Path Integral Methods for Continuum Quantum Systems

D. Ceperley
University of Illinois Urbana-Champaign

- Imaginary time path integrals
- Path integrals for bosons
- Restricted path integral method for fermions
- Exchange of localized particles
- Examples:
    - Liquid ^{4}He and ^{3}He: superfluids
    - Solid ^{4}He and ^{3}He : supersolid & magnetic order

Liquid helium
the prototypic quantum fluid

- A helium atom is an elementary particle. A weakly interacting hard sphere. First electronic excitation is 230,000 K.

- Interatomic potential is known more accurately than any other atom because electronic excitations are so high.
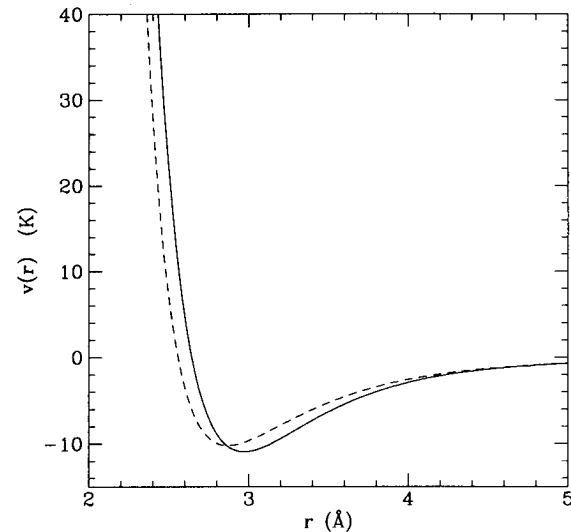

FIG. 1. The semiempirical pair potential between two helium atoms: solid line, Aziz *et al.* (1992); dashed line, Lennard-Jones 6-12 potential with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å.

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

Helium phase diagram

•Because interaction is so weak helium does not crystallize at low temperatures. Quantum exchange effects are important

•Both isotopes are quantum fluids and become superfluids below a critical temperature.

•One of the goals of computer simulation is to understand these states, and see how they differ from classical liquids starting from non-relativistic Hamiltonian:
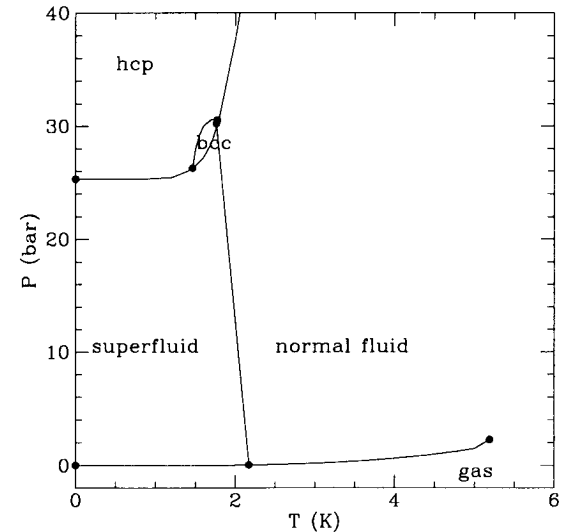

FIG. 2. The phase diagram of ^{4}He.

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

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

Imaginary Time Path Integrals

Atomic Theory of the λ Transition in Helium

R. P. FEYNMAN

California Institute of Technology, Pasadena, California

(Received May 15, 1953)

It is shown from first principles that, in spite of the large interatomic forces, liquid He⁴ should exhibit a transition analogous to the transition in an ideal Bose-Einstein gas. The exact partition function is written as an integral over trajectories, using the space-time approach to quantum mechanics. It is next argued that the motion of one atom through the others is not opposed by a potential barrier because the others may move out of the way. This just increases the effective inertia of the moving atom. This permits a simpler form to be written for the partition function. A rough analysis of this form shows the existence of a transition, but of the third order. It is possible that a more complete analysis would show that the transition implied by the simplified partition function is actually like the experimental one.

The thermal density matrix

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

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

$$\rho(R;\beta) = \sum_\alpha |\phi_\alpha(R)|^2 e^{-\beta E_\alpha} \quad \beta = 1/kT$$

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

off-diagonal density matrix:

- All equilibrium properties can be calculated in terms of thermal o-d density matrix

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

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

- Convolution theorem relates high temperature to lower temperature.

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

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

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

Notation

- Hamiltonian

$$\hat{H} = \hat{T} + \hat{V}$$

- Total potential energy

$$\hat{V} = V(R) = \sum_{i<j} v(r_{ij})$$

- Kinetic energy

$$-\lambda \sum_{i=1}^{N} \nabla_i^2 \quad \text{where } \lambda \equiv \frac{\hbar^2}{2m}$$

- Individual coordinate of a particle r_i
- All 3N coordinates $R = (r_1, r_2, \ldots r_N)$

PIMC Simulations

- We do Classical Monte Carlo simulations to evaluate averages such as:

$$< V >= \frac{1}{Z} \int dR V(R) e^{-\beta V(R)}$$

$$\beta = 1/(k_B T)$$

- Quantum mechanically for T>0, we need both to generate the distribution and do the average:

$$< V >= \frac{1}{Z} \int dR V(R) \rho(R; \beta)$$

$$\rho(R; \beta) = \text{diagonal density matrix}$$

- Simulation is possible since the density matrix is positive.

Trotter's formula (1959)

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

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

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

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

$$\tau = \beta / n$$

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

- Do by FT's

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

- V is "diagonal"

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

- Error at finite n comes from commutator

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

Using this for the density matrix.

- We sample the distribution:

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

Where the "primitive" <u>link action</u> is:

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

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

"Distinguishable" particles

- Each atom is a ring polymer; an exact representation of a quantum wavepacket in imaginary time.

- Trace picture of 2D helium. The dots represent the "start" of the path. (but all points are equivalent)

- The lower the real temperature, the longer the "string" and the more spread out the wavepacket.
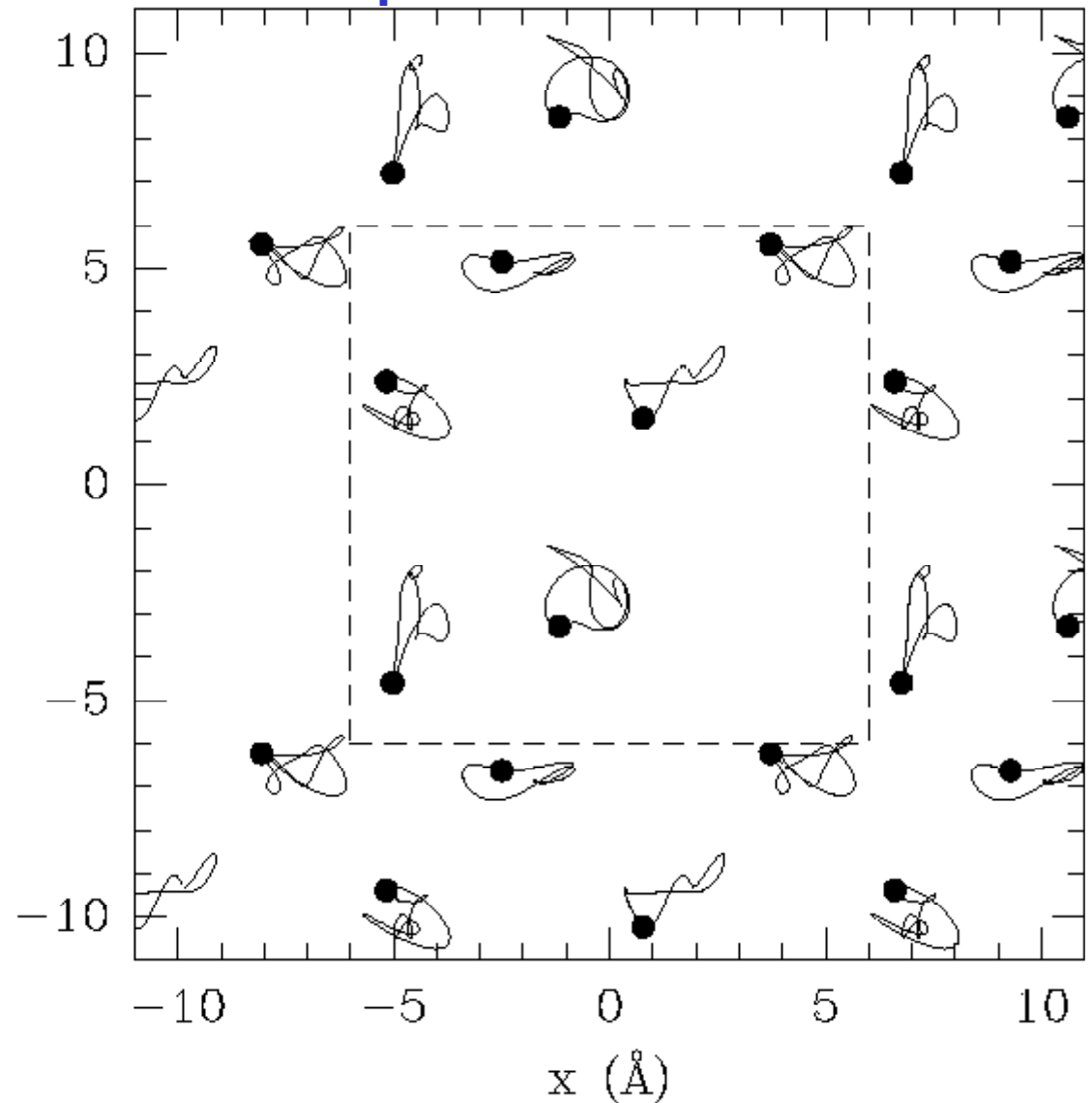
Main Numerical Issues of PIMC

- **How to choose the action**. We don't have to use the primitive form. Higher order forms cut down on the number of slices by a factor of 10. We can solve the 2-body problem exactly.

- **How to sample the paths** *and the permutations*. Single slice moves are too slow. We move several slices at once. *Permutation moves are made by exchanging 2 or more endpoints.*

- **How to calculate properties**. There are often several ways of calculating properties such as the energy.

If you use the simplest algorithm, your code will run 100s or 1000s of times slower than necessary.

Calculations of 1000 He atoms can be done on a laptop-- if you are patient.

Details see: RMP **67**, 279 1995.

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 "<u>bridge</u>": construct a path starting at R_0 and ending at R_t.
- How do we sample $R_{t/2}$? GUIDING RULE. Probability is:

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

- Do an entire path by recursion from this formula.
- Worm algorithms (sampling in space of open paths) can be more efficient.
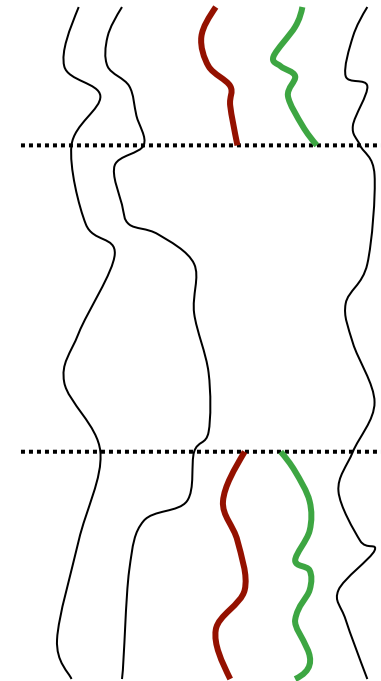
How to sample a single slice.

- 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.

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

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

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

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

$$\overset{=}{\sigma}^2 = \lambda t / 2 \overset{=}{I} + (\lambda t)^2 \overset{\leftrightarrow}{\nabla\nabla} U_s (R_{t/2}^0) = \left\langle \vec{\eta}\vec{\eta} \right\rangle$$

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

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
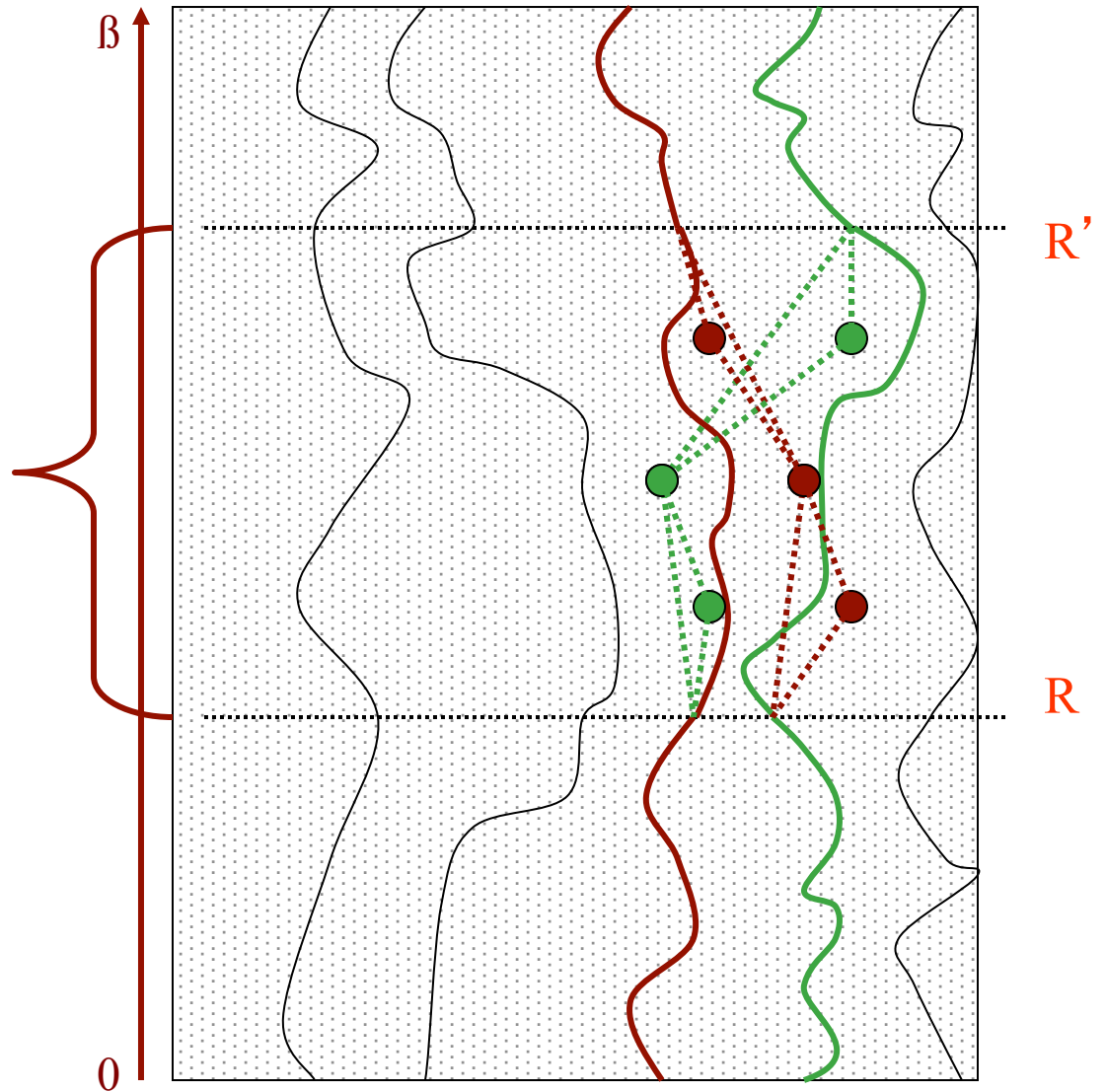
Improved Action

- If we make better actions, we can drastically cut down on the number of time slices.

- This saves lots of time, because the number of variables to integrate over is reduced

- but also because the correlation time of the walk is reduced since "polymers" are less entangled

- Possible approaches to better actions:
    - Harmonic approximation
    - Semi-classical approximation (WKB)
    - Cumulant approximation
    - Pair-product approximation

- Improved actions are also used in lattice gauge theory: the "perfect action."

Calculating properties

- Procedure is simple: write down observable:

$$< O >= \frac{\int dR dR' \left\langle R|\hat{O}|R' \right\rangle \left\langle R|e^{-\beta\hat{H}}|R' \right\rangle}{Z}$$

- Expand density matrix into a "path":

$$< O >= \left\langle\!\left\langle R|\hat{O}|R' \right\rangle\!\right\rangle_{\text{path average}}$$

$$< O >= \left\langle\!\left\langle \hat{O}(R_k) \right\rangle\!\right\rangle_{\text{path average}} \quad \text{for "diagonal operators}$$

- Density, density-density, …. the potential energy are diagonal operators.   Just take average values as you would classically.
- All time slices are the same – can use all for averages.

Calculation of Energy

- Thermodynamic estimator: differentiate partition function

$$E = -\frac{dZ}{Zd\beta} = \frac{1}{Z}\int dR e^{-S}\left[\frac{dS}{d\beta}\right] = \left\langle\frac{dS_k}{d\tau}\right\rangle_{path}$$

$$\frac{dS}{d\tau} = \frac{dU}{d\tau} + \frac{3N}{2\tau} - \frac{(R-R')^2}{4\lambda\tau^2}$$

Potential   n*NI-KE   spring energy

Problem: variance diverges as small time step.

- Virial Estimator: differentiate in "internal coordinates"

does not diverge at small time steps (Herman, Berne)

$$E_{virial} = \left\langle \frac{dU}{d\tau} + \frac{3N}{2\beta} + \frac{1}{2\tau}(R_i - C)\cdot\nabla_i U \right\rangle$$

Potential NI-KE   deviation from centroid   .force

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:

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

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

- Means the path closes on itself with a permutation. **$R_1 = PR_{M+1}$**

- Too many permutations to sum over; we must <u>sample</u> them.

- PIMC task: sample path { $R_1, R_2, ... R_M$ 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.
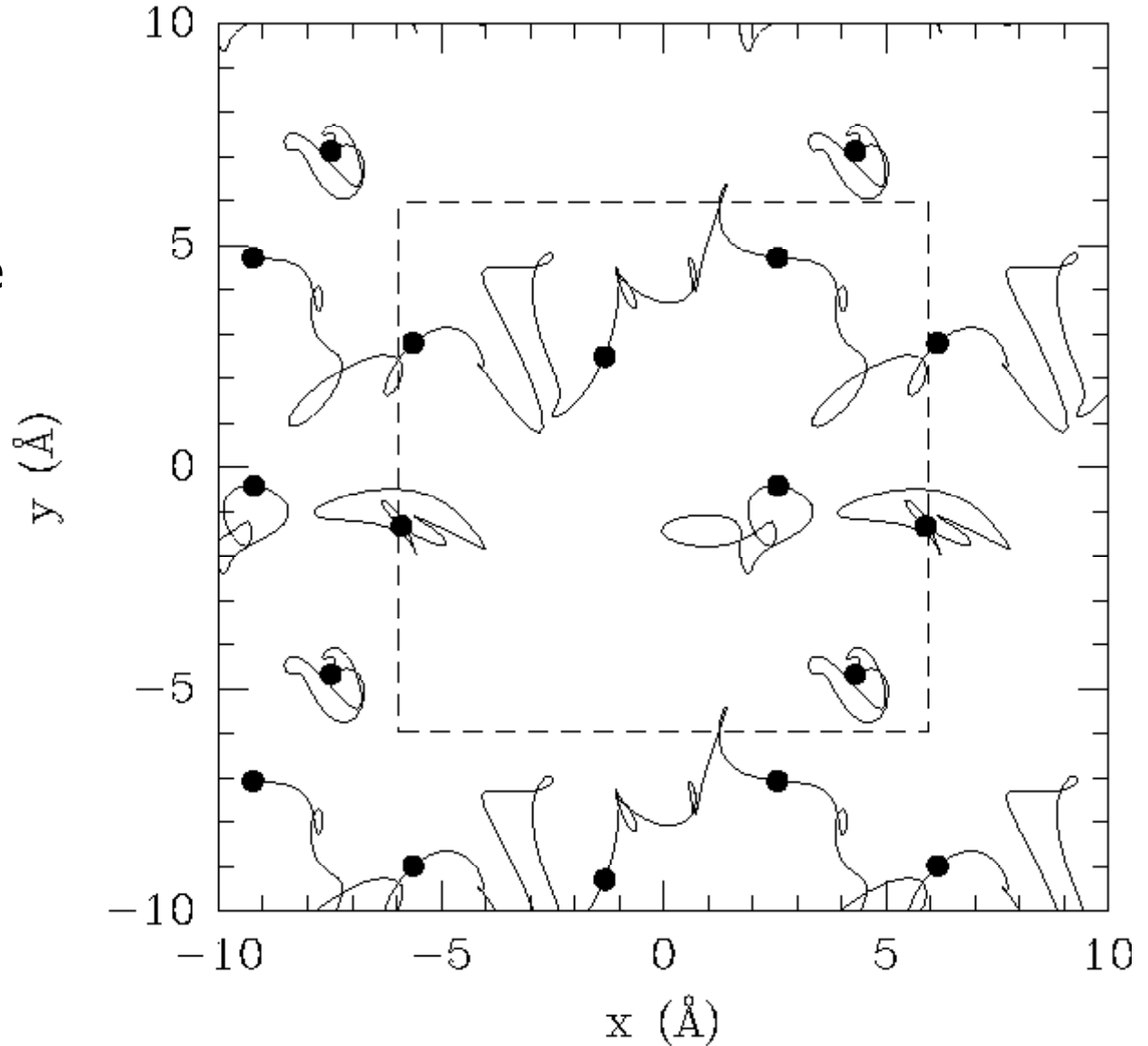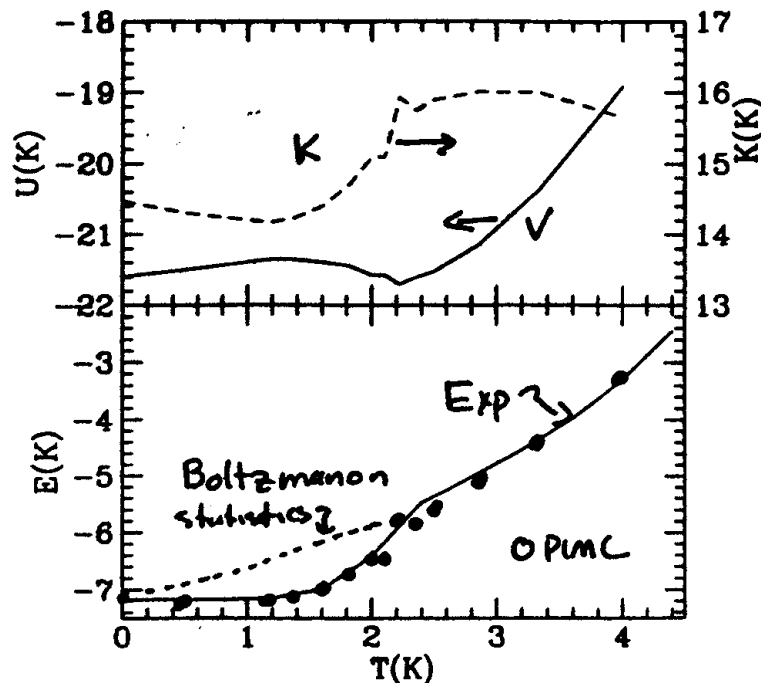
Path Integral explanation of Boson superfluidity

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

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

- Localization in a solid or glass can prevent exchange.
- Macroscopic exchange (long permutation cycles) is the underlying phenomena leading to:
  - Phase transition: bump in specific heat: entropy of long cycles
  - Superfluidity winding paths
  - Offdiagonal long range order--momentum condensation separation of cut ends
  - Absence of excitations (gaps)
- Some systems exhibit some but not all of these features.
- Helium is not the only superfluid. (2001 Nobel Prize for BEC)

ENERGY

Bose statistics have a small effect on the energy

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

SPECIFIC HEAT

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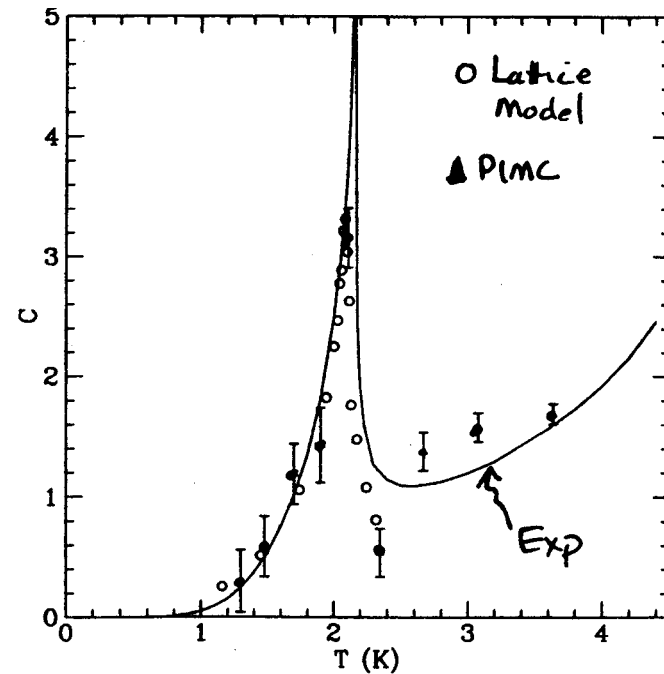- Finite size effects cause rounding above transition

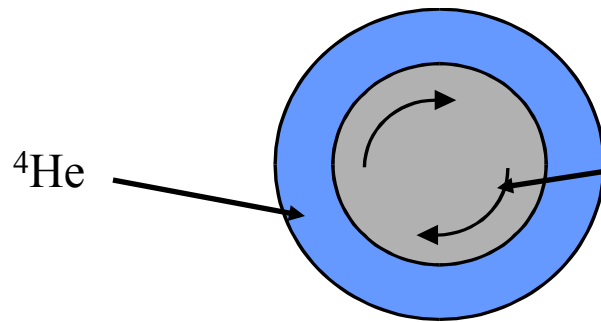$$E = \left\langle V + \frac{3N_{cycles}}{2\beta} + \frac{1}{2}(r_i - c_i)\cdot\nabla_i V \right\rangle$$

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

Superfluidity and PIMC

^{4}He

rotating disks:

- We define superfluidity as a linear response to a velocity perturbation (the energy to rotate the system) Landau definition.

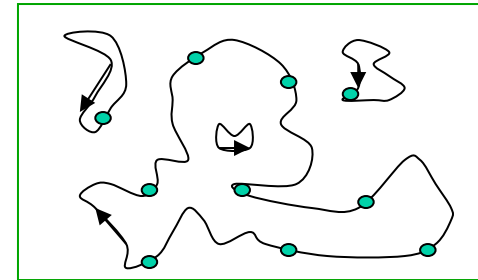$$\frac{\rho_s}{\rho} = 1 - \frac{I}{I_c} = \left.\frac{dF}{d\omega^2}\right|_{\omega=0} \qquad \rho_s + \rho_N \equiv \rho$$

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

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

$$\frac{\rho_s}{\rho} = 1 - \frac{1}{I_c} \left\langle \int_0^\beta dt\, \hat{L}_z\, e^{-(\beta-t)\hat{H}_0}\, \hat{L}_z\, e^{-t\hat{H}_0} \right\rangle$$
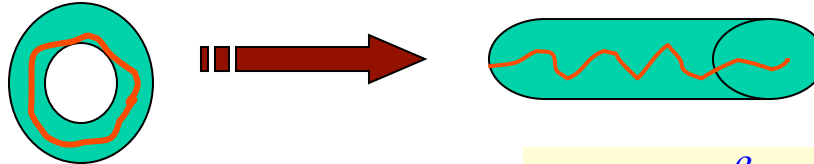
$$\frac{\rho_s}{\rho} = \frac{2m\, \langle A_z^2 \rangle}{\beta\, \lambda\, I_c}$$

A = signed area of imaginary-time paths

Winding numbers in periodic boundary conditions

- Distort annulus

- The area becomes the **winding**
  (average center of mass velocity)

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

- The superfluid density is now estimated as:

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

- Exact linear response formula. Analogous to relation between $\chi \sim <M^2>$ for the 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.

Bose condensation

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

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

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

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

- 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.
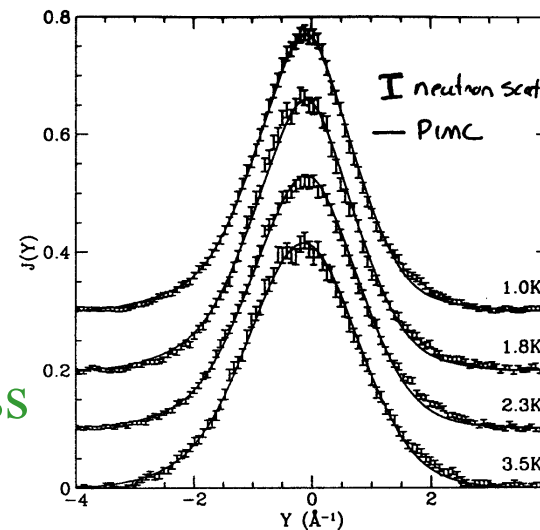
Comparison with experiment

Single particle density matrix
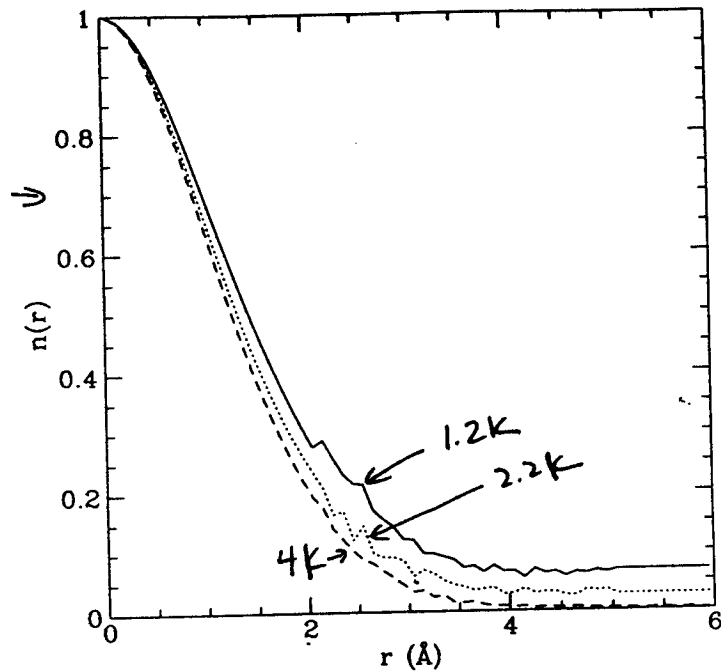
Condensate fraction
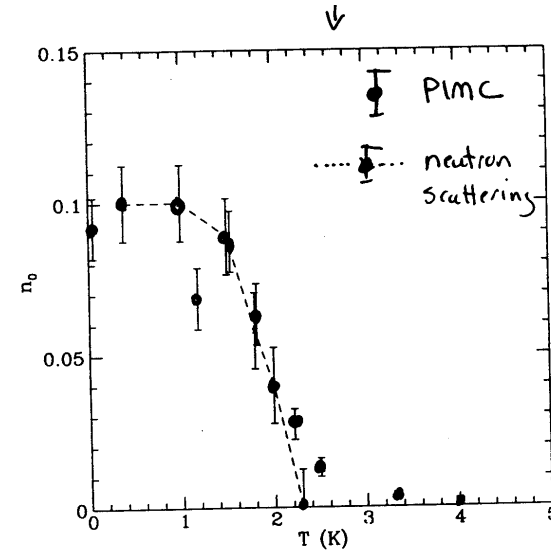
Neutron scattering cross section

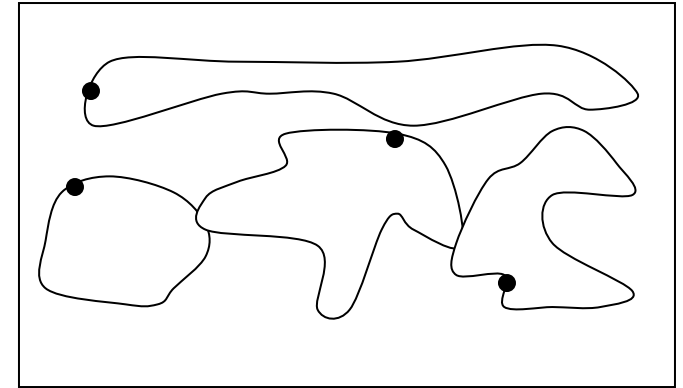
$$Y = \frac{m}{K}\left(\omega - \lambda k^2\right)$$

"Direct" Fermion Path Integrals

- Path integrals map quantum mechanics into a system of cross-linking closed "polymers."

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

$R_0 = PR_M$, P permutation,
$S(R_i, R_{i+1})$ is "boltzmannon action"

4 quantum paths

- Bosons are easy: simply sample **P**.
- Fermions: sample the "action" and carry **$(-1)^P$** as a weight.
- Observable is **even P - odd P.** scales exponentially in N and T^{-1}!

$$CPUtime \quad \propto \varepsilon^{-2} e^{2N[F_F - F_B]/k_B T}$$

Fermion variance

- Compute a fermion observable by sampling the boson probability and taking the sign as a weight

$$\langle O \rangle_F = \frac{\langle \sigma(P)O(R) \rangle_B}{\langle \sigma(P) \rangle_B} \quad \sigma(P) = (-1)^P$$

- The variance of O for this choice can be separated into a bosonic and fermionic contribution.

$$\upsilon_F(O) = \upsilon_B(O) \left[\frac{Z_B}{Z_F} \right]^2$$

- The fermion efficiency is

$$\xi = \left[\frac{Z_F}{Z_B} \right]^2 = \left[\frac{M_+ - M_-}{M} \right]^2 = e^{-2\beta N(\mu_F - \mu_B)}$$

- Big problem once N becomes large OR temperature becomes low-precisely when fermi statistics matter.

The Sign Problem

The expression for Fermi particles, such as He^3, is also easily written down. However, in the case of liquid He^3, the effect of the potential is very hard to evaluate quantitatively in an accurate manner. The reason for this is that the contribution of a cycle to the sum over permutations is either positive or negative depending on whether the cycle has an odd or even number of atoms in its length L. At very low temperature, the contributions of cycles such as L=51 and L=52 are very nearly equal but opposite in sign, and therefore they very nearly cancel. It is necessary to compute the difference between such terms, and this requires very careful calculation of each term separately. It is very difficult to sum an alternating series of large terms which are decreasing slowly in magnitude when a precise analytic formula for each term is not available. Progress could be made in this problem if it were possible to arrange the mathematics describing a Fermi system in a way that corresponds to a sum of positive terms. Some such schemes have been tried, but the resulting terms appear to be much too hard to evaluate even qualitatively.

The (explanation) of the superconducting state was first answered in a convincing way by Bardeen, Cooper, and Schrieffer. The path integral approach played no part in their analysis, and in fact has never proved useful for degenerate Fermi systems.

Feynman and Hibbs,1965.

Fixed-Node method with PIMC

- Get rid of negative walks by canceling them with positive walks. We can do this if we know where the density matrix changes sign. Restrict walks to those that stay on the same side of the node.

- Fixed-node identity. Gives exact solution if we know the places where the density matrix changes sign: the nodes.

$$\rho_F(R_\beta, R_*; \beta) = \frac{1}{N!} \sum_P (-1)^P \int_{\rho_F(R_t, R_*; t) > 0} dR_t \, e^{-S(R(t))} \text{ with } R_0 = PR_*$$

- Classical correspondence exists!!

- Problem: fermion density matrix appears on both sides of the equation. We need nodes to find the density matrix.

- But still useful approach. (In classical world we don't know V(R).)

Proof of the fixed node method

1. The density matrix satisfies the Bloch equation with initial conditions.

$$\frac{\partial \rho(R,t)}{\partial t} = \lambda \nabla^2 \rho(R,t) - V(R)\rho(R,t) \quad \rho(R,0) = \frac{1}{N!}\sum_P (-1)^P \delta(R - PR_0)$$

2. One can use more general boundary conditions, not only initial conditions, because solution at the interior is uniquely determined by the exterior-just like the equivalent electrostatic problem.

3. Suppose someone told us the surfaces where the density matrix vanishes (the nodes). Use them as boundary conditions.

4. Putting an infinite repulsive potential at the barrier will enforce the boundary condition.

5. Returning to PI's, any walk trying to cross the nodes will be killed.

6. This means that we just restrict path integrals to stay in one region.

β

neg   pos   neg

R_0 PR_0

R
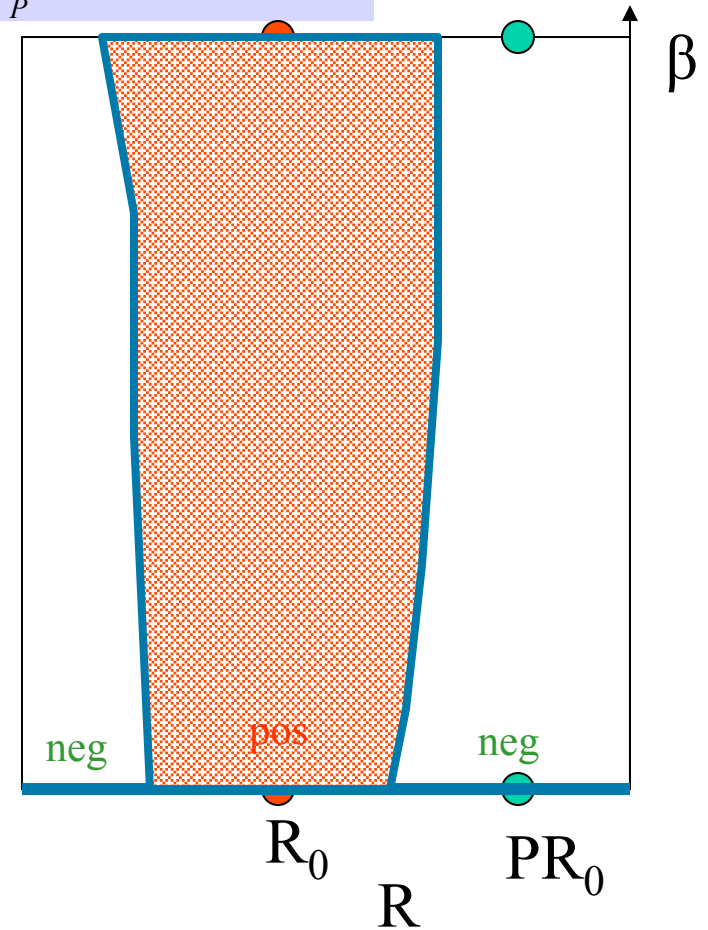
Ortho-para H_2 example

In many-body systems it is hard to visualize statistics.

- The simplest example of the effect of statistics is the H_2 molecule in electronic ground state.

- Protons are fermions-must be antisymmetric.

1. Spins symmetric (↑↑). spatial wf antisymmetric (ortho) "fermions"
2. Spins antisymmetric (↓↑- ↑↓). spatial wf symmetic (para) "bosons"
3. Non symmetrical case (HD)   "boltzmannons"

All 3 cases appear in nature!

- Go to relative coordinates: $r= r_1-r_2$

- Assume the bond length is fixed |r|=a. Paths are on surface of sphere of radius a.

PIMC task is to integrate over such paths with given symmetries.

For a single molecule there is no potential term, a "ring polymer" trapped on the surface of a sphere.

# Paths on a sphere

1. "boltzmannons" Ring polymers on sphere O(r ➜ r)

2. "bosons" 2 types of paths allowed. O(r ➜ r) + O(r ➜ -r)

3. "fermions" 2 types of paths allowed O(r ➜ r) - O(r ➜ -r)
   Low efficiency as

$$\zeta = e^{-\beta(E_1 - E_0)}$$
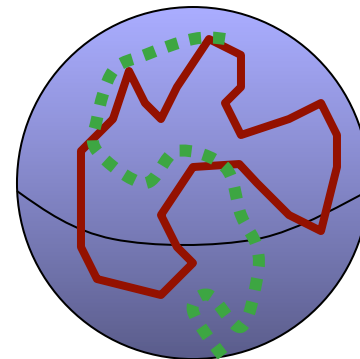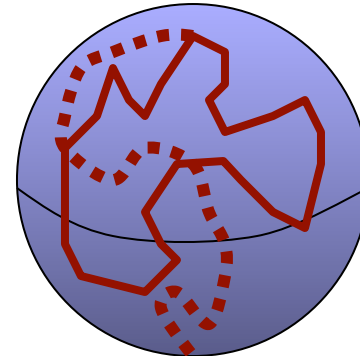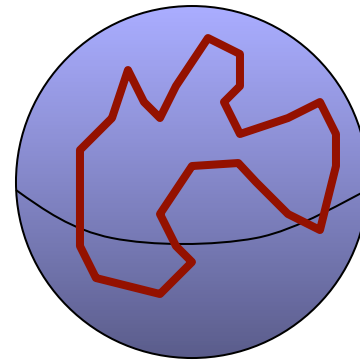
Restricted paths for ortho H$_2$

- Fix origin of path: the <u>reference point</u>.
- Only allow points on path with a positive density matrix. paths staying in the northern hemisphere: r(t)·r(0)>0
- Clearly negative paths are thrown out.
- They have cancelled against positive paths which went south and then came back north to close.
- The symmetrical rule in "t": r(t)·r(t')>0 is incorrect.
- Spherical symmetry is restored by averaging over the reference point: the north pole can be anywhere.
- Can do many H$_2$ the same way.
- Ortho H$_2$ is much more orientable than either HD or para H$_2$.
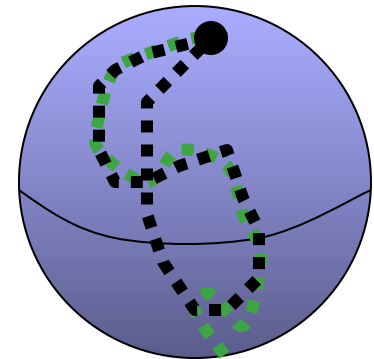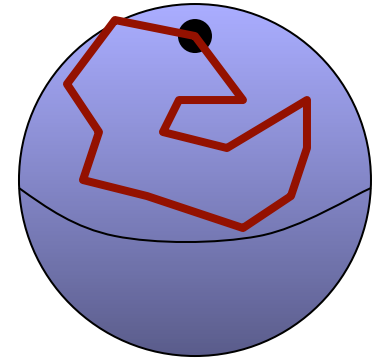
Nodal Properties

*If we know the sign of the exact density matrix(the nodes), we can solve the fermion problem with the fixed-node method.*

- If $\rho(R)$ is real, nodes are $\rho(R)=0$ where **R** is the **3N** dimensional vector.

- Nodes are a **3N-1** dimensional surface. (Do not confuse with single particle orbital nodes!)

- Coincidence points $\mathbf{r}_i = \mathbf{r}_j$ are **3N-3** dimensional hyper-planes

- In **1** spatial dimension these "points" exhaust the nodes. *fermion problem is easy to solve in 1D* with the "no crossing rule."

- Coincidence points (and other symmetries) only constrain nodes in higher dimensions, they do not determine them.

- The nodal surfaces define nodal volumes. How many nodal volumes are there? **Conjecture**: there are typically *only* 2 different volumes (+ and -) except in 1D. (but only demonstrated for free particles.)

- At high T, nodes are free particle-like, Vornoi polyhedra.

For a density matrix
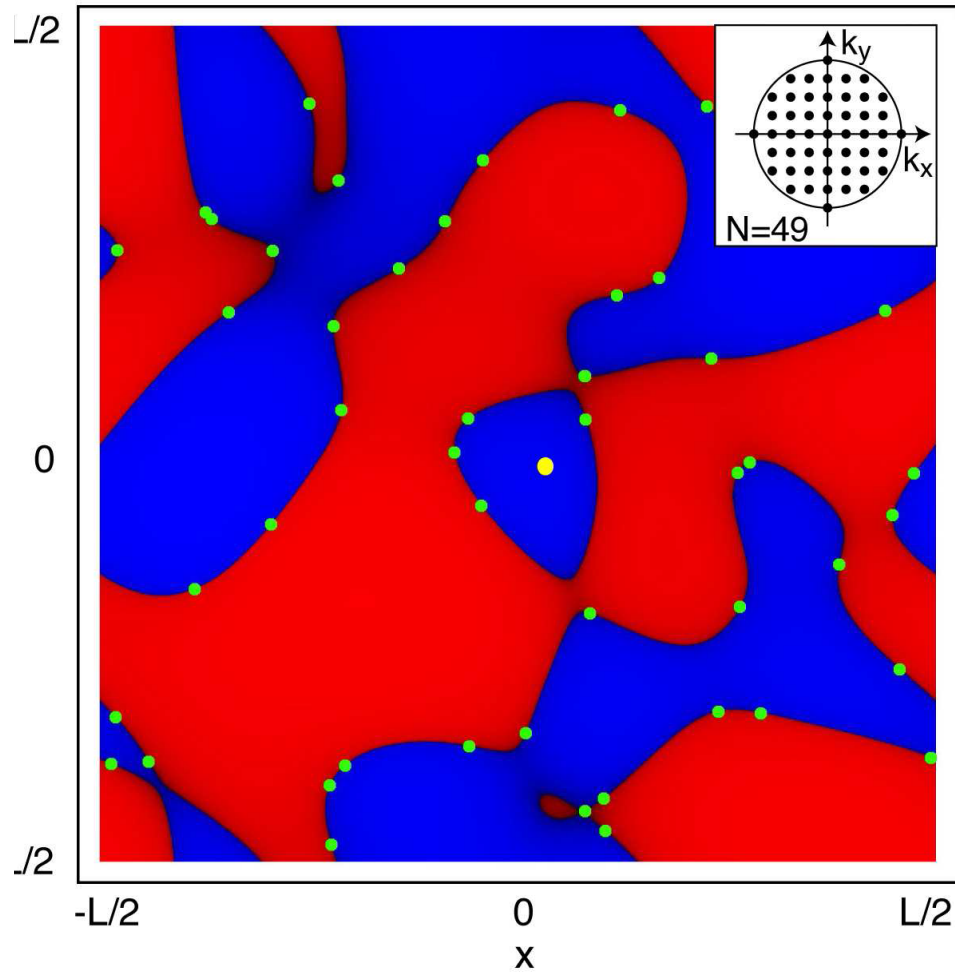
b)
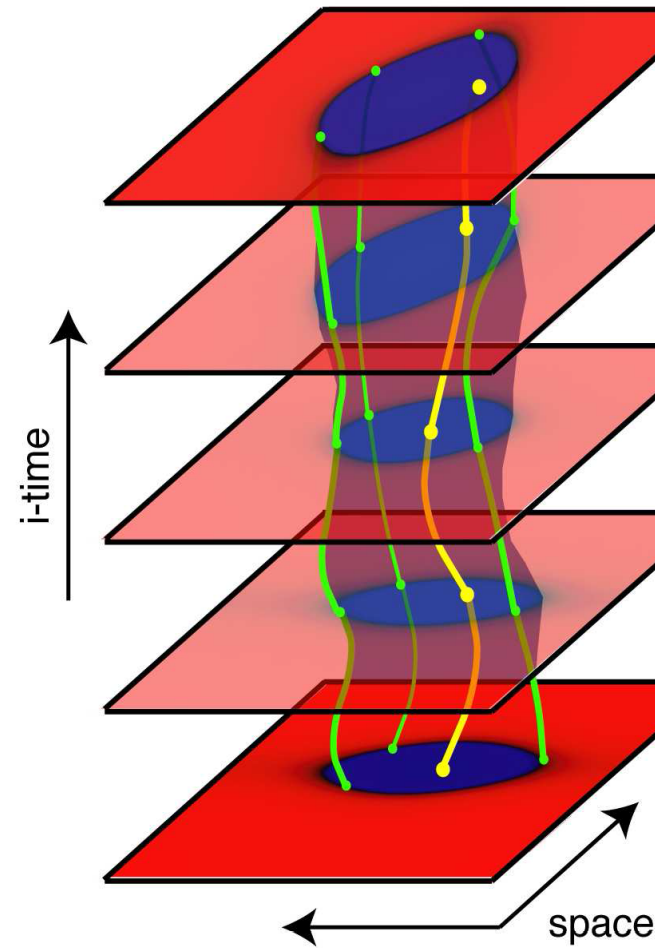
RPIMC with approximate nodes

- In almost all cases, we do not know the "nodal" surfaces.
- We must make an an ansatz.
- This means we get a fermion density matrix (function with the right symmetry) which satisfies the Bloch equation at all points except at the node.
- That is, it has all the exact "bosonic" correlation
- There will be a derivative mismatch across the nodal surface unless nodes are correct.
- In many cases, there is a free energy bound. Proved at high temperature and at zero temperature and when energy is always lower.
- Maybe one can find the best nodes using the variational principle. (variational density matrix approach)

Fermion superfluidity

- Liquid ^{3}He becomes superfluid at very low temperatures ($T_c \sim 1mK$).
- With the exact nodal restriction this must also happen within RPIMC, because we can calculate the free energy.
- What happens to the paths at this phase transition?
- SPECULATION: there is a "Cooper" pairing of up and down spin exchanges, similar to a polymer blend
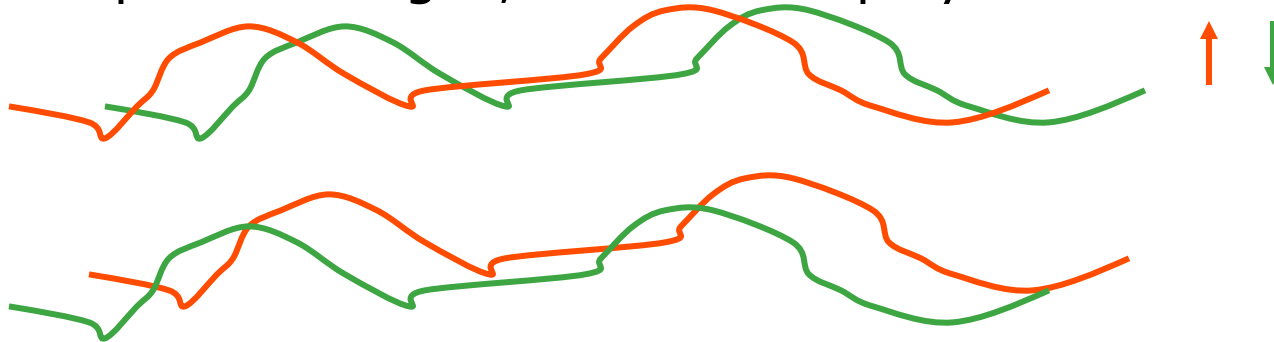

- Not tried in ^{3}He because of formidable practical difficulties (length, temperature scale) and lack of knowledge of nodal topology required.

Thouless theory of magnetic order

- At low temperature there are **very** few defects, phonons, etc.
- The many body wavefunction has N! peaks, corresponding to possible electron relabelings.
- Expand exact wavefunction in terms of localized wavefunctions.
- System remains in one peak, then tunnels to another, very rarely.
- Dominant tunneling rates are few particle cyclic exchanges.
- Exchange frequencies (J_P) determine the magnetic order.
- The resulting Hamiltonian is:

$$H = H_{phonon} - \sum_p (-1)^p J_p \hat{P}$$

Unimportant at low temperatures
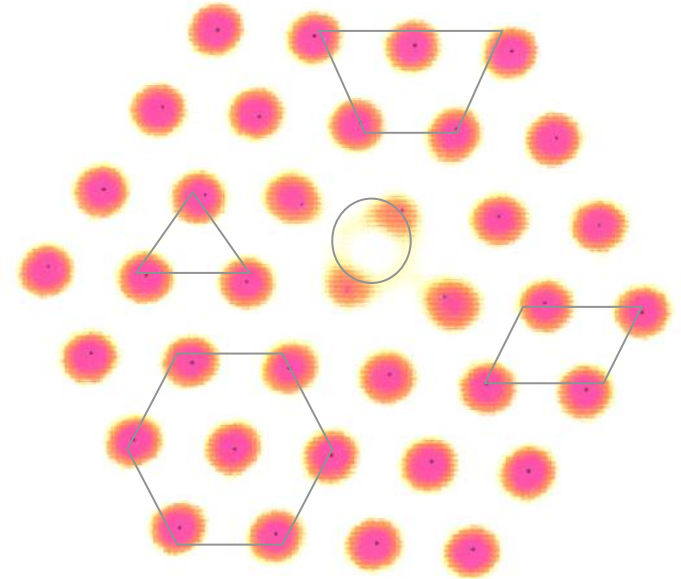
Solid ^{3}He

- Exchanges of 2,3,4,5 and 6 particles are important because of Metro effect.
- Large cancellation of effects of various exchanges leads to a frustrated broken symmetry ground state (u2d2).
- Main problem with MEM: there are too many parameters! But if they are determined with PIMC, they are no longer parameters!

- We have calculated *(Ceperley & Jacucci PRL 58, 1648, 1987)* exchange frequencies in bcc and hcp ^{3}He for 2 thru 6 particle exchanges.
- PIMC gives convincing support for the empirical multiple exchange model. *(Roger, Delrieu and Hetherington)*
- Agrees with experiment measurements on magnetic susceptibility, specific heat, magnetic field effects, ….

Path Integral Method to determine exchange frequency

- We make a path extending from Z to PZ and evaluate the change in the action. Z=perfect crystal lattice.

- We estimate the ratio:

$$f_P(\beta) = \frac{Q_P(\beta)}{Q_I(\beta)} = \tanh(J_P(\beta - \beta_0))$$

$$Q_P(\beta) = \left\langle Z \left| e^{-\beta \hat{H}} \right| PZ \right\rangle$$

X

fit tanh(2t/0.038)
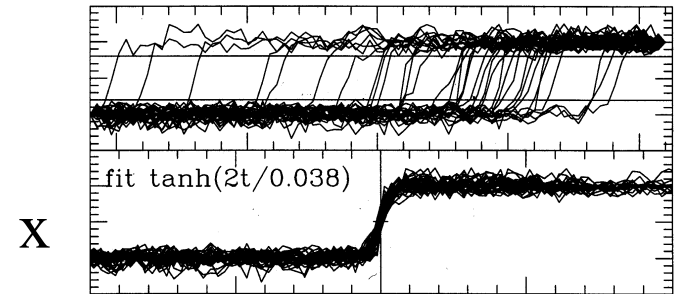
Imaginary time

- X is a "reaction coordinate" for the exchange.

- J_P is the imaginary time tunneling rate.

- β_0 is the width in imaginary time of the "instanton."

- How can we calculate a "free energy difference?": map paths from exchange to non-exchange (Bennett's method) and estimate the slope.

Exchange frequencies in bcc ³He

TABLE I. Calculated exchange frequencies (in μK) in bcc ^{3}He at two densities with the statistical error in % next to it. The density (in cc/mole) is shown at the top of the column. The exchange notation gives the set of $p(p-1)/2$ pair distances among the p atoms exchanging, where 1 is a nearest neighbor, 2 a next-nearest neighbor, etc. The first set of numbers specifies the distances of adjacent atoms on the cycle, the next set the second neighbors, etc. Thus the planar and folded exchanges are both nearest-neighbor four-body exchanges, but differ in the distance between the second and fourth atoms of the exchange.

MEM

p	Exchange	Name	20.07		24.12		
2	(11)	nn	13.8	5%	453 **350**	3%
	(22)	nnn	1.0	6%	62	7%
3	(112)	t	4.8	6%	182 **140**	5%
	(113)				5.3	15%
4	$(1^4; 23)$	planar	9.8	7%	250 **300**	6%
	$(1^4; 22)$	folded	0.45	10%	32	11%
	$(1122; 31)$	diamond			6	25%
	$(1212; 11)$	eight			0.5	45%
	$(1212; 14)$	para			11	30%
	$(2^4; 33)$	square			1.9	30%
5	$(1^4 2; 52341)$	planar			5.3	15%
6	$(1^6; 3^6; 4^3)$	crown			34	22%
	$(1^6; 123^2; 417)$	planar			10	10%

From: DMC, Jacucci PRL 58, 1648(1987)

Supersolid

Will solid ^{4}He be a superfluid if we go to low enough T?

Ring exchange frequencies in hcp ^{4}He.

Probable observation of a supersolid helium phase

E. Kim & M. H. W. Chan

Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

When liquid ^{4}He is cooled below 2.176 K, it undergoes a phase transition—Bose–Einstein condensation—and becomes a superfluid with zero viscosity[1]. Once in such a state, it can flow without dissipation even through pores of atomic dimensions. Although it is intuitive to associate superflow only with the liquid phase[2], it has been proposed theoretically[3–5] that superflow can also occur in the solid phase of ^{4}He. Owing to quantum mechanical fluctuations, delocalized vacancies and defects are expected to be present in crystalline solid ^{4}He, even in the limit of zero temperature. These zero-point vacancies can in principle allow the appearance of superfluidity in the solid[3,4]. However, in spite of many attempts[6], such a 'supersolid' phase has yet to be observed in bulk solid ^{4}He. Here we report torsional oscillator measurements on solid helium confined in a porous medium, a configuration that is likely to be more heavily populated with vacancies than bulk helium. We find an abrupt drop in the rotational inertia[5] of the confined solid below a certain critical temperature. The most likely interpretation of the inertia drop is entry into the supersolid phase. If confirmed, our results show that all three states of matter—gas[7], liquid[1] and solid—can undergo Bose–Einstein condensation

TABLE II. Calculated exchange frequencies in hcp ^{4}He at a molar volume of 21.04 cc. The notation of the exchange is from Roger (1984).

p	Name	J (μK)	% error
2	nn	3.2	13%
	nn'	3.4	13%
3	T	2.3	12%
	$T*$	0.5	13%
	T'	2.3	12%
4	K'	1.4	20%

- How can we have a supersolid?
- We would need:

$$\frac{\rho_s}{\rho} = \lim_{N\to\infty} \frac{m}{h^2 N} \sum_P J_P W_P^2 > 0$$

$$\beta_{0P} < \beta < J_P$$

- Local loops have no winding (do not transport mass)
- Need frequent long exchange
- Seems to require unbound vacancies and interstitials.
- BEC would also require delocalized paths.
- PIMC $E_{vac} \sim 16K$
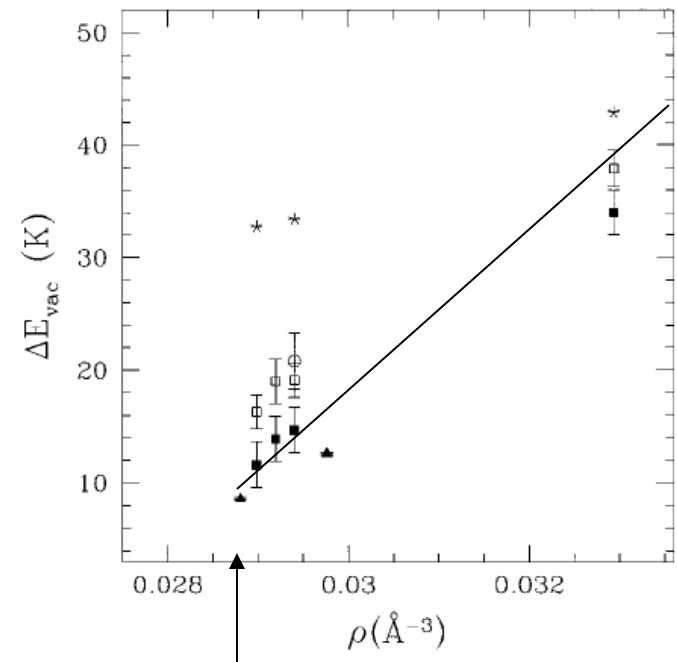- Pederiva et al find $E_{vac} \sim 10K$.

FIG. 1. Vacancy formation energy ΔE_{vac} vs reduced density. Solid triangles: data from Ref. 3, open squares: variational estimates for the fcc phase; filled squares: for the hcp phase; open circle: for the bcc phase. Stars: formation energy of a static vacancy [see Eq. (10) in text].

Calculation of density matrix of solid helium
Clark & DMC cond-mat/0512547
Boninsegni, Prokof'ev & Svistunov cond-mat/0512103

- n(r) from PIMC gets very small at large r. No BEC

- Oscillations are due to lattice effects

- Separating 2 ends costs a constant "energy" per unit length (string tension).

- If you pull the string too hard, you create vacancy-interstitial pairs.

- Can you have a superfluid even if there is no BEC?
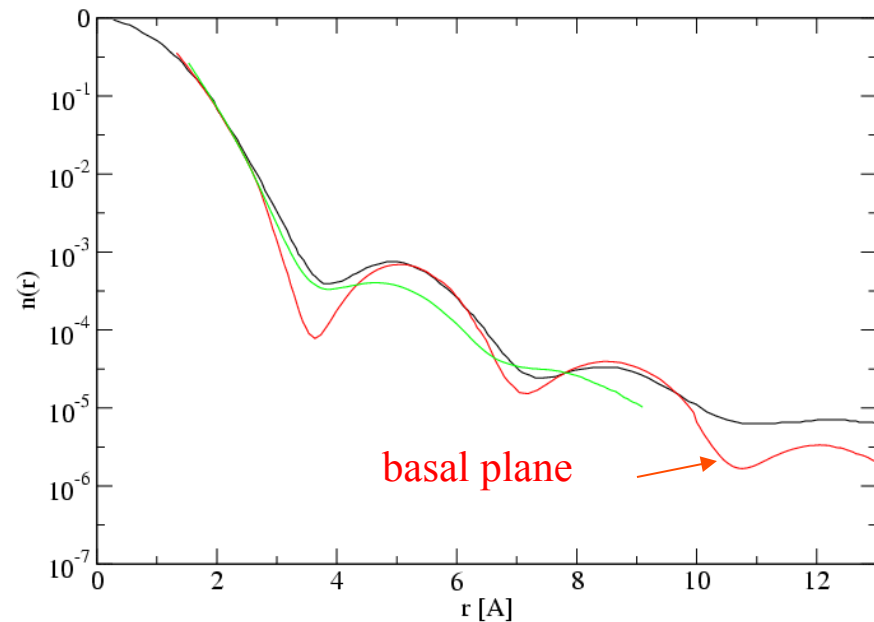
basal plane

Winding exchanges

- Winding exchanges are much more probable because they are straight.
- PIMC exchange frequencies in the basal plane decrease exponentially

$$J = J_0 \exp\left[-\alpha L_p\right] \quad \alpha = 2.7$$

- Consider exchanges with various angles
- Coordination number in hcp lattice is 12; 11=exp(2.4)
- Can this compensate for the exponential drop?
- To find out, we did calculations of 50 different exchanges in solid ^{4}He with 4<L<9.

26 bars
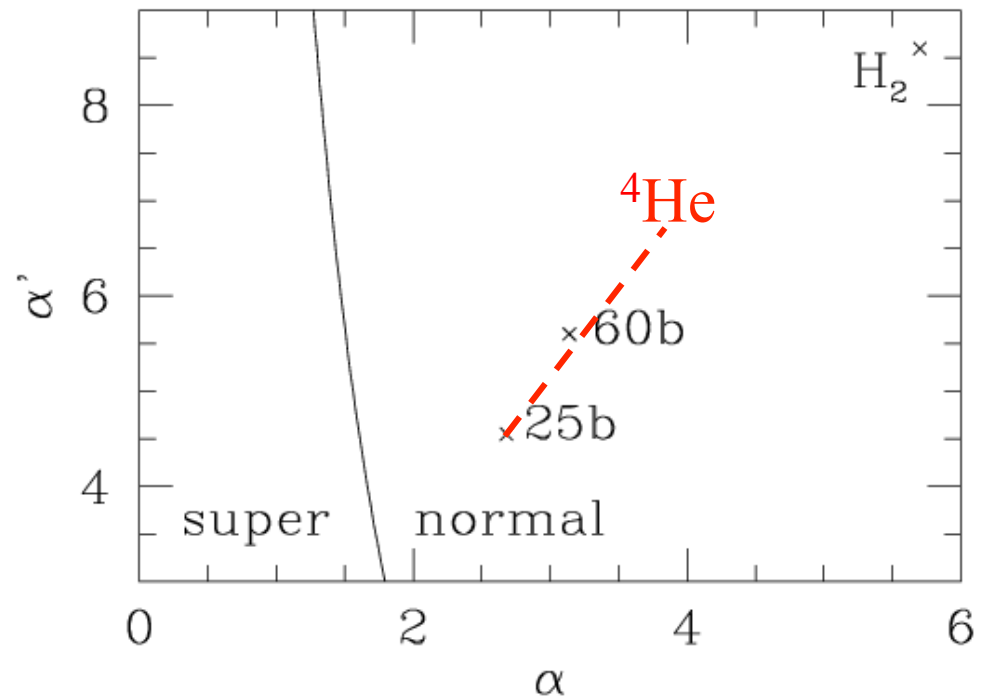
60 bars
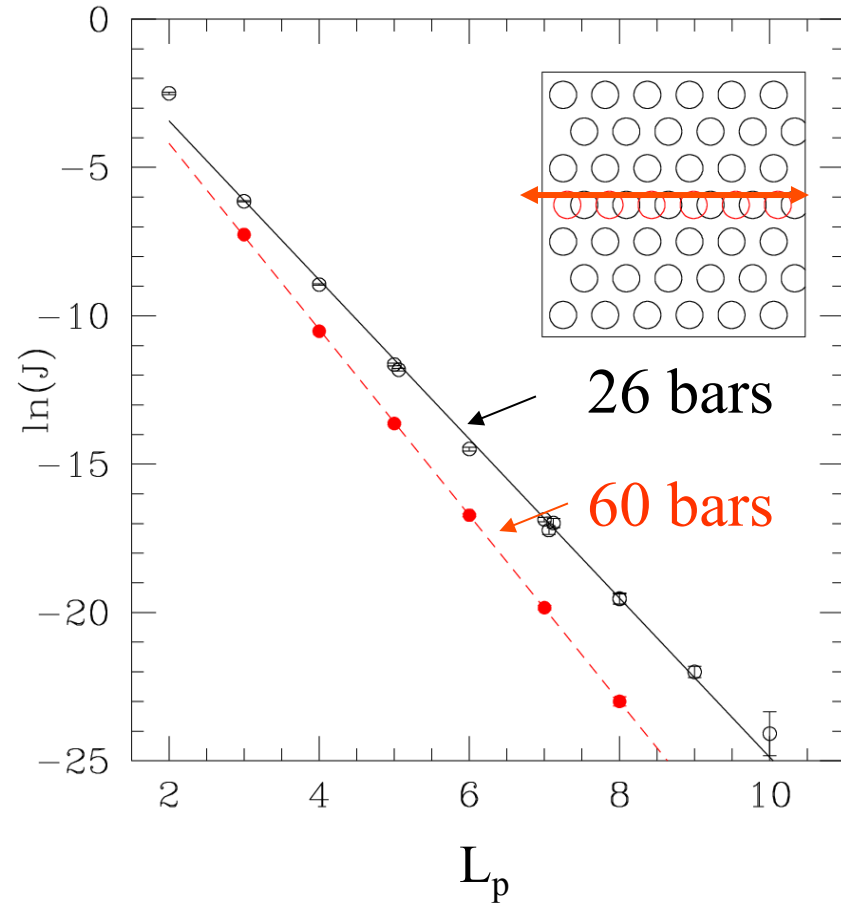
Phase diagram of lattice model

- Ring exchange model with parameters from fit, is not a supersolid
- Probability of long exchanges *decreases* faster than number of polygons increases
- Increasing the density makes it worse!

$$J_p = J_0 e^{-\alpha L_p - \alpha' \sum_{k=1}^{L_p} \cos^4(\theta_k/2)}$$

Dictionary of the Quantum-Classical Isomorphism

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
Pauli Principle	Restricted Paths
Cooper Pairing	Paired Fermion Paths
Fermi Liquid	Winding restricted paths
Insulator	Nonexchanging paths

"fermion dictionary"?