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CONTINUUM QUANTUM MONTE CARLO METHODS

12 - 23 January 2004

PATH INTEGRAL MONTE CARLO:

BOSONIC PATH INTEGRALS

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These are preliminary lecture notes, intended only for distribution to participants.

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
6. MAXENT calculation of real time information from imaginary time correlation functions.

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:

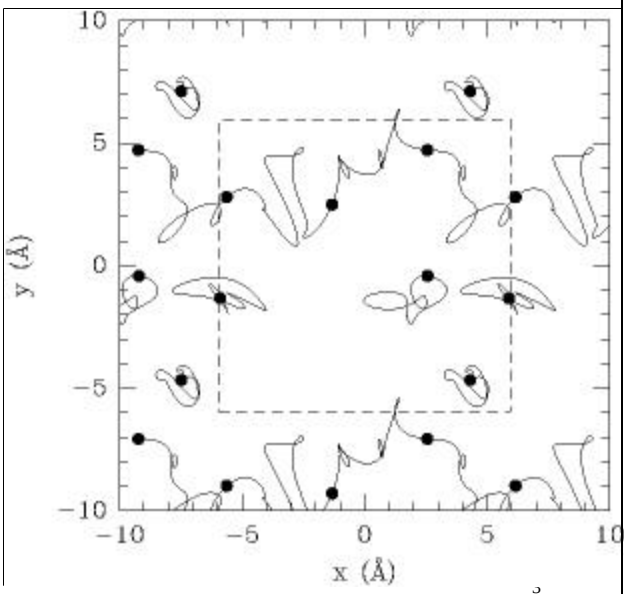
$$\hat{P} f(R) = \sum_{p=1}^{N!} \frac{1}{N!} f(PR)$$

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

- 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.



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3 boson example

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

$$\left\langle R\left|e^{-bH}\right|R'\right\rangle = e^{-\sum_i (r_i - r_i')^2} \prod_{i<j} f\left(r_{ij}, r_{ij}'\right) \qquad \text{units with } 4bl = 1$$

$$r_{bose}(R) = \sum_P \left\langle R\left|e^{-bH}\right|PR\right\rangle \sim \left[\sum_P \left\langle R\left|e^{-bH_0}\right|PR\right\rangle\right] \prod_{i<j} f\left(r_{ij}, r_{ij}\right)$$

$$r_{bose}(R) = \left|\Psi(R)\right|^2 \left[1 + e^{-r_{12}^2} + e^{-r_{13}^2} + e^{-r_{23}^2} + 2e^{-r_{12}^2 - r_{23}^2 - r_{13}^2}\right]$$

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

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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

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

- 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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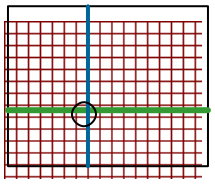
Heat Bath Method

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

$$T(s \to s') = \frac{p(s')}{C(s)}$$

$$C(s) = \sum_{s' \in N(s)} p(s'')$$



Then the acceptance probability will be: $A(s \to s') = \min\left(1, \frac{C(s)}{C(s')}\right)$

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).

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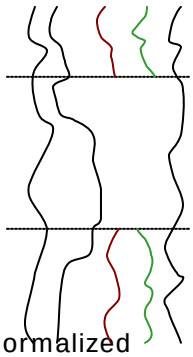
How to select permutation

- Heat bath probability of move being accepted is:

$$T(p) \propto \left\langle pR \left| e^{-\pi t H} \right| R' \right\rangle \approx \exp\left[-\frac{\sum_j \left(r_j - r_{pj}' \right)^2}{4nl\,t} \right] = \prod_j h_{jp_j}$$

$$h_{i,j} = \exp\left[-\frac{\left(r_j - r_i' \right)^2}{4nl\,t} \right] = \text{distance table}$$

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



- 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: $\hat{T} = \frac{T}{C}$ where $C = \sum_p T(p)$
- This gives an addition rejection rate.

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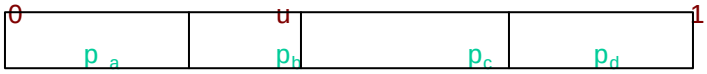
Discrete Distributions

Any discrete distribution p_k can be sampled by constructing the cumulant.

$$c_k = \sum_{i=1}^{k} p_i$$



- Sample 0<u<1.
- Find which region it is in. i.e. find k: $c_{k-1} < u < c_k$
- Return label "k".

- The search operation can be done by bisection in $\log_2(N)$ steps.

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Bisection method

1. Select time slices

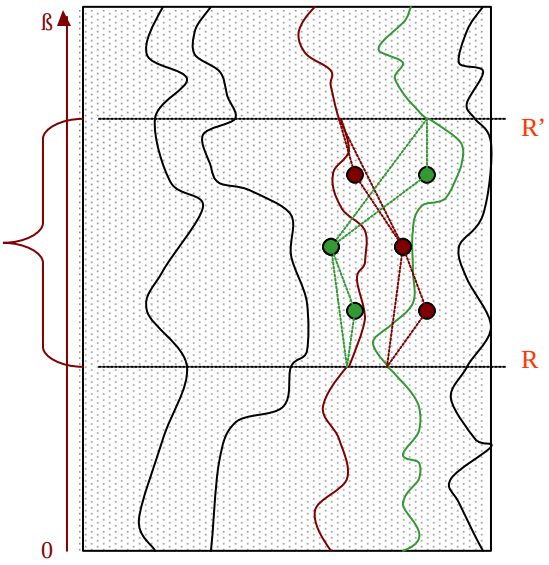
2. Select permutation from possible pairs, triplets, from:

$$r(R, PR'; 4t)$$

3. Sample midpoints

4. Bisect again, until lowest level

5. Accept or reject entire move



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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:

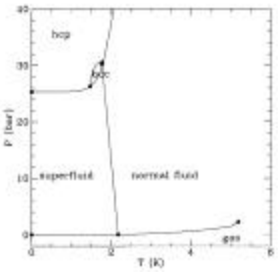

FIG. 3. The phase diagram of ^{4}He.

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

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

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Path Integral explanation of Boson superfluidity

- Exchange can occur when thermal wavelength is greater than interparticle spacing $k_B T \le h^2 r^{2/d} / m$
- 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)

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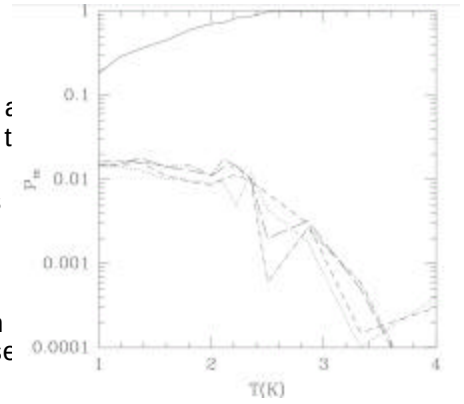
Permutation Distribution

- As paths get longer probability of permutation gets significant.
- Shown is the probability of a given atom attaching itself t 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.



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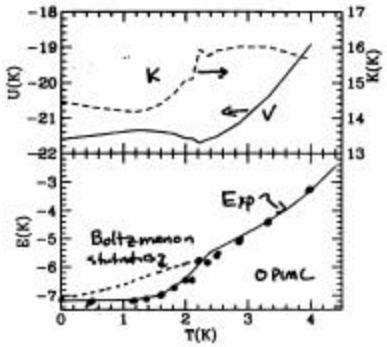
ENERGY

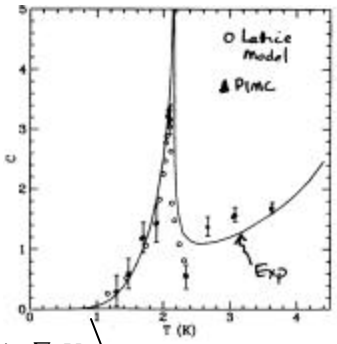
Bose statistics have a small effect on the energy

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



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

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

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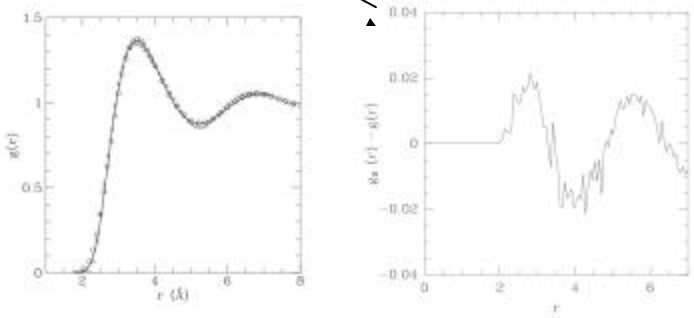
- Transition is not in the static distribution functions like S(k) or g(r). They do not change much at the transition. NON-CLASSICAL TRANSITION
- Effect of turning off bose statistics at the transition:



- Transition is in the imaginary-time connections of the paths-the formation of the macroscopic exchange.

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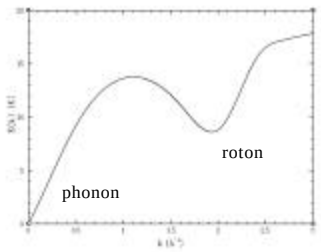
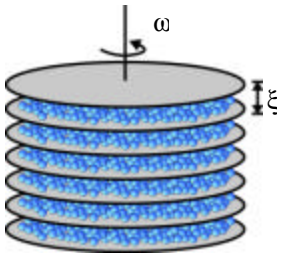
Superfluidity: Two-Fluid Model

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.





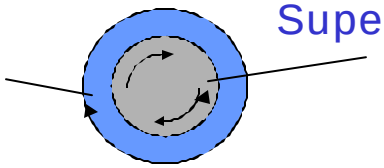
Andronikashvili Experiment:

normal fluid between disks rotates rigidly with system

viscous penetration depth $\xi = \sqrt{\frac{2\nu}{\rho\omega}}$?: kinematicviscosity, ω: angular velocity

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

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 to rotate the system) Landau definition.

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

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

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

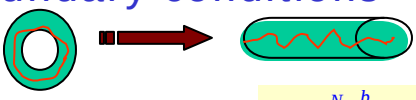
$$\frac{\rho_s}{\rho} = 1 - \frac{1}{I_c}\left\langle \int_0^\beta dt\, \hat{L}_z\, e^{-(\beta-t)\hat{H}_0}\, \hat{L}_z\, e^{-t\hat{H}_0} \right\rangle$$

$$\frac{r_s}{r} = \frac{2m}{b\ l\ I_c}\left\langle A_z^2 \right\rangle$$

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)

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

- The superfluid density is now estimated as:

$$\frac{r_s}{r} = \frac{\langle W^2 \rangle}{2lbN}$$

- 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.

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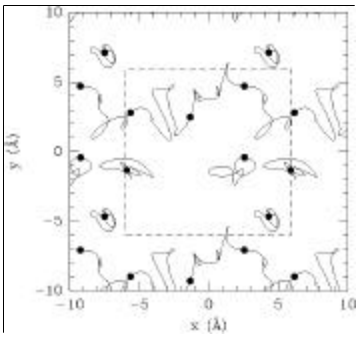
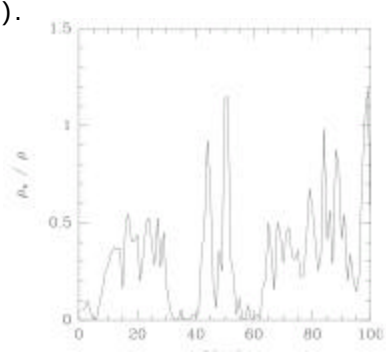
Ergodicity of Winding Number

- 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).





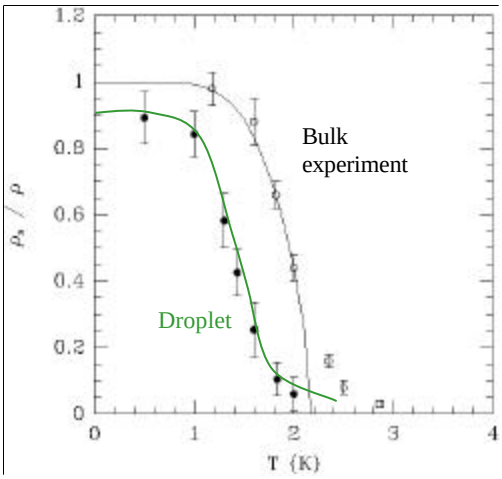
Superfluidity in pure Droplets

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

  NOT A PHASE TRANSITION!
- But almost completely superfluid at 0.4K (according to response criteria.)
- Superfluidity of small droplets recently verified.

Sindzingre et al 1990

$$\frac{r_s}{r} = \frac{2m}{b} \frac{\left\langle A_z^2 \right\rangle}{l} \frac{}{I_c}$$



Determination of T_c

Runge and Pollock PRB.

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

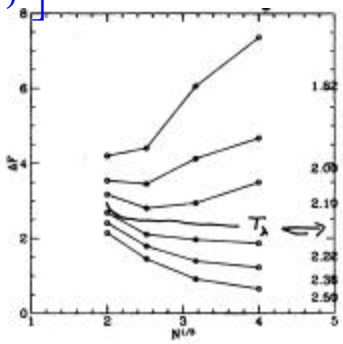
$$F = \int dr \left[l \left| \nabla f(r) \right|^2 + m \left| f(r) \right|^2 + V f(r)^4 \right]$$

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

$$F = \frac{m l p^2 L^{d-2}}{V} = -k_B T \left\langle e^{iWp/L} \right\rangle$$

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

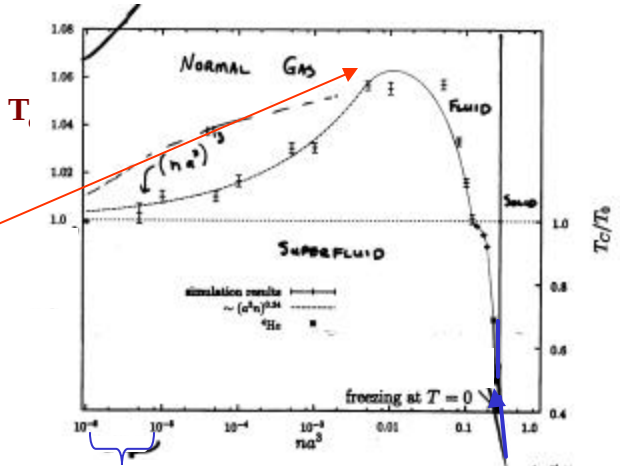
For N~100 , T_c correct to ~1%.



Phase Diagram of Hard Sphere Bosons

- Atomic traps are at low density
- With PIMC we mapped out range of densities
- There is an enhancement of T_c by 6% because of density homogenization.

Gruter et al PRL 99.



$T_c / T_{c0} \sim 1 + n^{1/3} a$

Density of atom traps

Liquid ^{4}He

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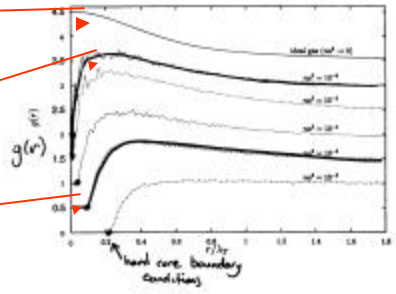
Pair correlations at low density

Free boson pair correlation.

Peak caused by attraction of bosonic exchange.

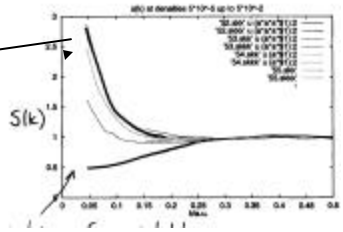
Zero is hard core interaction.



Structure Factor S(K)

(FT of density)

Large compressiblity near T_c (clustering)



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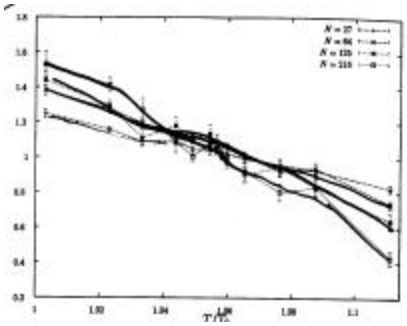
Determination of T_c using superfluid density. Finite size scaling.

$$r_s = \frac{1}{L} Q\left(\frac{L}{z}\right)$$

z = bulk correlation length

$$z \rightarrow \left(\frac{T - T_c}{T_c}\right)^{-n}$$



- 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.

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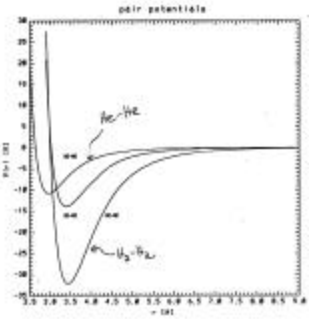
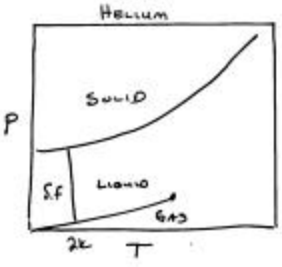
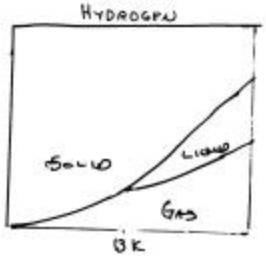
Why is H_2 not a superfluid?

- H_2 is a spherically symmetric boson like He.
- However its intermolecular attraction is three times larger
- Hence its equilibrium density is 25% higher ⇒ 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 high⇒$H_2$is spherical.

$$E(J_1) - E(J_0) = 170K$$
$$E(J_2) - E(J_0) = 510K$$

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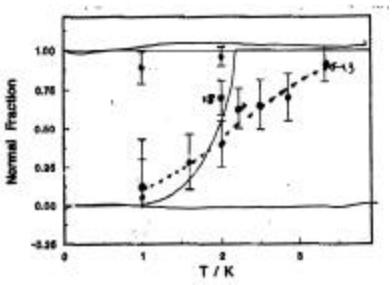
H_2 droplets

- In droplet or at surfaces, many bonds are broken.
- We found that small droplets are superfluid.
- Recently verified in experiments of ^4He-H_2-OCS clusters: When a complete ring of H_2 surrounds OCS impurity, it no longer acts as a rigid body, but decouples from the motion of the OCS.

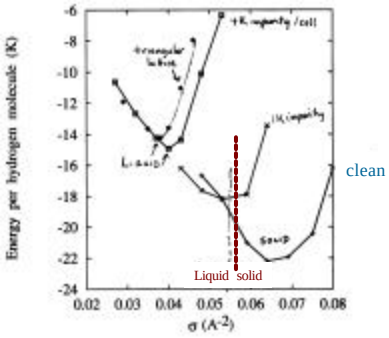


Sindzingre et al. PRL 67, 1871 (1991).

H_2 on Ag-K surfaces

Gordillo, DMC PRL 79, 3010, 1997.

- Formation of solid H_2 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.



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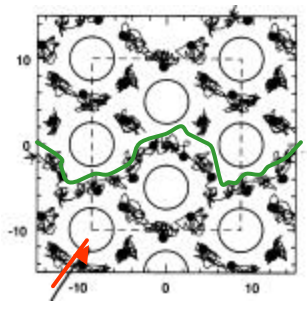
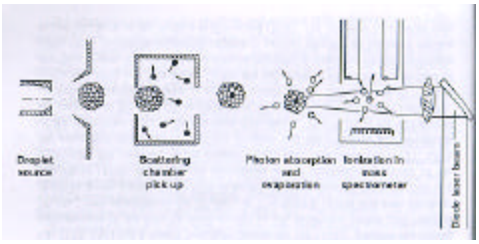


Winding H_2 path.

K atoms



Experimental Setup for He droplets

Toennies and Vilesov,
Ann. Rev. Phys. Chem. 49, 1 (1998)

- Adiabatic expansion cools helium to below the critical point, forming droplets.
- Droplets then cool by evaporation to:
  T=0.38 K, $N \approx 10^4$ (^{4}He)
  T=0.15 K, $N \approx 10^3$ (^{3}He)
- 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.

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Droplets and PIMC

E. Draeger (LLNL) D. Ceperley(UIUC)

- Provide precise microscopic probes for phenomenon such as superfluidity and vortices.
- Provide a nearly ideal "spectroscopic matrix" for studying molecular species which 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.

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Demonstration of droplet superfluidity

Grebenev, Toennies, Vilesov: *Science 279, 2083 (1998)*

- An OCS molecule in a ^{4}He droplet shows rotational bands corresponding to free rotation, with an increased moment of inertia (2.7 times higher)

  → ^{4}He are "coat" the impurity allowing it to freely rotate in the superfluid

- They replaced boson ^{4}He with fermion ^{3}He. If Bose statistics are important, then rotational bands should disappear. → they didn't!
- However, commercial ^{3}He has ^{4}He impurities, which would be more strongly attracted to an impurity.

  → How much ^{4}He does it take to "coat" the impurity and get free rotation?
- They found that it takes around 60 ^{4}He atoms.

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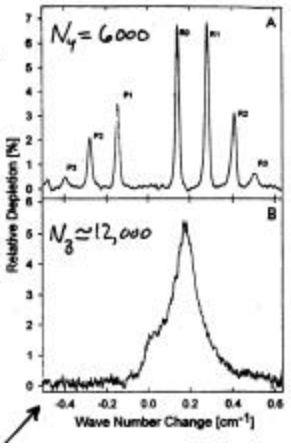
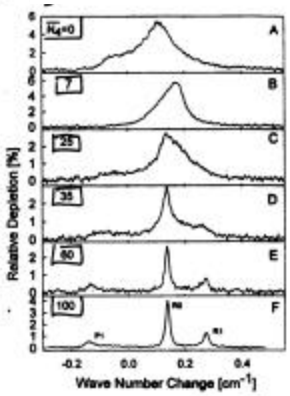
^{4}He

^{3}He



Small impurities of ^{4}He in ^{3}He



^{4}He is more strongly attracted to impurity because of zero point effects, so it coats the impurity, insulating it from the ^{3}He.

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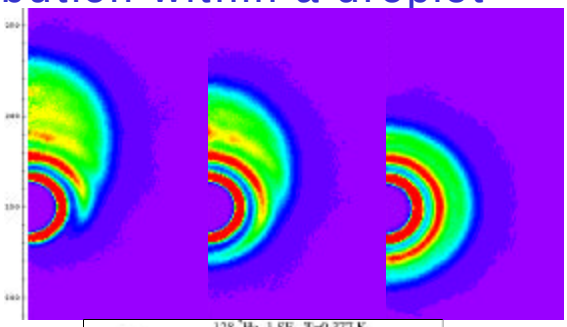
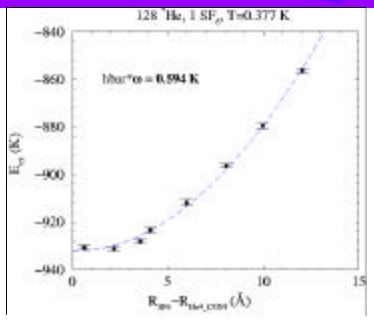
Density distribution within a droplet

- Helium forms shells around impurity (SF_6)
- 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.



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Local Superfluid Density Estimator

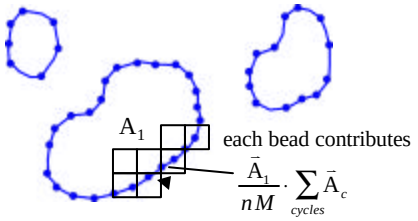
Although superfluid response is a non-local property, we can calculate the local contribution to the total response.

$$\rho_s = \frac{4m^2\rho}{3\hbar^2\beta I_c \Omega^2}\int d\vec{r}\, d\vec{r}'\, \vec{A}(\vec{r})\cdot\vec{A}(\vec{r}') = \frac{1}{\Omega}\int d\vec{r}\, \rho_s(\vec{r})$$

Where A is the area.

$$\vec{A}(\vec{r}) \equiv \int_0^\beta dt \sum_i (\vec{r}_{it}\times\vec{v}_{it})\delta(\vec{r}_{it}-\vec{r})$$

$$\Rightarrow \quad \rho_s(\vec{r}) = \frac{4m^2 N}{3\hbar^2\beta I_c}\int d\vec{r}'\, \vec{A}(\vec{r})\cdot\vec{A}(\vec{r}')$$



$$r_s(\vec{r}) \propto \frac{\vec{A}_1}{n\ M}\cdot\sum_{cycles}\vec{A}_c = \frac{A_1^2}{n\ M} + \frac{\vec{A}_1}{n\ M}\cdot\sum_{c\neq 1}\vec{A}_c$$

approximation: use only diagonal terms

not positive definite could be noisy

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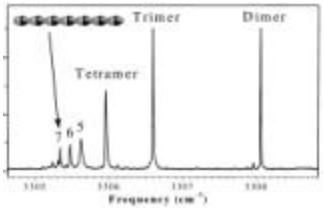
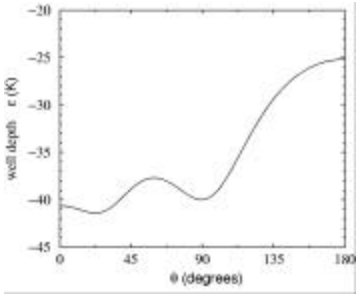
$(HCN)_x$: Self-Assembled Linear Isomers

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 stablize and pin them.



K. Nauta, R. E. Miller, Science **238**, 1895 (1999).



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.

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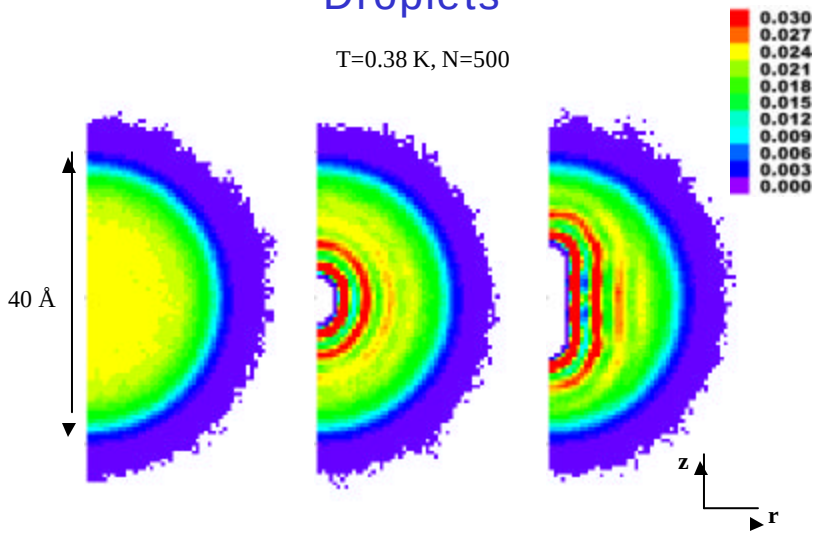
Density Distribution of ^{4}He+$(HCN)_x$ Droplets

T=0.38 K, N=500



pure 1 HCN 3 HCN

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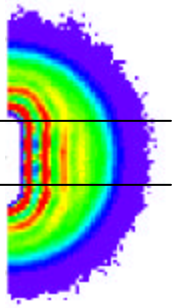
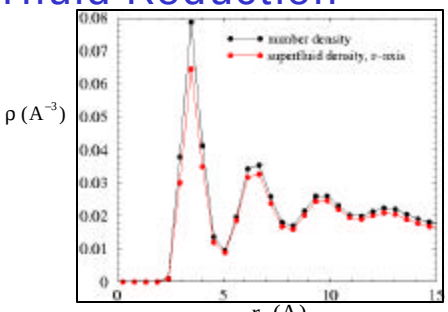
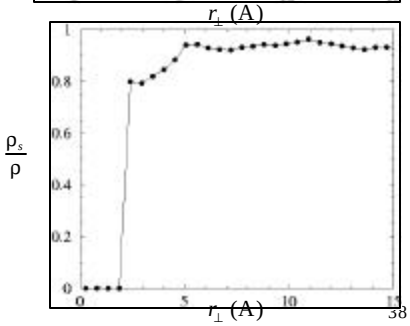
Local Superfluid Reduction



T=0.38 K, N=500
$(HCN)_3$





The local superfluid estimator shows a decrease in the superfluid response throughout the first solvation layer.

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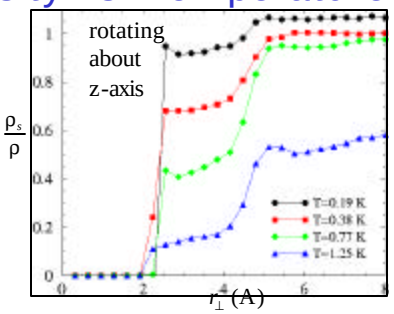
Local Superfluid Density vs. Temperature

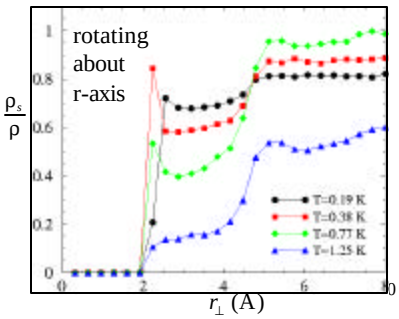
We calculated the superfluid density distribution of N=128 ^{4}He droplets with an $(HCN)_3$ isomer at several temperatures

The superfluid density in the first layer is temperature dependent!

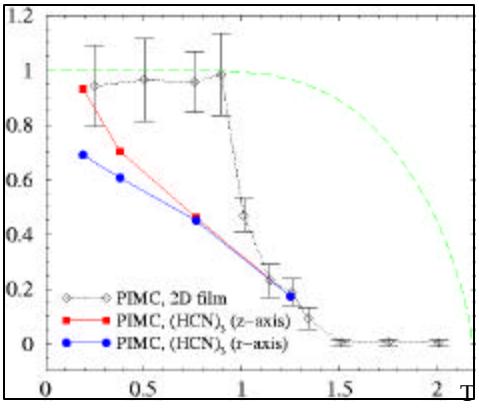
Bulk ^{4}He is 100% superfluid below 1.0 K. Both experimental measurements on helium films and PIMC studies of 2D helium show transition temperatures T_c which are significantly lower than bulk helium.

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





First Layer Superfluid Density vs. T



$\frac{\rho_s}{\rho}$

M. C. Gordillo and D. M. Ceperley, Phys. Rev. B **58**, 6447 (1998)

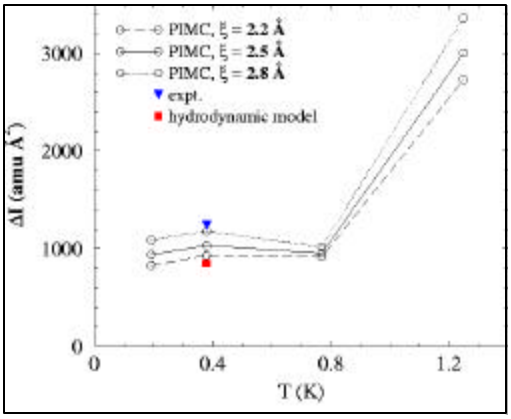
- Very broad transition, due to the small number of atoms in first layer (around 30)
- How will this affect the moment of inertia?

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.



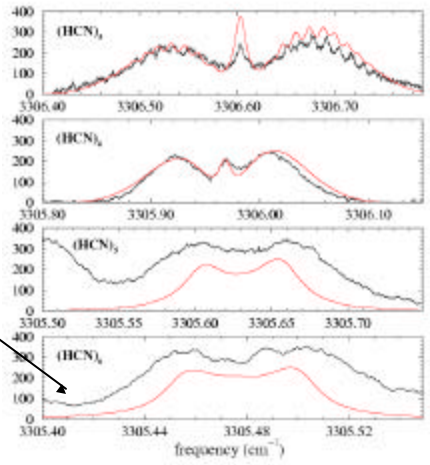
$$\Delta I = \int_{V(\rho)} d\vec{r}\, m_4 r_\perp^2 \left(\rho(\vec{r}) - \rho_s(\vec{r})\right)$$

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:

Lehmann, Draeger, Miller (unpublished 2003)



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Bose condensation

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

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

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

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

- 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.

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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

$$\Pr(k_1,..k_N) = \left| \int dR\, e^{-i(k_1 r_1 + ... + k_N r_N)} \Psi(R) \right|^2$$

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

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

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

Where: $$n(r,s) = \frac{V}{Q} \int dr_2 ... dr_N \left\langle r, r_2 .. r_N \left| e^{-bH} \right| s, r_2 ... r_N \right\rangle$$

occupy the states with the Boltzmann distribution.

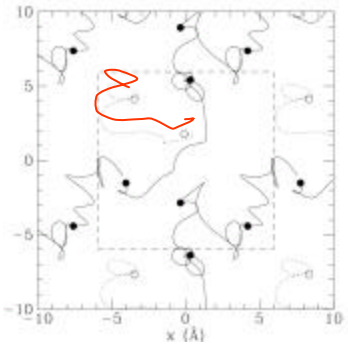
How to calculate n(r)

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>Λ.

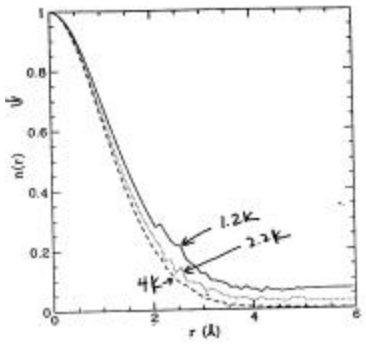
2. Do simulation off the diagonal and measure end-end distribution. Will get condensate when free end hooks onto a long exchange.

- advantage: works for any r
- Disadvantage:
  - Offdiagonal simulation not good for other properties
  - Normalization problem.

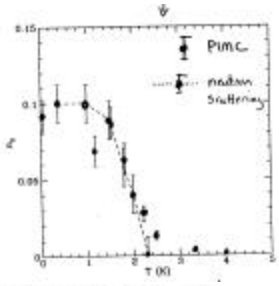


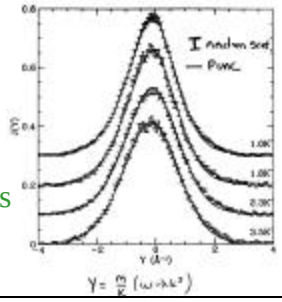
Comparison with experiment

Single particle density matrix



Condensate fraction





Neutron scattering cross section

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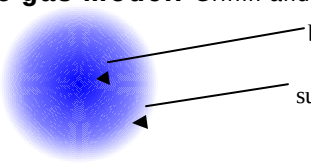
Surface of Liquid Helium

2 possible pictures of the surface

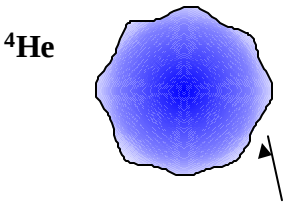
- **Dilute Bose gas model:** Griffin and Stringari, PRL 76, 259 (1996).

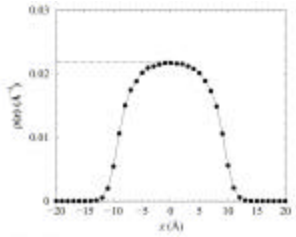


- **Ripplon model:** Galli and Reatto, J. Phys. CM 12,6009 (2000).

Can smeared density profile be caused by ripplons alone?

Density profile does not distinguish





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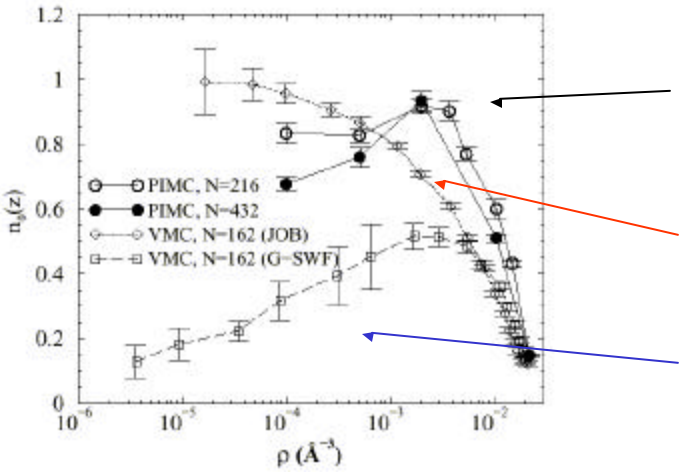
Condensate Fraction at the Surface of ^{4}He



- PIMC supports dilute gas model.
- Jastrow wavefunction
- Shadow wavefunction

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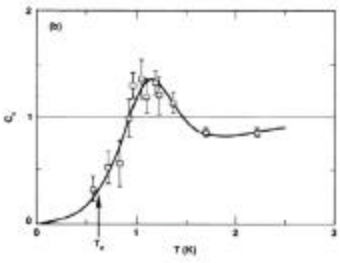
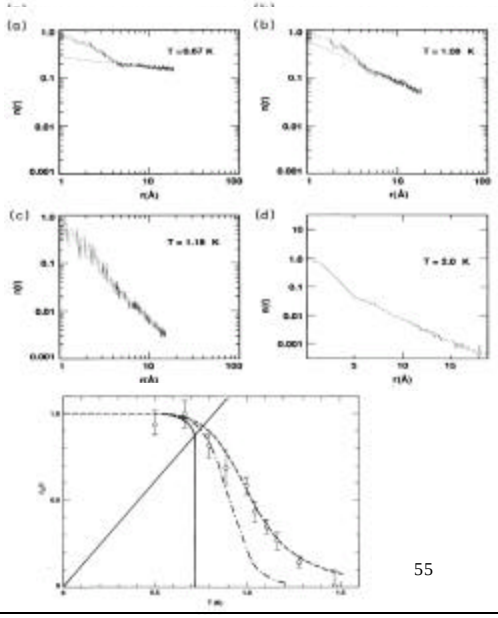
2D superfluids
Kosterlitz-Thouless transition

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





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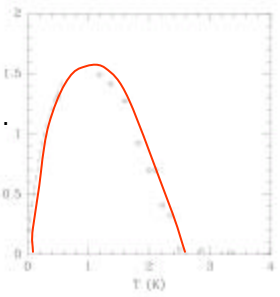
Exchange energy

- 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



$$e^{-bm_3} = \frac{Z_{N-1,1}}{Z_N} = \Pr(\text{atom 1 does not exchange})$$

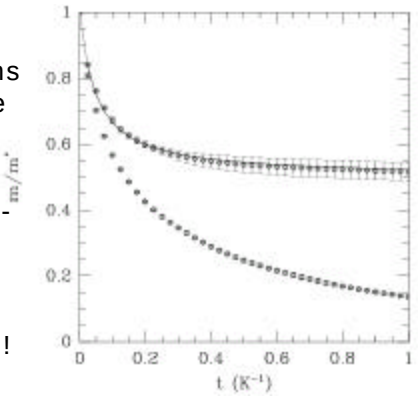
$$m_3 = m_4 - kT\ln(P_1) + \int_{\ln(3)}^{\ln(4)} d\ln(m)K(m)$$

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

Effective mass

- Effective mass is gotten from the diffusion constant at low temperature
- 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!

$$\frac{m}{m^*} = \frac{\left\langle [r(t) - r(0)]^2 \right\rangle}{6lt}$$



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

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Introduction to the UPI code

- Does an arbitrary collection of classical or quantum (bolzmannons,bosons and fermions) at finite temperature (restricted path for fermions)
- 2 or 3 dimensions in periodic boundary conditions
- Only pair potentials, and long-ranged charged interactions. Uses pair density matrix.
- Point, line or plane “particles”
- Calculates energy, pressure, density pair correlation, structure factor, superfluid density, …
- Various analysis codes, such as MAXENT.
- F77 code freely available. Extension to order(N) parallel version.
- Basic code written by D. Ceperley + others 1990-94. Few updates since then.

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General scheme

- Input file is name.in "name" identifies run
- Code opens "name.out" or appends to it if it exists already
- Code goes thru input file, responding to each keyword
- Order matters
- Output files append information (or overwrite)

General keywords:

- SEED sets rng (to repeat a run)
- RESTART (NONE, PARTIAL or FULL)
  - PARTIAL Read name.rs for state
  - FULL: also space down to correct line and resume
- TIMER: stop excecution if time > xxx
- DEBUG: higher level of printouts.

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File structure

- Create project space with a link to upi, squarer,….
- Upi version number
  - pimc contains "global routines" common blocks
  - fnlib contains independent routines (no common blocks)
  - forsub contains library routines: blas, linpack,..
  - xxxrtl contains vendor specific routines
  - Setup routines to construct input
  - Analysis routines to read output
  - sqdir: squarer directory for density matrix
  - doc: some documentation
  - uscript: some scripts
  - makefile goes into directories

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Common parameters variables

- Upi.p controls all dynamic dimensions

```
      parameter (ndim=3,mnc=1,mnp=180,mnspin=1,mslices=35,mnmovers=1
     +,mlevels=5,mspermt=10000,mterms=6,mntab=551,mpfile=2,lptable=201
     +,mnkv=600,mnsh=50,mmsize=2
     &,mwrapd=7,mfpdm=101,msamp=1,mstimes=1,mlong=1)
c lptable is the size of the g(r) grid
c ndim is the spatial dimensionality
```

- m*** is “maximum, n*** is actual value.
- If code stops, one of the parameters is too small. Look at last line of the output file.
- Upi.cm holds the global common
- Names must be unique for routines in directory pimc!
- Everything is typed.

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Averages

- Scalars are written to the .bsc file
- “report” or “dataspork” to examine the output
- qid.out file just has execution “notes”
- How do averages get there?
  - Call setav reserves a global pointer, e.g. “jenergy”
  - In some routine we add to avtemp(jenergy) and anorm(jenergy) during upi execution.
  - Adding a new scalar is easy
  - Library takes care of initialization(s), output,…
- Many “vector” averages
  - Histograms: g(r),density
  - Tables: s(k,i,j), winding numbers,cycle lengths …
  - Efficiency measures: acceptance ratios, diffusion
  - All these are handled separately.

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UPI System information

- BETA xxx is the inverse temperature
- BOXSIZE x y z
- NSLICES n = number of time slices
- UNITS (energy and length) is to label output files
- ENORM reported energy is divided by ENORM

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Particle information

TYPE “name” nspins number hbs2m nppss “file” [charge]

Creates particles with this name, spin, etc
hbs2m=0 for classical particles (external potential)
“file” contains initial coordinates
nspins=0 bosons, -1 “boltzmanons”

LINE and PLANE are similar keywords, but the particles are of lower dimensionality. E.g. Can be used to treat vortex lines, surfaces, tubes, slabs

- Subroutine addtype initializes data for a new type.

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Markov State is:

r(mdim,mparts,mslices) iperm(mparts) join

iperm gives the permutation

join says at which slice it acts

rperm(*,I,join)=r(*,p(I),join)

velocity (*,*,t)=r(*,*,t+1)-r(*,*,t) t.ne.join
=r(*,*,t+1)-rperm(*,*) t=join

- More complicated data structure needed for parallelization or for off-diagonal simulations

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Find_velocity

```
do k=1,nslices
   kp1=iwrap(k+1l)
   do it=1,ntypes
   if(hbs2m(it).gt.0.) then
        do it=1,ntypes
        do l=1,ndim

         if(k.eq.join) then
          do i=nfpty(it),nlpty(it)
           vel(l,i,js)=fpbc(r(l,i,kp1)-rperm(l,i),l)
          enddo
         else
          do i=nfpty(it),nlpty(it)
           vel(l,i,js)=fpbc(r(l,i,kp1)-r(l,i,k),l)
          enddo
         endif
```

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Squarer produces *.dm file

Huge file contains several subfiles

- Description of grids
- Potential
- Action in various approximations
- Action at various time slices
- Beta or mass derivatives of the action
- Sampling tables

- Radial grid has several options. Can vary for each type of pair interaction to put more grid points in some region.
  - GRID n LINEAR r1 r2
  - GRID n LOG r1 r2
  - …..

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Density matrices used in PUPI

- Pair density matrix: generated by squarer, (see new simpler code on WEB) Includes expansion for offdiagonal components. Action is evaluated in **dmeval** (calls **dstnce** and **offd**). Energy is evaluated in **pairact**. Calls radial tables for variety of grid types.
- Single particle propagator in periodic boundary conditions: **fpdmg.f** uses a table set up in **setfpdm.f** Used for fermion and boson density matrix. Also to determine permutations.
- Free fermion density matrix. **Ofill** sets up the matrix, calls **invert or newup** to calculate the determinant.
- Particle near a plane (image method). **Dleak.f** (related computations in the nodal action, **dnode.f**)
- Long range potential: (in k-space) (**ewald.f**) setup code generates the expansions. Uses fourier coefficents (rhok).

Functionality:

- Action at specified temperatures differing by powers of 2 in temperature
- beta derivative
- spatial derivative
- has to be flexible with respect to grid type, analytic features …
- update formulas for all cases—how we compute changes with respect to a single variable and derivatives.

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Potentials

POT PAIR name1 name2 file.dm [n m]

Potential between these types of particles is on file.
File is output of squarer
N and M control accuracy of expansion of action.
USR(r,4,type1,type2,levels,expansion,derivative)

Subroutine addpot initializes a new potential

Does only the range in r as existing in table, with the grid, etc hidden in the file.

POT EWALD cutk file
defines a k-space potential, cutoff=cutk, data on “file”
ULR(k,type1,type2,levels, derivative)

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Computation of pair interaction

- Tentry calculates table entries for radial tables
  Determines: index and remainders (I,P)
- Vsum looks up adds them together

```
function vsum0(m,i,p,t,n)
      vsum0=0.
     do j=1,m
       vsum0 = vsum0 + t(i(j),1)
    &                + p(j)*(t(i(j),2)
    &                       + p(j)*(t(i(j),3)
    &                              + p(j)*t(i(j),4)))
     end do
     return
     end
```

- Dmeval determines the action
  - Dstnce computes diagonal action
  - Offd the off-diagonal portion (expansion)

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CODE LEVELS

Driver -> setsys	Does system setup
incom	control driver, checkpointing output
Permute, select, omove	drivers for MC
Weave, displace	constructs a move
sampfr samcg codrift ptable	sampling routines
dmeval	routines for action,energy
Dstnce offd ewald	details of action
Tentry vsum deltar cossin	numerically intensive routines
skadd,gradd,anal,wind,area	averages

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Moving probabilities

- With option SELECT one searches over all 1-4 particle moves for ones likely to be accepted.
- GAMMA allows you to fine tune the selection probabilities
- "GAMMA n type x"
  sets the relative probability for a move of n particles of "type" to be x: $1 \le n \le 4$
- "DISPLACE type dx gamma" : makes a whole chain move (if not involved in a permutation) of particle type inside a cube of size dx with probability gamma.
- PERMUTE is more complex, but can allow larger moves.

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