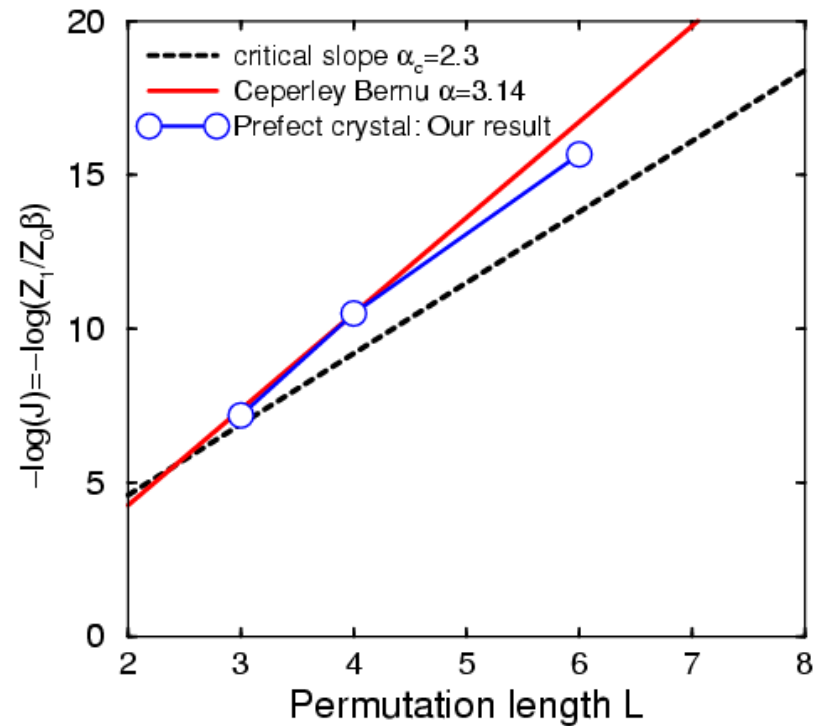


Let us look in 2D first:
6 particle exchange cycles
(B. Bernu)

Ceperley-Bernu approach: Exchange frequency calculation in perfect crystal



$$\frac{Z_P}{Z_0} = \frac{\int dR \langle R | (e^{-\tau \hat{H}})^M | PR \rangle}{\int dR \langle R | (e^{-\tau \hat{H}})^M | R \rangle} \equiv J_P \beta$$



- For a **fixed** permutation, the free energy cost, J , is calculated using a switching method (Bennett).
- Kikuchi model: The slope of $J(L)$ must be less than **2.3** to support superfluidity.
- Ceperley & Bernu (PRL 2004) showed that a **perfect helium crystal** cannot become a superfluid.

Boninsegni, Prokofev, Svistunov: Worm Algorithm for Grand Canonical PIMC

PRL 96, 070601 (2006)

PHYSICAL REVIEW LETTERS

week ending
24 FEBRUARY 2006

Worm Algorithm for Continuous-Space Path Integral Monte Carlo Simulations

Massimo Boninsegni,¹ Nikolay Prokof'ev,^{1,2,3,4} and Boris Svistunov^{2,3}

- Introduce one open polymer
- Allow it change length
- Introduce a chemical potential that controls the length of the path

This introduces more flexibility and allows for a higher efficiency in the permutation sampling

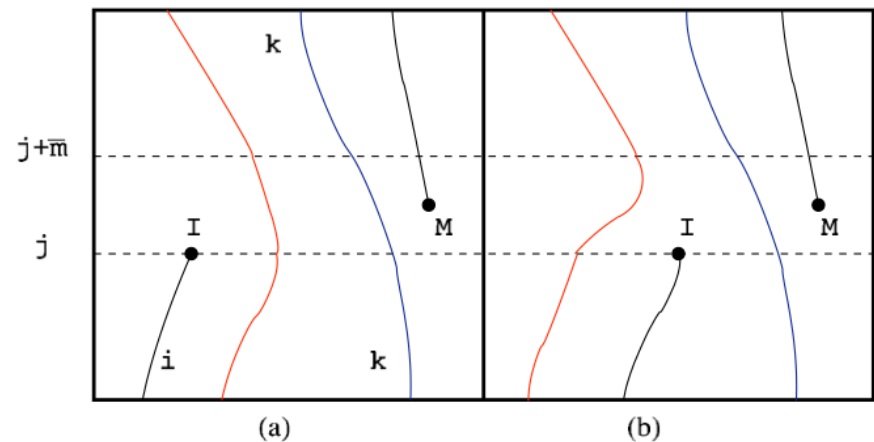


FIG. 1 (color online). Schematic illustration of *swap* move described in the text. (a) before the move. (b) after the move.

Boninsegni, et al. (2007)

Screw Dislocation proposed

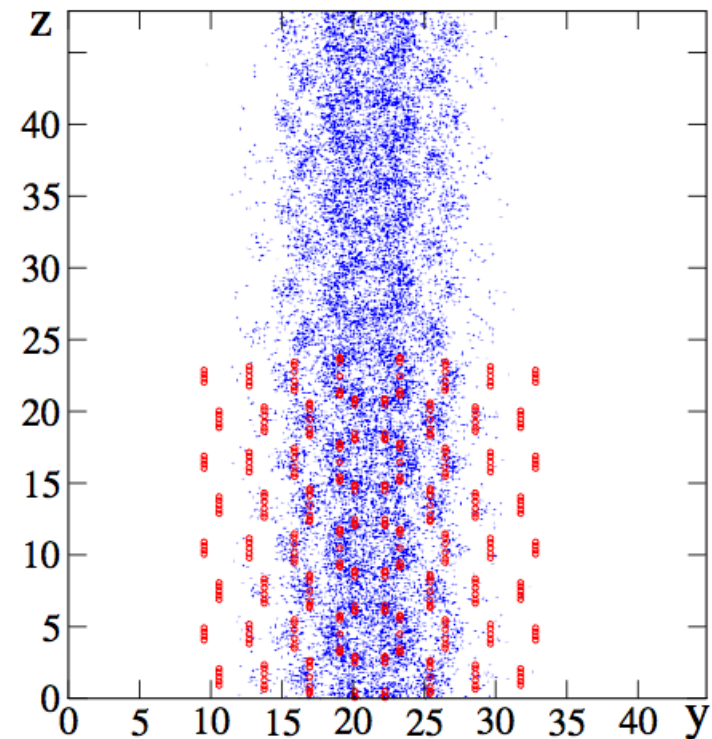
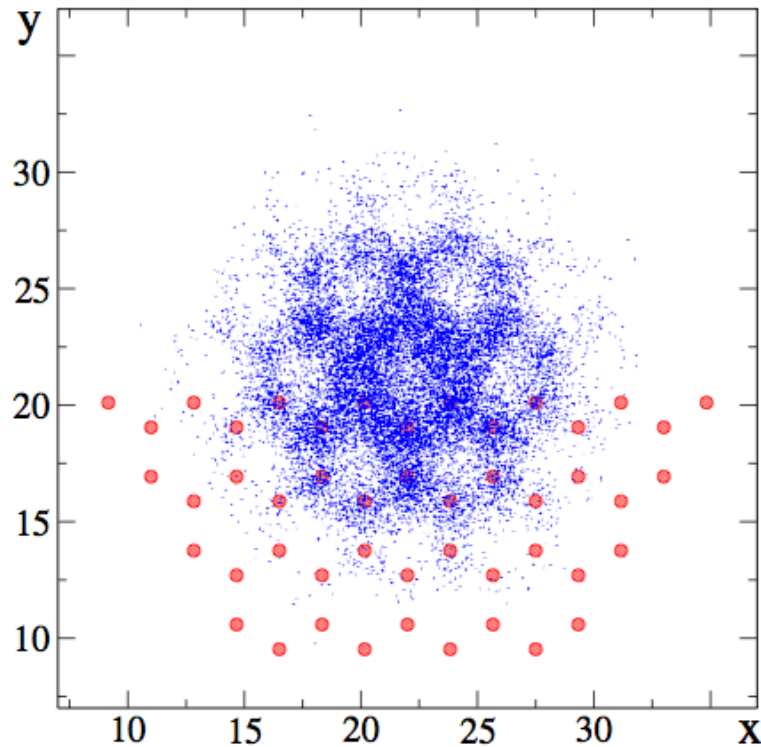
PRL **99**, 035301 (2007)

PHYSICAL REVIEW LETTERS

week ending
20 JULY 2007

Luttinger Liquid in the Core of a Screw Dislocation in Helium-4

M. Boninsegni,¹ A. B. Kuklov,² L. Pollet,³ N. V. Prokof'ev,^{4,5} B. V. Svistunov,^{4,5} and M. Troyer³



Experiments find: “Supersolid” signal (NCRI) depends on cooling rate

PRL 98, 175302 (2007)

PHYSICAL REVIEW LETTERS

week ending
27 APRIL 2007

Disorder and the Supersolid State of Solid ^4He

Ann Sophie C. Rittner and John D. Reppy*

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Ithaca, New York 14853-2501, USA*

(Received 13 March 2007; published 26 April 2007)

We report torsional oscillator supersolid studies of highly disordered samples of solid ^4He . In an attempt to approach the amorphous or glassy state of the solid, we prepare our samples by rapid freezing from the normal phase of liquid ^4He . Less than two minutes is required for the entire process of freezing and the subsequent cooling of the sample to below 1 K. The supersolid signals observed for such samples are remarkably large, exceeding 20% of the entire solid helium moment of inertia. These results, taken with the finding that the magnitude of the small supersolid signals observed in our earlier experiments can be reduced to an unobservable level by annealing, strongly suggest that the supersolid state exists for the disordered or glassy state of helium and is absent in high quality crystals of solid ^4He .

The End