Bosonic Path Integrals

1. Overview of effect of bose statistics
2. Permutation sampling considerations
3. Calculation of superfluid density and momentum distribution.
4. Applications of PIMC to liquid helium and helium droplets.
5. Momentum distribution calculations

Quantum statistics

- For quantum many-body problems, not all states are allowed: allowed are totally symmetric or antisymmetric. Statistics are the origin of BEC, superfluidity, lambda transition.
- Use permutation operator to project out the correct states:
  \[ \hat{P} f(R) = \sum_{p=1}^{N!} \frac{1}{N!} f(PR) \]
  \[ Z = \sum_{p=1}^{N!} \int dR_1 \ldots dR_M e^{-\sum_{i=1}^{M} S(R_i, R_{i+1})} \]
- Means the path closes on itself with a permutation. \( R_1 = PR_{M+1} \)
- Too many permutations to sum over; we must sample them.
- **PIMC task**: sample path \( \{ R_1, R_2, \ldots, R_M \text{ and } P \} \) with Metropolis Monte Carlo (MCMC) using “action”, \( S \), to accept/reject.
Exchange picture

- Average by sampling over all paths and over connections.
- Trial moves involve reconnecting paths differently.
- At the superfluid transition a "macroscopic" permutation appears.
- This is reflection of Bose condensation within PIMC.

Ceperley PIMC for bosons

3 boson example

- Suppose the 2 particle action is exact.
- Make Jastrow approximation for spatial dependance (Feynman form)

\[
\langle R | e^{-\beta H} | R' \rangle = e^{-\sum_p f(r^p, r'^p)} \prod_{i<j} f(r^p_i, r'^p_j) \quad \text{units with } 4\beta\lambda = 1
\]

\[
\rho_{\text{bose}}(R) = \sum_p \langle R | e^{-\beta H} | PR \rangle \approx \sum_p \langle R | e^{-\beta H} | PR \rangle \prod_{i<j} f(r^p_i, r'^p_j)
\]

\[
\rho_{\text{bose}}(R) = |\Psi(R)|^2 \left[ 1 + e^{-\beta\lambda} + e^{-\beta\lambda} + e^{-2\beta\lambda} + 2e^{-\beta\lambda - \beta\lambda} - \beta\lambda \right]
\]

- Spatial distribution gives an effective attraction (Bose condensation).
- For 3 particles we can calculate the "permanent," but larger systems require us to sample it.
- Anyway permutations are more physical.
PIMC Sampling considerations

- Metropolis Monte Carlo that moves a single variable is too slow and will not generate permutations.
- We need to move many time slices together.
- Key concept of sampling is how to sample a “bridge”: construct a path starting at $R_0$ and ending at $R_t$.
- How do we sample $R_{t/2}$? GUIDING RULE. Probability is:

$$P(R) = \frac{\langle R_0 | e^{-iHt/2} | R_{t/2} \rangle \langle R_{t/2} | e^{-iHt/2} | R_t \rangle}{\langle R_0 | e^{-iHt} | R_t \rangle}$$

- Do an entire path by recursion from this formula.
- Related method: fourier path sampling.

How to sample a single slice.

- pdf of the midpoint of the bridge: (a pdf because it is positive, and integrates to 1)
- For free particles this is easy - a Gaussian distribution

PROVE: product of 2 Gaussians is a Gaussian.
- Interaction reduces $P(R)$ in regions where spectator atoms are.
- Better is correlated sampling: we add a bias given by derivatives of the potential (for justification see RMP pg 326)
- Sampling potential $U_s$ is a smoothed version of the pair action.
**Bisection method**

1. Select time slices
2. Select permutation from possible pairs, triplets, from: $\rho(R, PR'; 4\tau)$
3. Sample midpoints
4. Bisect again, until lowest level
5. Accept or reject entire move

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**Multilevel Metropolis/ Bisection**

- Introduce an approximate level action and sampling.
- Satisfy detailed balance at each level with rejections (PROVE)

$$A_i(s \rightarrow s') = \min \left[ 1, \frac{T_i(s' \rightarrow s)(s')\pi_i(s')\pi_{i-1}(s)}{T_i(s \rightarrow s')(s)\pi_i(s)\pi_{i-1}(s')} \right]$$

- Only accept if move is accepted at all levels.
- Allows one not to waste time on moves that fail from the start (first bisection).
**Permutation Sampling**

For bosons we also have to move through permutation space. A "local" move is to take an existing permutation and multiply by a k-cycle

\[ P_{\text{trial}} = \hat{p}(i_1, i_2, ..., i_k)P \]

- Sometimes need more than 2-particle exchanges—for fermions 3 particle exchanges are needed
- Need more than 1 time slice because of hard core.

Two alternative ways:

1. Make a table of possible exchanges and update the table. Good for up to 4 particle exchanges “SELECT”
2. Have a virtual table and sample permutation from that table. Good for longer exchanges (up to 10 body exchanges). "PERMUTE"

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**Heat Bath Method**

Sample a neighborhood of a given point so that it is in local equilibrium.

\[ T(s \rightarrow s') = \frac{\pi(s')}{C(s)} \]

\[ C(s) = \sum_{s'' \in N(s)} \pi(s'') \]

Then the acceptance probability will be:

\[ A(s \rightarrow s') = \min \left( 1, \frac{C(s)}{C(s')} \right) \]

Can only be used if it is possible to quickly compute the normalization.

Acceptance ratio=1 if C(s) is independent of s.

For a given neighborhood, convergence is as fast as possible (it equilibrates in one step).
How to select permutation

- Heat bath probability of move being accepted is:

\[ T(p) = \left( \rho_R e^{-\beta H} \right) \approx \exp \left[ -\frac{\sum (c_j - r_j')}{4 n \lambda \tau} \right] = \prod h_{j, j'} \]

\[ h_{i,j} = \exp \left[ -\frac{(c_j - r_i')}{4 n \lambda \tau} \right] = \text{distance table} \]

Example: \( T(1,2) \approx h_{1,2} h_{2,1} \)

- Set up “h” matrix
- Loop over all pairs and find all \( T(i,j) \)’s
- Loop over triplets and find \( T(i,j,k) \)’s ...
- In acceptance probability we need the normalized probability:

\[ \hat{T} = \frac{T}{C} \text{ where } C = \sum_p T(p) \]

- This gives an addition rejection rate.

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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.

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

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

\[
\lambda \equiv \frac{\hbar^2}{2m_i}
\]

Path Integral explanation of Boson superfluidity

- Exchange can occur when thermal wavelength is greater than interparticle spacing
  \[
k_B T \leq \hbar^2 \rho^{2/d} / m
\]
- Localization in a solid or glass can prevent exchange.
- Macroscopic exchange (long permutation cycles) is the underlying phenomena leading to:
  - Phase transition: bump in specific heat: entropy of long cycles
  - Superfluidity: winding paths
  - Offdiagonal long range order --momentum condensation separation of cut ends
  - Absence of excitations (gaps)
- Some systems exhibit some but not all of these features.
- Helium is not the only superfluid. (2001 Nobel Prize for BEC)
Permutation Distribution

- As paths get longer probability of permutation gets significant.
- Shown is the probability of a given atom attaching itself to a permutation of length n.
- Superfluid transition occurs when there is a non-zero probability of cycle length N=size of system.
- Permutations are favored in the polymer system because of entropy. In the quantum system because of kinetic energy.
- Impurities can be used to "measure" the permutations.
ENERGY

Bose statistics have a small effect on the energy
Below 1.5K $^4$He is in the ground state.

\[ E = \left\langle V + \frac{3N_{\text{cycles}}}{2\beta} + \frac{1}{2}(\mathbf{r}_i - \mathbf{c}_j) \cdot \nabla \mathbf{V} \right\rangle \]

Kinetic term becomes smaller because $N_{\text{cycle}} \approx N$. Springs stretched more.

SPECIFIC HEAT

• Characteristic $\lambda$ shape when permutations become macroscopic
• Finite size effects cause rounding above transition

• Transition is not in the static distribution functions like $S(k)$ or $g(r)$. They do not change much at the transition.

NON-CLASSICAL TRANSITION

• Effect of turning offbose statistics at the transition:

• Transition is in the imaginary-time connections of the paths-the formation of the macroscopic exchange.
Superfluidity: Two-Fluid Model

Landau Two-Fluid Model: \( \rho = \rho_s + \rho_n \)
- superfluid: irrotational, aviscous fluid. Does not couple to boundaries because of the absence of states.
- normal fluid: created by thermal excitations of superfluid and density gradients.

Andronikashvili Experiment:
normal fluid between disks rotates rigidly with system viscous penetration depth
\[ \xi = \frac{2v}{\sqrt{\rho \omega}} \]  
\( v \): kinematic viscosity  
\( \omega \): angular velocity

Two-fluid model is phenomenological -- what happens on a microscopic scale?

Superfluidity and PIMC

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

\[ \frac{\rho_s}{\rho} = 1 - \frac{I}{I_c} = \frac{dF}{d\omega^2} \bigg|_{\omega=0} \]

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

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

\[ \frac{\rho_s}{\rho} = 1 - \frac{1}{I_c} \left\langle \int_0^T dt \hat{L}_z e^{-i(\beta-\frac{\omega}{c}t)\hat{L}_z} e^{-i\hat{L}_z} \right\rangle \]

\[ \frac{\rho_s}{\rho} = \frac{2m}{\beta \lambda I_c} \]

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)
- The superfluid density is now estimated as:

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

$$\rho_s = \frac{\langle W^2 \rangle}{2\lambda \beta N}$$

- 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.

Ergodicity of Winding Number

- Because winding number is topological, it can only be changed by a move stretching all the way across the box.
- For cubic boundary conditions we need $m \geq N^{1/3}$
- Problem to study finite size scaling: we get stuck in a given winding number sector.
- Advanced algorithms needed such as worm or directed loops (developed on the lattice).
Superfluidity in pure Droplets

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

**NOT A PHASE TRANSITION!**

- But almost completely superfluid at 0.4K (according to response criteria.)
- Superfluidity of small droplet recently verified. *Sindzingre et al 1990*

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

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**Determination of \(T_c\)**

*Runge and Pollock PRB.*

At long wavelength, the free energy is given by the functional:

\[
F = \int dr \left[ \lambda |\nabla \phi(r)|^2 + \mu |\phi(r)|^2 + V\phi(r)^4 \right]
\]

The energy to go from PBC to ABC is given by:

\[
F = \frac{4\lambda \pi^2 L_\perp^2}{V} = k_B T \langle e^{i2\pi L_\perp} \rangle
\]

We determine \(T_c\) by where \(F\) is constant with respect to number of atoms \(N\).

For \(N \sim 100\), \(T_c\) correct to \(~1\%).
Phase Diagram of Hard Sphere Bosons

- Atomic traps are at low density
- With PIMC we mapped out range of densities
- There is enhancement of $T_c$ by 6% because of density homogenization.
  Gruter et al PRL 99.

$$\frac{T_c}{T_c^0} \sim 1 + n^{1/3} a$$

Pair correlations at low density

Free boson pair correlation.
Peak caused by attraction of bosonic exchange.
Zero is hard core interaction.

Structure Factor $S(K)$
(FT of density)
Large compressibility near $T_c$ (clustering)
Determination of $T_c$ using superfluid density. Finite size scaling.

\[ \rho_s = \frac{1}{L} Q \left( \frac{L}{\zeta} \right) \]

\[ \zeta = \text{bulk correlation length} \]

\[ \zeta \to \left( \frac{T - T_c}{T_c} \right)^{-\nu} \]

- Near $T_c$ a single length enters into the order parameter.
- Write superfluid density in terms of the available length.
- Determine when the curves cross to get $T_c$ and exponent.
- Exponent is known or can be computed.

Why is $H_2$ not a superfluid?

- $H_2$ is a spherically symmetric boson like He.
- However its intermolecular attraction is three times larger.
- Hence its equilibrium density is 25\% higher $\Rightarrow$ solid at $T<13K$.
- To be superfluid we need to keep the density lower or frustrate the solid structure.

At low $T$ and density, orientational energies are higher $\Rightarrow H_2$ is spherical.

\[ E(J_1) - E(J_0) = 170K \]
\[ E(J_2) - E(J_0) = 510K \]
**H₂ droplets**

- In droplet or at surfaces, many bonds are broken.
- We found that small droplets are superfluid.
- Recently verified in experiments of ⁴He-H₂-OCS clusters: When a complete ring of H₂ surrounds OCS impurity, it no longer acts as a rigid body, but decouples from the motion of the OCS.

*Sindzingre et al. PRL 67, 1871 (1991).*

**H₂ on Ag-K surfaces**

*Gordillo, DMC PRL 79, 3010, 1997.*

- Formation of solid H₂ is frustrated by alkali metal atoms.
- Lowers the wetting density-result is liquid (superfluid) ground state with up to 1/2 layer participating.
- Has not yet been seen experimentally.
Droplets and PIMC
E. Draeger (LLNL)  D. Ceperley (UIUC)

- Provide precise microscopic probes for phenomena such as superfluidity and vortices.
- Provide a nearly ideal “spectroscopic matrix” for studying molecular species that 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.

Experimental Setup for He droplets
Toennies and Vilesov,

- Adiabatic expansion cools helium to below the critical point, forming droplets.
- Droplets then cool by evaporation to:
  
  \[
  \begin{align*}
  T &= 0.38 \text{ K}, \quad N = 10^4 \quad (^4\text{He}) \\
  T &= 0.15 \text{ K}, \quad N = 10^3 \quad (^3\text{He})
  \end{align*}
  \]
- 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


- An OCS molecule in a $^4\text{He}$ droplet shows rotational bands corresponding to free rotation, with an increased moment of inertia (2.7 times higher)
- $^4\text{He}$ “coat” the impurity allowing it to freely rotate in the superfluid
- They replaced boson $^4\text{He}$ with fermion $^3\text{He}$. If Bose statistics are important, then rotational bands should disappear. They didn’t!
- However, commercial $^3\text{He}$ has $^4\text{He}$ impurities, which would be more strongly attracted to an impurity.
- How much $^4\text{He}$ does it take to “coat” the impurity and get free rotation?
- They found that it takes around 60 $^4\text{He}$ atoms.

$^4\text{He}$ is more strongly attracted to impurity because of zero point effects, so it coats the impurity, insulating it from the $^3\text{He}$.
Density distribution within a droplet

- Helium forms shells around impurity (SF₆)
- During addition of molecule, it travels from the surface to the interior boiling off 10-20 atoms.

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

Hydrodynamic Model

Callegari et al:
- Helium inertia due primarily to density anisotropy in superfluid
- Assume the system is 100% superfluid, and the many-body wavefunction has the form:
  \[ \psi(r₁, r₂, \ldots, rₙ) = |\psi| \exp(-i \sum_j \phi_j) \]
  density time-indep.
  in rotating frame
- Then, for systems in the adiabatic limit:
  \[ \nabla \cdot (\rho \nabla \phi) = \frac{\partial \rho}{\partial t} = -\left(\nabla \rho \right) \cdot (\tilde{\omega} \times \vec{r}) \]
  continuity equation
- For a known \( \rho(\vec{r}) \) (adiabatic limit), calculate \( \nabla \phi(\vec{r}) \) from this equation using Gauss-Seidel relaxation. Hydrodynamic inertia is given by
  \[ K.E. = \frac{1}{2} I_c \omega^2 = \frac{1}{2} m \int dV \rho(\nabla \phi) \cdot (\nabla \phi) \]
Local Superfluid Density Estimator

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

\[
\rho_s = \frac{4 m^2}{3 \hbar ^2 B_1 \Omega^2} \int d\vec{r} d\vec{r}' \vec{A}(\vec{r}) \cdot \vec{A}(\vec{r}') = \frac{1}{\Omega} \int d\vec{r} \rho_s(\vec{r})
\]

Where \( A \) is the area.

\[
\vec{A}(\vec{r}) = \int_0^\beta d\tau \sum_i (\vec{r}_i \times \vec{v}_i) \delta(\vec{r}_i - \vec{r})
\]

\[
\rho_s(\vec{r}) = \frac{4 m^2 N}{3 \hbar ^2 B_1 \Omega^2} \int d\vec{r}' \vec{A}(\vec{r}) \cdot \vec{A}(\vec{r}')
\]

\[
\rho_s(\vec{r}) \propto \frac{\hat{A}}{n M} \sum_{\text{cycles}} \hat{V} \left[ \frac{\hat{A}}{n M} + \frac{\hat{A}}{n M} \sum_{\text{cycles}} \hat{V} \right]
\]

approximation: use only diagonal terms

not positive definite could be noisy

(NCN)_x: Self-Assembled Linear Isomers

Nauta and Miller: HCN molecules in \(^4\)He droplets self-assemble into linear chains

- They measured the rotational constants for (HCN)_1, (HCN)_2, and (HCN)_3.
- Adiabatic following holds for (HCN)_3, allowing us to compare both models to experiment.
- Line vortices are unstable in pure helium droplets. Linear impurity chains may stabilize and pin them.

Atkins and Hutson: Calculated the anisotropic \(^4\)He-HCN pair potential from experimental scattering data. This fit can be reproduced within error bars by a sum of three spherical Lennard-Jones potentials and a small anisotropic term.

Superfluidity around a linear molecule

- K. Nauta and R.E. Miller (Science 283, 1895 (1999)) found that HCN molecules will line up in a linear chain in a helium droplet, and measured the HCN-HCN spacing.
- In vacuum they form rings!
- Systems with up to 10 molecules observed.
- Use area formula to find superfluid response.
- We find almost complete superfluid system, even near the impurity.
The local superfluid estimator shows a decrease in the superfluid response throughout the first solvation layer.

Hydrodynamic model prediction: rotating the molecule about its symmetry axis will produce no change in the free energy.

Our local superfluid calculations show a clearly defined decrease in the superfluid density in the first layer!
We calculated the superfluid density distribution of $N=128$ $^4$He droplets with an (HCN)$_3$ isomer at several temperatures.

The superfluid density in the first layer is temperature dependent!

Bulk $^4$He is 100% superfluid below 1.0 K. Both experimental measurements on helium films and PIMC studies of 2D helium show transition temperatures $T_c$ which are significantly lower than bulk helium.

The first layer is a two-dimensional system with important thermal excitations at 0.4K: "vortex-antivortex excitations".

- Very broad transition, due to the small number of atoms in first layer (around 30)
- How will this affect the moment of inertia?
Moment of Inertia

The moment of inertia due to the normal helium does not depend on temperature below 1.0 K.

This is in agreement with experimental results, which found that the moment of inertia of an OCS molecule was the same at $T=0.15$ K and $T=0.38$ K.

We only looked at the superfluid density in the cylindrically-symmetric region of the first layer, not the entire first layer.

\[ \Delta I = \int d\vec{r} \, m_s \, r^2 \left( \rho(\vec{r}) - \rho_s(\vec{r}) \right) \]

Ceperley PIMC for bosons

Moment of Inertia

Separate contribution from cylindrically-symmetric region and spherical endcaps to moment of inertia

The contribution from the endcaps is temperature-independent below 1.0 K. In this region, the induced normal fluid is due primarily to the anisotropic density distribution.

Ceperley PIMC for bosons
Temperature Dependence observed

- Unexplained measurements of Roger Miller of Q branch.
- No Q branch \((\Delta J=0)\) is allowed at \(T=0\) for linear molecules.
- But possible for \(T>0\).

Lines are PIMC based model calculations:

- We have calculated the condensate fraction and density-density correlation functions throughout the free surface. We find that the surface is well-represented as a dilute Bose gas, with a small ripplon contribution.

- We have derived a local superfluid estimator, and directly calculated the normal response of helium droplets doped with HCN molecules.

- We find that the helium in the first solvation layer is a two-dimensional system, with a thermal excitations at \(T=0.38\) K. Explains observation of Q-branch.

- The moment of inertia due to the normal fluid is dominated by the contribution from helium at the ends of the linear molecule, which is independent of temperature below \(T=1.0\) K.
Bose condensation

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

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

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

\[ n(r,s) = \frac{V}{Q} \int dr_2...dr_N \left< r_1r_2...r_N \mid e^{-\beta H} \mid s_1s_2...s_N \right> \]

- 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) \((\text{The FT of a constant is a delta function.})\)

- The condensate fraction gives the linear response of the system to another superfluid.

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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

\[ Pr(k_1,..k_N) = \left| \int dR e^{-i(k_1r_1+...+k_Nr_N)}\psi(R) \right|^2 \]

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

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

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

\[ n(r,s) = \frac{V}{Q} \int dr_2...dr_N \left< r_1r_2...r_N \mid e^{-\beta H} \mid s_1s_2...s_N \right> \]

Where: \( n(r,s) \) 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.

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**Comparison with experiment**

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).

Surface of Liquid Helium

2 possible pictures of the surface

- **Dilute Bose gas model:** Griffin and Stringari, PRL 76, 259 (1996).
  
  $^4$He
  
  bulk: $n_0 = 9\%$
  
  surface: $n_0 = 100\%$


  Can smeared density profile be caused by ripplons alone?

  $^4$He

  Density profile does not distinguish

  surface: $n_0 = 50\%$
ODLRO at the Surface of Liquid $^4$He

Simulation supports the dilute bose gas model.

Condensate Fraction at the Surface of $^4$He

- PIMC supports dilute gas model.
- Jastrow wavefunction
- Shadow wavefunction
Non-condensed distribution

![Graph showing non-condensed distribution](image)

- \( \rho = 0.0218 \text{ Å}^{-3} \)
- \( \rho = 0.0149 \text{ Å}^{-3} \)
- \( \rho = 0.0105 \text{ Å}^{-3} \)
- \( \rho = 0.0054 \text{ Å}^{-3} \)

2D superfluids
Kosterlitz-Thouless transition

- Reduced dimensionality implies no bose condensate (except at \( T=0 \)).
- Exchange responsible
- Specific heat bump only
- But still a good superfluid.

Ceperley PIMC for bosons
Exchange energy

- Let’s calculate the chemical potential of a $^3$He atom in superfluid $^4$He.
- First suppose that we neglect the difference in mass but only consider effect of statistics.
- The “tagged particle” is should not permute with the other atoms.
- How does this effect the partition function?
- We do not need to do a new calculation

$$e^{-\beta \mu_1} = \frac{Z_{N-1,1}}{Z_N} = \text{Pr(atom 1 does not exchange)}$$

$$\mu_1 = \mu_4 - kT \ln\left(\frac{P_1}{P_0}\right) + \int_{\ln(3)}^{\ln(4)} d\ln(m)K(m)$$

- Cycle length distribution is measurable, not just a theoretical artifact.

Effective mass

- Effective mass is gotten from the diffusion constant at low T.
- At short time KE dominates and $m=m^*$.
- At large times, neighboring atoms block the diffusion increasing the mass by a factor of 2.
- Same formula applies to DMC!
- Lower curve is for Boltzmannons-they have to return to start position so they move less.
- Diffusion in imaginary time has something to do with excitations!
Dictionary of the Quantum-Classical Isomorphism

Properties of a quantum system are mapped into properties of the fictitious polymer system

Attention: some words have opposite meanings.

<table>
<thead>
<tr>
<th>Quantum</th>
<th>Classical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bose condensation</td>
<td>Delocalization of ends</td>
</tr>
<tr>
<td>Bose statistics</td>
<td>Joining of polymers</td>
</tr>
<tr>
<td>Exchange frequency</td>
<td>Free energy to link polymers</td>
</tr>
<tr>
<td>Free energy</td>
<td>Free energy</td>
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<tr>
<td>Imaginary velocity</td>
<td>Bond vector</td>
</tr>
<tr>
<td>Kinetic energy</td>
<td>Negative spring energy</td>
</tr>
<tr>
<td>Momentum distribution</td>
<td>FT of end-end distribution</td>
</tr>
<tr>
<td>Particle</td>
<td>Ring polymer</td>
</tr>
<tr>
<td>Potential energy</td>
<td>Iso-time potential</td>
</tr>
<tr>
<td>Superfluid state</td>
<td>Macroscopic polymer</td>
</tr>
<tr>
<td>Temperature</td>
<td>Polymer length</td>
</tr>
</tbody>
</table>

Some current applications of PIMC

- Helium 4:
  - “supersolid,”
  - Vortices
  - Droplets
  - Metastable high pressure liquid
- 2D and 3D electron gas:
  - Phase diagram
  - Stripes
  - Disorder
  - Polarization
- Hydrogen at high pressure and temperature
- Vortex arrays
- Pairing in dilute atom gases of fermions
- Liquid metals near their critical point