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Research Workshop on Condensed Matter Physics
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MINIWORKSHOP ON
QUANTUM MONTE CARLO SIMULATIONS OF LIQUIDS AND SOLIDS
30 JUNE - 11 JULY 1997
and
CONFERENCE ON
QUANTUM SOLIDS AND POLARIZED SYSTEMS
3 - 5 JULY 1997

"Variational monte carlo: shadow wave function for boson ground state"

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

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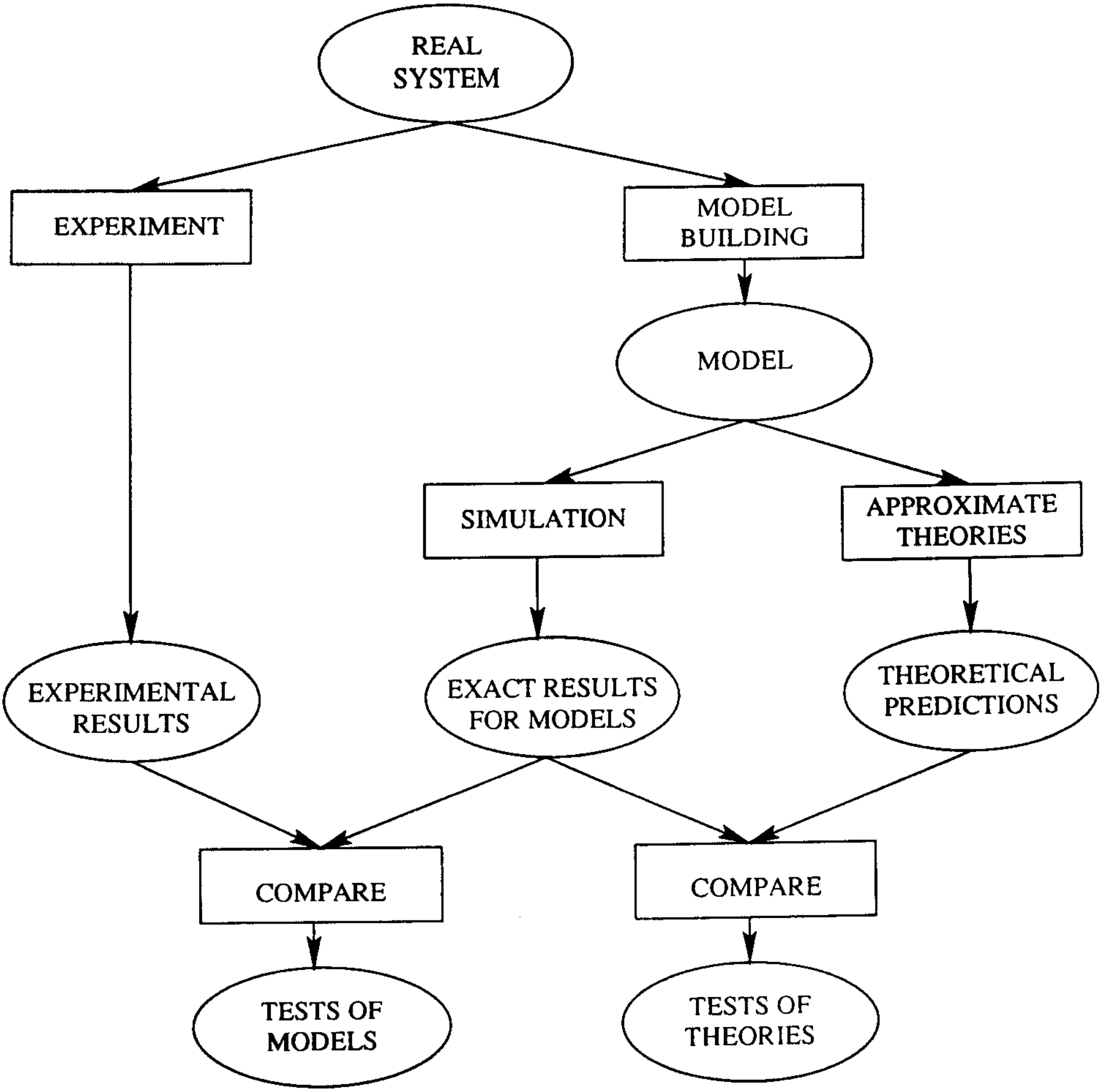
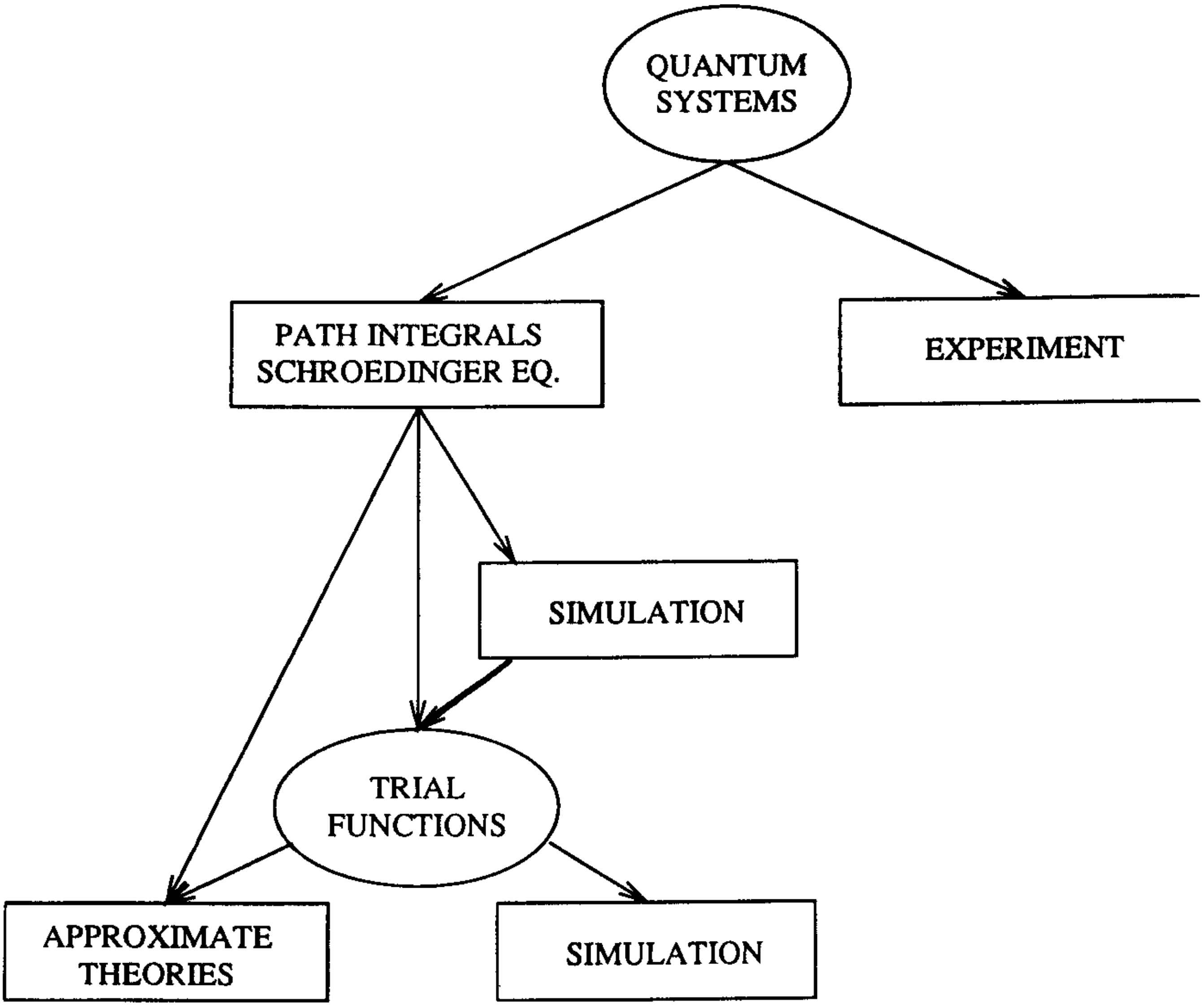
VARIATIONAL MONTE CARLO:
SHADOW WAVE FUNCTION FOR
BOSON GROUND STATE

INTERPLAY AMONG EXPERIMENT, COMPUTER SIMULATION AND THEORY



INVESTIGATIONS OF QUANTUM MANY-BODY SYSTEMS



Aims: To study quantum many-body systems from a microscopic point of view using first principles
To fully understand a given aspect of a phenomenon by analyses of results, building and refinement of models

The Monte Carlo Method

Estimate of multiple integrals

$$\theta = \int_{\Omega_0} f(x)\, \phi(x)\, dx$$

Suppose $f(x)$ a pdf $\begin{cases} f(x) \geq 0 & \forall x \\ \int_{\Omega_0} f(x)\,dx = 1 \end{cases}$

- Sample $X_1, \dots, X_M$ from $f(x)$
- To estimate θ form

$$\hat{\theta} = \frac{1}{M} \sum_{i=1}^{M} \phi(X_i)$$

- Compute

$$Var(\hat{\theta})_f = \frac{1}{M} \int (\phi(x) - \theta)^2 f(x)\, dx$$

- Precision

MC estimate of $\theta \rightarrow \mathcal{O}(M^{-1/2})$

Crude Monte Carlo

1-D $$\theta = \int_0^1 u(x)\, f(x)\, \phi(x)\, dx$$

$\Omega_0 \equiv [0,1]$

$$u(x) = \begin{cases} 1 & \text{if } 0 < x < 1 \\ 0 & \text{otherwise} \end{cases}$$

- Generate $\xi_1, \dots \xi_M$ random numbers

- Form $\hat{\theta} = \frac{1}{M} \sum f(\xi_i)\, \phi(\xi_i)$

$$\mathrm{var}(\hat{\theta})_u = \frac{1}{M} \int (f(x)\phi(x) - \theta)^2 dx$$

→ $\mathrm{Var}(\hat{\theta})_u \gg \mathrm{Var}(\hat{\theta})_f$

→ If f is chosen to make $\phi(x)$ nearly constant

Metropolis Method

- A random walk with transition K will have equilibrium distribution f iff

$$f(x) = \int K(x|y) f(y)\, dy$$

- It is reversible if

$$K(x|y) f(y) = K(y|x) f(x)$$

→ Reversibility implies that f is stationary

$$\int K(x|y) f(y) dy = \int K(y|x) f(x)\, dy$$
$$= f(x) \int K(y|x)\, dy = f(x)$$

- To sample from f
  - → Select any transition K satisfying detailed balance
  - → Run it until it has settled down to equilibrium

Generalized Metropolis Algorithm

- Choose any transition distribution $T(X|Y)$
- Sample X from $T(\cdot|Y)$
- Move from Y to X with probability

$$A(X|Y) = \min\left\{1, \frac{T(Y|X)f(X)}{T(X|Y)f(Y)}\right\}$$

- Otherwise remain at Y

$$X = \begin{cases} X & \text{if } A(X|Y) \geq \xi \\ Y & \text{otherwise} \end{cases}$$

The acceptance probability is such that detailed balance holds

$$\begin{aligned} A(X|Y)T(X|Y)f(Y) &= \min\left\{T(X|Y)f(Y), T(Y|X)f(X)\right\} \\ &= \min\left\{\frac{T(X|Y)f(Y)}{T(Y|X)f(X)}, 1\right\}T(Y|X)f(X \\ &= A(Y|X)T(Y|X)f(X) \end{aligned}$$

The equilibrium distribution is <u>unique</u>
if K is irreducible $\Longrightarrow K(X|Y) > 0$

Any initial distribution <u>converge</u> to f
if K is aperiodic $\Longrightarrow K(X|X) > 0$

A sufficient condition is to check that it is possible to move from any state to any other in some number of steps under K ($f \neq$ const.)

Advantages of Metropolis algorithm

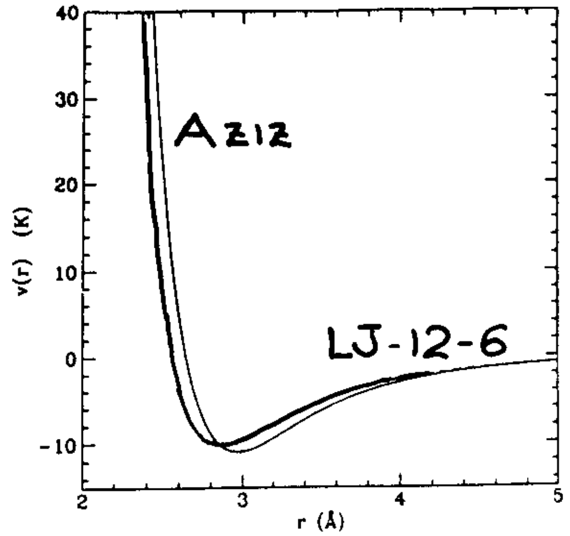
- Almost any density function f can be sampled
- No restriction in the number of dimensions

Basic Facts Concerning Helium

^{3}He	spin $\frac{1}{2}$	Fermion
^{4}He	spin 0	Boson

Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|)$$



v(r) Known from

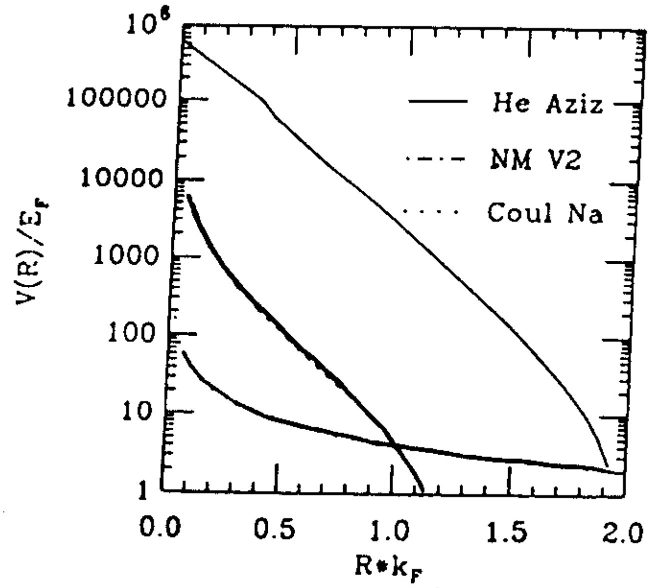
- theoretical calculation
- experiments in the gas phase

Binding Energies (K/atom)
At The Equilibrium Densities

		E_0	K	U
^{3}He	Exp.:	-2.52	12	-14
^{4}He	Exp.:	-7.14	14.5	-21.7
	GFMC:	-7.12	14.5	

Small binding energies due to cancelation betwee Kinetic and potential energie

Typical Interaction Potential For Three Different Quantum Many-Body Systems



E_F - Fermi Energy

K_F - Fermi momentum

Potential		strong-coupling
- Atomic - Nuclear	strong repulsive core	high density
- Conduction electrons	falls off very slowly at large r	low density

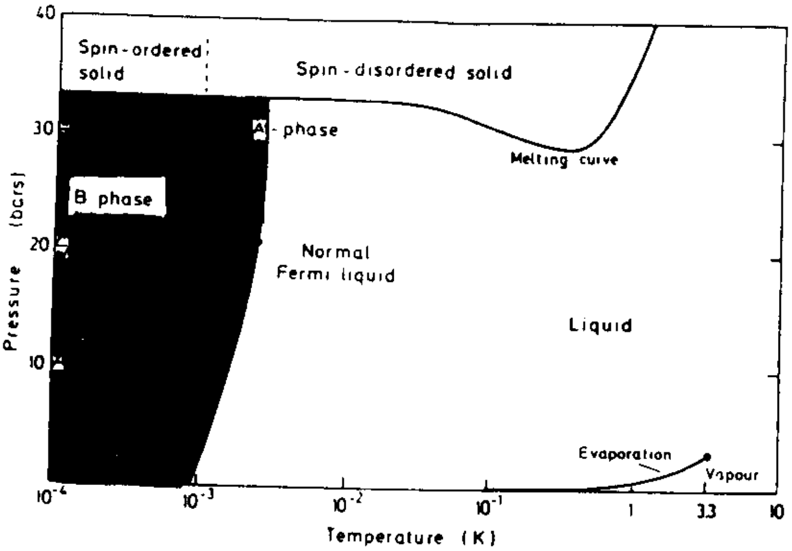
Equilibrium Density

	ρ	V_{hc}/V_{total}	effective r_c	equilibrium relative separation
NM	$0.156\ fm^{-3}$	0.7 %	0.45 fm	$4\ r_c$
^3He	$0.0166\ Å^{-3}$	7 %	2.1 Å	$1.9\ r_c$
^4He	$0.0219\ Å^{-3}$	11 %	2.1 Å	$1.7\ r_c$

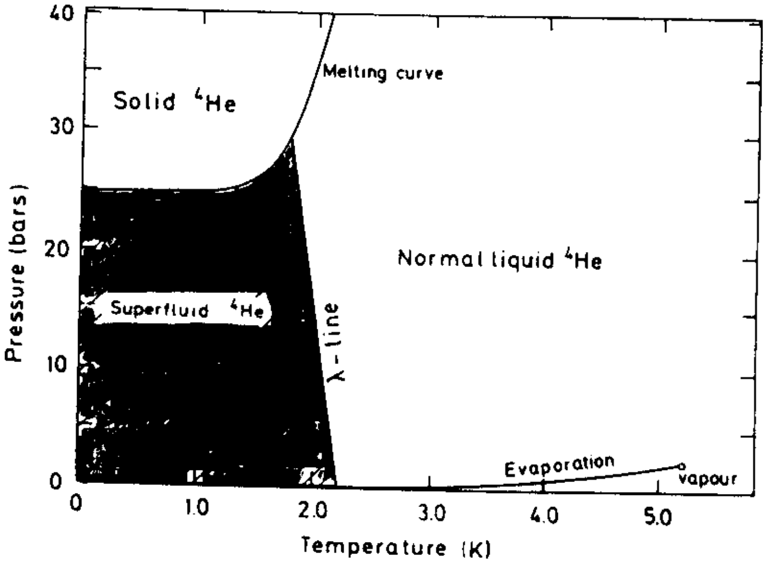
Helium liquids are far higher in density than nuclear matter

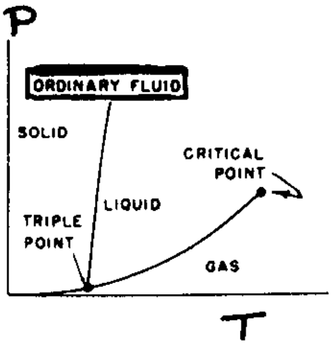
Phase Diagrams

^{3}He



^{4}He





Helium is a strongly interacting system

- The hard core repulsion dominates the interaction
- Usual perturbation theory cannot treat the particle - particle interaction
- Straightforward application of mean field theories is not possible

As consequences

- Theories for the helium systems are not simple
- We do not have a closed and compact theory
- Present theories deal only with specific aspects of these systems

Monte Carlo Methods for Quantum Many-Body Systems

→ Path Integrals [Ceperley-Pollock]

- General Principles: A random walk is used to sample the path space created by Feynman's path integrals
- Results: microscopic properties of the system at $T > 0$
- Pratical problems: Cannot yet treat exactly a Fermi system

→ Green's Function [Kalos]

- General Principles: A random walk is constructed to generate a Green's Function that transforms Schrödinger equation into an integral Eq. Than it is used to project out the ground state
- Results: microscopic properties of the system at $T = 0$
- Pratical problems: Needs importance sampling. Not yet completely developed for Fermions

Variational [McMillam]

- General Principles: A random walk is used to sample the configuration space spanned by a variational function
- Results: for the model (trial function) at $T=0$
- Aims: To develop a model of the system in order to compute its properties
- Pratical problems:
  - Leave open the exact values of the computed quantities
  - Needs parameter optimizatio
- Aditional Features
  - It is easy to understand and to program
  - Calculations an order of magnitude faster than PI or GFMC
  - Computations of ground state properties of Fermi systems can be standard
  - Excited states can be treated by appropriated trial functions
  - Different physical insights are readily tested

The Variational Principle

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geqslant E_0$$

Minimize E_T with respect to the Trial function parameters

$$E_T = \frac{\int dR \, \Psi_T^*(R) \, H \, \Psi_T(R)}{\int dR \, |\Psi_T(R)|^2} \qquad \begin{cases} dR = d^3r_1 \ldots d^3r_N \\ R \equiv \{ \mathbf{r}_i \mid i = 1, \ldots N \} \end{cases}$$

Local Energy: $E_L(R) = \dfrac{H \Psi_T(R)}{\Psi_T(R)}$

$$f(R) = \frac{|\Psi_T(R)|^2}{\int dR \, |\Psi_T(R)|^2}$$

$$E_T = \int dR \, f(R) \, E_L(R)$$

Variational Monte Carlo

- Sample $f(R)$ (usually by Metropolis)
- Form $E_M = \frac{1}{M} \sum_i^M E_L(R_i)$ $\qquad E_T = \lim E_M$
- Compute $\mathrm{Var}(E_M)$ and other properties

Bulk Quantum Liquid

The Pair Product Trial Function

$$\Psi_J(R) = \prod_{i<j} f(r_{ij})\, \phi(R)$$

Bijl - Dingle - Jastrow

The one-body model wave function

$\Phi(R) \equiv 1$ - Bose Liquid

The correlation factor

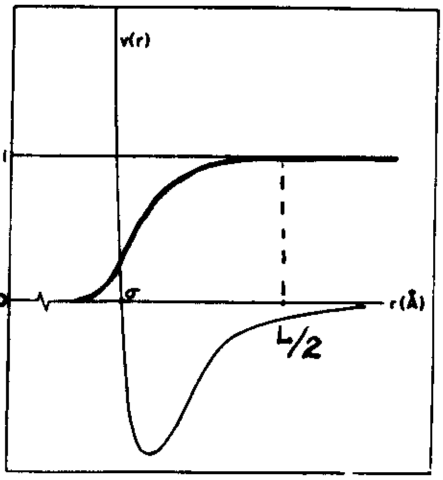
$$f(r) = e^{-\frac{1}{2}\left(\frac{b}{r}\right)^5}$$

Solution of Schrödinger Eq. at small r

$$-\frac{\hbar^2}{m}\nabla^2 f(r) + \left(V(r) - \cancel{\lambda}\right) f(r) = 0$$

$$V(r) = 4\varepsilon\left\{\left(\frac{\sigma}{r}\right)^{12} - \cancel{\left(\frac{\sigma}{r}\right)^{6}}\right\}$$

$$b = \begin{cases} \frac{16}{25}\,\frac{m}{\hbar^2}\,\varepsilon\sigma \simeq 1.13\sigma \\ 1.16\sigma \quad \text{MC minimization} \end{cases}$$



Two-particle correlation factor $f(r)$ for liquid helium.

However $f\left(\frac{L}{2}\right) = 1$, $f'(r)\big|_{r=\frac{L}{2}}$ continuos

Liquid ^{4}He

$$\Psi_J(R) = \prod_{i<j} e^{-\frac{1}{2}\left(\frac{b}{r_{ij}}\right)^5}$$

$$\left.\begin{array}{l} E_J \simeq -5.7 \,\frac{K}{\text{atom}} \\ \\ E_{exp} = -7.14 \,\frac{K}{\text{atom}} \end{array}\right\} \text{At the equilibrium density}$$

$g_J(r)$ lower tham $g_{exp}(r)$ by 5 – 10 %

The T=0 Bose fluid can be mapped onto a classical particle system

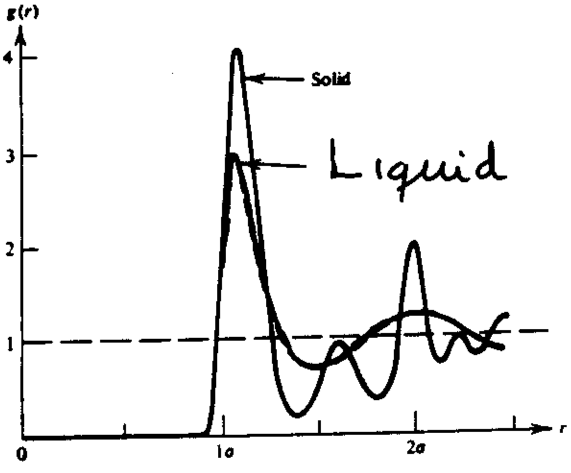
$$E_T = \frac{1}{\mathcal{N}} \int dR \; e^{-\sum_{i<j} u(r_{ij})} E_L(R)$$

$u(r) = \frac{1}{r^5}$ is the interacting potentia

$b = \frac{1}{k_B T}$ gives an effective T

Classical System

Ar

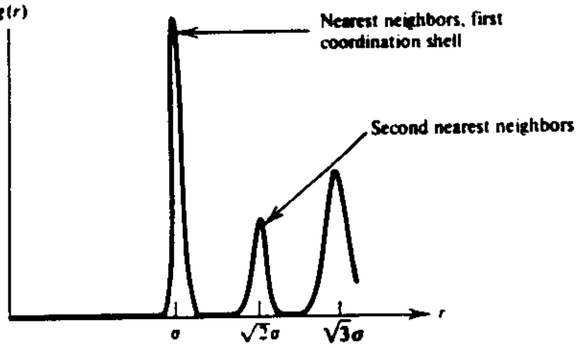


Radial distribution functions for liquid and solid argon ($\sigma = 3.4$ Å).

Solid ^{4}He

$$\Psi_J(R) = \prod_{i<j} f(r_{ij})$$

Is NOT an appropriate trial function for solid ^{4}He



Radial distribution function for a highly ordered solid.

The particles are too localized

The variational energy is too high

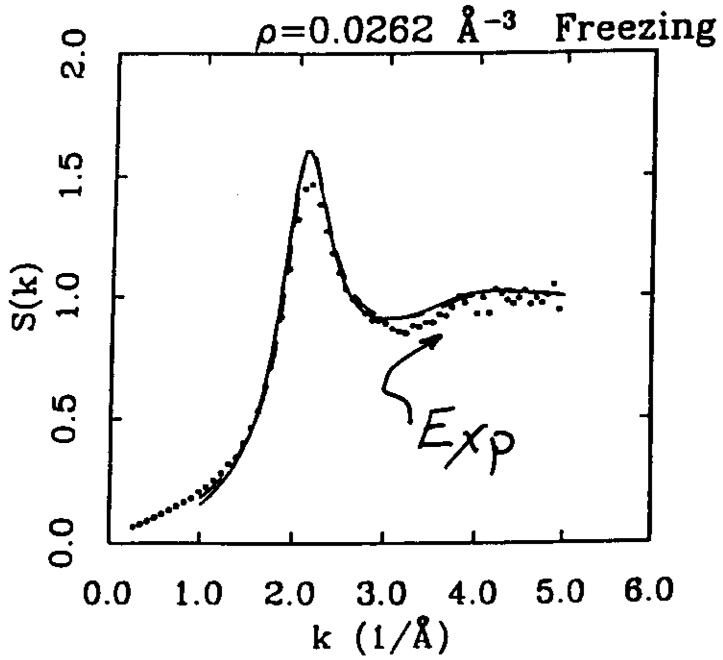
Solid ^{4}He is termed a quantum crystal
the quantum zero-point motions extend
through out the available atomic volumes

The Structure Factor

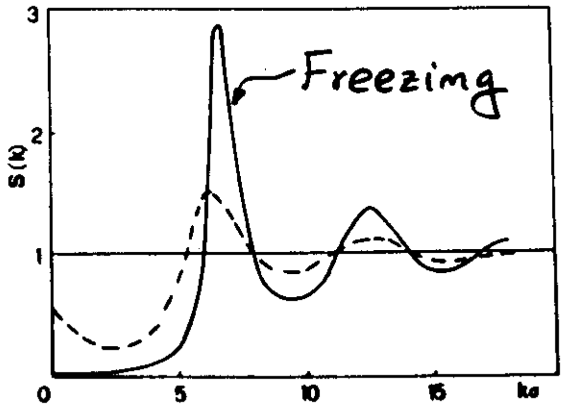
$$S(\mathbb{k}) = \frac{1}{N}\langle \rho_{\mathbb{k}}^{+} \rho_{\mathbb{k}} \rangle, \qquad \rho_{\mathbb{k}} = \sum_{j} e^{i\mathbb{k}\cdot\mathbb{r}_j}$$

density fluctuation operator

^{4}He



Classical Fluid



Solid ^{4}He Trial function

It needs to consider

- Short range collisions due to the large zero-point motion
- Large displacements from an equilibrium position

The Nosanow-Jastrow Trial Function

$$\Psi_{NJ}(R) = \prod_{i<j} f(r_{ij}) \prod_{i} e^{-\frac{c}{2}|\mathbf{r}_i - \mathbf{z}_i|^2}$$

$\mathbf{z}_i$ sites of an ad hoc lattice

- Reasonable quantitative results
- Conceptually Ψ_{NJ} is a bad choice:
  - Not symmetric under permutation of 2 particles
  - Not translational invariant
  - Does not allow exchange
  - Prevents the existence of a condensate

A Base Set Approach to Optimize Quantum Fluid and Solid Wave Functions

Jastrow Basis

$$\Psi_J(R) = \prod_{i<j} f(r_{ij})$$

- Parametrize f as

$$f(r) = \sum c_i f_i(r)$$

- $f_i(r)$ are solutions of

$$-\frac{\hbar^2}{m}\nabla^2 f_i(r) + v(r) f_i(r) = \lambda_i f_i(r)$$

$v(r)$ is the He-He interacting potenti

- $f_i(r)$ satisfy

$$f_i(L/2) = 1 \quad \text{and} \quad f_i'(r)\Big|_{r=\frac{L}{2}} = 0$$

- Motivation: To varie the functional form of $f(r)$

Three-Body Correlations

$$\Psi_T(R) = \prod_{i<j<k} f_{ijk} \prod_{i<j} f(r_{ij})$$

$$f_{ijk} = \exp\left(-\sum_{\text{cyclic}} \lambda\, \xi_{ij}\, \xi_{ik}\, \mathbf{r}_{ij}\cdot \mathbf{r}_{ik} \right)$$

$\xi(r)$ a variational function (Gaussian)

λ a parameter

Motivation: To minimize fluctuations in the local energy

$$\frac{\nabla_i^2 \Psi_J}{\Psi_J} \propto \frac{\nabla_i^2 f(r_{ij})}{f(r_{ij})} \quad \text{and} \quad \frac{\nabla_i f(r_{ij})}{f(r_{ij})} \cdot \frac{\nabla_i f(r_{ik})}{f(r_{ik})}$$

To eliminate the three-body terms: $\mathbf{r}\,\xi(r) = \nabla \log f(r$

Consequences

- Much better agreement between experience and theory
- It is not able to describe solid ^{4}He
  A product of one-body terms are still needed

Path Integrals in Imaginary Time

The density matrix at $T = 1/\beta$

$$\rho(R, R'; \beta) = \langle R | e^{-\beta H} | R' \rangle = \sum_i \phi_i^*(R)\, \phi_i(R)\, e^{-\beta E_i}$$

The average of an operator O

$$\langle O \rangle = Z^{-1} \int dR\, dR'\, \rho(R, R'; \beta) \langle R | O | R' \rangle$$

where z is the partition function

$$z = \int dR\, \rho(R, R; \beta)$$

The density matrix satisfy

$$\rho(R, R'; \beta) = \int dR_1 \cdots dR_{M-1}\, \rho(R, R_1; \tfrac{\beta}{M}) \cdots \rho(R_{M-1}, R; \tfrac{\beta}{M})$$

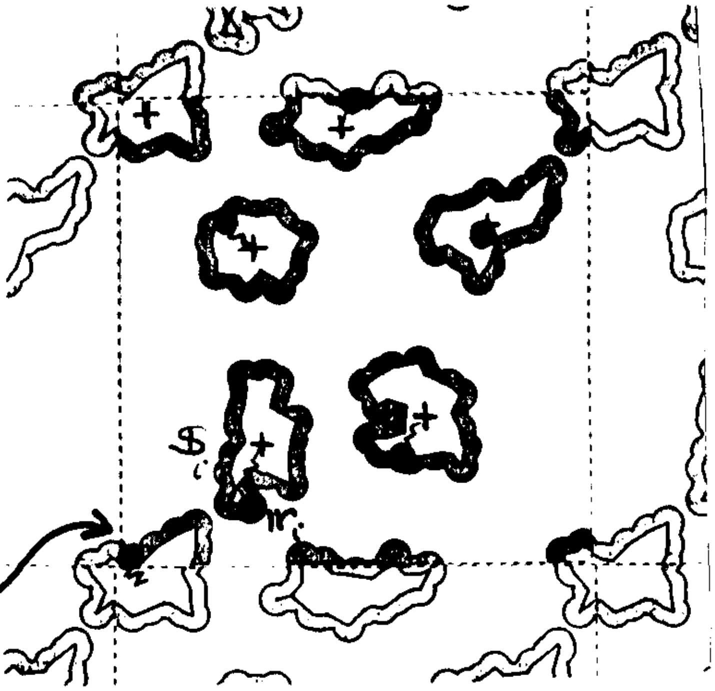
For Bosoms

$$\rho(R, R'; \beta) = \frac{1}{N!} \sum_P \rho(R, PR'; \beta)$$

The primitive approximation

$$\rho(R, R'; \beta) = e^{-\frac{\beta}{M} V(R) - c|R-R'|^2 - \frac{\beta}{M} V(R')}$$

Six He atoms in a periodic square at 2K



The shaded areas
- are points within a distance α of the beads
- indicate which points could have been visited

Markers for the (arbitrary) beginning of the path

The Shadow Wave Function Ansatz

Decompose a particle path into its
- center of massa or average position
- fluctuations about this point

Consider
- a Gaussian model for the fluctuations around the CM
- an average over the fluctuations that dresses the interactions between the centers of mass

The shadow Wave function

$$\Xi(R,S) = \exp\Big(-\sum_{i<j}\frac{1}{2}\Big(\frac{b}{r_{ij}}\Big)^5 - \sum_i c|\mathbf{r}_i - \mathbf{s}_i|^2 - \sum_{i<j}\beta v(\gamma s_{ij})\Big)$$

$$\Psi_{sh}(R) = \int dS\, \Xi(R,S) \qquad dS = d^3s_1 \cdots d^3s_N$$

b, c, β and γ are variational parameters

v is the He-He interaction potential

$S \equiv \{\mathbf{s}_i \mid i = 1, \ldots, N\}$ is isomorphic to coordinates of particles interacting pair-wise throught βv

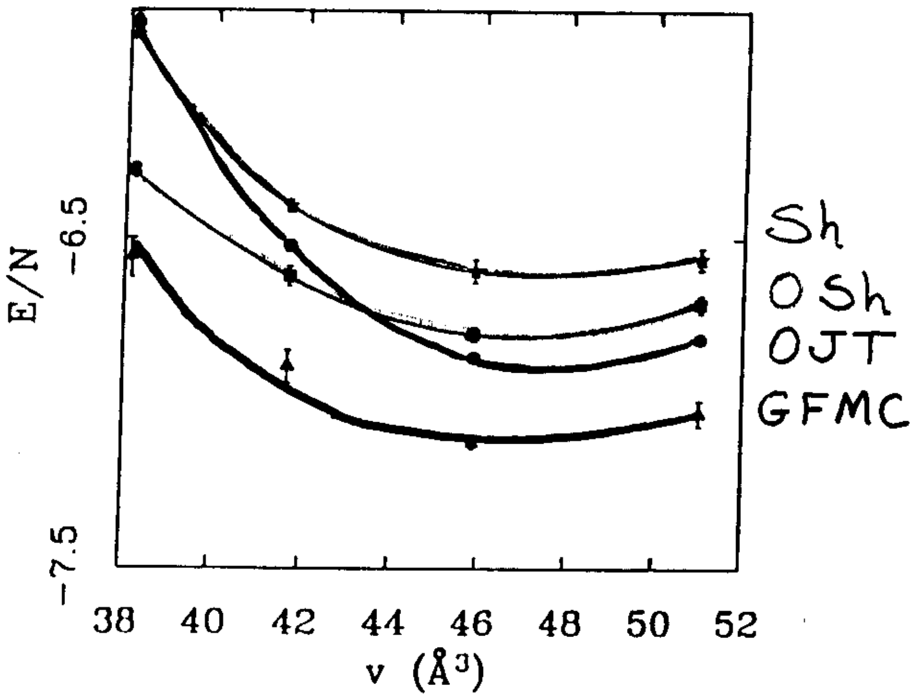
$$\left.\begin{array}{l}\text{zero-point motion}\\ \text{hard core}\end{array}\right\}\ \begin{array}{l}\text{quantum hole or}\\ \text{SHADOW PARTICLE}\end{array}$$

Consequences

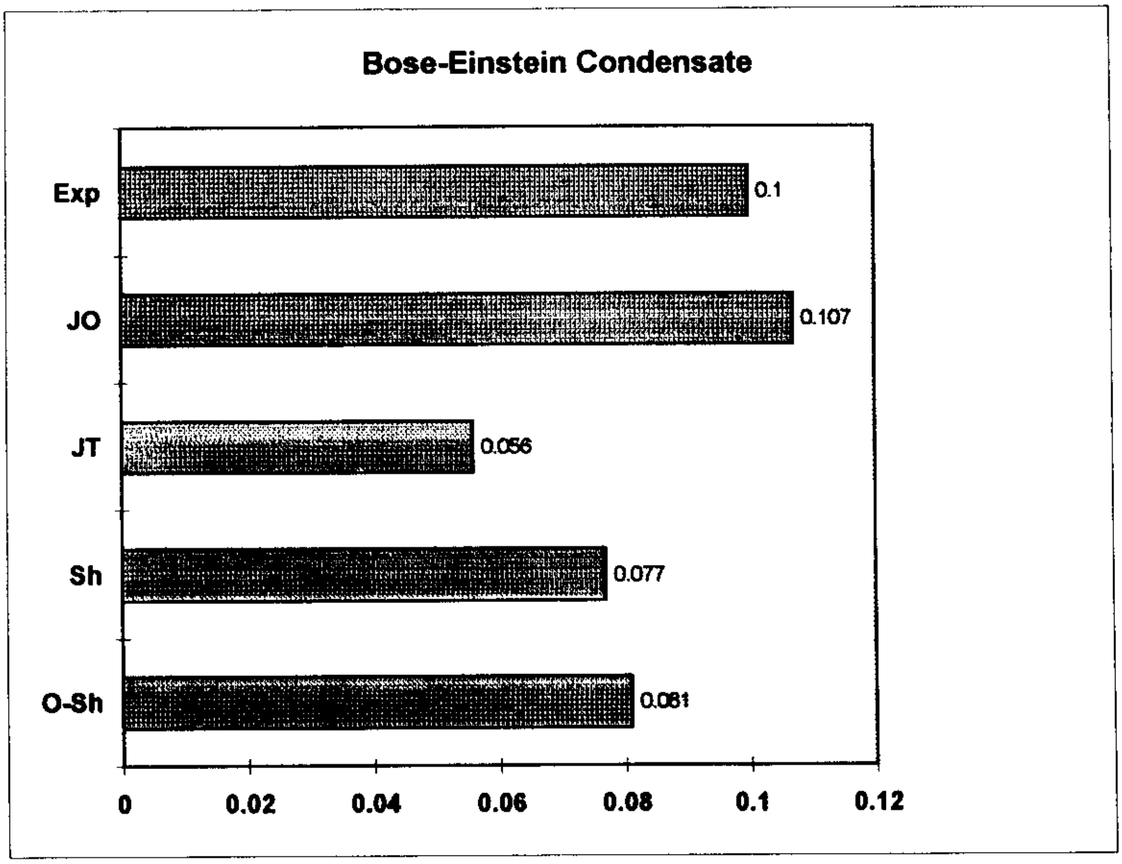
- Correlations due to the quantum delocalization ("polymer - polymer")
- Correlations of arbitrary order in the number of particles

  - Ψ_{sh} is one of the possible Feemberg representation

Ground State Energies for Liquid ^{4}He



High order correlations become increasely important as the density grows



The condensate fraction

The fraction of particles occupying the $\mathbb{k}=0$ state

$$\rho_1(r) = \left\langle \frac{\Psi_T(\mathbb{r}_1, \dots, \mathbb{r}_i + \mathbb{r}, \dots \mathbb{r}_N)}{\Psi_T(\mathbb{r}_1, \dots, \mathbb{r}_i, \dots \mathbb{r}_N)} \right\rangle$$

$$n_0 = \lim_{r \to \infty} \rho_1(r)$$

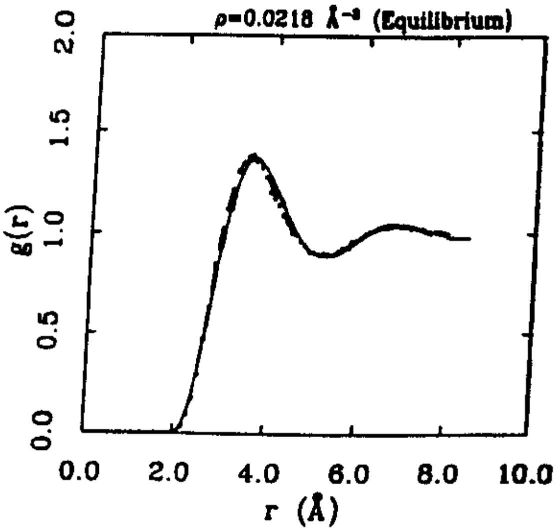
The Radial Distribution Function

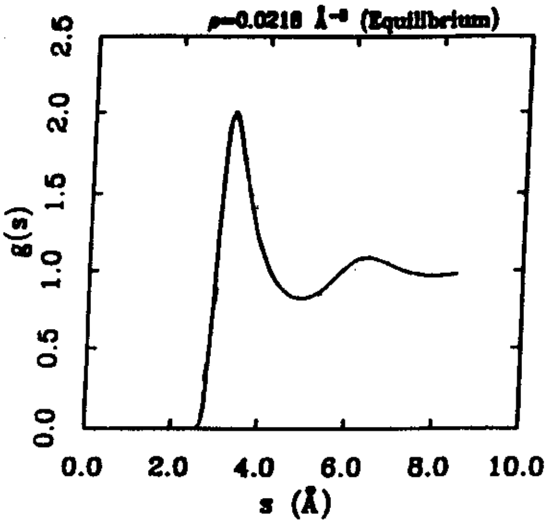
$$g(r) = \frac{1}{N\rho} \sum_{i \neq j} \langle \delta(|\mathbf{r}_i - \mathbf{r}_j - \mathbf{r}|) \rangle$$

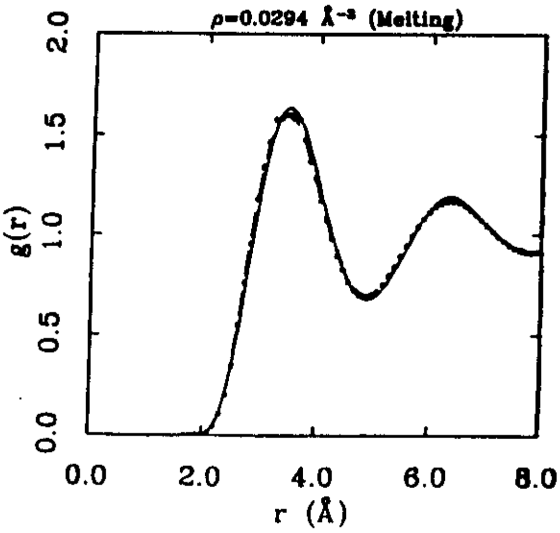
Particles

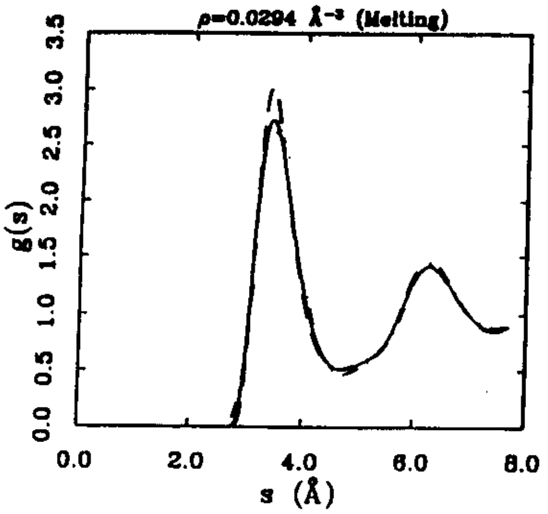
Shadows

^{4}He



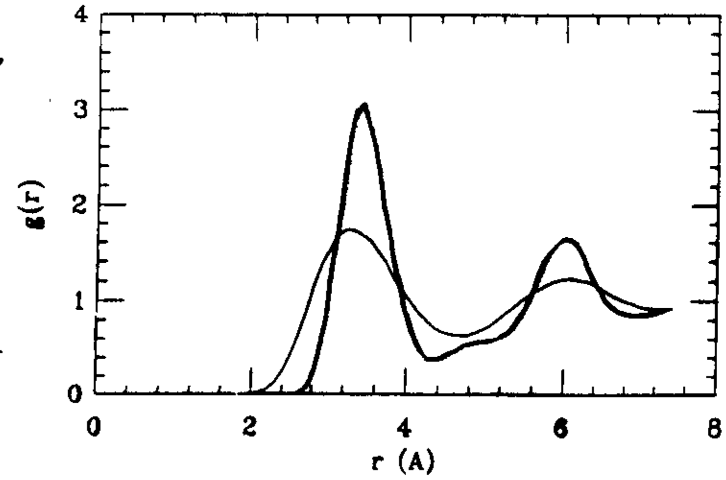






High density solid ^{4}He

Long-range order imposed through the shadows



Shadow correlations are somewhat closer to those of a classical system

Lindemann Ratio

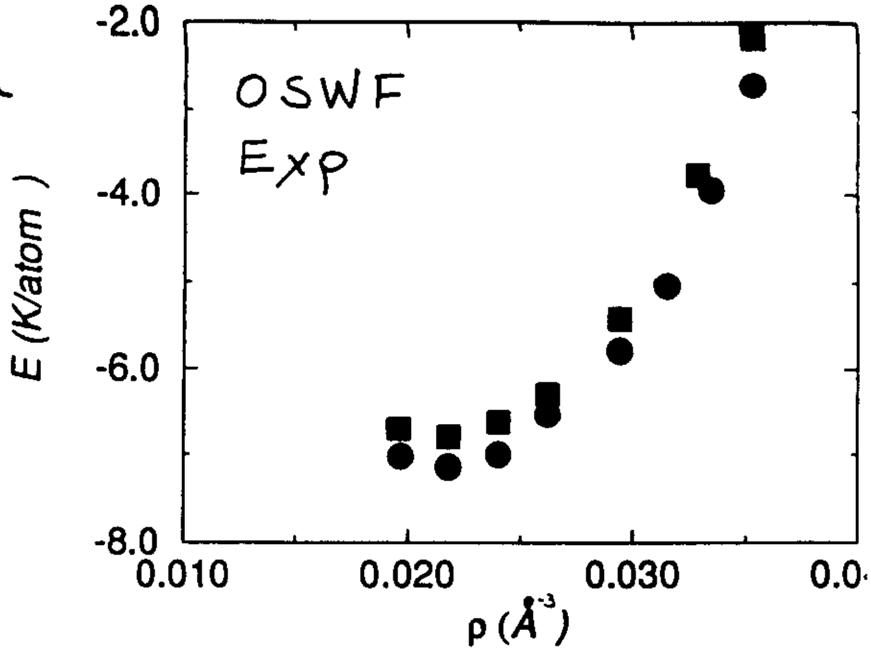
$$\gamma = \frac{\sqrt{\langle |\mathbf{r}_i - \bar{\mathbf{r}}_i| \rangle}}{d}$$

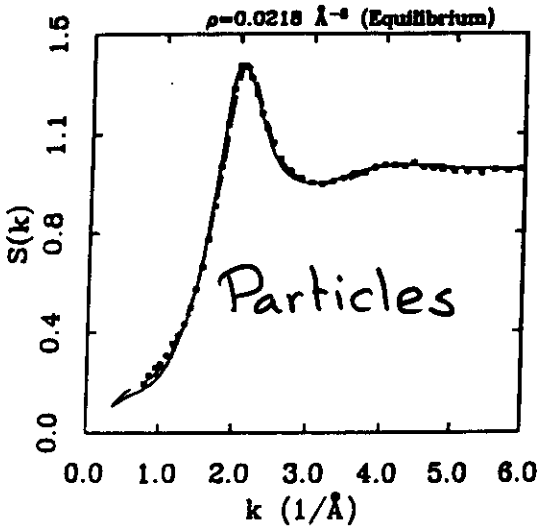
Melting

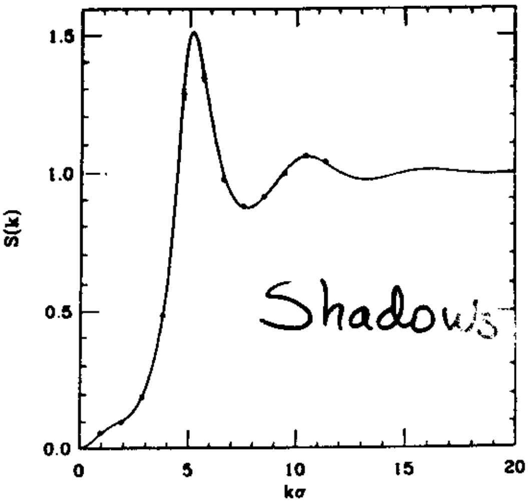
Particles	Shadows	Classical LJ
0.26	0.15	0.14

Shadow Wave Function Results

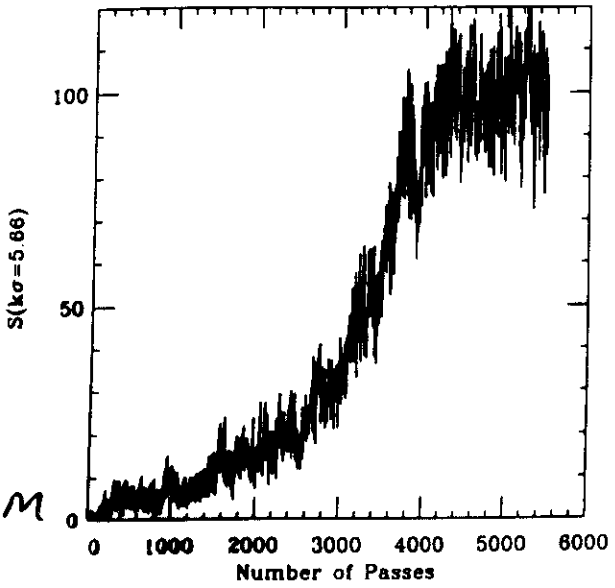
Liquid and Solid phases of ^{4}He







Particles



Shadow Wave Function a single functional form for the liquid and solid phases

⟹ Crystalization of a liquid-like configuration

Crystalization

Classical Liquid

$$f(R) \propto e^{-\beta \sum_{i<j} V(r_{ij})}$$

steric comstraints

$\Rightarrow$ pair interaction

$\Rightarrow$ crystalization

Quantum Liquid

$$f(R) \propto |\Psi(R)|^2$$

zero point motion

$$\Rightarrow \left\{ \begin{array}{l} \text{pair} \\ \text{three-body} \end{array} \right\} \text{interaction.}$$

are NOT emought to describe crystalization

$\Rightarrow$ high order correlations

$\Rightarrow$ crystalization

Inhomogeneous systems: ^{4}He droplets

The shadow wave approach

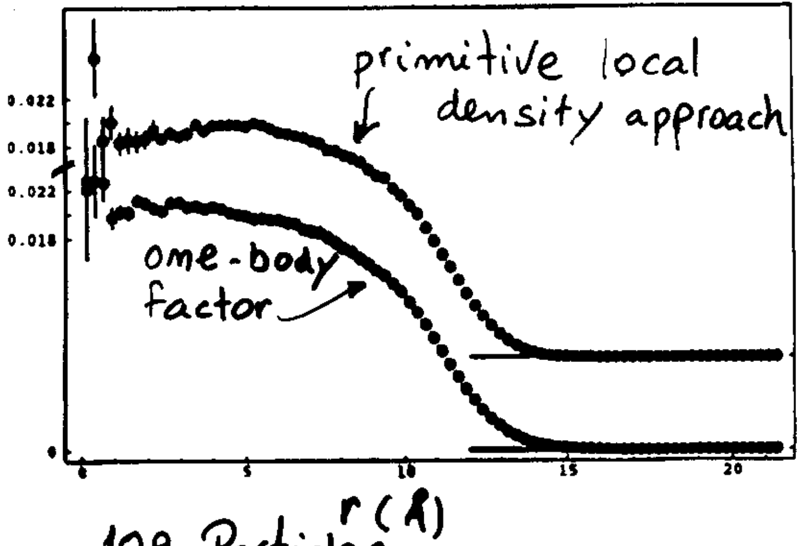
- To allow particle modulations in a flexible way
- To study self-bound clusters

How?

Modify the shadow-shadow interaction to reflect the varying local density in the system

N	Ψ_{sh}	JT
20	-1.61	-1.57
108	-3.43	-3.47

Density Profile



108 Particles

Variational Path Integrals

$$|\Psi_{PI}|^2 = \Psi_J^*(R_{-M})\, e^{-\sum_i S(R_{i-1}, R_i; \frac{\beta}{M})}\, \Psi_J(R_M)$$

- Improves a resonable trial function by projecting out the ground state
- Any number of links might be used

Comparison with the Shadow Wave Function

- Ψ_{sh} is a model of the system with a physical insight
- It is not only projecting out the ground state (An attractive pseudopotential is used for the shadow variables)

Why use a Shadow Wave Function?

- To model the crystalization of a quantum many-body system
- To understand quantitative differences between theory and experiment
- To impose particle modulations in a very flexible way

Conclusions

The Shadow Wave Function

- Introduces quantum delocalization of the particles explicitly in a variational description
- Describes the crystalline order as a spontaneously broken symmetry
- Allows the investigation of self-bound states of inhomogeneous systems
- A simple way of introducing high-order correlations