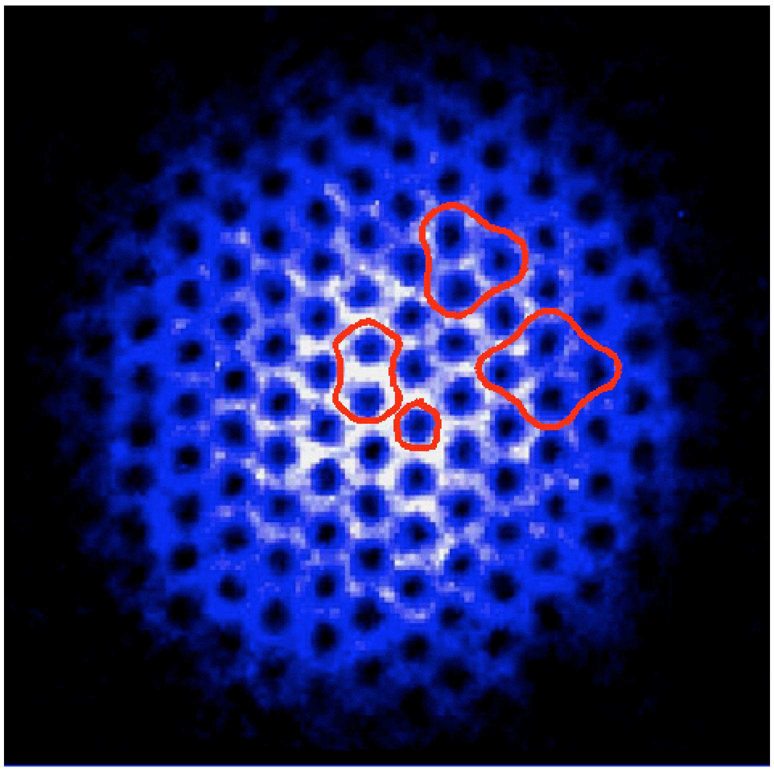
Path Integral Monte Carlo II

Summer school "QMC from Minerals and Materials to Molecules"



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Bosonic and Fermionic Density Matrices

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.

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Project out symmetric and antisymmetric states:

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

Bosonic and Fermionic Path Integrals

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Apply projection to the density matrix:

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

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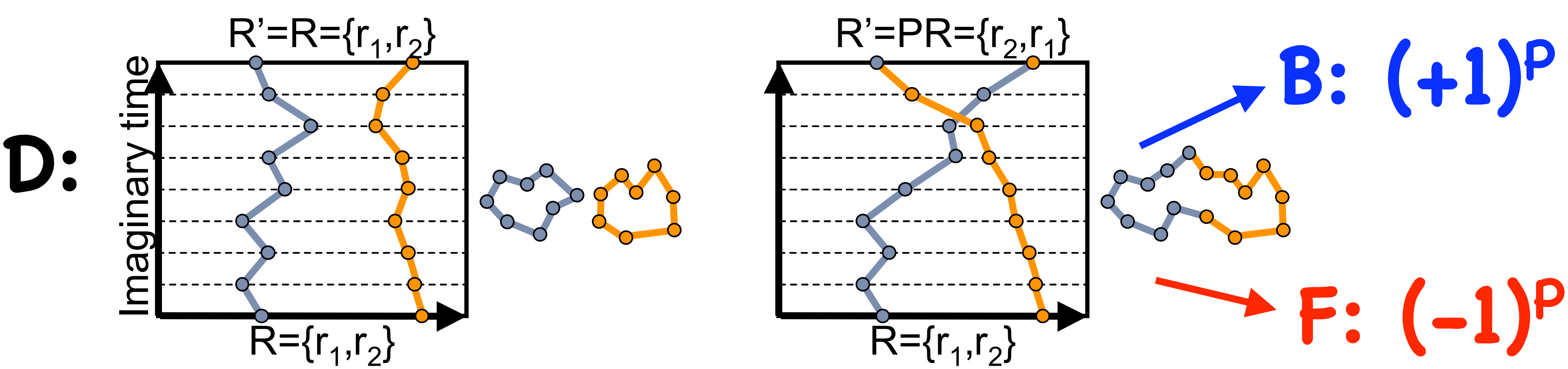
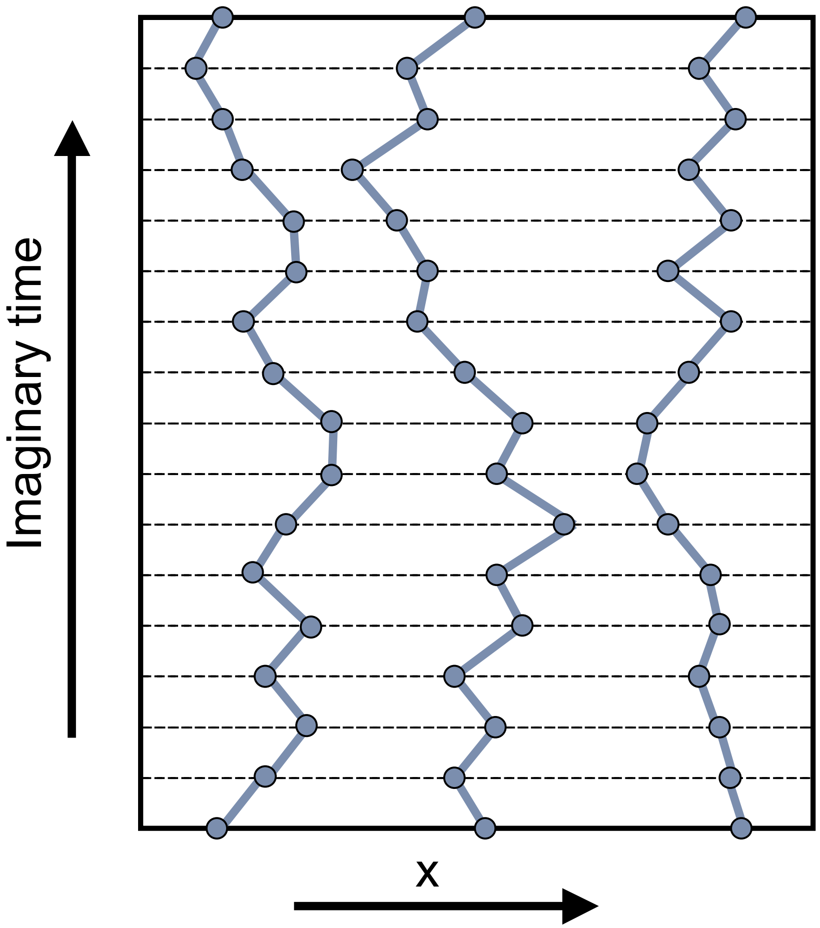


How do we sample the permutation space?



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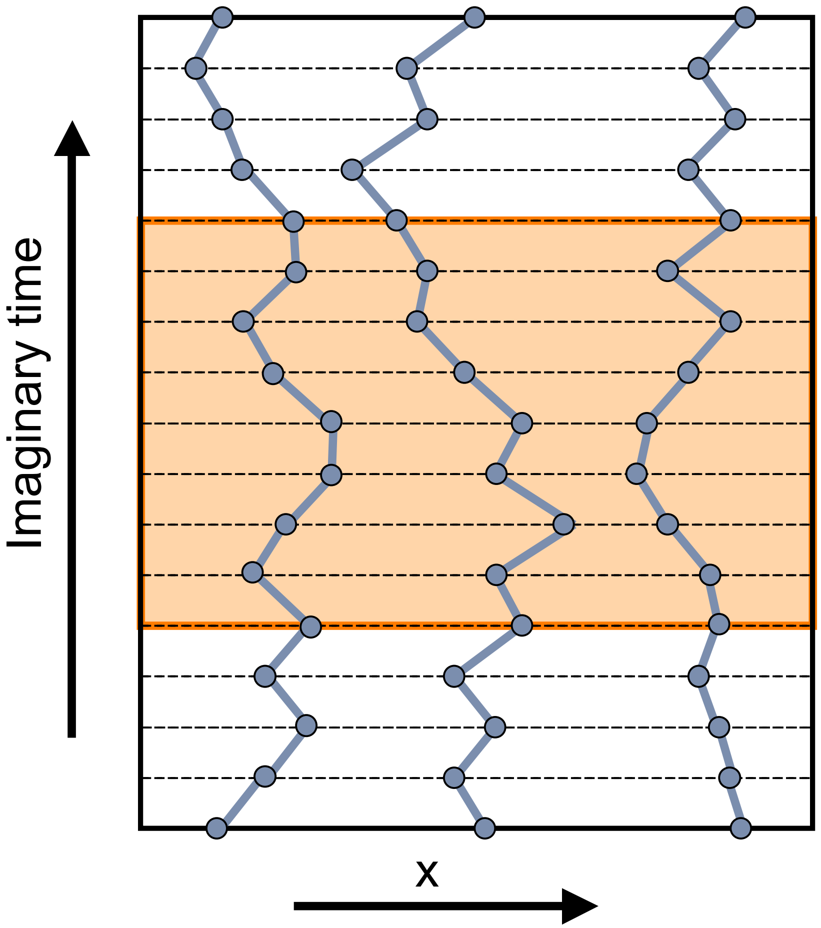

Step 0: Pick an imaginary time window

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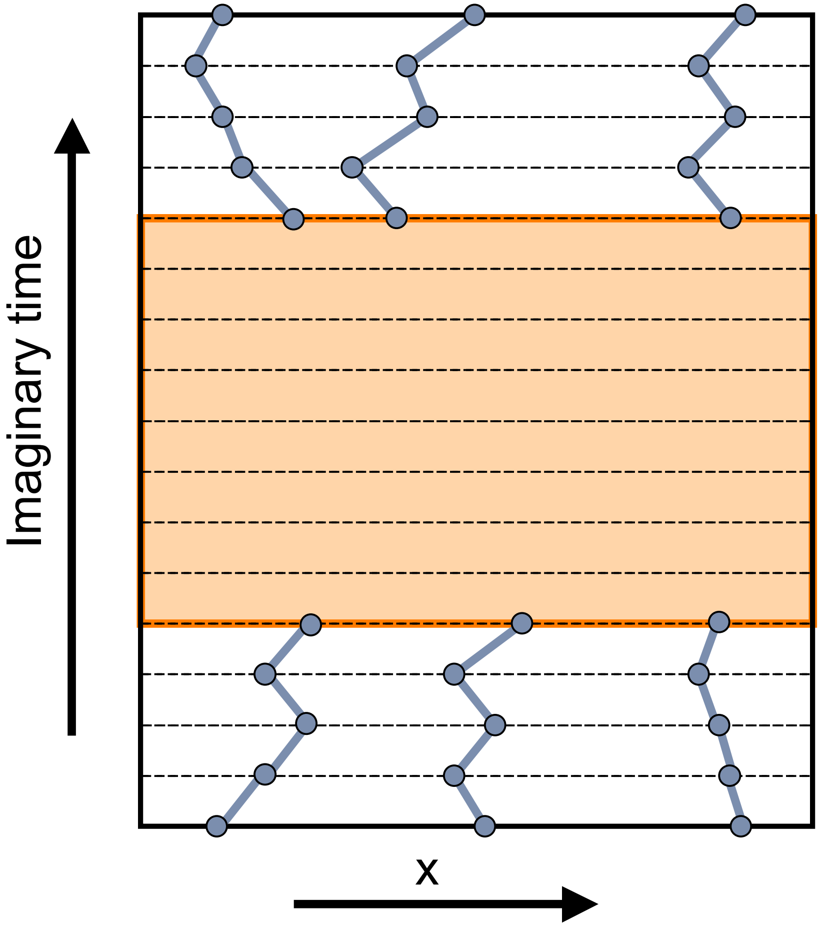

Step 0: Pick an imaginary time window
Step 1: Study all possible permutations
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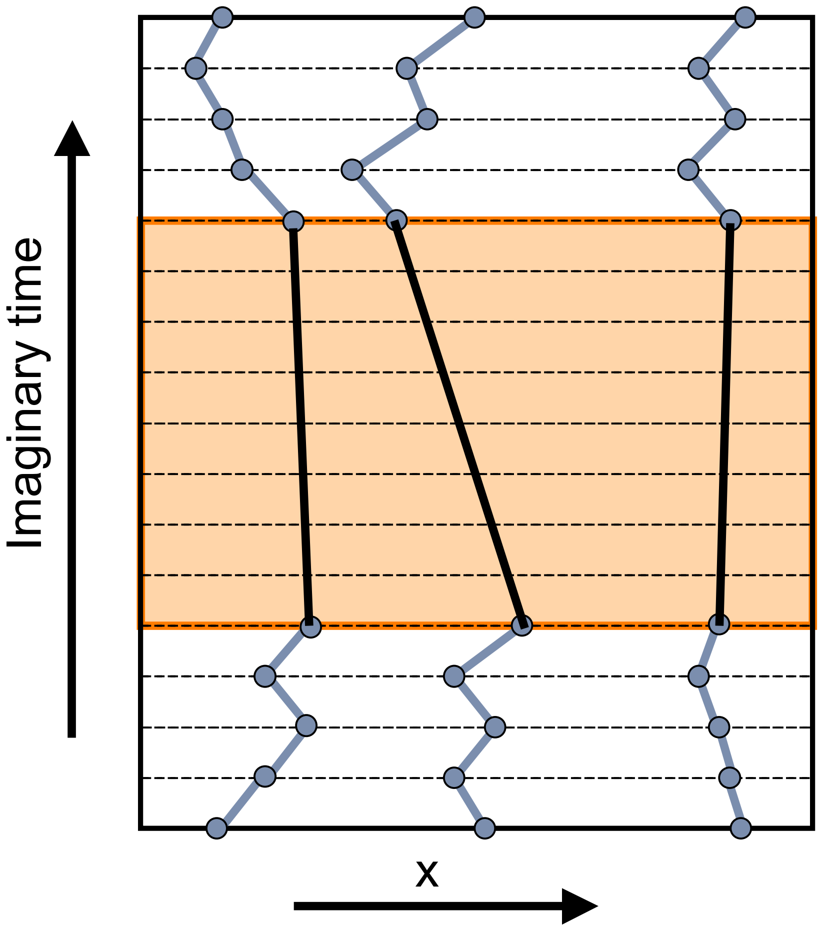

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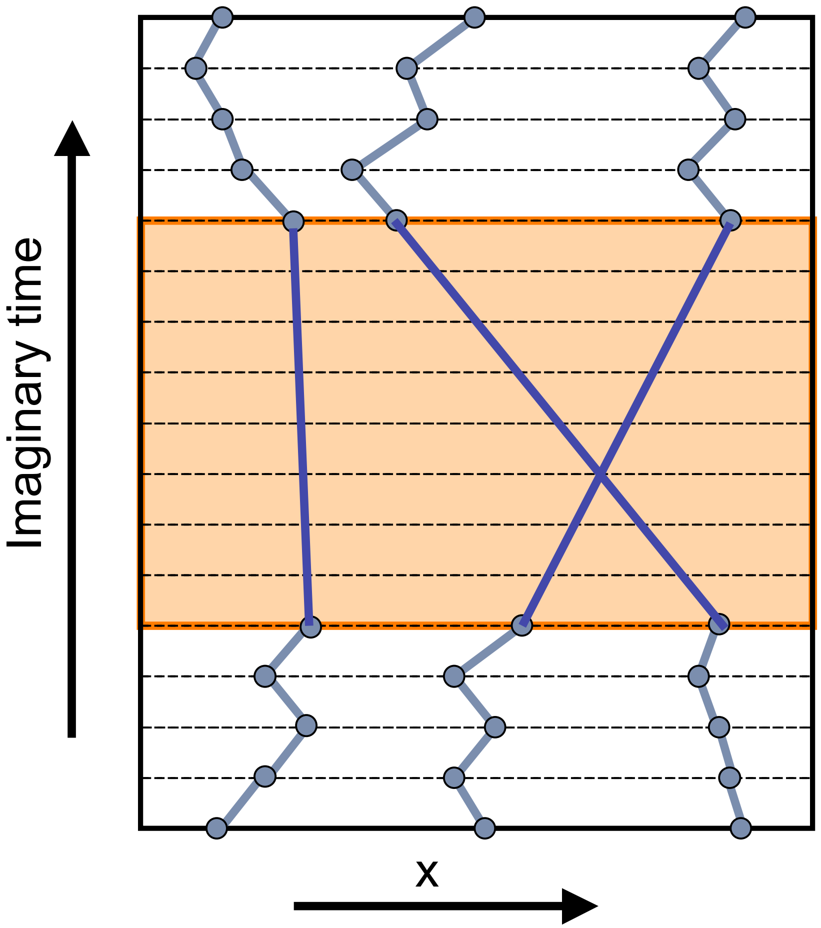
(1 2 3)
↓
(1 2 3)
P=+1

Identity permutation (1)

How do we sample the permutation space?



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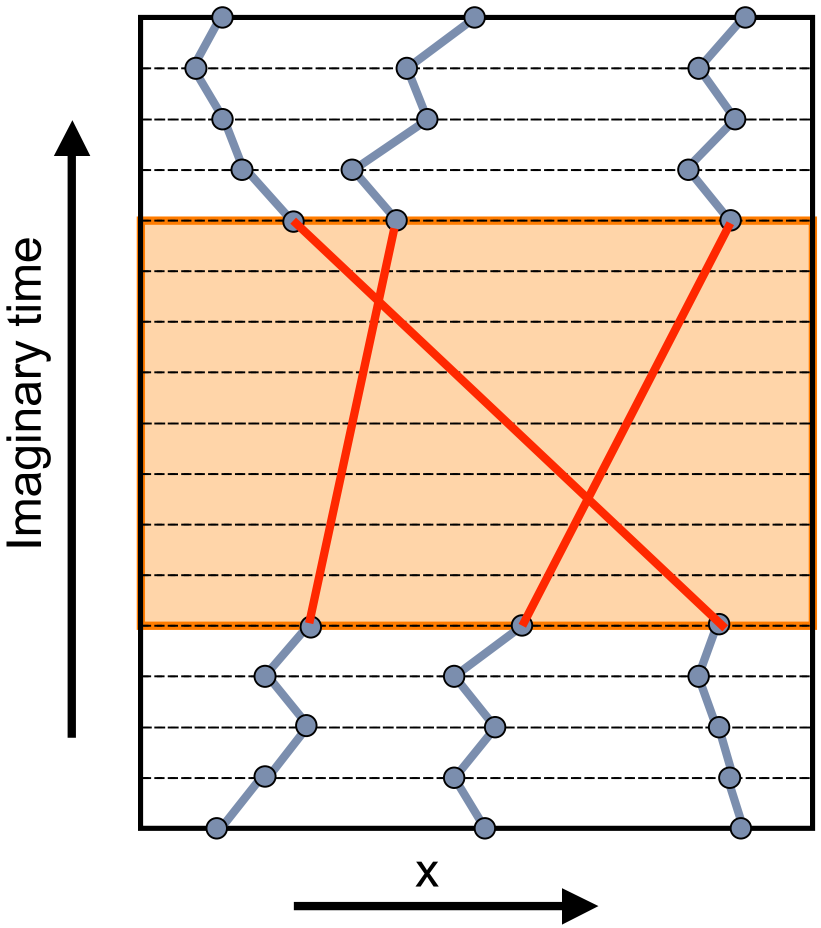

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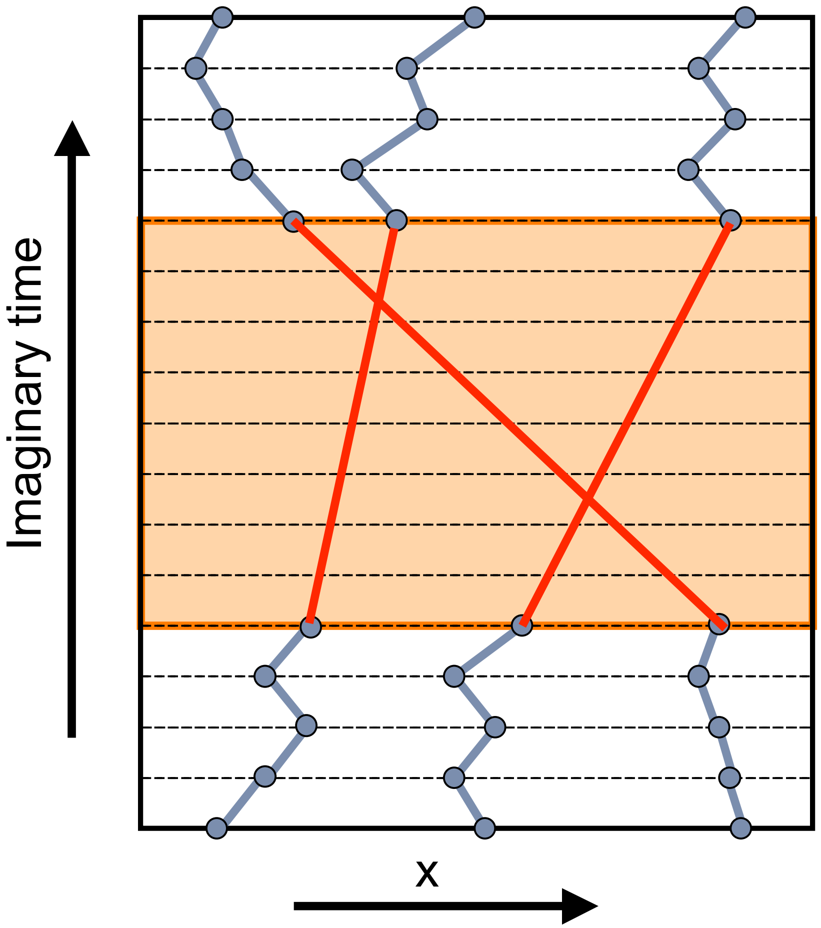

Step 0: Pick an imaginary time window

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:

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

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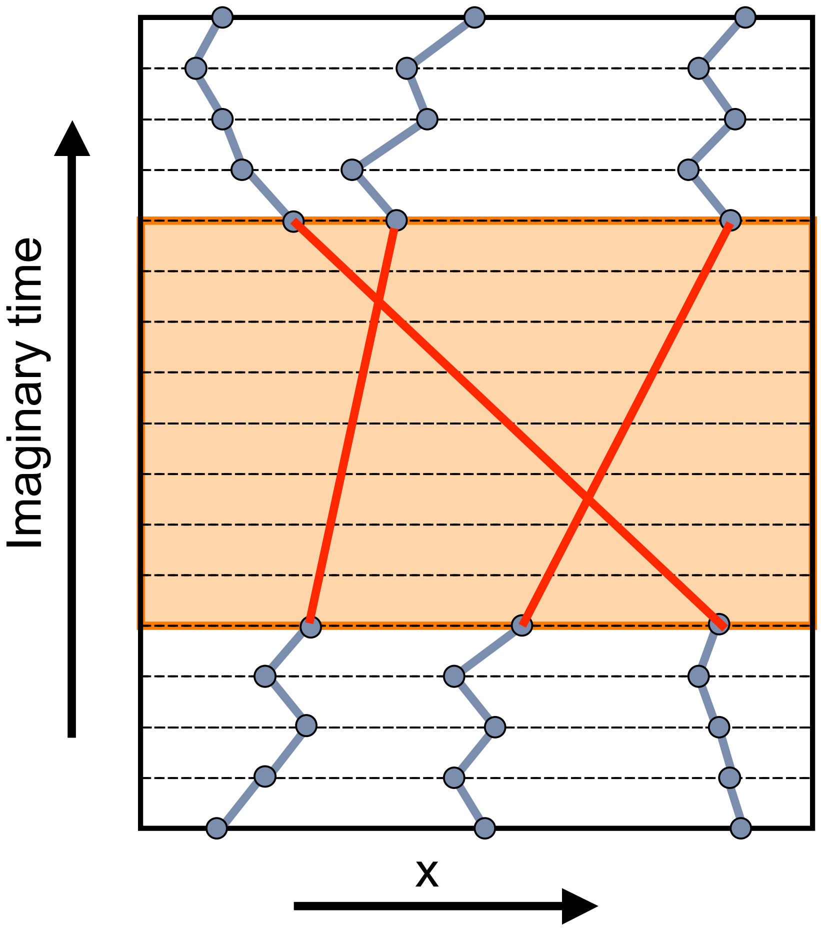

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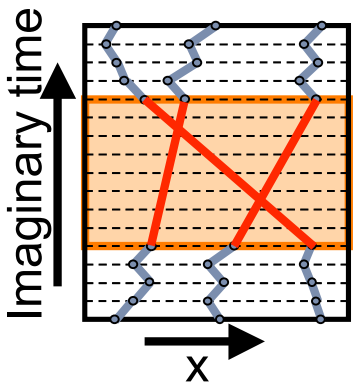
Step 3: Pick from permutation table
Step 4: Regrow the permuted path using the bisection or Levy flight method.
Step 5: Accept or Reject based on action.

How to construct a table containing all likely permutations?



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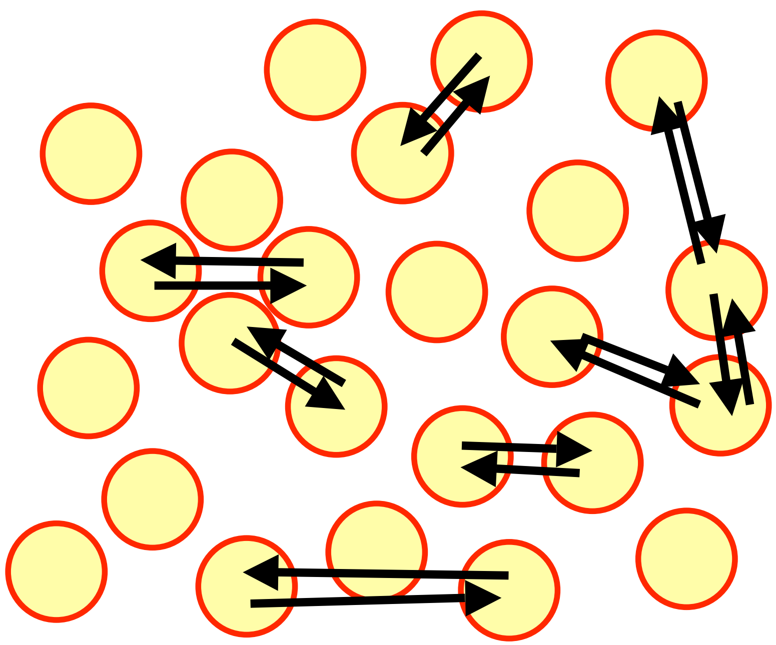

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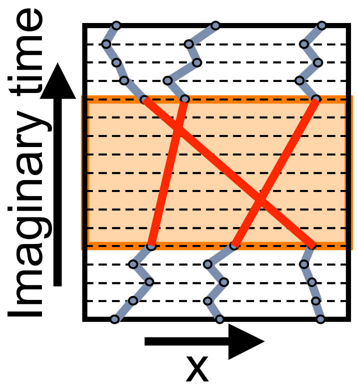

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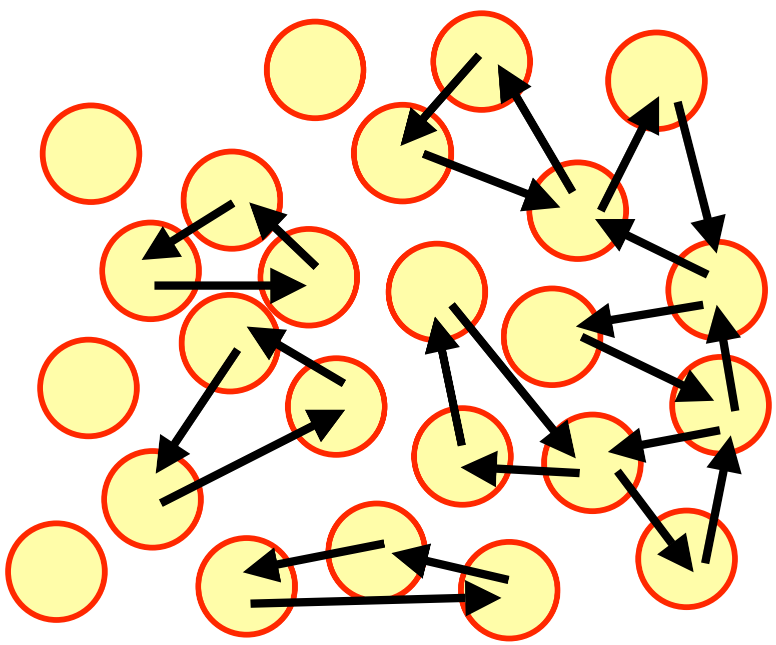

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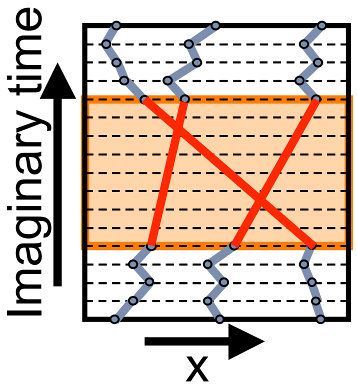

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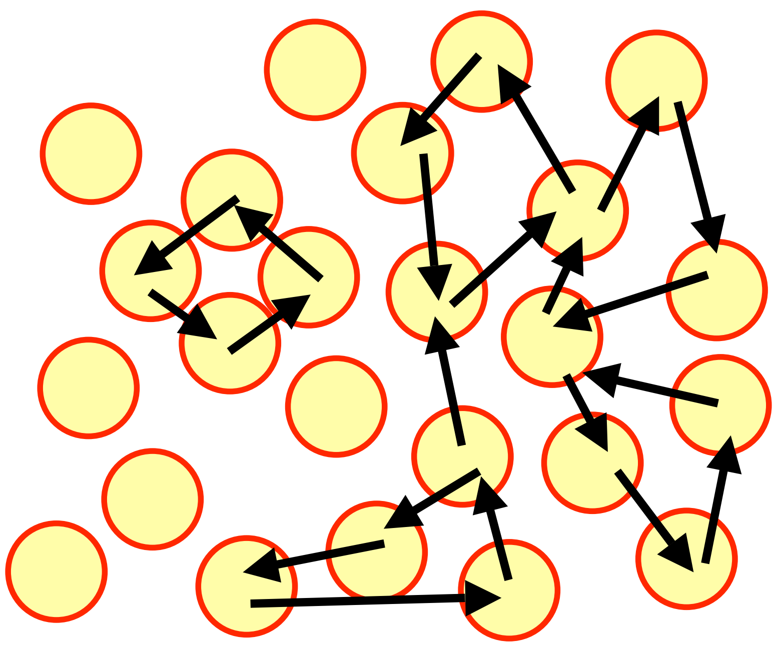

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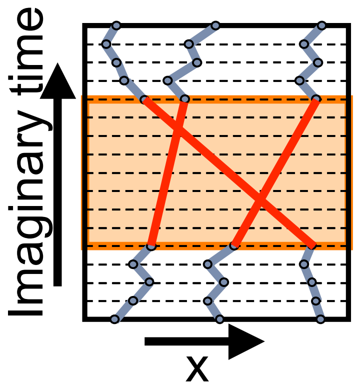

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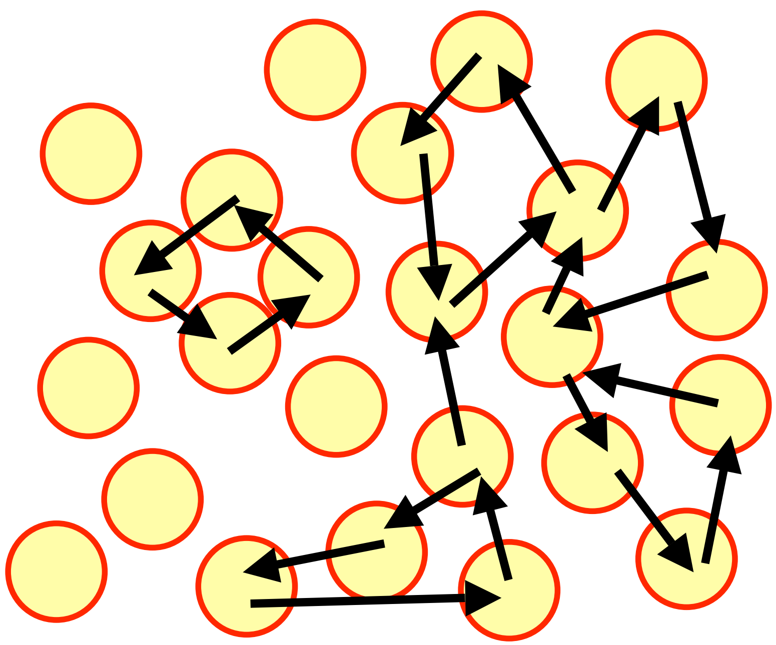

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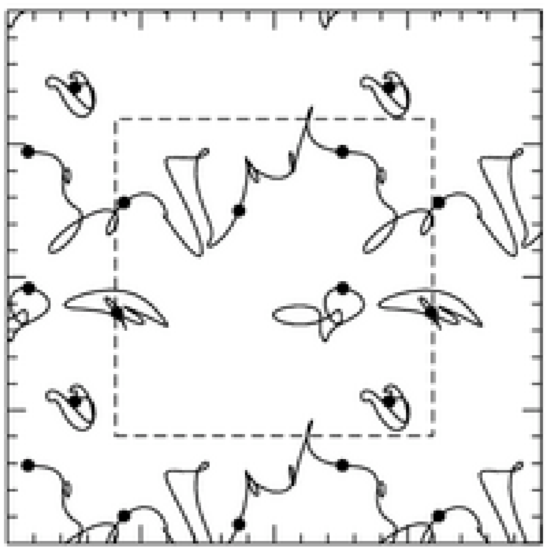
Permutations in bosonic path integrals can explain superfluidity in ^{4}He

Symmetry leads to bosonic and fermionic path integrals

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

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



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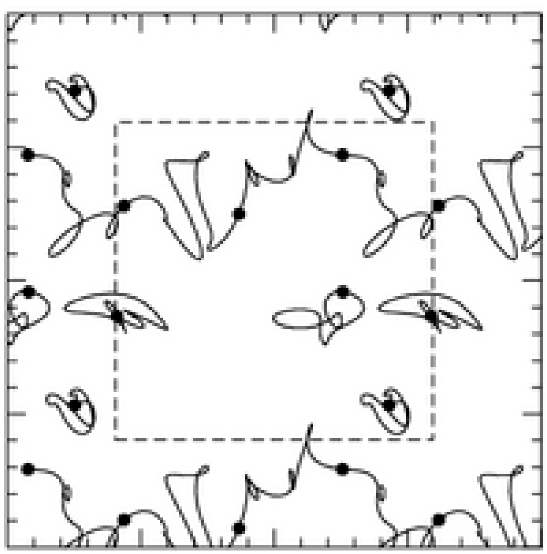
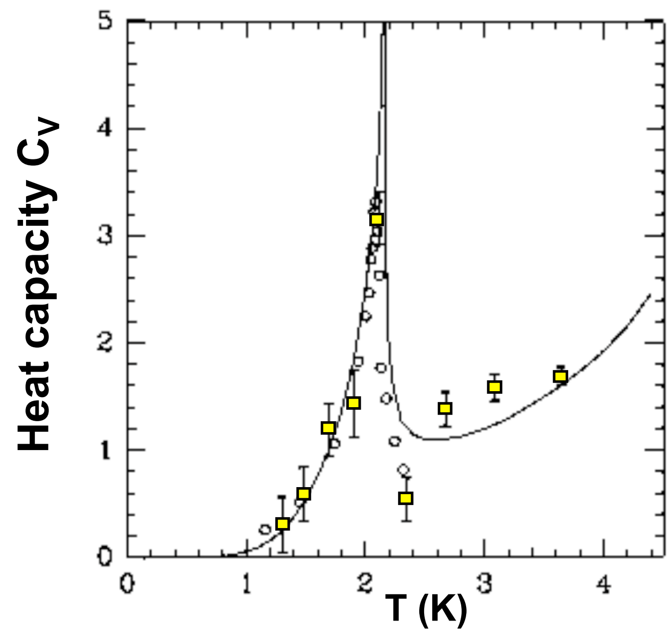
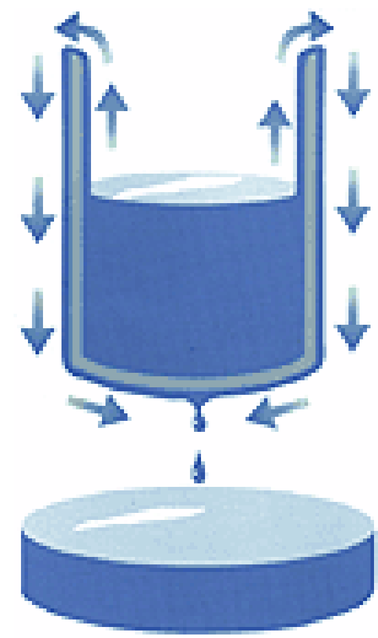


PIMC reproduces λ-transition in ^{4}He
[Ceperley, Pollock (1986)]



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.

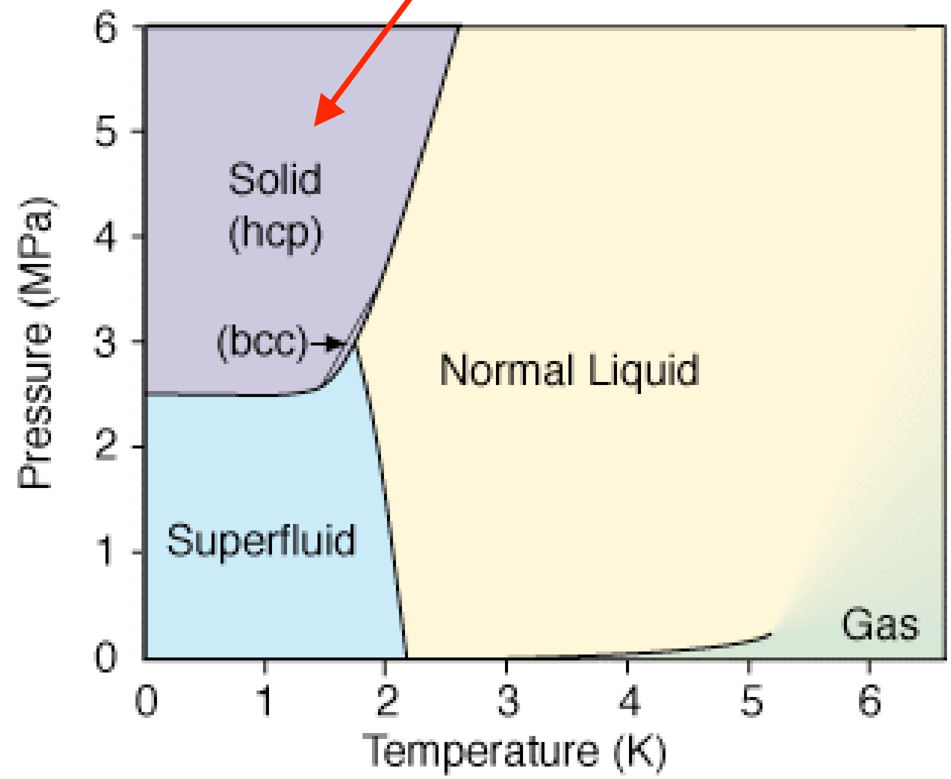
What materials exhibit superfluidity?

1.
2.
3.
4.
5.

What materials exhibit superfluidity?

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

Not superfluid!



What materials exhibit superfluidity?

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2. Fluid ^{3}He (pairing)
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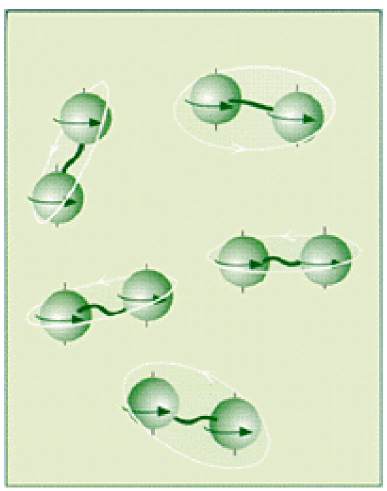

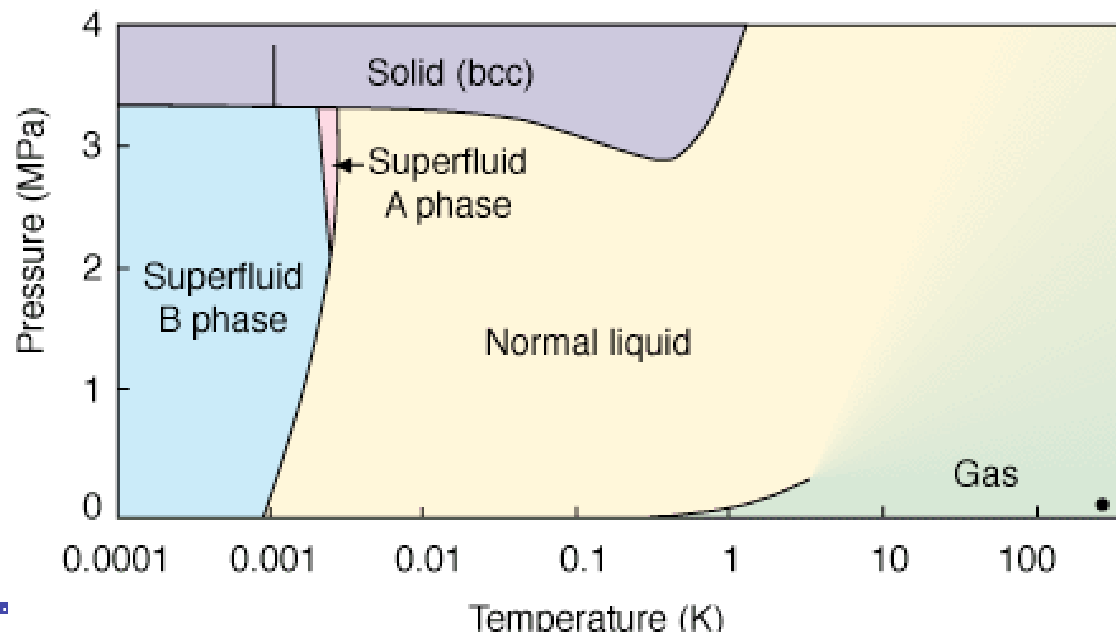

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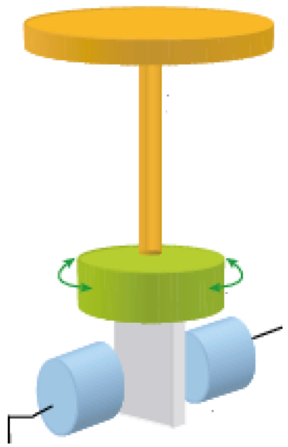
5. Supersolid ^{4}He ?

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:

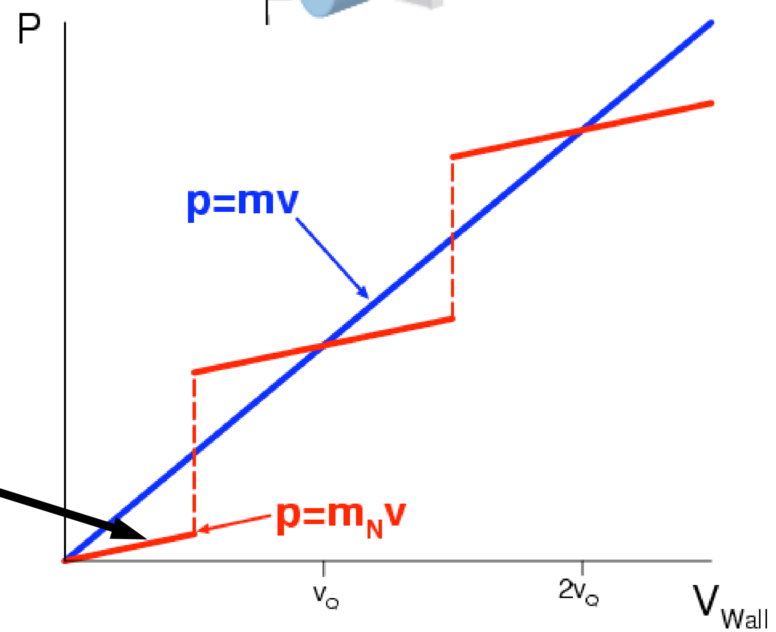


$$I = \left.\frac{dF}{d\omega^2}\right|_{\omega \to 0} = \left.\frac{d\langle \hat{L}_Z \rangle}{d\omega}\right|_{\omega \to 0}$$

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

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 of inertia (NCRI).** This is the definition of a superfluid.

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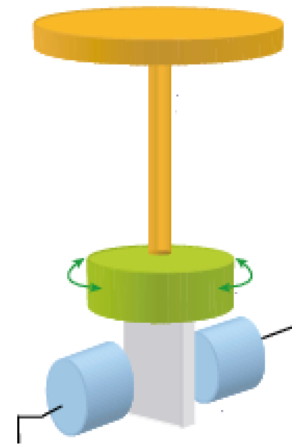

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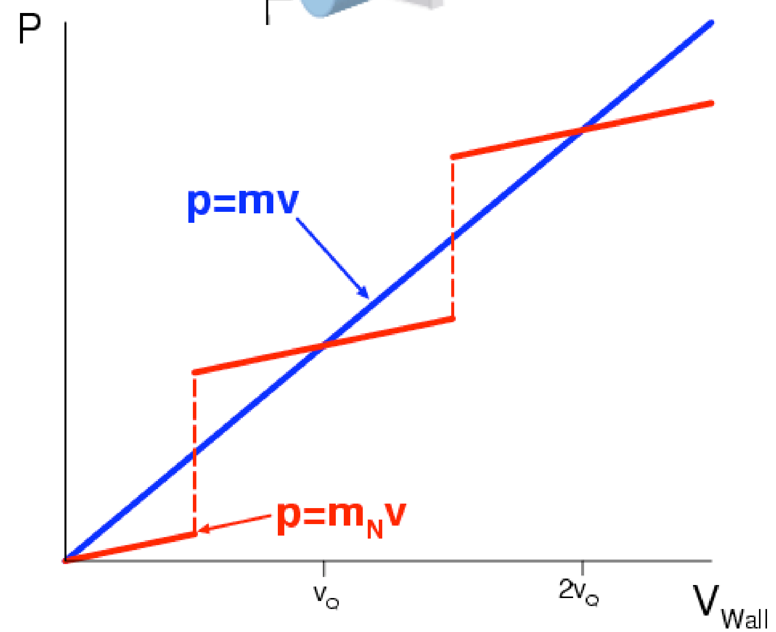
This is "interpreted" as a fraction of the particle became superfluid and stopped spinning.

→ Two fluid model (Landau)

$$\rho = \rho_S + \rho_N \qquad m = m_S + m_N$$

Normal fluid: $\vec{L}(T) = I(T)\ \vec{\omega}$ $\qquad \dfrac{\rho_N}{\rho} = \dfrac{I(T)}{I_{cl}}$



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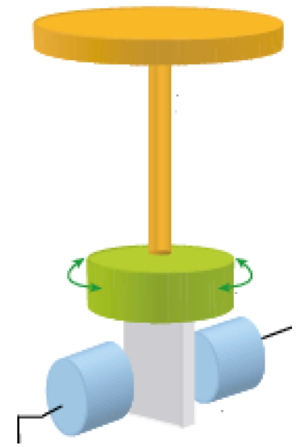

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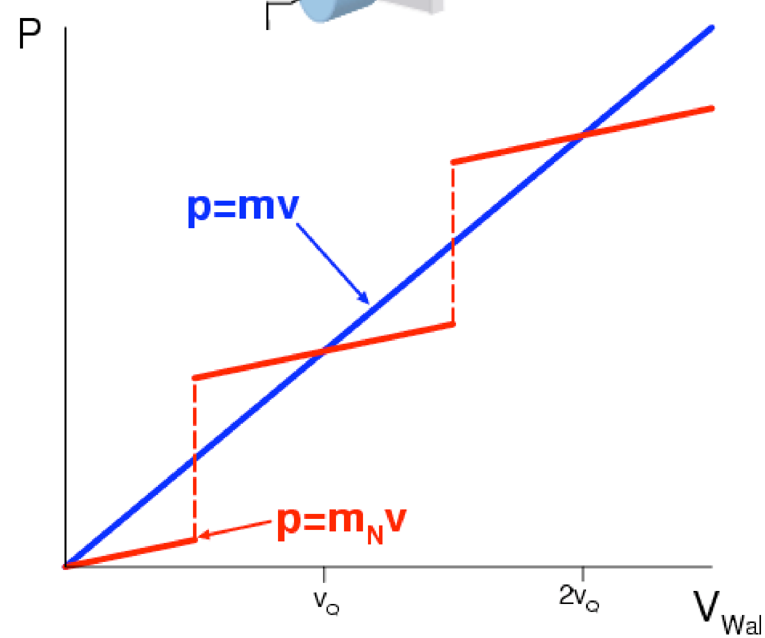
Superfluid:

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



Superfluid moves frictionless, which leads to persistent currents

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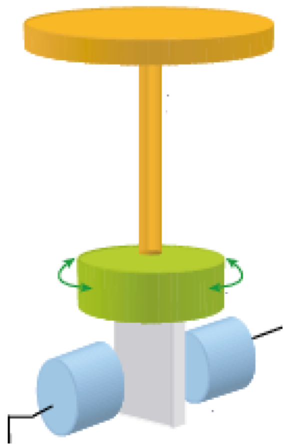


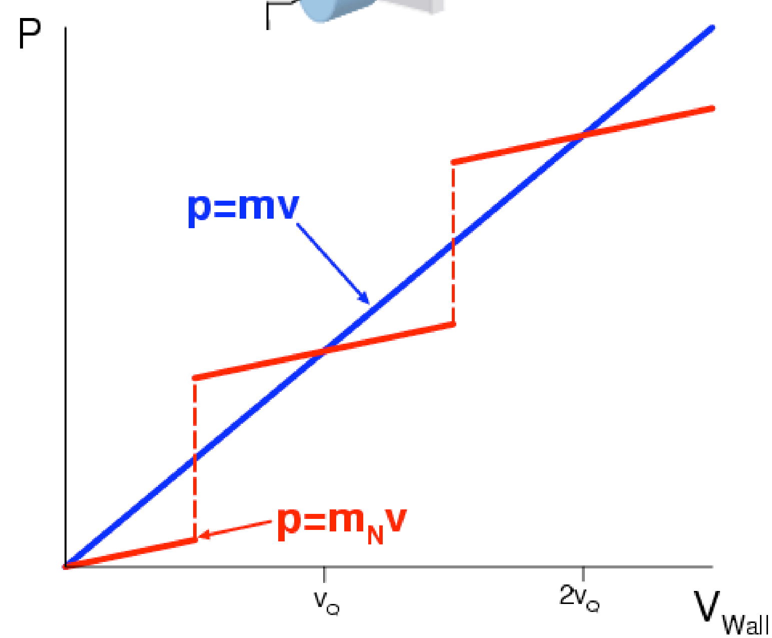
Different experiment: Spin the bucket and cool the system below transition temperature. Then stop the bucket.

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

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:

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

ρ_V statisfies periodic boundary conditions.

$$\rho_V(r_1,\ldots,r_N\ ;\ r_1'\ ,\ \ldots\ ,\ r_j' + L\ ,\ \ldots\ ,\ r_N')$$
$$= \rho_V(r_1\ ,\ \ldots\ ,\ r_N\ ;\ r_1'\ ,\ \ldots\ ,\ r_j'\ ,\ \ldots\ ,\ r_N')$$

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$$\begin{aligned} &\rho_V(r_1,\ldots,r_N\ ;\ r_1',\ \ldots,\ r_j'+L,\ \ldots,\ r_N') \\ &= \rho_V(r_1,\ \ldots,\ r_N\ ;\ r_1',\ \ldots,\ r_j',\ \ldots,\ r_N') \end{aligned}$$

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

$$\frac{\rho_N}{\rho} Nm\ \vec{v} = \left\langle \vec{P} \right\rangle_V = \frac{Tr[\vec{P}\hat{\rho}_V]}{Tr[\hat{\rho}_V]} = -\frac{\partial F_V}{\partial \vec{v}} + Nm\ \vec{v}$$

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

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$$\rho_V(r_1,\ldots,r_N \; ; \; r_1' \, , \; \ldots \, , \; r_j' + L \, , \; \ldots \, , \; r_N') = \rho_V(r_1 \, , \; \ldots \, , \; r_N \; ; \; r_1' , \; \ldots \, , \; r_j' \, , \; \ldots \, , \; r_N')$$

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

$$\frac{\rho_N}{\rho} Nm\,\vec{v} = \left\langle \vec{P} \right\rangle_V = \frac{Tr[\vec{P}\hat{\rho}_V]}{Tr[\hat{\rho}_V]} = -\frac{\partial F_V}{\partial \vec{v}} + Nm\,\vec{v}$$

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

Equivalent to system with stationary walls:

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

with modified boundary conditions

$$\rho(r_1,\ldots,r_N \; ; \; r_1' \, , \; \ldots \, , \; r_j' + L \, , \; \ldots \, , \; r_N') = \exp\left[i\; m\; \vec{v} \circ \vec{L} / \hbar\right] * \rho(r_1 \, , \; \ldots \, , \; r_N \; ; \; r_1' , \; \ldots \, , \; r_j' \, , \; \ldots \, , \; r_N')$$

PIMC computation of the superfluid fraction [Pollock, Ceperley, *Phys. Rev.* B 36 (1987) 8343]

Hamiltonian in a system with moving walls:

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

ρ_V statisfies periodic boundary conditions.

$$\rho_V(r_1,\ldots,r_N \; ; \; r_1' \; , \; \ldots \; , \; r_j' + L \; , \; \ldots \; , \; r_N') = \rho_V(r_1 \; , \; \ldots \; , \; r_N \; ; \; r_1' , \; \ldots \; , \; r_j' \; , \; \ldots \; , \; r_N')$$

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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:

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

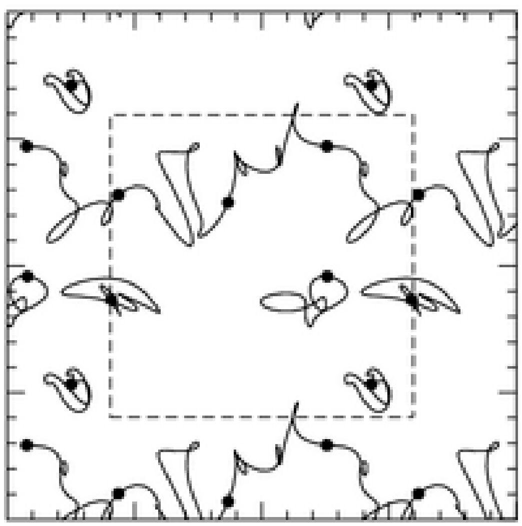
Computation of the Superfluid Fraction with PIMC

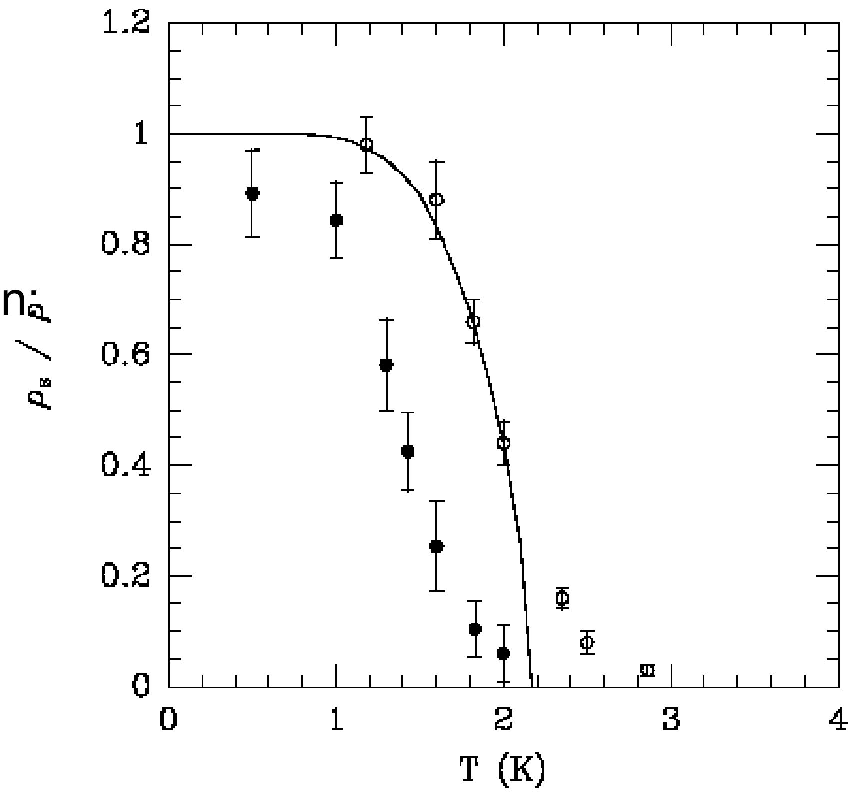
Definition of winding number:

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

PIMC estimator for the superfluid fraction:

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





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

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

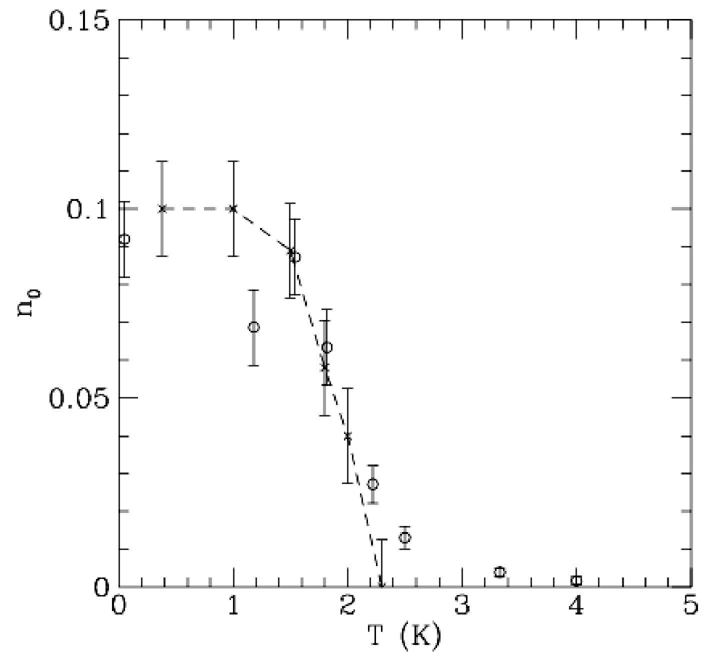
Definition of the *condensation fraction*

London (1938) suggested that superfluidity is Bose condensation.
The quation is whether this is the *zero-momentum state* 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 measured and computed.

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



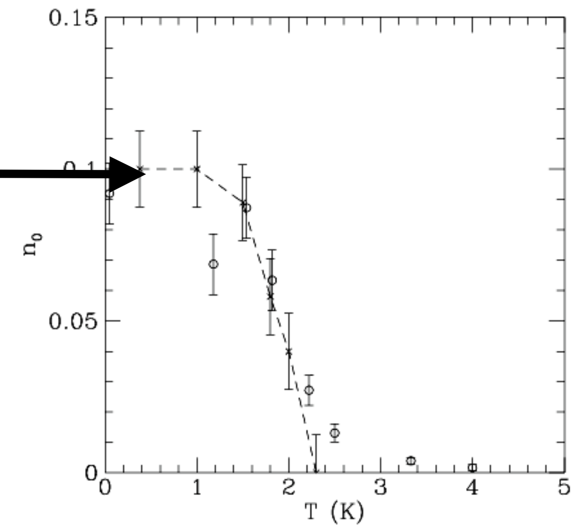
For interacting systems, the T=0 limit of the condensate fraction less than 1 (10% for ^{4}He).

How to compute the momentum distribution in PIMC?

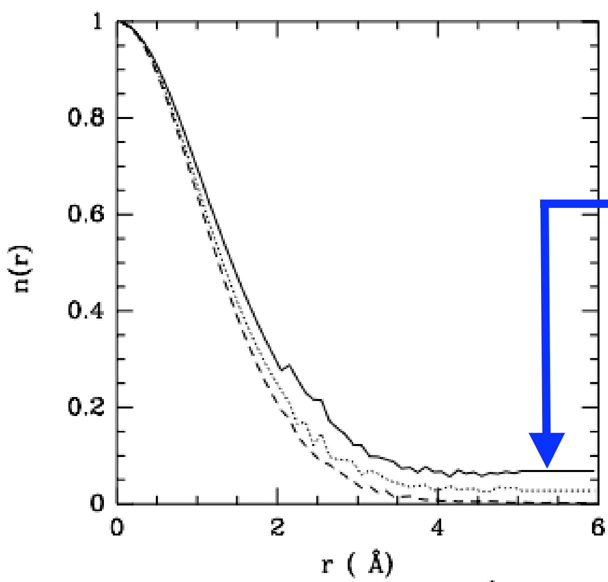
The momentum distribution can also be expressed in terms of the thermal density matrix. However, this requires **off-diagonal density matrix elements**

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

$$n(k) \sim \int dR\, dr_1'\, e^{i(r_1 - r_i')\circ k}\, \rho(r_1 \ldots r_N, r_1' \ldots r_N)$$



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.**

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

Probable observation of a supersolid helium phase

E. Kim & M. H. W. Chan

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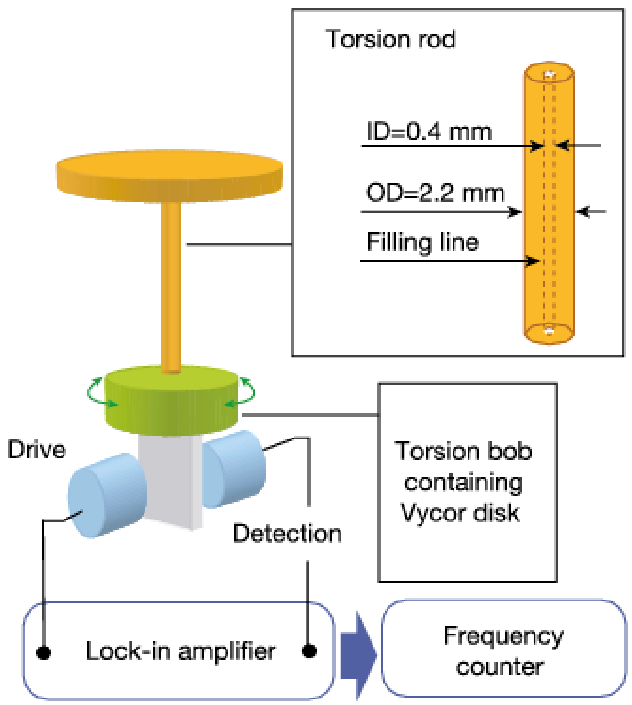
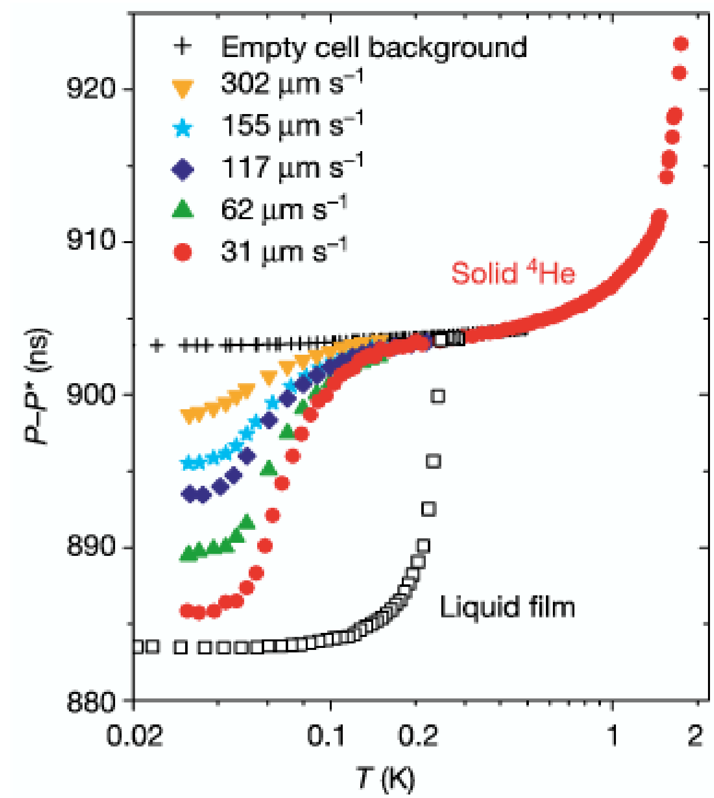
Below T_C, a fraction becomes superfluid.
This lowers the moment of inertia I.
This lowers the oscillation period P.





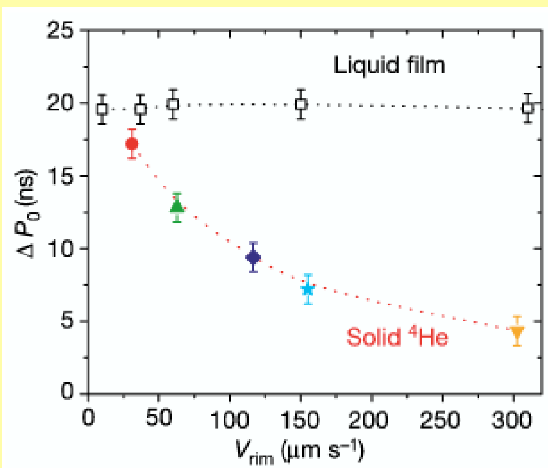
Possible interpretations of the experiment:

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?

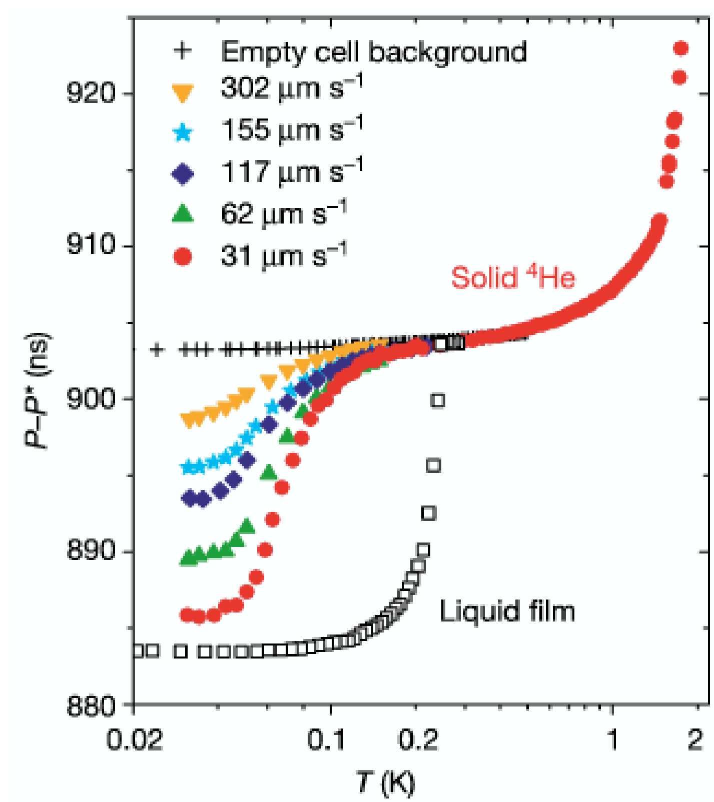
- Results are not consistent of picture of a film:



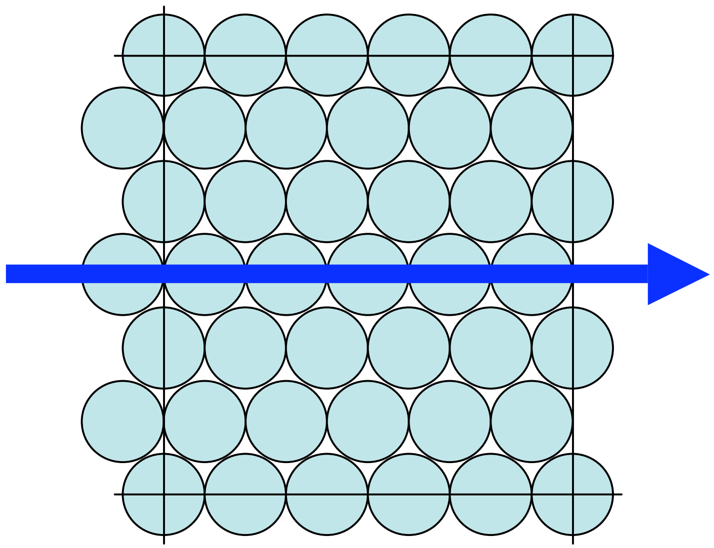
How can we explain the experiment:

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

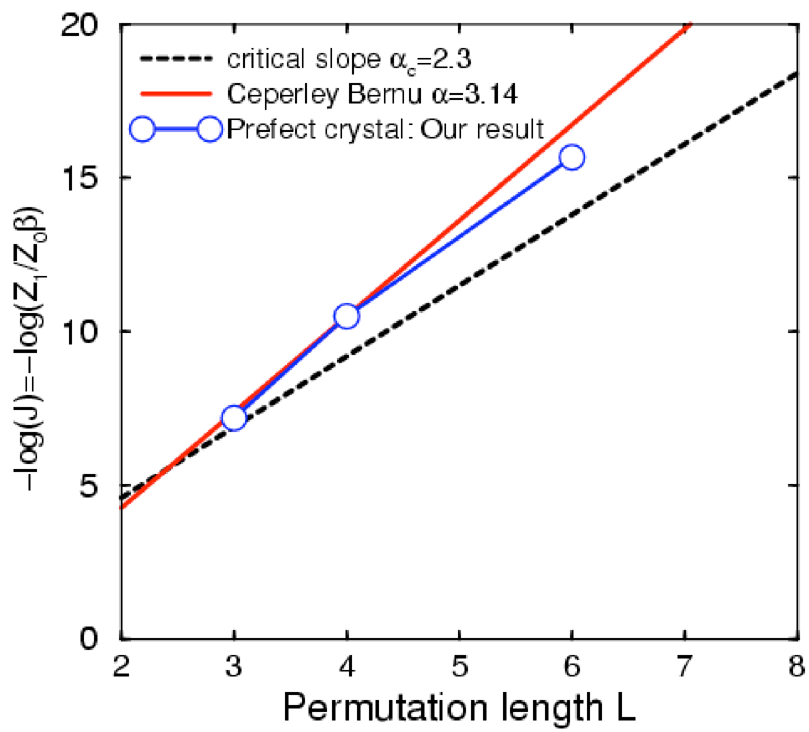
Below T_C, a fraction becomes superfluid.
This lowers the moment of inertia I.
This lowers the oscillation period P.



Ceperley-Bernu approach: Exchange frequency calculation in perfect crystal



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



•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 then **2.3** to support superfluidity.
•Ceperley & Bernu (PRL 2004) showed that a perfect crystal cannot become superfluid.