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.

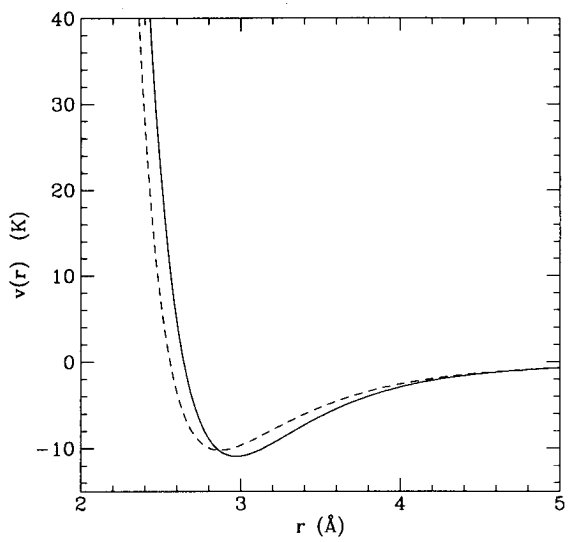


FIG. 1. The semiempirical pair potential between two helium atoms: solid line, Aziz *et al.* (1992); dashed line, Lennard-Jones 6-12 potential with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å.

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

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:

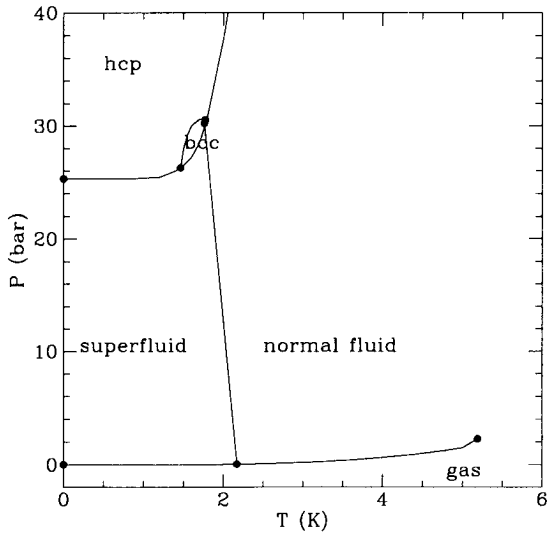


FIG. 2. The phase diagram of ^{4}He.

$$\widehat{H} = -\sum_i \frac{\hbar^2}{2m_i}\nabla_i^2 + V(R)$$

$$\lambda \equiv \frac{\hbar^2}{2m_i}$$

Path Integral explanation of Boson superfluidity

- Exchange can occur when thermal wavelength is greater than interparticle spacing

$$k_B T \le h^2 \rho^{2/d} / m$$

- 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)

Superfluidity: Two-Fluid Model

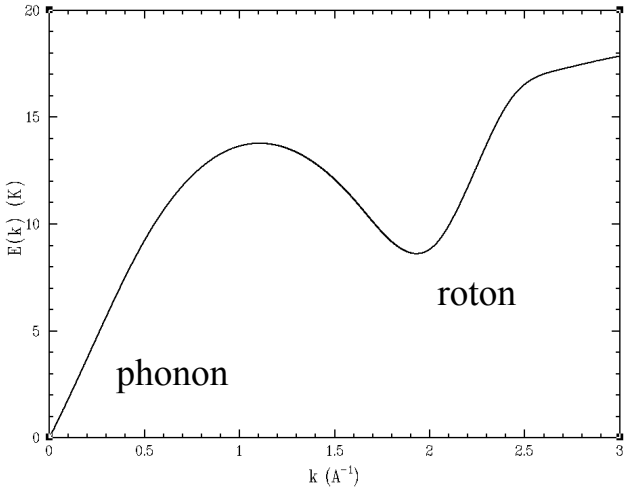
Landau Two-Fluid Model: $\rho = \rho_n + \rho_s$

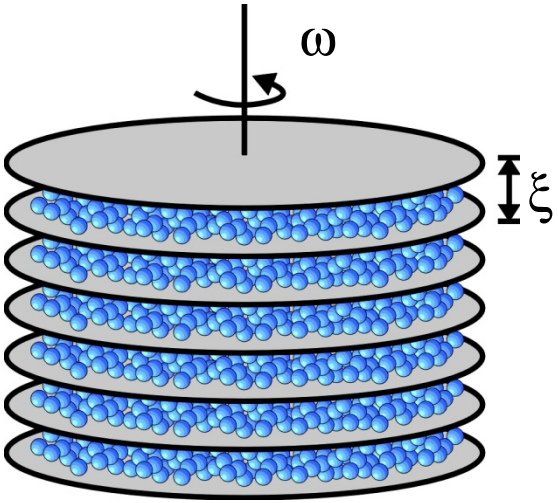
superfluid:

- 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 $\xi = \sqrt{\frac{2\nu}{\rho\omega}}$

ν: kinematic viscosity

ω: angular velocity

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

Imaginary Time Path Integrals

PHYSICAL REVIEW

A journal of experimental and theoretical physics established by E. L. Nichols in 1893

SECOND SERIES, VOL. 91, NO. 6 SEPTEMBER 15, 1953

Atomic Theory of the λ Transition in Helium

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(Received May 15, 1953)

It is shown from first principles that, in spite of the large interatomic forces, liquid He^4 should exhibit a transition analogous to the transition in an ideal Bose-Einstein gas. The exact partition function is written as an integral over trajectories, using the space-time approach to quantum mechanics. It is next argued that the motion of one atom through the others is not opposed by a potential barrier because the others may move out of the way. This just increases the effective inertia of the moving atom. This permits a simpler form to be written for the partition function. A rough analysis of this form shows the existence of a transition, but of the third order. It is possible that a more complete analysis would show that the transition implied by the simplified partition function is actually like the experimental one.

The thermal density matrix

- Find exact many-body eigenstates of H.
- Probability of occupying state α is $\exp(-\beta E_\alpha)$

- All equilibrium properties can be calculated in terms of thermal o-d density matrix
- Convolution theorem relates high temperature to lower temperature.

$$\hat{H}\phi_\alpha = E_\alpha \phi_\alpha$$

$$\rho(R;\beta) = \sum_\alpha \left|\phi_\alpha(R)\right|^2 e^{-\beta E_\alpha}$$

$$\hat{\rho}_\beta = e^{-\beta \hat{H}} \quad \text{operator notation}$$

off-diagonal density matrix:

$$\rho(R,R';\beta) = \sum_\alpha \phi_\alpha^*(R')\phi_\alpha(R)e^{-\beta E_\alpha}$$

$$\rho(R,R';\beta) \geq 0 \quad \text{(without statistics)}$$

$$\rho(R_1,R_2;\beta_1+\beta_2) =$$

$$= \int dR' \rho(R_1,R';\beta_1)\rho(R',R_2;\beta_2)$$

or with operators: $e^{-(\beta_1+\beta_2)\hat{H}} = e^{-\beta_1\hat{H}} e^{-\beta_2\hat{H}}$

Trotter's formula (1959)

- We can use the effects of operators separately as long as we take small enough time steps.

$$\hat{\rho} = e^{-\beta(\hat{T}+\hat{V})}$$

$$\hat{\rho} = \lim_{M\to\infty}\left[e^{-\tau\hat{T}}e^{-\tau\hat{V}}\right]^M$$

$$\tau = \beta / M$$

- M is number of time slices.
- τ is the "time-step"

- We now have to evaluate the density matrix for potential and kinetic matrices by themselves:

- Do by FT's

$$\left\langle r\left|e^{-\tau\hat{T}}\right|r'\right\rangle = \left(4\pi\lambda\tau\right)^{-3/2} e^{-(r-r')^2/4\lambda\tau}$$

- V is "diagonal"

$$\left\langle r\left|e^{-\tau\hat{V}}\right|r'\right\rangle = \delta(r-r')e^{-\tau V(r)}$$

- Error at finite n is roughly: comes from communtator

$$e^{-\frac{\tau^2}{2}\left[\hat{T},\hat{V}\right]}$$

Using this for the density matrix.

- We sample the distribution:

$$e^{-\sum_{i=1}^{M} S(R_i, R_{i+1}; \tau)} / Z \qquad \text{with} \quad Z = \int dR_1 \ldots dR_M \, e^{-\sum_{i=1}^{M} S(R_i, R_{i+1}; \tau)}$$

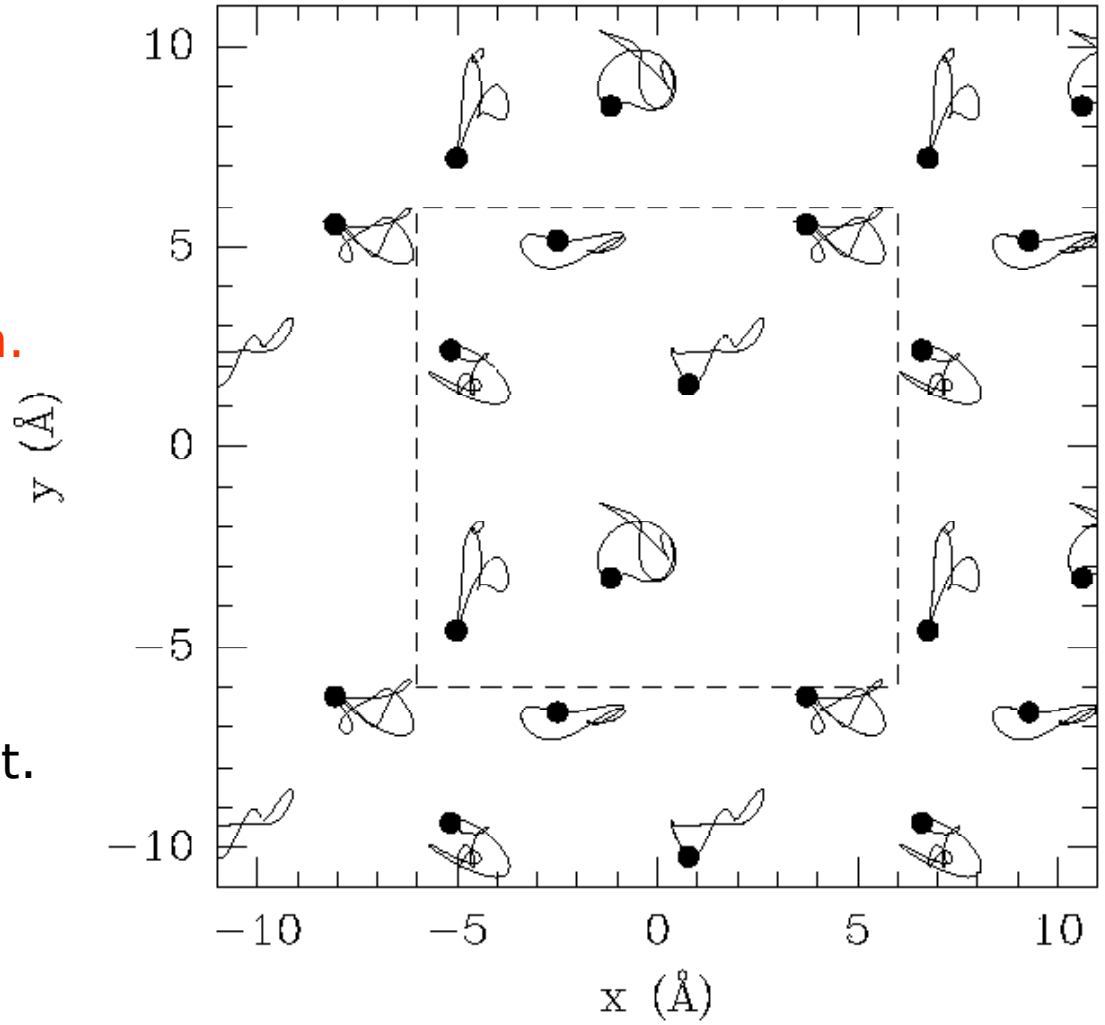
Where the "primitive" link action is:

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

- Similar to a classical integrand where each particle turns into a "polymer."
  - K.E. is spring term holding polymer together.
  - P.E. is inter-polymer potential.
- Trace implies $R_1 = R_{m+1}$ ⇨ closed or ring polymers

“Distinguishable” particles

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



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:

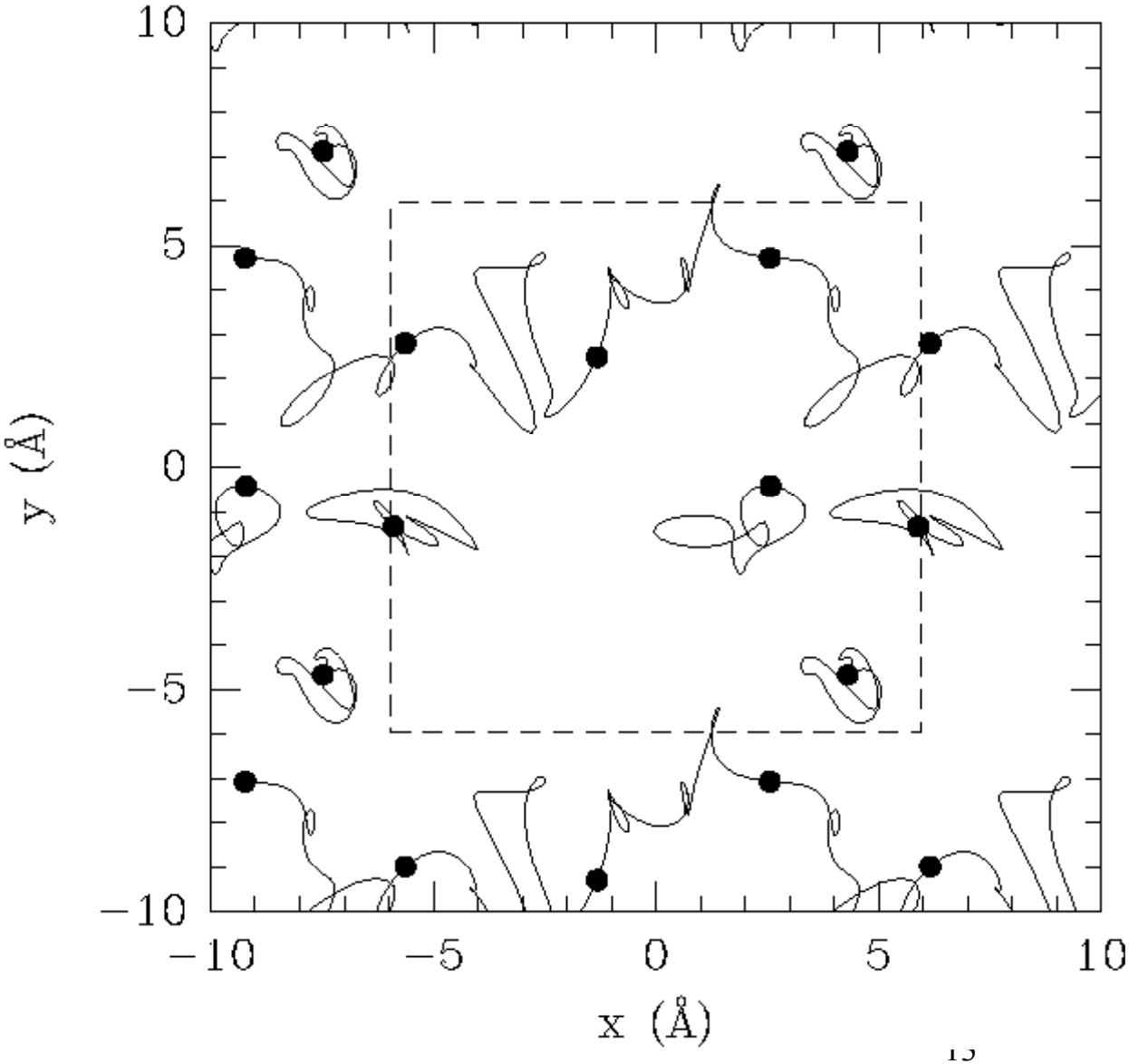
$$\hat{P} f(R) = \sum_{P=1}^{N!} \frac{1}{N!} f(PR)$$

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

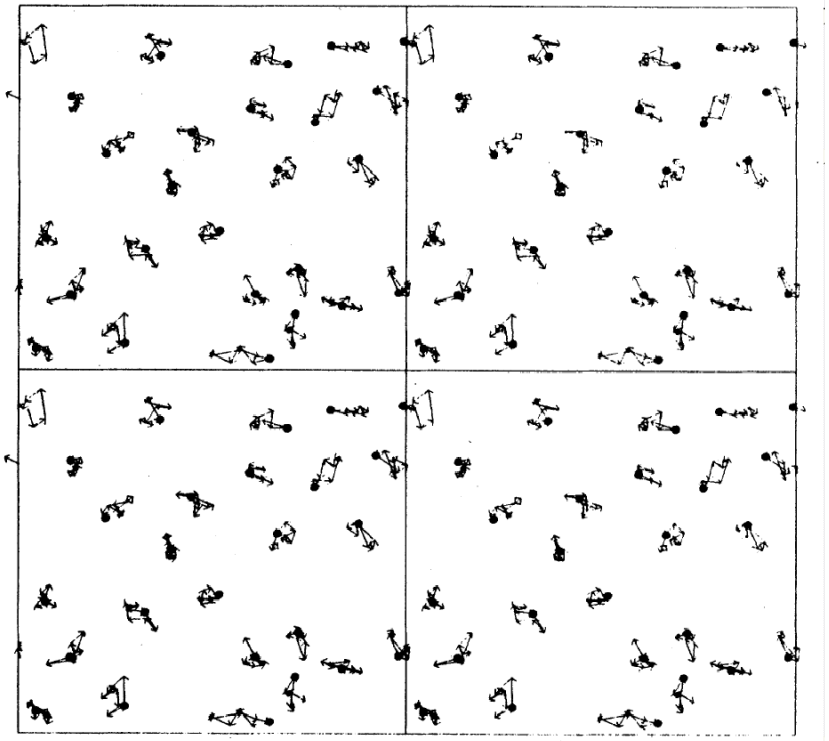
- Means the path closes on itself with a permutation. $R_1 = PR_{M+1}$
- Too many permutations to sum over; we must sample them.
- PIMC task: sample path $\{ R_1, R_2, \ldots R_M$ and $P\}$ with Metropolis Monte Carlo (MCMC) using "action", S, to accept/reject.

Exchange picture

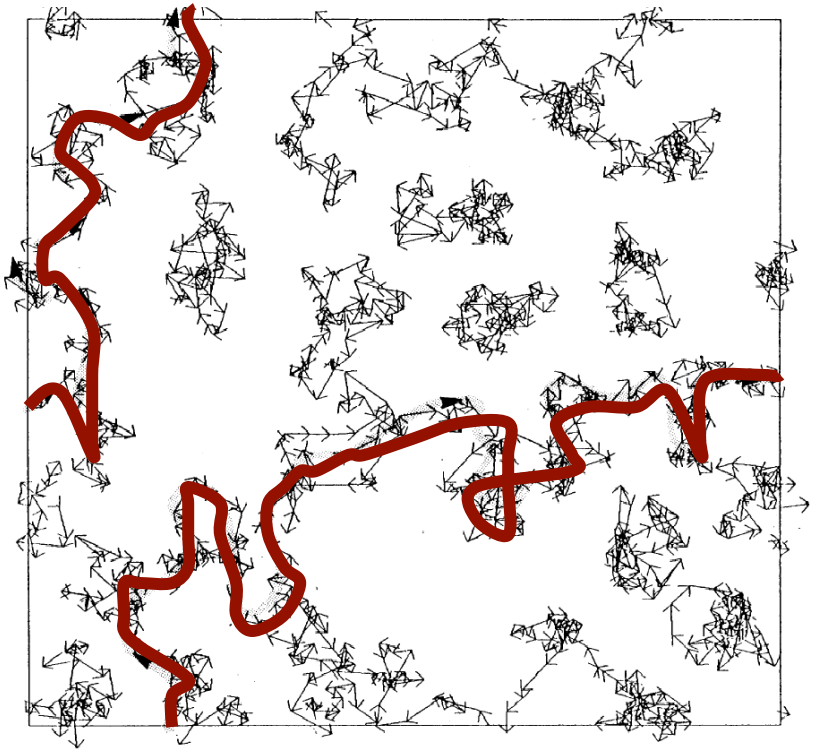
- Average by sampling over all paths and over connections.
- Trial moves involve reconnecting paths differently.
- At the superfluid transition a “macroscopic” permutation appears.
- This is reflection of bose condensation within PIMC.



T=2.5K



T=1K



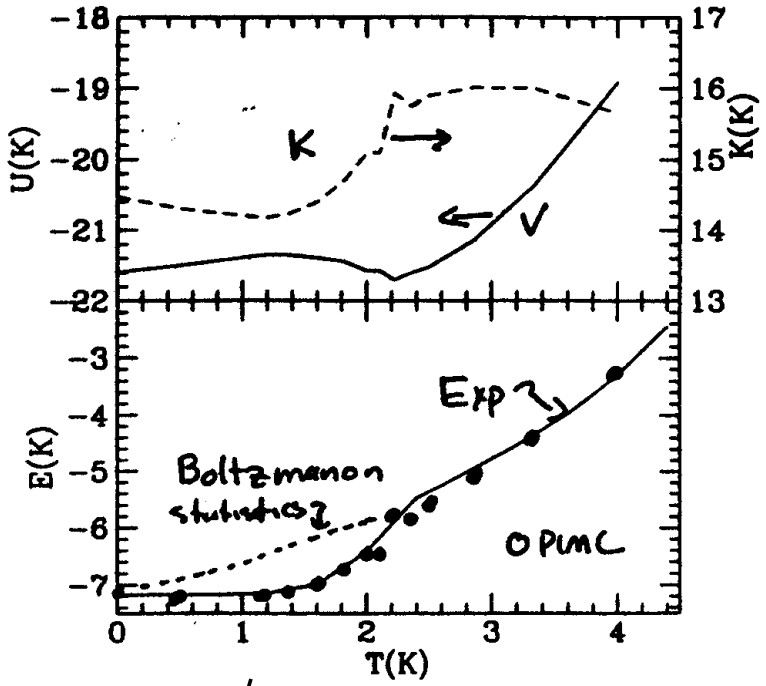
Normal “atomic” state

“entangled” liquid

ENERGY

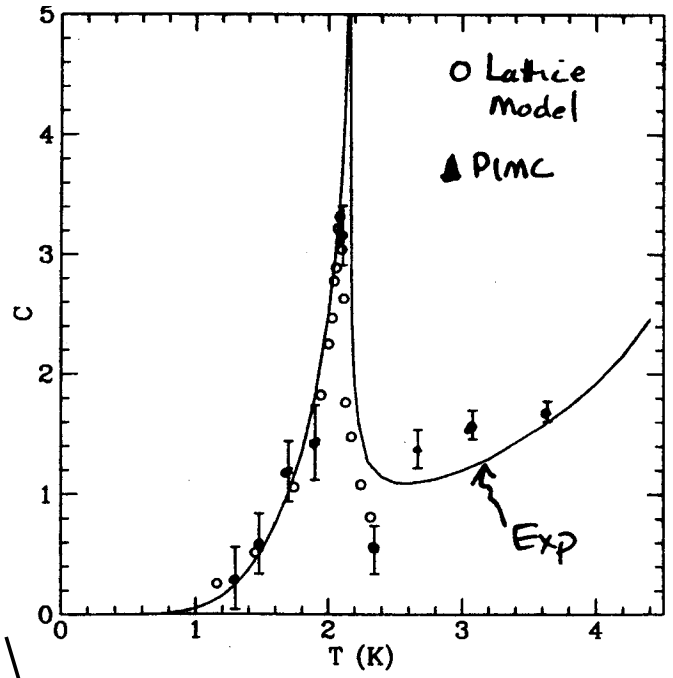
Bose statistics have a small effect on the energy

Below 1.5K ^{4}He is in the ground state.



SPECIFIC HEAT

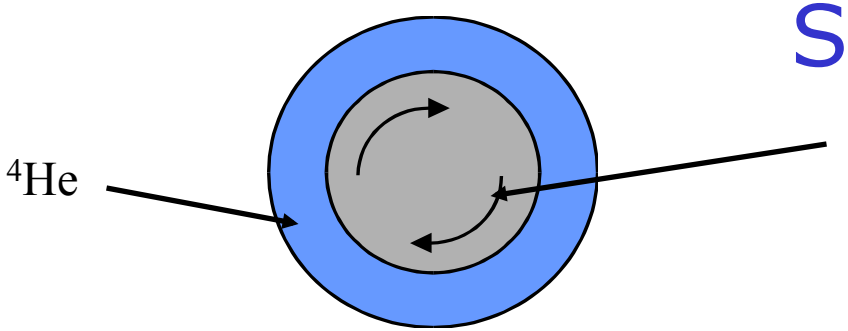
- Characteristic λ shape when permutations become macroscopic
- Finite size effects cause rounding above transition



$$E = \left\langle V + \frac{3N_{cycles}}{2\beta} + \frac{1}{2}(r_i - c_i)\cdot\nabla_i V \right\rangle$$

Kinetic term becomes smaller because $N_{cycle}<N$. Springs stretched more.

Superfluidity and PIMC



rotating disks:

Andronikashvili's expt (1946)

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

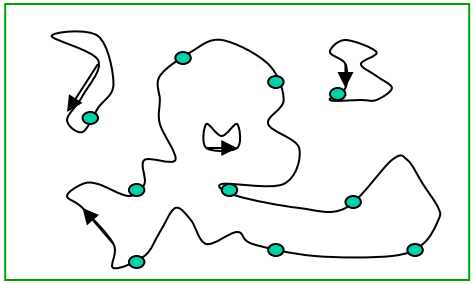
- We define superfluidity as a linear response to a velocity perturbation (the energy needed to rotate the system) "NCRI=nonclassical rotational inertia"

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

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

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

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

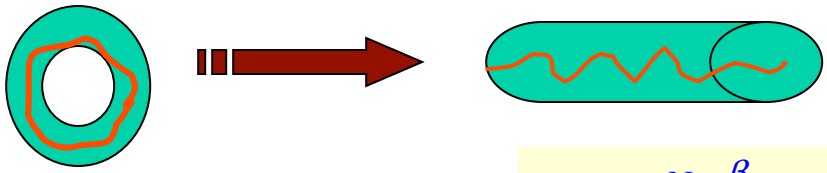


$$\frac{\rho_s}{\rho} = \frac{2m\ \left\langle A_z^2 \right\rangle}{\beta\ \lambda\ I_c}$$

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)

$$W = \sum_{i=1}^{N} \int_0^{\beta} dt \, \frac{dr_i(t)}{dt}$$

- The superfluid density is now estimated as:

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

- 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.

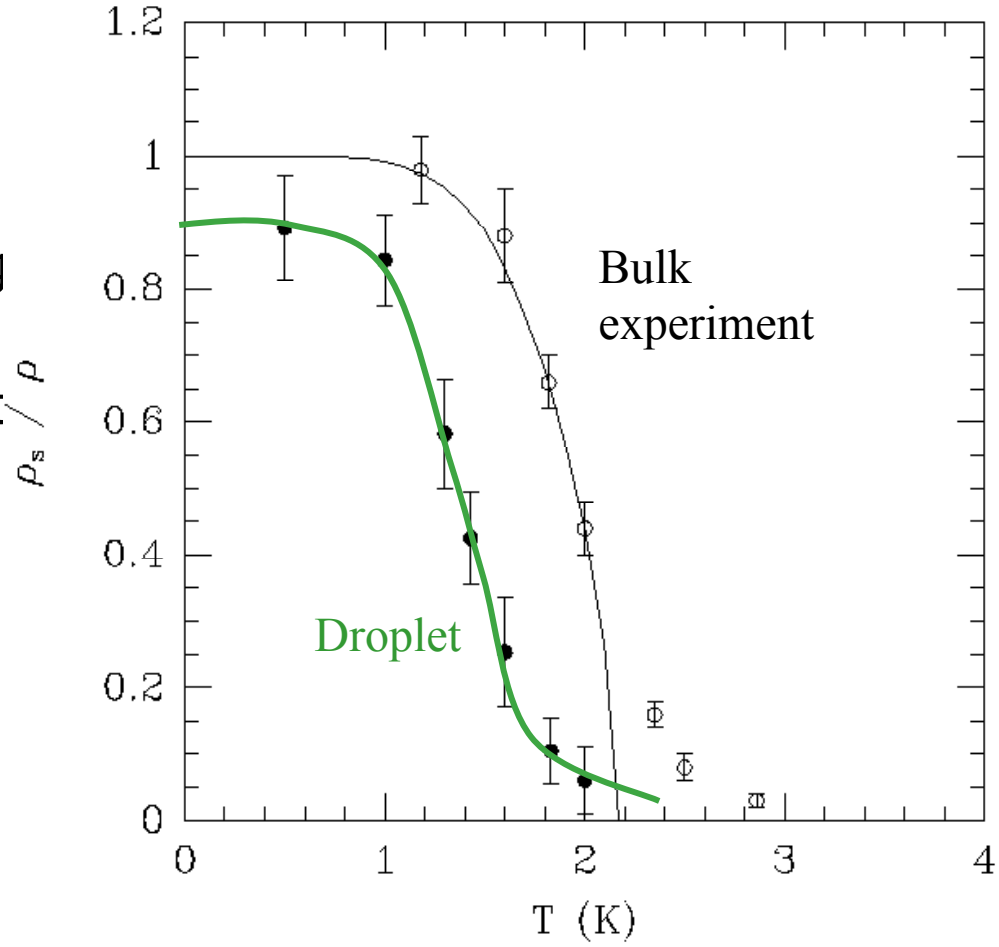
Superfluidity in pure Droplets

- 64 atom droplet goes into the superfluid state in temperature range 1K <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

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



Bose condensation

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

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

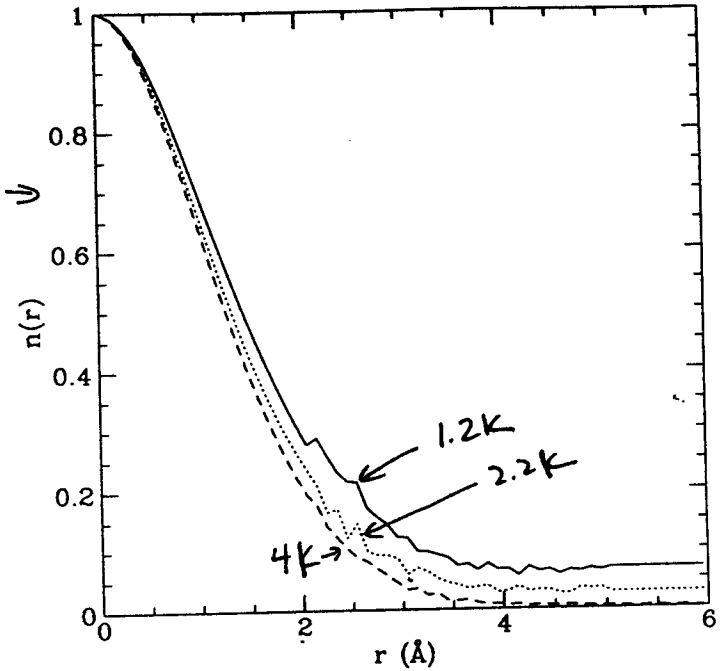
- The one particle density matrix is defined in terms of open paths:

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

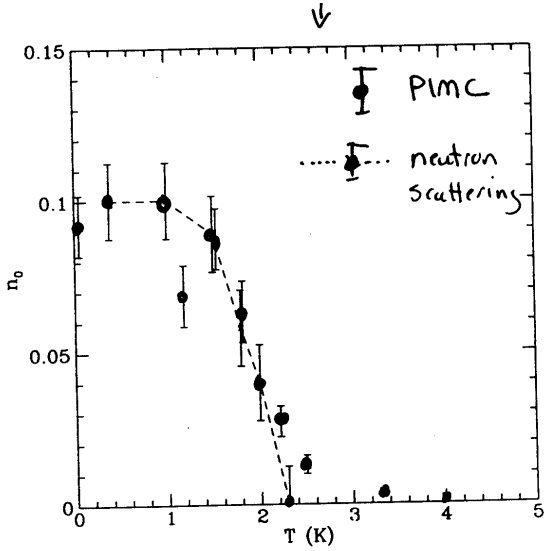
- We cannot calculate n(r,s) on the diagonal. We need one open path, which can then exchange with others.
- Condensate fraction is probability of the ends being widely separated versus localized. **ODLRO** (off-diagonal long range order) (*The FT of a constant is a delta function.)*
- The condensate fraction gives the linear response of the system to another superfluid.

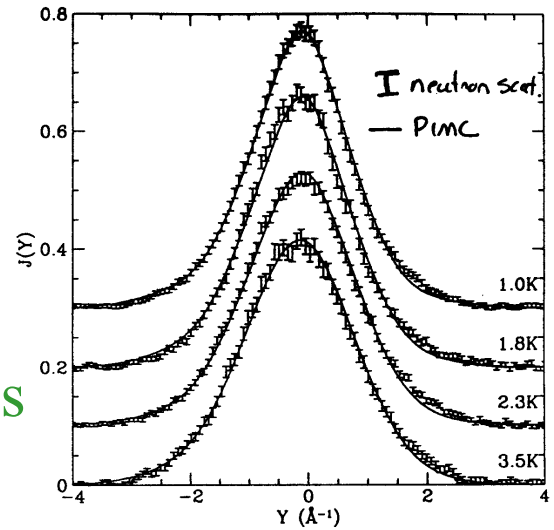
Comparison with experiment

Single particle density matrix



Condensate fraction





$Y = \frac{m}{K}(\omega - \lambda k^2)$

Neutron scattering cross section

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.*

Quantum	**Classical**
Bose condensation	Delocalization of ends
Boson statistics	Joining of polymers
Exchange frequency	Free energy to link polymers
Free energy	Free energy
Imaginary velocity	Bond vector
Kinetic energy	Negative spring energy
Momentum distribution	FT of end-end distribution
Particle	Ring polymer
Potential energy	Iso-time potential
Superfluid state	Macroscopic polymer
Temperature	Polymer length

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 H_2O at high pressure and temperature
- Vortex arrays
- Pairing in dilute atom gases of fermions
- BEC in atom trap experiments
- Liquid metals near their critical point