

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:

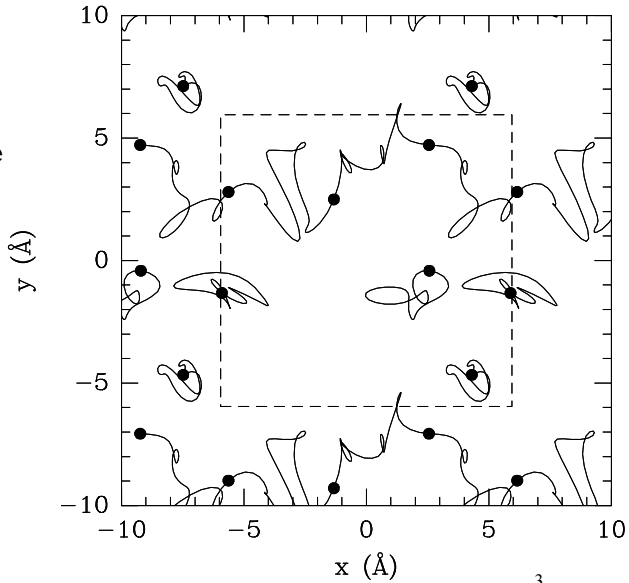
$$\hat{P}f(R) = \sum_{p=1}^{N!} \frac{1}{N!} f(PR)$$

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

- 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 $\{R_1, R_2, \dots, R_M$ and $P\}$ with Metropolis Monte Carlo (MCMC) using "action", S_i , 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 dependence (Feynman form)

$$\langle R | e^{-\beta H} | R' \rangle = e^{-\sum_i (r_i - r'_i)^2} \prod_{i < j} f(r_{ij}, r'_{ij}) \quad \text{units with } 4\beta\lambda = 1$$

$$\rho_{bose}(R) = \sum_P \langle R | e^{-\beta H} | PR \rangle \sim \left[\sum_P \langle R | e^{-\beta H_0} | PR \rangle \right] \prod_{i < j} f(r_{ij}, r_{ij})$$

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

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

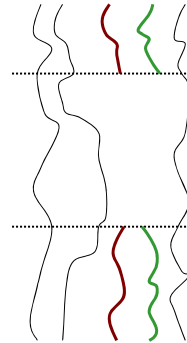
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PIMC Sampling considerations

- 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:

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



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

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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.

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

$$R_{t/2} = \frac{1}{2}(R_0 + R_t) + \eta$$

$$\sigma^2 = \lambda t / 2 = \langle \eta^2 \rangle$$

$$R_{t/2} = \frac{1}{2}(R_0 + R_t) + \lambda t \nabla U_s(R_{t/2}^0) + \eta$$

$$\sigma^2 = \lambda t / 2 \bar{I} + (\lambda t)^2 \bar{\nabla} \bar{\nabla} U_s(R_{t/2}^0) = \langle \bar{\eta} \bar{\eta} \rangle$$

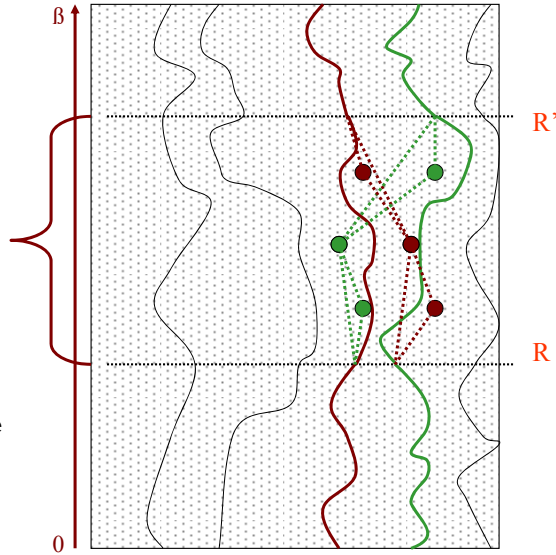
$$U_s(R) = \text{sampling potential}$$

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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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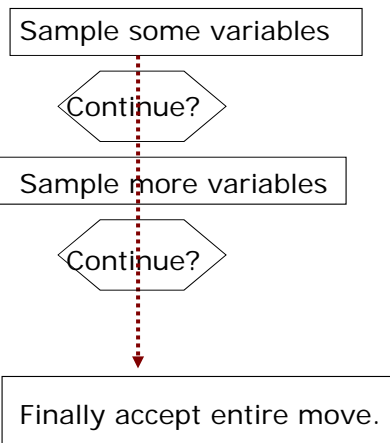
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Multilevel Metropolis/ Bisection

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

$$A_k(s \rightarrow s') = \min \left[1, \frac{T_k(s' \rightarrow s) \pi_k(s') \pi_{k-1}(s)}{T_k(s \rightarrow s') \pi_k(s) \pi_{k-1}(s')} \right]$$

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



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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

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

- 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:

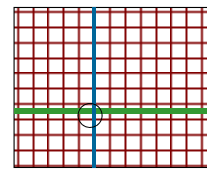
1. Make a table of possible exchanges and update the table. Good for up to 4 particle exchanges "SELECT"
2. Have a virtual table and sample permutation from that table. Good for longer exchanges (up to 10 body exchanges). "PERMUTE"

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:

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

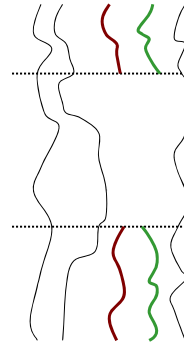
$$h_{i,j} = \exp \left[-\frac{(r_j - r_i')^2}{4n\lambda\tau} \right] = \text{distance table}$$

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:

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

- 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.

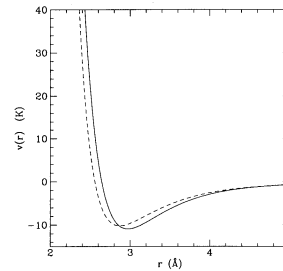


FIG. 1. The semiempirical pair potential between two helium atoms: solid line, Aziz *et al.* (1992); dashed line, Lennard-Jones 6-12 potential with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å.

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

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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:

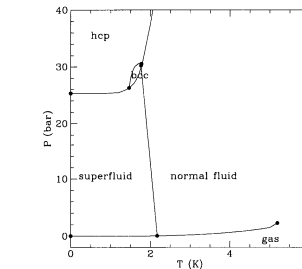


FIG. 2. The phase diagram of ${}^4\text{He}$.

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

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

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Path Integral explanation of Boson superfluidity

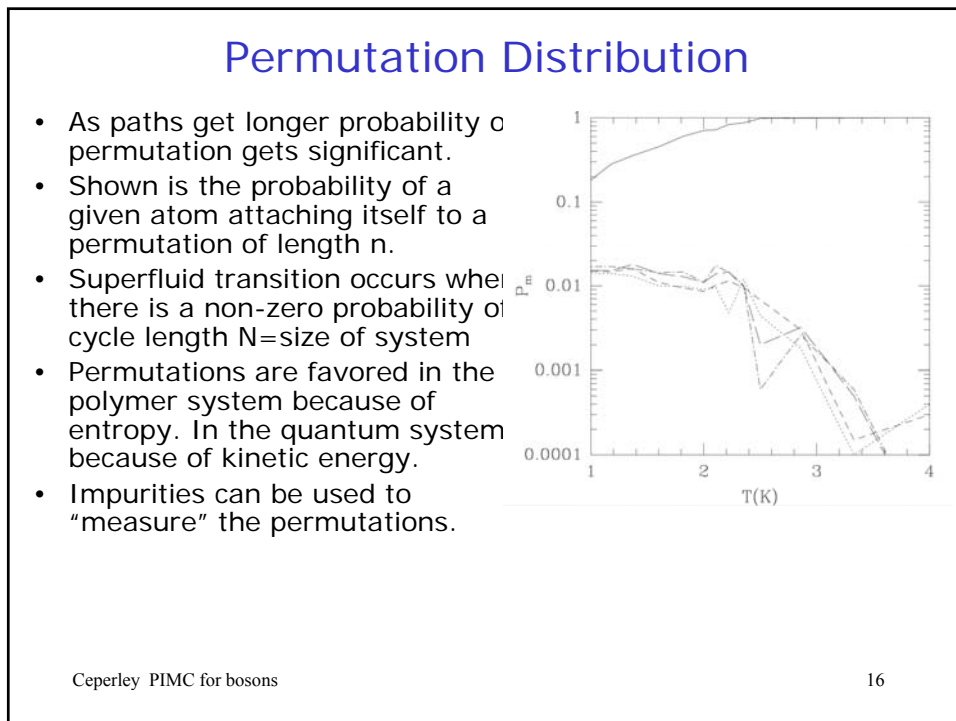
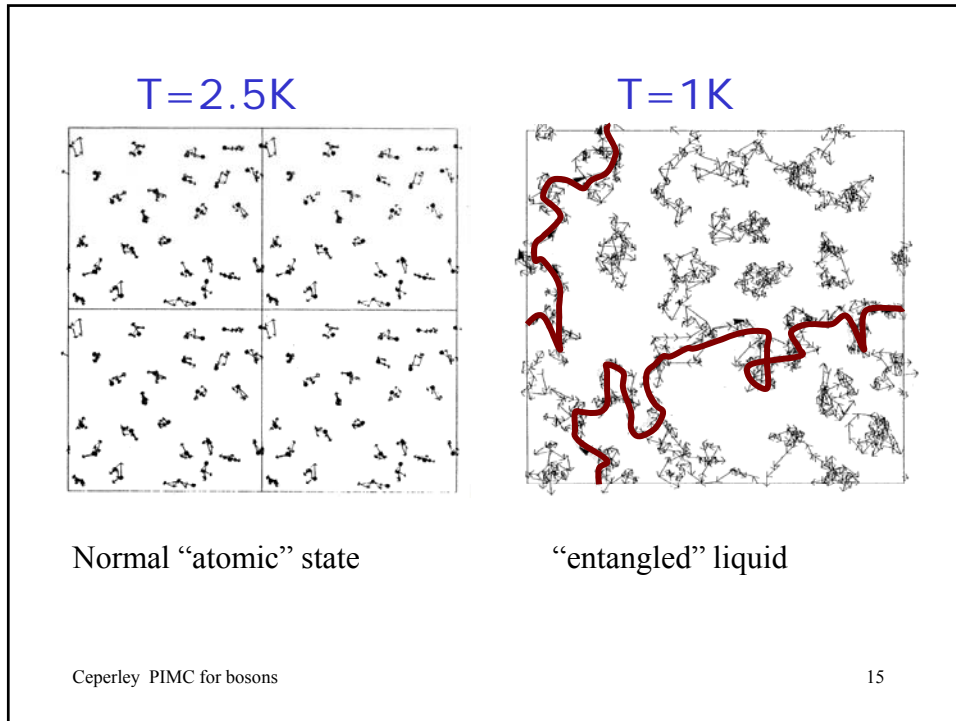
- Exchange can occur when thermal wavelength is greater than interparticle spacing

$$k_B T \leq \hbar^2 \rho^{2/d} / m$$

- 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)

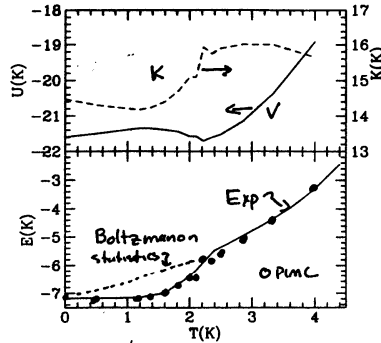
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ENERGY

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



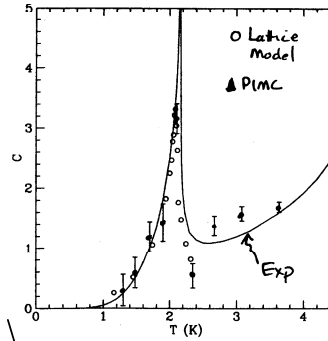
$$E = \left\langle V + \frac{3N_{\text{cycles}}}{2\beta} + \frac{1}{2} (r_i - c_i) \cdot \nabla_i V \right\rangle$$

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

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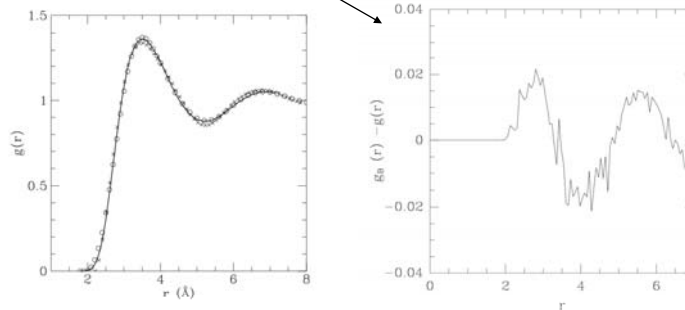
SPECIFIC HEAT

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



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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

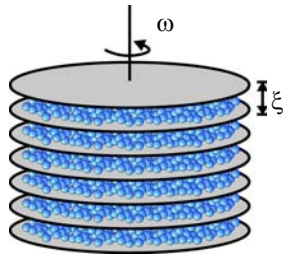
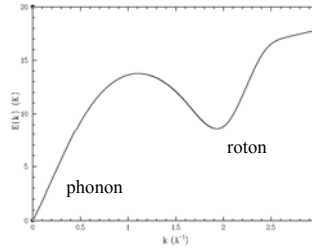
Landau Two-Fluid Model: $\rho = \rho_n + \rho_s$

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

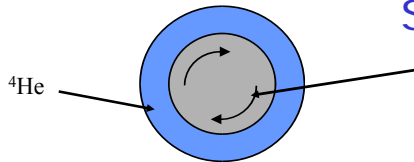
$$\xi = \sqrt{\frac{2\nu}{\rho\omega}} \quad \begin{array}{l} \nu: \text{kinematic viscosity} \\ \omega: \text{angular velocity} \end{array}$$

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

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Superfluidity and PIMC



rotating disks:

Andronikashvili's expt (1946)

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

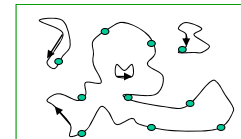
- We **define** superfluidity as a linear response to a velocity perturbation (the energy needed to rotate the system) "NCRI=nonclassical rotational inertia"

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

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

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

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



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

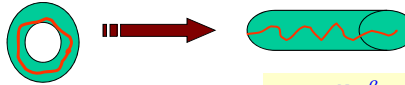
A = signed area of imaginary-time paths

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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:

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

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

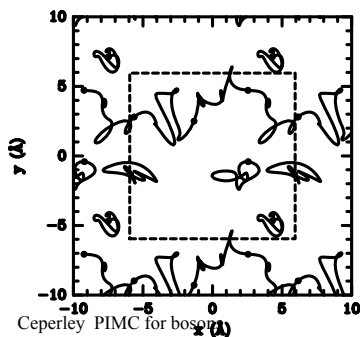
- Exact linear response formula. (analogous to relation between $\chi \sim \langle M^2 \rangle$ for Ising model.)
- Relates **topological** property of paths to dynamical response. Explains why superfluid is "protected."
- Imaginary time dynamics is related to real time response.
- How the paths are connected is more important than static correlations.

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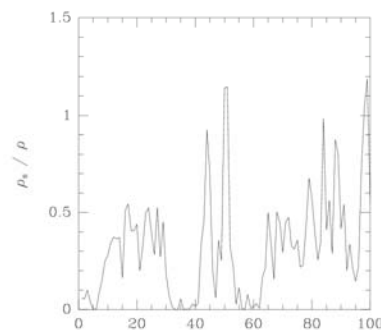
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Ergodicity of Winding Number

- 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).



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Superfluidity in pure Droplets

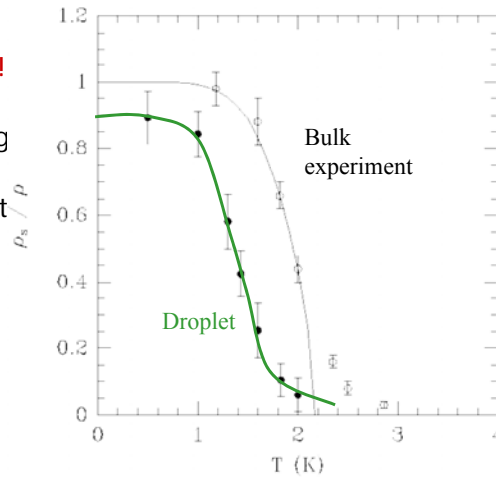
- 64 atom droplet goes into the superfluid state in temperature range $1\text{K} < T < 2\text{K}$.

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

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



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Determination of T_c

Runge and Pollock PRB.

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

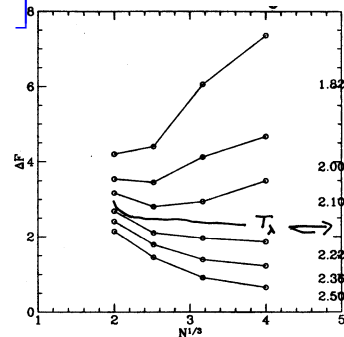
$$F = \int dr \left[\lambda |\nabla \phi(r)|^2 + \mu |\phi(r)|^2 + V \phi(r)^4 \right]$$

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

$$F = \frac{\mu \lambda \pi^2 L^{d-2}}{V} = -k_B T \langle e^{iW\pi/L} \rangle$$

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

For $N \sim 100$, T_c correct to $\sim 1\%$.



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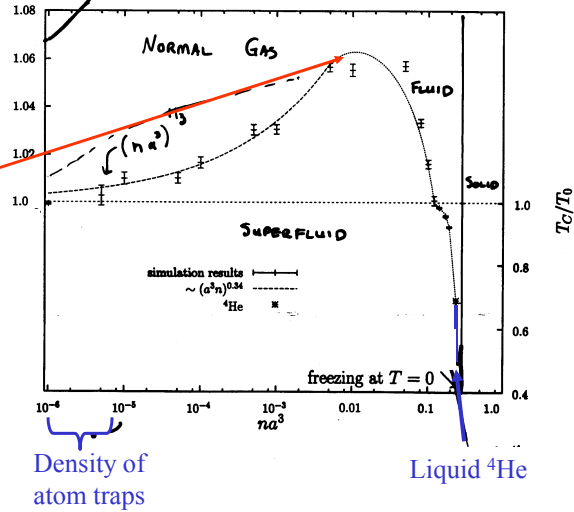
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Phase Diagram of Hard Sphere Bosons

- 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.

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



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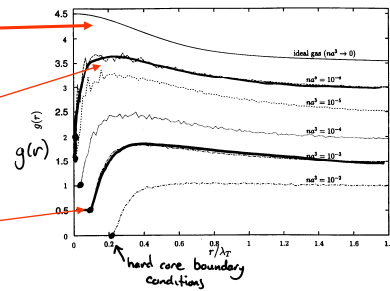
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Pair correlations at low density

Free boson pair correlation.

Peak caused by attraction of bosonic exchange.

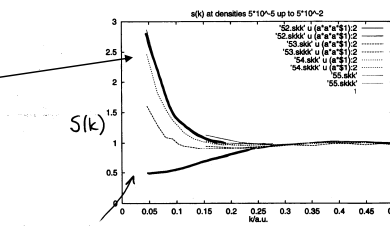
Zero is hard core interaction.



Structure Factor S(K)

(FT of density)

Large compressibility near T_c (clustering)



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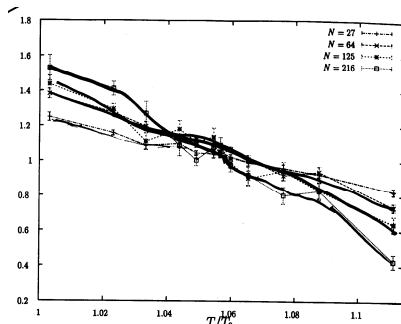
Determination of T_c using superfluid density. Finite size scaling.

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

ζ = bulk correlation length

$$\zeta \rightarrow \left(\frac{T - T_c}{T_c}\right)^{-\nu}$$

- 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.

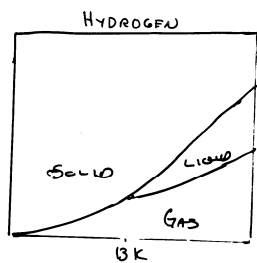
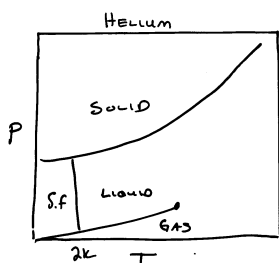
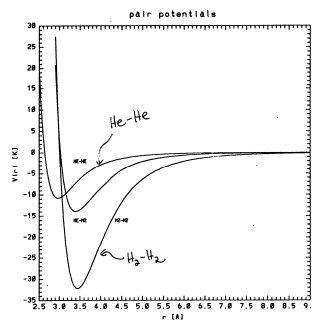


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Why is H_2 not a superfluid?

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

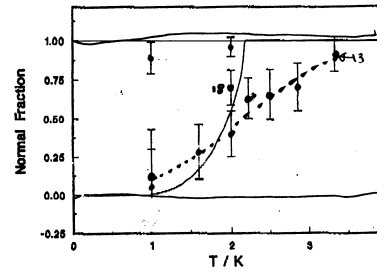
$$E(J_1) - E(J_0) = 170K$$

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

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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).

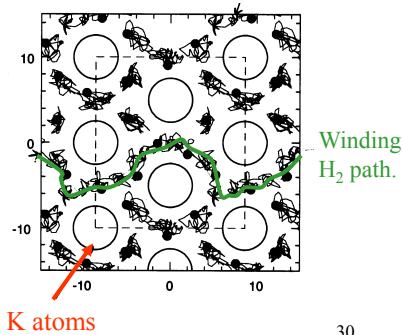
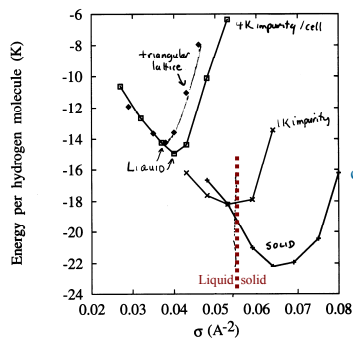
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H₂ on Ag-K surfaces

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.



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Droplets and PIMC

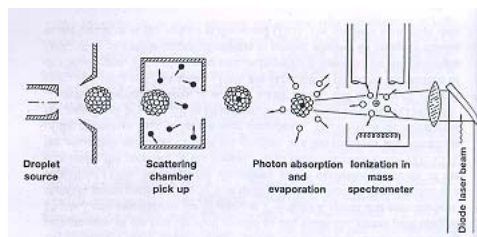
E. Draeger (LLNL) D. Ceperley (UIUC)



- Provide precise microscopic probes for phenomenon such as superfluidity and vortices.
- Provide a nearly ideal “spectroscopic matrix” for studying molecular species that may be unstable or weakly interacting in the gas phase.
- PIMC can be used to simulate ^4He 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 ($T=0.38\text{ K}$)
 - Bose statistics (no sign problem)
 - Finite size effects are interesting.

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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:

$T=0.38\text{ K},$	$N \approx 10^4$	(^4He)
$T=0.15\text{ K},$	$N \approx 10^3$	(^3He)
- 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 $0.01/\text{cm}$. Almost free rotation in superfluid helium **but increase of MOI of rotating impurities.**

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Demonstration of droplet superfluidity

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

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

—————→ ^4He “coat” the impurity allowing it to freely rotate in the superfluid

- They replaced boson ^4He with fermion ^3He . If Bose statistics are important, then rotational bands should disappear. —————→ they didn't!

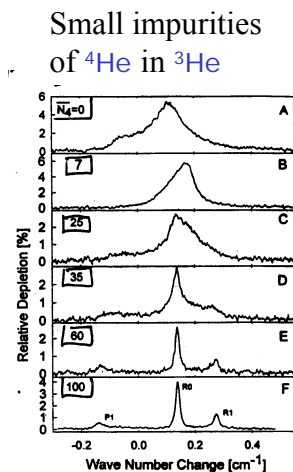
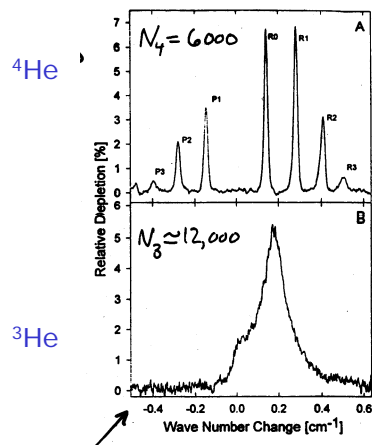
- However, commercial ^3He has ^4He impurities, which would be more strongly attracted to an impurity.

—————→ How much ^4He does it take to “coat” the impurity and get free rotation?

- They found that it takes around 60 ^4He atoms.

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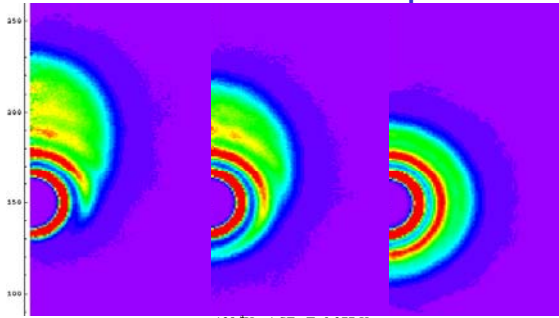
^4He is more strongly attracted to impurity because of zero point effects, so it coats the impurity, insulating it from the ^3He .

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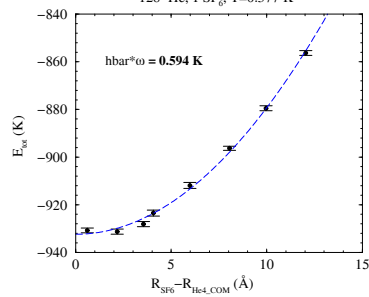
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Density distribution within a droplet

- 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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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:

$$\Psi(r_1, r_2, \dots, r_N) = |\psi| \exp(-i \sum_j \phi_j)$$

density time-indep.
in rotating frame

- Then, for systems in the adiabatic limit:

$$\underbrace{\bar{\nabla} \cdot (\rho \bar{\nabla} \phi)}_{\text{continuity equation}} = \frac{\partial \rho}{\partial t} = -(\bar{\nabla} \rho) \cdot (\bar{\omega} \times \bar{r})$$

- For a known $\rho(\bar{r})$ (adiabatic limit), calculate $\bar{\nabla} \phi(\bar{r})$ from this equation using Gauss-Seidel relaxation. Hydrodynamic inertia is given by

$$K.E. = \frac{1}{2} I_h \omega^2 = \frac{1}{2} m \int dV \rho(\bar{\nabla} \phi) \cdot (\bar{\nabla} \phi)$$

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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.

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

Where A is the area.

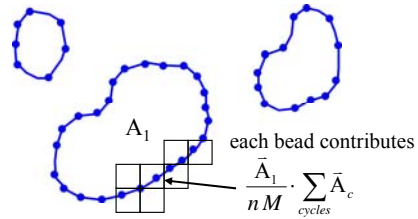
$$\bar{A}(\vec{r}) \equiv \int_0^\beta dt \sum_i (\vec{r}_{it} \times \vec{v}_{it}) \delta(\vec{r}_{it} - \vec{r})$$

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

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

approximation: use only diagonal terms

not positive definite
could be noisy



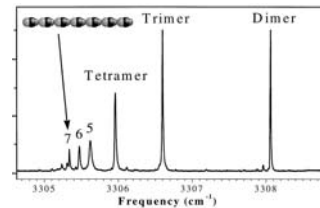
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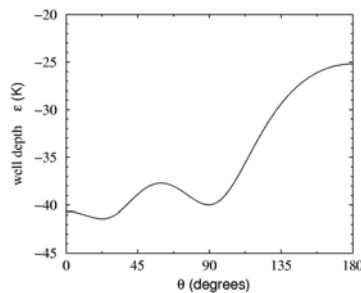
(HCN)_x: Self-Assembled Linear Isomers

Nauta and Miller: HCN molecules in ⁴He 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.



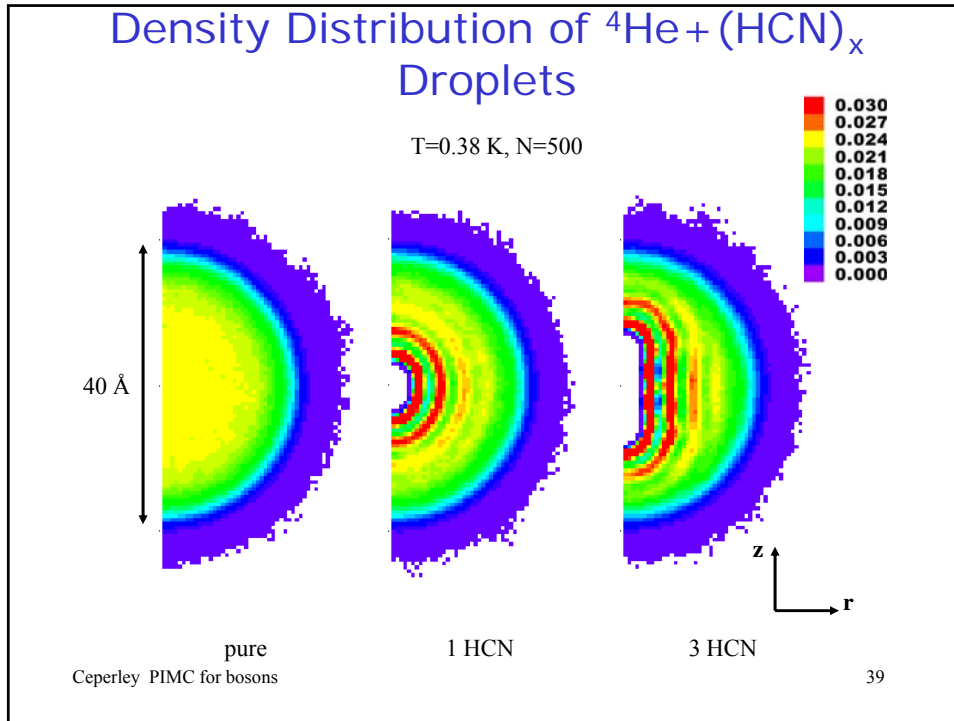
K. Nauta, R. E. Miller, Science 238, 1895 (1999).



Ceperley PIMC for bosons

Atkins and Hutson: Calculated the anisotropic ⁴He-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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Superfluidity around a linear molecule

Draeger + DMC

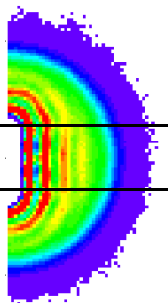
- K. Nauta and R.E. Miller (*Science* **283**, 1895 (1999)) found that HCN molecules will line up in a linear chain in a helium droplet, and measured the HCN-HCN spacing.
- In vacuum they form rings!
- Systems with up to 10 molecules observed.
- Use area formula to find superfluid response.
- We find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

(HCN)₁₀ (He)₁₀₀₀

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Local Superfluid Reduction

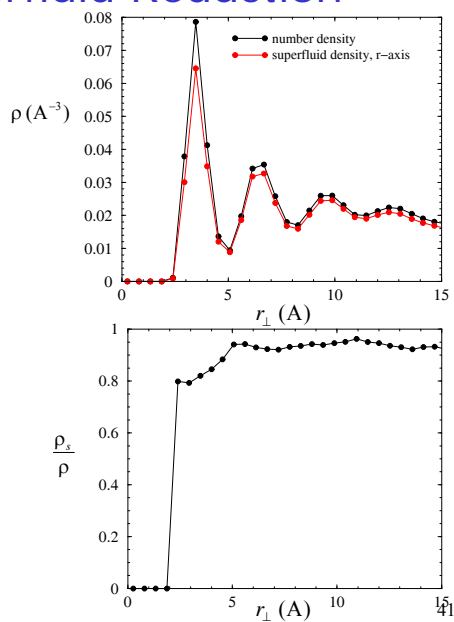
Average over region with cylindrical symmetry



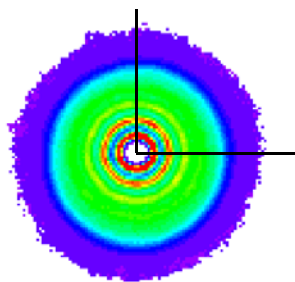
$T=0.38$ K, $N=500$
(HCN)₃

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

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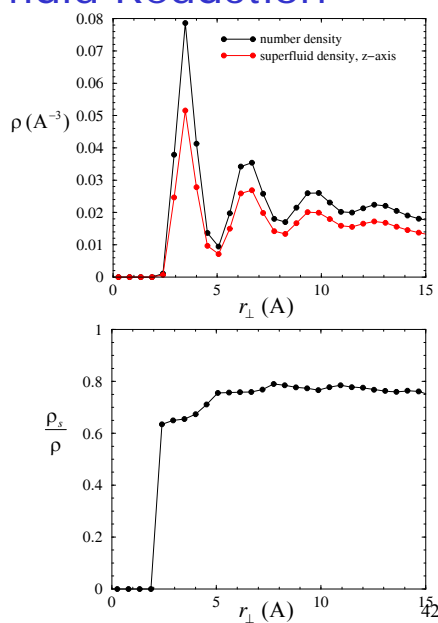
Local Superfluid Reduction



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!

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Local Superfluid Density vs. Temperature

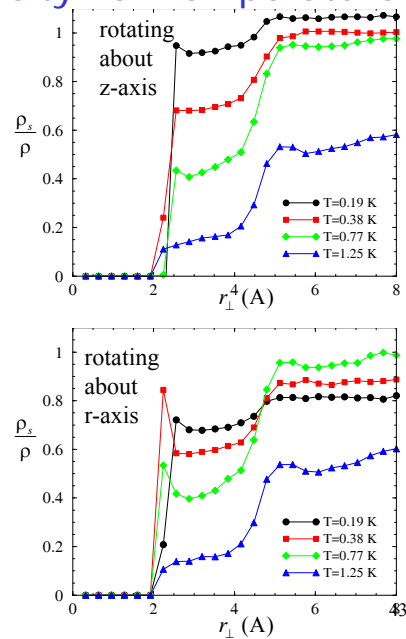
We calculated the superfluid density distribution of $N=128$ ^4He droplets with an $(\text{HCN})_3$ isomer at several temperatures

The superfluid density in the first layer is **temperature dependent!**

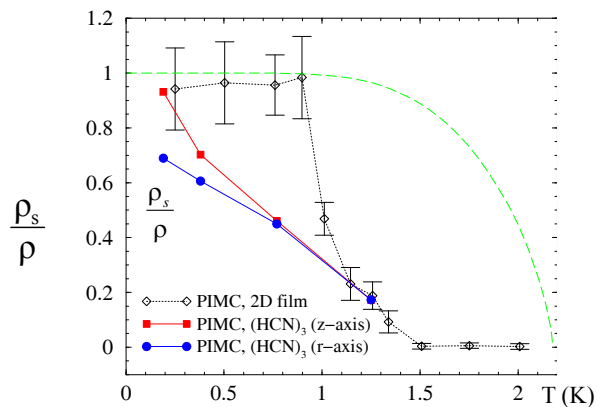
Bulk ^4He is 100% superfluid below 1.0 K. Both experimental measurements on helium films and PIMC studies of 2D helium show transition temperatures T_c which are significantly lower than bulk helium.

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

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First Layer Superfluid Density vs. T



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?

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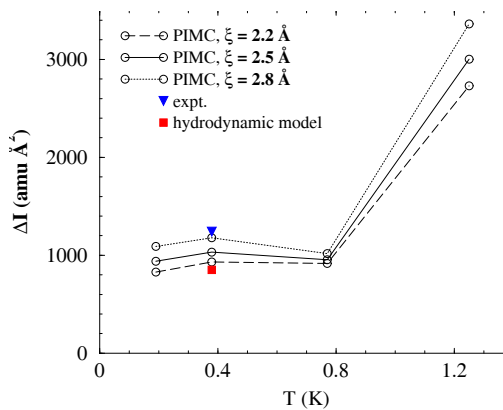
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Moment of Inertia

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.



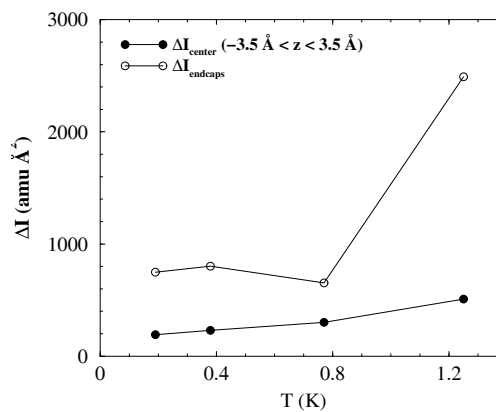
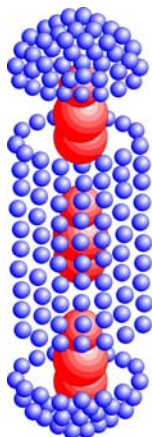
$$\Delta I = \int_{v(\xi)} d\vec{r} m_4 r_{\perp}^2 (\rho(\vec{r}) - \rho_s(\vec{r}))$$

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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.

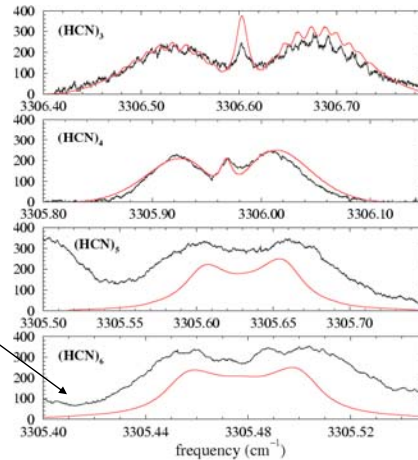
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Temperature Dependence observed

- 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)*



- 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).

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

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

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

- 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.

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

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

$$n_k = \int dk_2 \dots dk_N \text{Pr}(k, k_2, \dots, k_N)$$

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

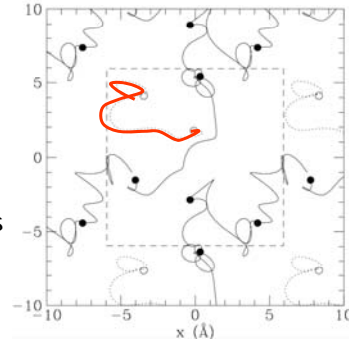
$$n_k = \int \frac{d^3r d^3s}{(2\pi)^3 V} \exp(-ik(r-s)) n(r,s)$$

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

occupy the states with the Boltzmann distribution.

How to calculate $n(r)$

- Take diagonal paths and find probability of displacing one end.
 - advantage:
 - simultaneous with other averages,
 - all time slices and particle contribute.
 - disadvantage: unreliable for $r > \Lambda$.
- 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.

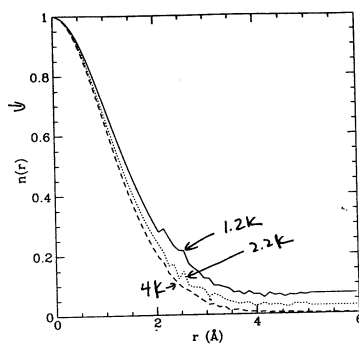


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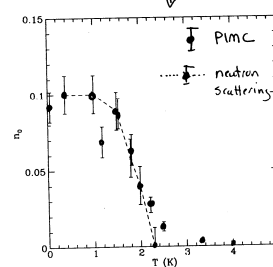
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Comparison with experiment

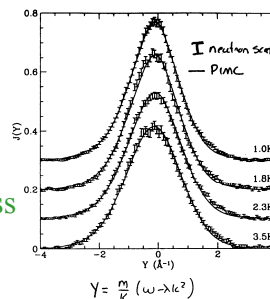
Single particle density matrix



Condensate fraction

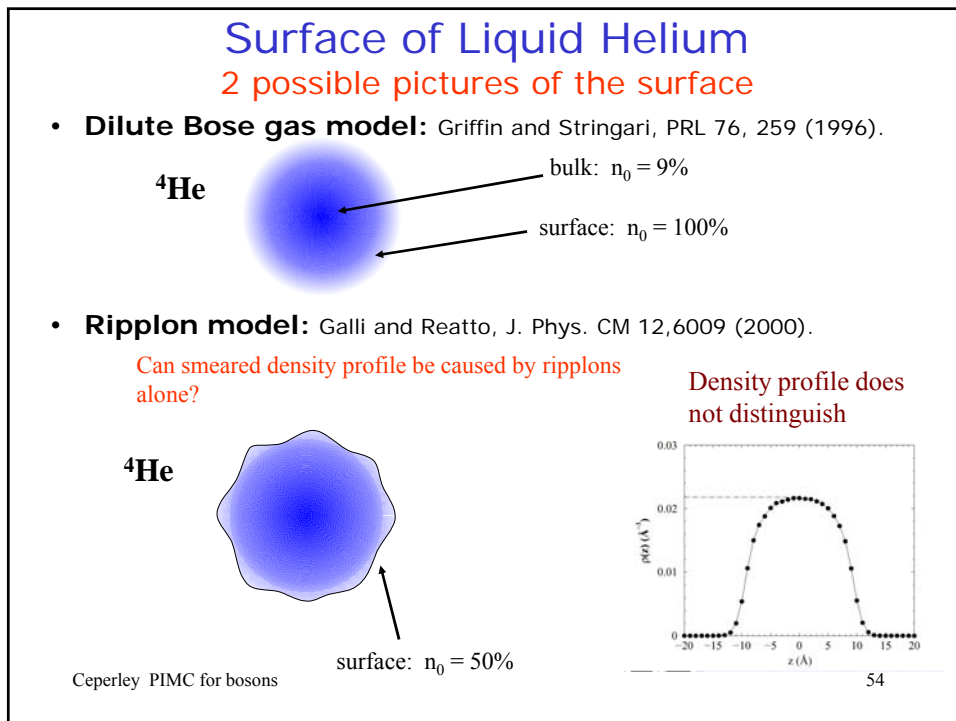
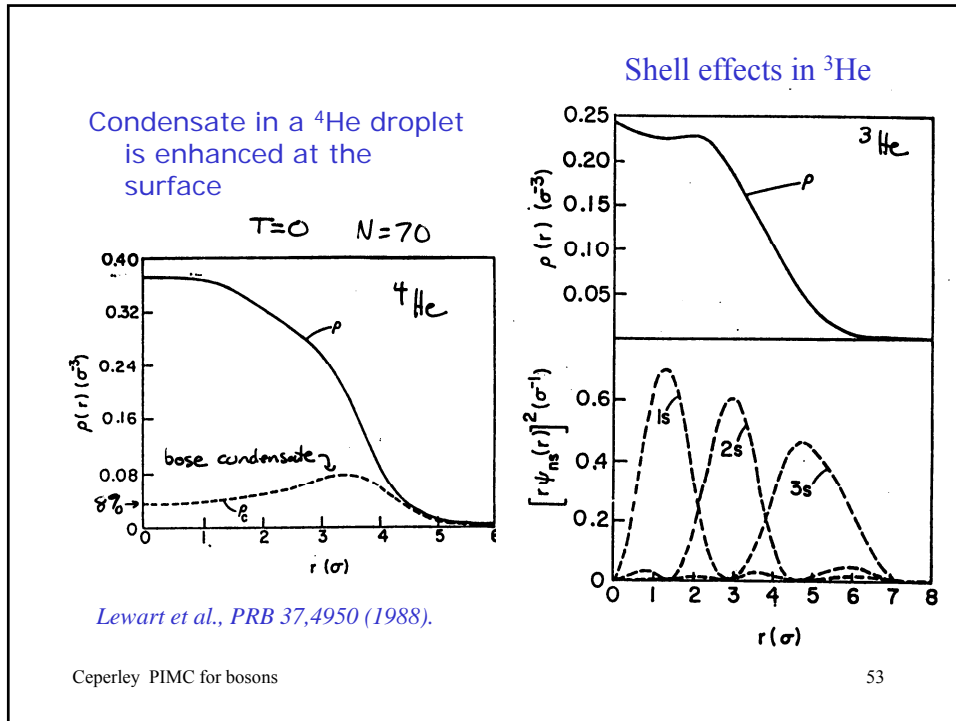


Neutron scattering cross section



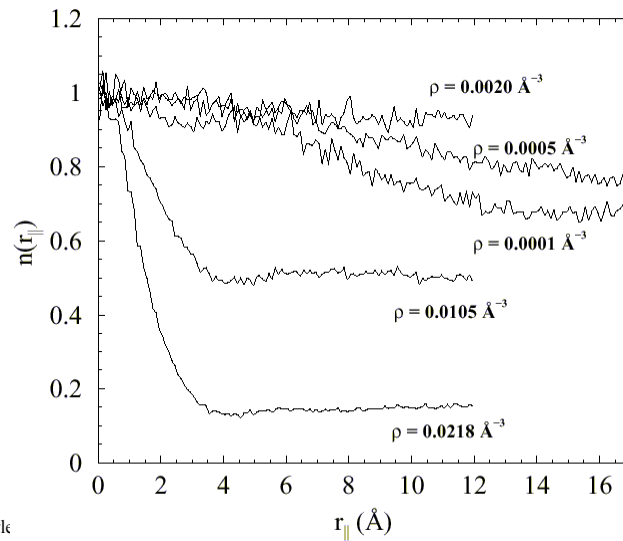
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ODLRO at the Surface of Liquid ^4He

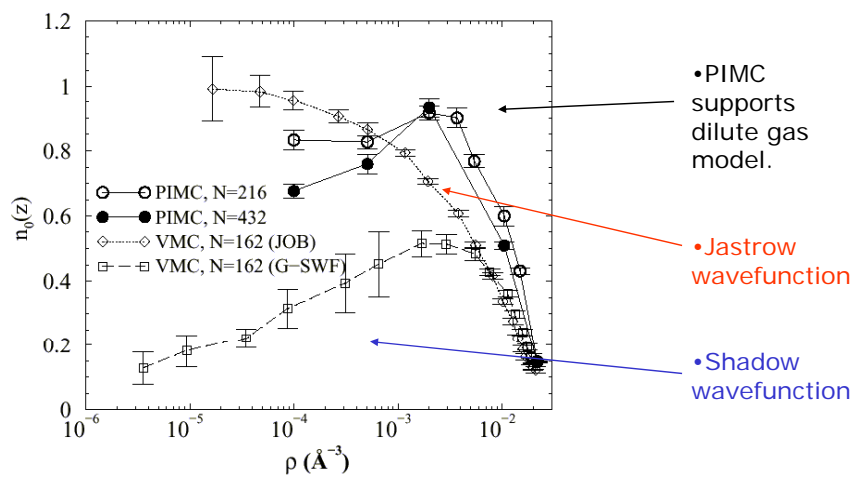
Simulation supports the dilute bose gas model.



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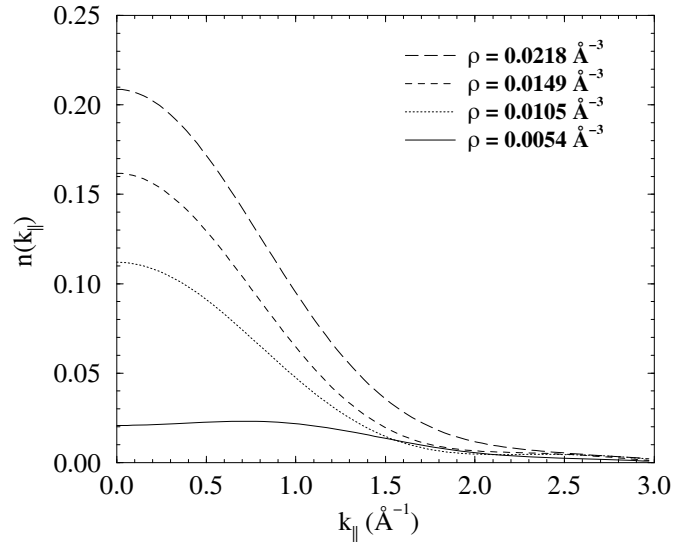
Condensate Fraction at the Surface of ^4He



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Non-condensed distribution

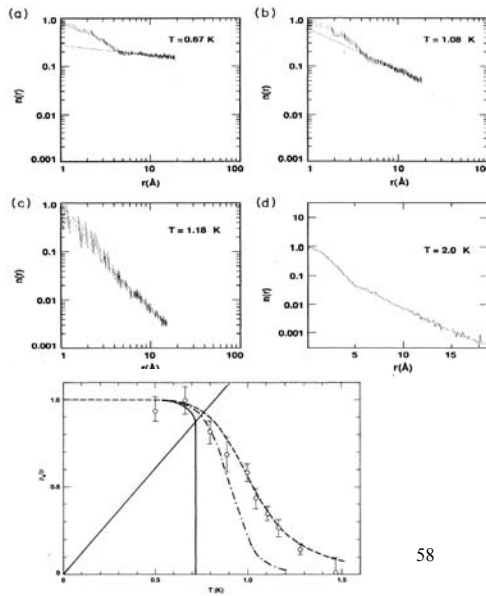
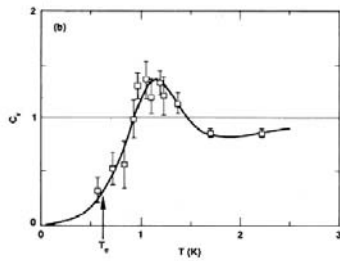


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2D superfluids Kosterlitz-Thouless transition

- 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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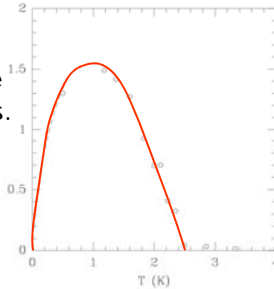
Exchange energy

- Let's calculate the chemical potential of a ^3He atom in superfluid ^4He .
- 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

$$e^{-\beta\mu_3} = \frac{Z_{N-1,1}}{Z_N} = \text{Pr}(\text{atom 1 does not exchange})$$

$$\mu_3 = \mu_4 - kT \ln(P_1) + \int_{\ln(3)}^{\ln(4)} d \ln(m) K(m)$$

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



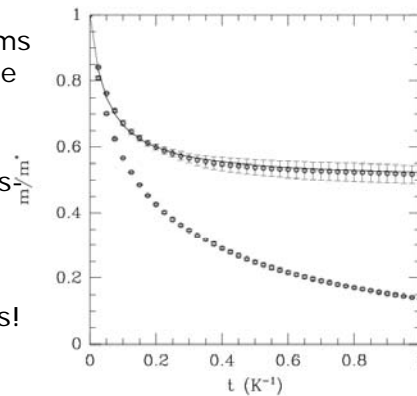
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Effective mass

- 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!

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



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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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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

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