Path Integral Monte Carlo for Bosons

Summer school 2012 “QMC Theory and Fundamentals”

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# Properties of Bosons and Fermions

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_Burkhard Militzer, UC Berkeley: “Path Integral Monte Carlo”, 2012_
### 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:

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

---

Apply projection to the density matrix:

\[
\rho_B(R,R',\beta) = \sum_P (\pm 1)^P \rho_D(R,PR',\beta)
\]

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

\[
\langle R \mid \hat{\rho}_{F/B} \mid R' \rangle = \sum_P (\pm 1)^P \int dR_1 \ldots \int dR_{M-1} \langle R \mid e^{-\tau \hat{H}} \mid R_1 \rangle \ldots \langle R_{M-1} \mid e^{-\tau \hat{H}} \mid PR' \rangle
\]
Bosonic and Fermionic Path Integrals

Bosonic density matrix:
Sum over all symmetric eigenstates.

$$\rho_B(R,R',\beta) = \sum_i e^{-\beta E_i} \Psi^i_s(R) \Psi^i_s(R')$$

Project out the symmetric states:

$$\rho_B(R,R',\beta) = \sum_p (+1)^p \rho_D(R,PR',\beta)$$

$$\langle R | \hat{\rho}_F/B | R' \rangle = \sum_p (\pm)^p \int dR_1...\int dR_{M-1} \langle R | e^{-\tau \hat{H}} | R_1 \rangle...\langle R_{M-1} | e^{-\tau \hat{H}} | PR' \rangle$$

D:

\[ R' = R = \{r_1, r_2\} \]

\[ R = \{r_1, r_2\} \]

Fermionic density matrix:
Sum over all antisymmetric eigenstates.

$$\rho_F(R,R',\beta) = \sum_i e^{-\beta E_i} \Psi^i_{AS}(R) \Psi^i_{AS}(R')$$

Project out the antisymmetric states:

$$\rho_F(R,R',\beta) = \sum_p (-1)^p \rho_D(R,PR',\beta)$$

B: \((+1)^p\)

F: \((-1)^p\)
Particle Statistics
leads to exchange effects represented by permutations

Symmetry leads to bosonic and fermionic path integrals

\[
\langle R \mid \hat{\rho}_{F/B} \mid R' \rangle = \sum_{p} (\pm 1)^{p} \int dR_{1} \ldots \int dR_{M-1} \langle R \mid e^{-\tau \hat{H}} \mid R_{1} \rangle \ldots \langle R_{M-1} \mid e^{-\tau \hat{H}} \mid PR' \rangle
\]

Bosons: Long permutation cycles, only positive contributions
\[\rightarrow \text{superfluidity in } ^{4}\text{He}\]

Fermions: Cancellation of positive and negative contributions
\[\rightarrow \text{Fermion sign problem, efficiency } e^{-\beta N}\]

Fixed node approximation

\[
\langle R \mid \hat{\rho}_{F} \mid R' \rangle = \sum_{p} (-1)^{p} \oint dR_{i} e^{-S[R_{i}]} \quad \rho_{T} \geq 0
\]

Burkhard Militzer, UC Berkeley: “Path Integral Monte Carlo”, 2012
I. Permutation sampling
How do we sample the permutation space?

Step 0: Pick an imaginary time window

Imaginary time

x
How do we sample the permutation space?

Step 0: Pick an imaginary time window
Step 1: Study all possible permutations and determine their sign.
How do we sample the permutation space?

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

(1 2 3)

Identity permutation (1)

P=+1
How do we sample the permutation space?

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

Identity permutation (1)
(1 2 3)
P=+1

2-particle permutation (3)
(1 2 3)
P=-1

(1 2 3)
(1 3 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.

Identity permutation (1)

2-particle permutation

How many 2-particle permutations are there?
How do we sample the permutation space?

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

- **Identity permutation (1)**
  - (1 2 3) \( P=+1 \)

- **2-particle permutation (3)**
  - (1 2 3) \( P=-1 \)

- **3-particle cyclic permutation**
  - (1 2 3) \( P=-1 \)
How do we sample the permutation space?

Step 0: Pick an imaginary time window

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

(1 2 3)  P=+1

Identity permutation (1)

(1 2 3)  P=-1

2-particle permutation (3)

(1 3 2)  P=-1

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 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?

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.

\[
\pi(P) = \frac{\rho(R_0, PR_8, 8\tau)}{\sum_{P'} \rho(R_0, P'R_8, 8\tau)}
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Step 2: Include all likely three-particle permutations. Enter them with any increased probability to try to make move more often (to sample the superfluid state better). Detailed balanced remains satisfied.

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Step 3: 4 body-permutations

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How to construct a table containing all likely permutations?

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II. Superfluidity
Permutations in bosonic path integrals can explain superfluidity in $^4\text{He}$

Symmetry leads to bosonic and fermionic path integrals

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

Bosons: Long permutation cycles, only positive contributions

$\rightarrow$ superfluidity in $^4\text{He}$

PIMC reproduces $\lambda$-transition in $^4\text{He}$

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

Heat capacity $C_v$

$T$ (K)

[Ceperley, Pollock (1986)]
Permutations in bosonic path integrals can explain superfluidity in $^4$He

Symmetry leads to bosonic and fermionic path integrals

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

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

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

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

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 $^4$He (boson)
2. 
3. 
4. 
5. Not superfluid!
What materials exhibit superfluidity?

1. Fluid $^4\text{He}$ (boson)
2. Fluid $^3\text{He}$ (pairing)
3. 
4. 
5. 

![Diagram showing phase transitions in helium isotopes](image)
What materials exhibit superfluidity?

1. Fluid $^4\text{He}$ (boson)
2. Fluid $^3\text{He}$ (pairing)
3. Lasercooled atoms magnet traps
4.
5.
What materials exhibit superfluidity?

1. Fluid $^4$He (boson)
2. Fluid $^3$He (pairing)
3. Lasercooled atoms magnet traps
4. Molecules in magnetic traps.
What materials exhibit superfluidity?

1. Fluid $^4$He (boson)
2. Fluid $^3$He (pairing)
3. Lasercooled atoms magnet traps
4. Molecules in magnetic traps.
5. Supersolid $^4$He?
Definition of the superfluid fraction
Nonclassical rotational inertia (NCRI)

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

$$I = \frac{dF}{d\omega^2} \bigg|_{\omega \to 0} = \frac{d \langle \hat{L}_z \rangle}{d\omega} \bigg|_{\omega \to 0}$$

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

Quantized circulations define $v_0$

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

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

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

→ Two fluid model (Landau)

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

Normal fluid:

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

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

$$ \rho = \frac{m_N v}{\rho} $$
**Definition of the superfluid fraction**

Nonclassical rotational inertia (NCRI)

Experiment: spinning a bucket of fluid $^4$He:

Below $T_C$, $^4$He exhibits a **lowered moment of inertia**:

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\[
\rho = \rho_S + \rho_N \quad m = m_S + m_N
\]

Normal fluid:  \( \tilde{L}(T) = I(T) \tilde{\omega} \)

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

Superfluid: \[
\frac{\rho_S}{\rho} = 1 - \frac{\rho_N}{\rho} = 1 - \frac{I}{I_C}
\]

\[
\frac{\rho_S}{\rho} = 1 - \frac{m_N}{m}
\]

\[p = mv\]

\[p = m_N v\]
Superfluid moves frictionless, which leads to persistent currents

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

$$I = \frac{dF}{d\omega^2} \bigg|_{\omega \to 0} = \frac{d\langle \hat{L}_z \rangle}{d\omega} \bigg|_{\omega \to 0}$$

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

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

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

The superfluid keeps spinning. Normal component is at rest.

→ **Persistent currents.**

They disappear above the transition temp.
PIMC computation of the superfluid fraction


Hamiltonian in a **system with moving walls**:

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

\(\rho_V\) satisfies periodic boundary conditions.

\[
\rho_V(r_1, ..., r_N; r_1', ..., r_j + L, ..., r_N') = \rho_V(r_1, ..., r_N; r_1', ..., r_j', ..., r_N')
\]

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

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

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

\[
e^{-\beta(F_V - F_{V=0})} = \frac{\int dR \rho_V(R,R;\beta)}{\int dR \rho_{V=0}(R,R;\beta)} = \left\langle e^{i\vec{W} \cdot \vec{L}} \right\rangle
\]

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:

\[ \frac{\rho_s}{\rho} = \frac{mL^2}{\hbar^2 3\beta N \langle \vec{W}^2 \rangle} \]

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

Challenge: Compute winding number for large system, especially in \(^4\text{He}\) at higher pressures.
Computation of the Superfluid Fraction in Finite Systems with PIMC – Area Estimator

Hamiltonian in rotating frame:
\[ \hat{H}_\omega = \hat{H}_0 - \omega \hat{L}_z \]

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

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

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 \(^4\text{He}\)).
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

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

\[ n(k) \sim \int dR \, d' \, e^{i(r_i - r'_i) \cdot k} \rho(r_1 ... r_N, r'_1 ... r'_N) \]

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?

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 $^4$He 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:

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

How can we explain the experiment:
- e.g. superfluid defects
- disorder could also introduce s.f.
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

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

- 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 helium crystal cannot become a superfluid.
Boninsegni, Prokofev, Svistunov: Worm Algorithm for Grand Canonical PIMC

Worm Algorithm for Continuous-Space Path Integral Monte Carlo Simulations

Massimo Boninsegni,¹ Nikolay Prokof`ev,¹,²,³,⁴ and Boris Svistunov²,³

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

Disorder and the Supersolid State of Solid $^4$He

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(Received 13 March 2007; published 26 April 2007)

We report torsional oscillator supersolid studies of highly disordered samples of solid $^4$He. 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 $^4$He. 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 $^4$He.
The End