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"Shadow wave function calculations for solid 3He"

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SHADOW WAVE FUNCTION CALCULATIONS FOR SOLID ^3He

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OUTLINE

- G.S. PROPERTIES OF SOLID ^3He
- Shadow wave functions for ^3He
- ShSB results for solid ^3He
- FSWF and preliminary results
- Comparison with experiments : where is the problem ?
- Conclusions

GROUND STATE PROPERTIES OF SOLID ^{3}He

LOW PRESSURE PHASE: ($v < 20\ \mathrm{cm}^3/\mathrm{mol}$)

- structure is b.c.c.
- anarmonicity is dominant
- For $T < 1\,\mathrm{mK}$ magnetically ordered (LFP or u2d2)

HIGH PRESSURE PHASE: ($v > 20\ \mathrm{cm}^3/\mathrm{mol}$)

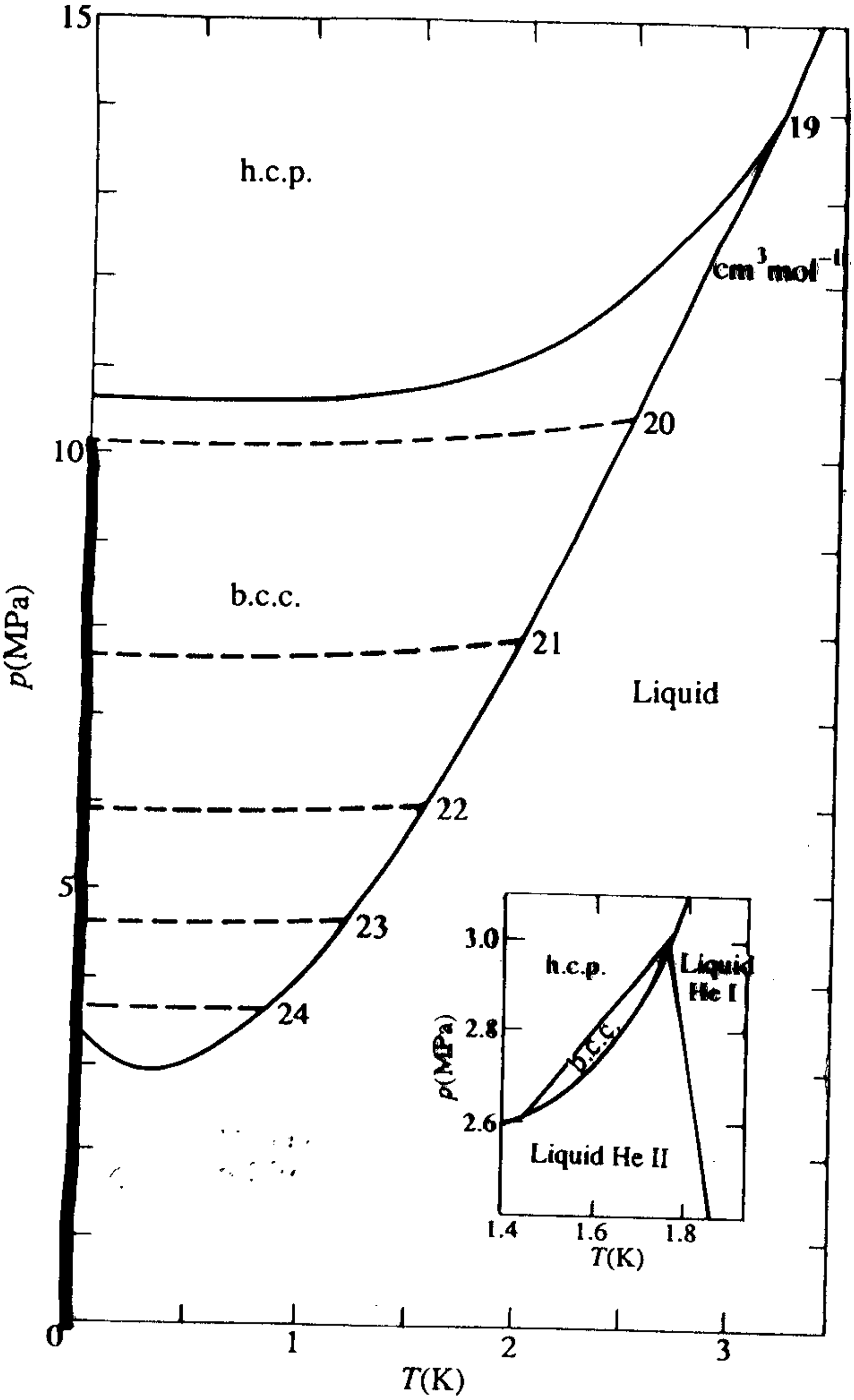
- structure is h.c.p. (as low density ^{4}He)
- [illegible] ?

MEASUREMENTS

- LPP: R.C. Pandorf, D.O. Edwards PR 169, 222 (1968)
- HPP: J.W. Stewart PR 129, 1950 (1963)

Magnetic phase diagram:

- D.D. Osheroff, Physica 109 & 110B, 1461 (1982)
- Y.H. Tang, E.D. Adams, K. Uhlig, PRL 57, 222 (1986)
- A. Sawada, H. Yano, M. Kato, K. Iwahashi, Y. Masuda, PRL 56, 1587 (1986)


15
10
5
0
p(MPa)
1
2
3
T(K)
h.c.p.
b.c.c.
Liquid
cm³mol⁻¹
19
20
21
22
23
24
3.0
2.8
2.6
p(MPa)
1.4
1.6
1.8
T(K)
h.c.p.
b.c.c.
Liquid He I
Liquid He II

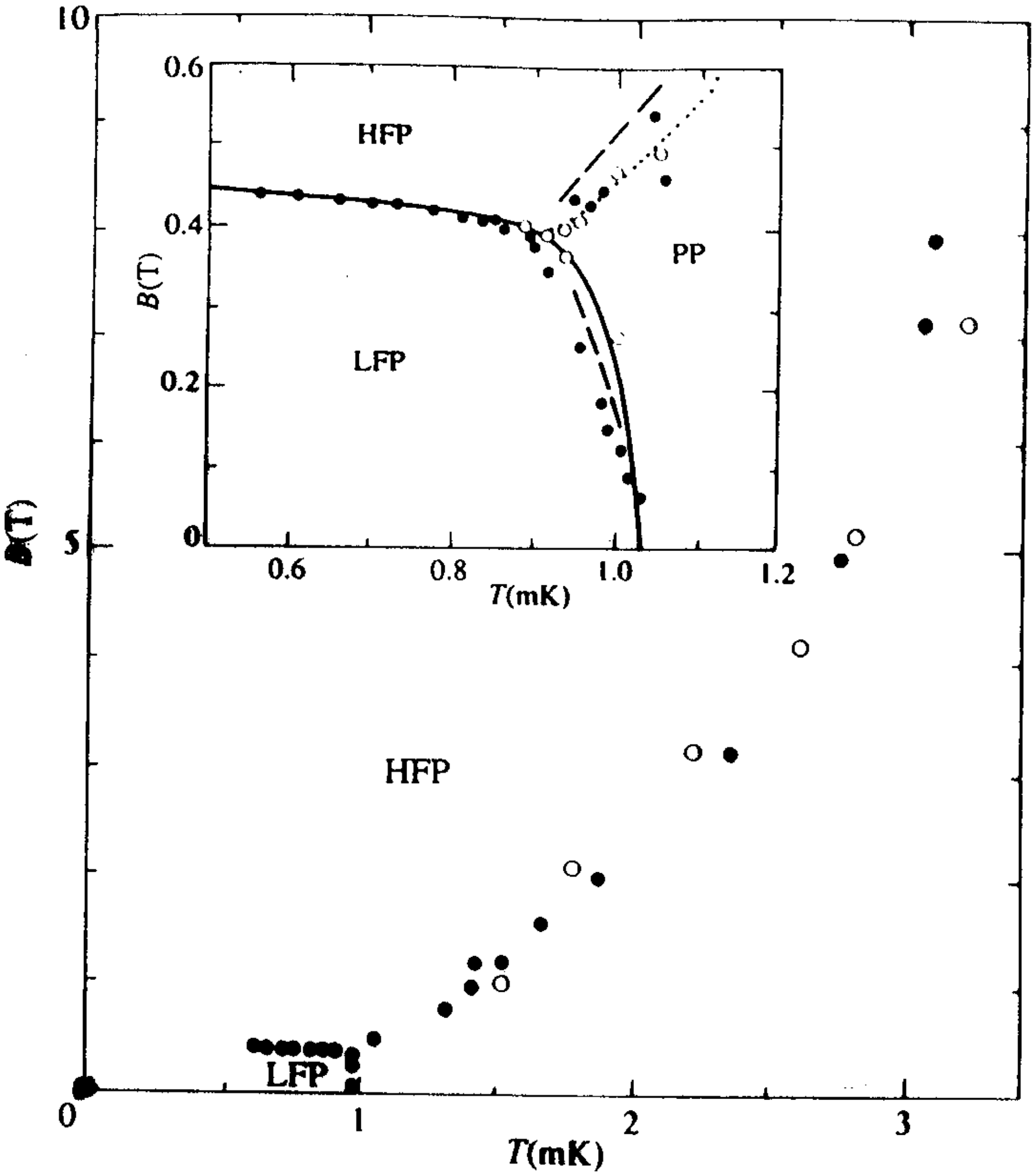


Fig. 5.8 The magnetic phase diagram of b.c.c. ^{3}He of molar volume 24.15 cm^3 from the measurements of (●) its nuclear magnetic heat capacity by Sawada *et al.* (1986) and (○) the melting curve in a range of magnetic fields by Godfrin *et al.* (1980). Inset: Details of the phase diagram at melting pressure measured by: (●) Osheroff (1982) from NMR data; (○) and dotted line, Tang *et al.* (1986) from high-resolution pressure data; broken line from Kummer *et al.* (1975). The transitions to the low-field antiferromagnetic phase (LFP) from either the paramagnetic phase (PP) or the high-field phase (HFP) are first order, but the transitions from the PP to HFP phases are not first-order (after Sawada *et al.* 1986; Tang *et al.* 1986).

THEORIES FOR SOLID ^{3}He

- Most of the theories for the ground state of solid ^{3}He are based on the variational approach.

Nosanow (1966)

Guess a solution for the many body Schrödinger equation:

$$\hat{H}\,\psi(\bar{r}_1 \ldots \bar{r}_N) = \mathcal{E}\,\psi(\bar{r}_1 \ldots \bar{r}_N)$$

in the form:

$$\psi_0 = \psi_H \psi_J$$

$$\psi_H(\bar{r}_1 \ldots \bar{r}_N) = \prod \phi(|\bar{u}_i|) \qquad u_i = \bar{r}_i - \bar{R}_i \qquad \{R_i\} \text{ is a lattice}$$

$$\phi(r) = \exp(-A r^2/2)$$

$$\psi_J = \prod_{i<j} f(|\bar{r}_{ij}|) \qquad f(r) = \exp[-b/r^5],$$

the function contains several parameters which are fixed according to the variational principle

$$E_v = \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} \geq \mathcal{E}$$

and the equality holds only if ψ_0 is the true ground state of the system. Several improvements to this simple scheme have been carried out (Holian, 1978, Locke, 1984, Svorstøl and Østgaard, 1986)

MAGNETIC PROPERTIES OF SOLID ^3He

Roger et al. (1983)

Exchange of 3 and 4 atoms are major processes to determine magnetic phases.

Exchange Hamiltonian:

$$\mathcal{H}_{ex} = -J_{nn} \sum_{\langle i,j \rangle} P^{\sigma}_{ij} + J_t \sum_{\langle i,j,k \rangle} \{ P^{\sigma}_{ijk} + (P^{\sigma}_{ijk})^{-1} \} -$$
$$- K_F \sum_{\langle i,j,k,l \rangle}^{F} \{ P^{\sigma}_{ijkl} + (P^{\sigma}_{ijkl})^{-1} \} - K_P \sum_{\langle ijkl \rangle}^{P} \{ P^{\sigma}_{ijkl} + (P^{\sigma}_{ijkl})^{-1} \}$$

K_F and K_P account for 4 particles ring exchanges

A model with only $J_t = -0.1$ mK and $K_P = -0.385$ mK is sufficient to describe the low field pf -> U2D2 transition.

In 1987 Ceperley and Jacucci developed a Path Integral Monte Carlo scheme to evaluate exchange frequencies. They have computed all the coefficients in $\mathcal{H}_{ex}$ plus six-spin exchange and next nearest neighbours. A model with J_t and K_P only appears to be justified (other terms are about 1/10 in magnitude)

Phenomenology of solid ^{3}He is extremely rich, involving several different magnetic and structural phases.

REQUIREMENTS FOR A COMPLETE MICROSCOPIC THEORY OF SOLID ^{3}He

1) IN ORDER TO ACCOUNT FOR MAGNETIC PROPERTIES ANTISYMMETRY OF THE WAVE FUNCTION MUST BE PRESERVED
(Most variational theories actually deal with "mass 3 bosons" and not with ^{3}He !
Good for g.s. energy but for nothing else...)

2) NO LATTICE HAS TO BE FIXED "A PRIORI"
(b.c.c. -> h.c.p)

3) LIQUID-SOLID PHASE TRANSITION SHOULD OCCUR IN A SPONTANEOUS WAY WITH THE CORRECT STRUCTURE
(what does He crystal remember of the liquid state ?)

VARIATIONAL CALCULATIONS FOR ^3He

NB: $T = 0$!

Several variational calculations for normal ^{3}He in the liquid phase are already present. The trial wave function used are usually of the form:

$$\Psi_T(\{r\}) = D^{\uparrow} D^{\downarrow} F(\vec{r}_1 \ldots \vec{r}_N)$$

where D is a Slater determinant of suitable single particle wave functions (we have one determinant for the spin up and one for the spin down particles), and F is a bosonic wave function expressing the usual two body (Jastrow) and three body (triplet) correlations.

Results for the variational energy obtained with such a wave function are as good as the analogous results in ^{4}He. Here following we report some results at equilibrium density ($\rho\sigma^3 = 0.273, \sigma = 2.556$Å)

Ψ_T	$E_0 \pm \Delta E_0$
Jastrow – Slater	-1.08 ± 0.03
JS+Triplet	-1.61 ± 0.03
JS+backflow	-1.55 ± 0.04
JS+T+B	-1.91 ± 0.03
Experiment	-2.47 ± 0.01

The situation for the mycroscopic description of the solid phase is still highly unsatisfactory.

SHADOW WAVE FUNCTION FOR ^{3}He

A shadow wave function is a sophisticated variational ansatz for the solution of the m.b. Schrödinger equation.

$$\psi_0(\vec{r}_1 \dots \vec{r}_N) = \phi_R(\vec{r}_1 \dots \vec{r}_N) \int k(S,R)\, \phi_S(\vec{s}_1 \dots \vec{s}_N)$$

$$\underbrace{S = \{\vec{s}_1 \cdots \vec{s}_N\}}_{\text{AUXILIARY VARIABLES}} \qquad \underbrace{R = \{\vec{r}_1 \cdots \vec{r}_N\}}_{\text{PARTICLES COORDINATES}}$$

The antisymmetry in ψ_0 can be enforced in two ways:

1) Making $\phi_R(\vec{r}_1 \dots \vec{r}_N)$ antisymmetric

2) Making $\phi_S(\vec{s}_1 \dots \vec{s}_N)$ antisymmetric

Both pictures have some advantages and drawbacks, although the choice #2 revealed to be definitely superior.

We use the following acronyms:

#1 : ShSB [Shadows - Slater - Backflow]

#2 : FSWF [Fermionic Shadow Wave Function]

The SHADOW-SLATER-BACKFLOW WAVE F.

(F.P. et al, PRB 76, 15162 (1996)

The explicit form of ShSB is the following

$$\psi_0(\vec{r}_1 \dots \vec{r}_N) = e^{-\sum_{i<j}(b/r_{ij})^5} \mathcal{A} \prod_{\substack{i \le i \le N \\ k \le k_F}} \phi_k(i) \times$$

$$\times \int e^{-C(\vec{r}_i - \vec{s}_i)^2} \, e^{-\sum_{i<j} U_s(s_{ij})}$$

where:

$$\phi_k(i) = \exp\left[i\vec{k} \cdot \left(\vec{r}_i + \lambda_B \sum_{\ell \ne i} \eta(r_{i\ell}) \vec{r}_{i\ell} \right) \right] \xi(i)$$

where $\eta(r)$ is a function accounting for the backflow correlations and $\xi(i)$ is the spin state. The antisymmetric product above is written as:

$$\phi(R) = \{ \det{}_\uparrow(\phi_k(i)) \det{}_\downarrow(\phi_k(j)) \mid i = 1 \dots N/2, \, j = 1 \dots N/2, \, k \in k_F \}$$

The shadow-shadow correlation pseudopotential is given by

$$U_s(s_{j\ell}) = U_s^{\uparrow\uparrow}(s_{j\ell}) \frac{1 + \sigma_z(i)\sigma_z(j)}{2} + U_s^{\uparrow\downarrow}(s_{j\ell}) \frac{1 - \sigma_z(i)\sigma_z(j)}{2}$$

and

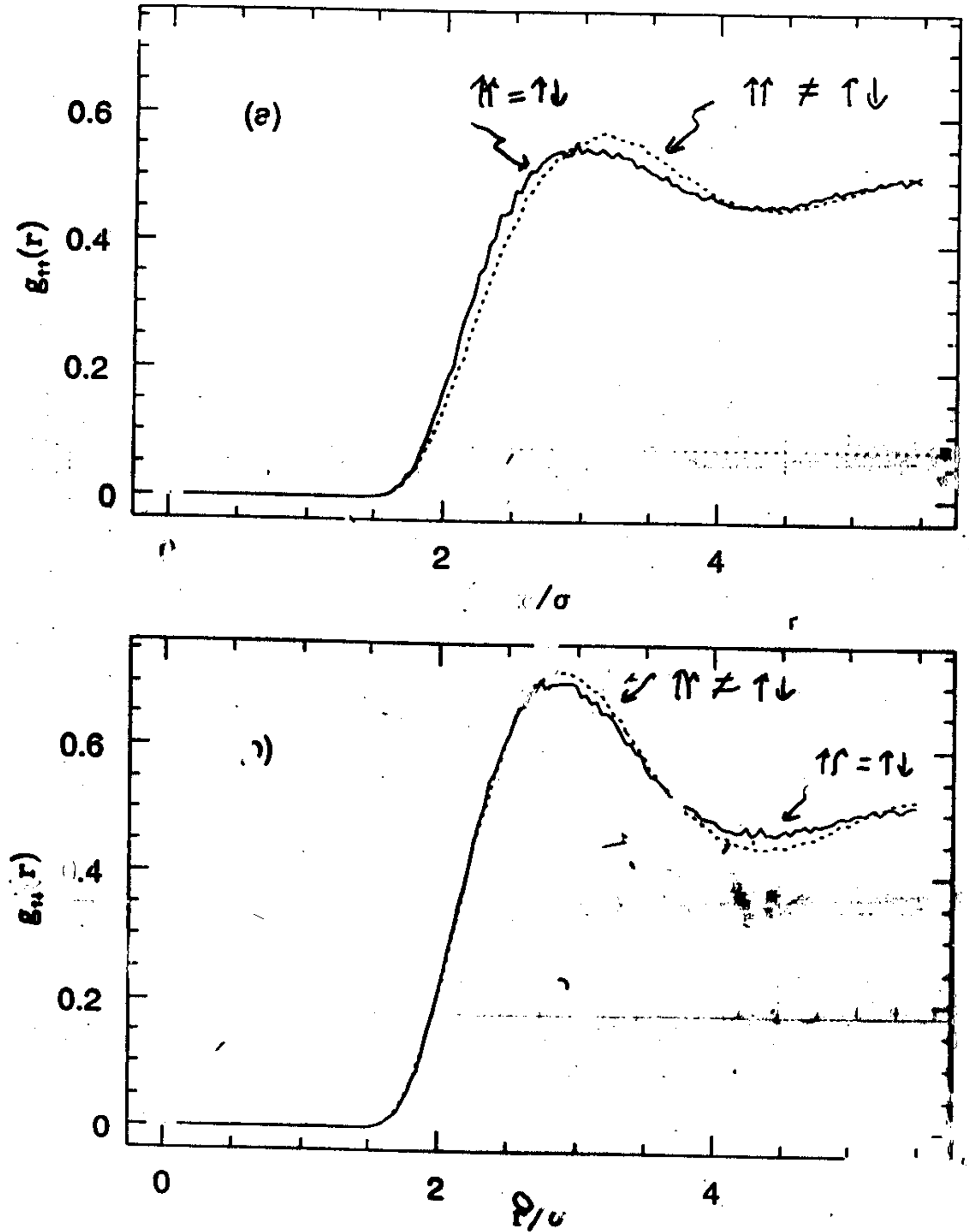
$$U_s^\sigma(s) = \delta^\sigma V(\alpha^\sigma s)$$

where $V(r)$ is the interatomic potential (namely Aziz I)

PAIR d. f.

$$g_{\uparrow\uparrow,\uparrow\downarrow}(r) = \frac{1}{N\rho}\left\langle \sum_{i,j}^{i\neq j} \frac{1\pm\sigma_z(i)\sigma_z(j)}{2}\,\delta(r_{ij}-r)\right\rangle$$

LIQUID PHASE, EQUILIBRIUM DENSITY, N = 54



$< E > /N\ (K)$	$< T >\ (K)$	wave function
-1.821 ± 0.029	11.881 ± 0.040	ShSB
-1.08 ± 0.03	—	JS[12]
-1.55 ± 0.04	—	JSB[12]
-1.91 ± 0.03	—	(J+T)SB[12]
-2.163 ± 0.006	12.271 ± 0.008	OJOTB[19]
-2.37 ± 0.01	—	DMC[19]

TABLE III. Total and kinetic energy at equilibrium density $\rho\sigma^3 = 0.273$ for different functional forms of the trial wave function. Calculations from Ref. 21 were done at $\rho\sigma^3 = 0.277$.

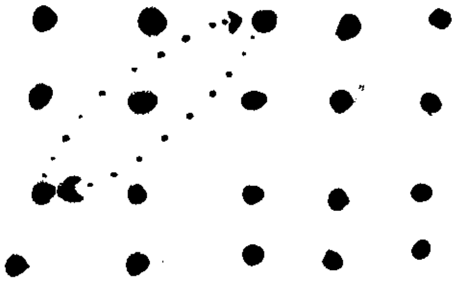
$\rho\sigma^3$	wave function	$\langle E\rangle/N(K)$	$\langle T\rangle(K)$	O_G (particles)	O_G (shadows)
0.427	ShSB–NAF	0.955±0.033	25.826±0.065	0.291	0.391
	ShSB+exchange	2.057±0.039	25.912±0.069	0.274	0.592
0.440	ShSB–NAF	1.382±0.023	26.511±0.047	0.496	0.785
	ShSB+exchange	2.405±0.042	26.952±0.076	0.426	0.679

TABLE IV. Total energy and kinetic energy per particle at two densities in the solid phase for different functional forms of the trial wave functions. The value of the order parameter proper for the liquid phase is $\simeq 0.136$.

"EXCHANGE" MOVES

In an ordinary MC simulation with SWT exchange of atoms in a crystal, although possible in principle, is extremely rare.

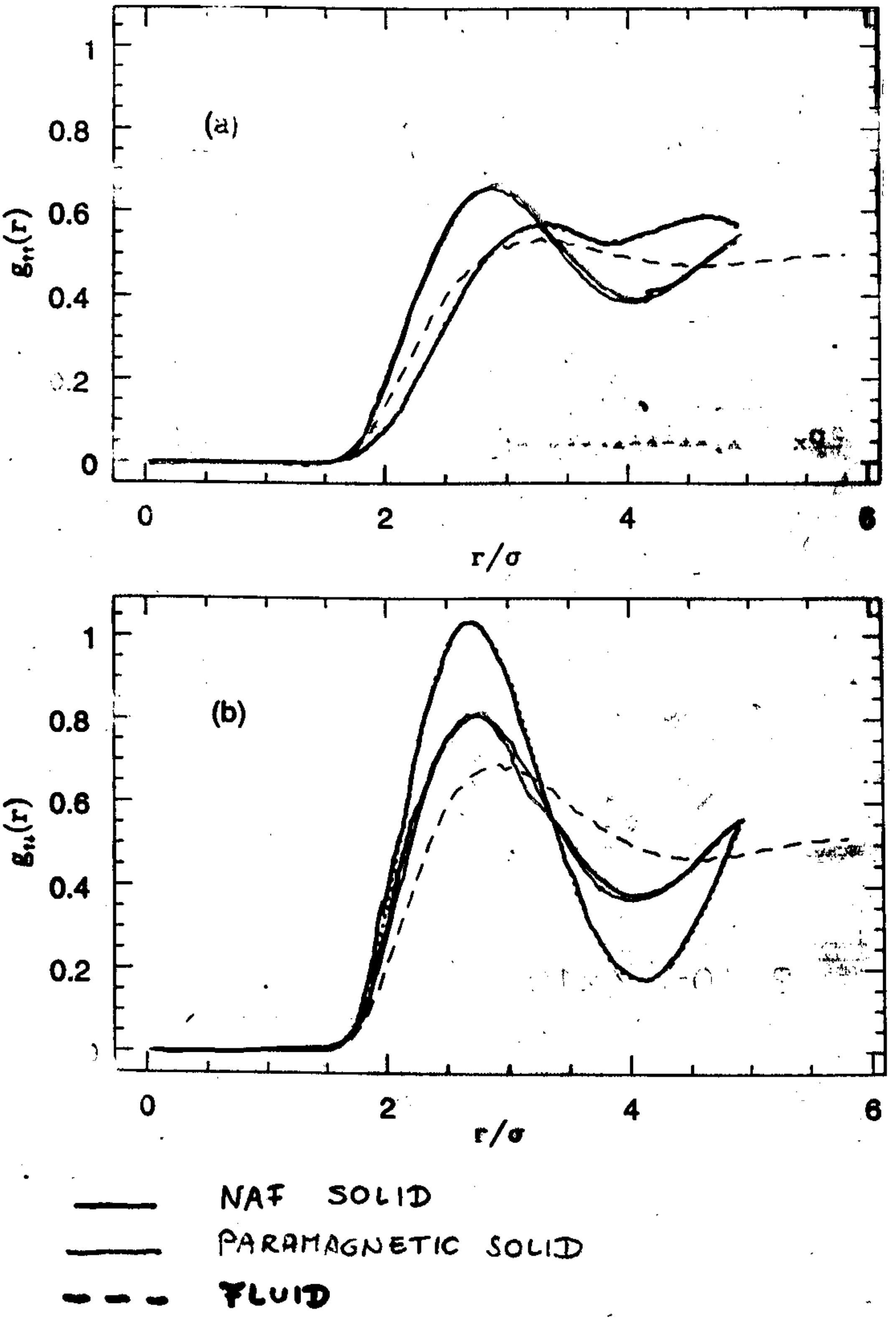
In order to improve the speed of convergence we can introduce "exchange trial moves"



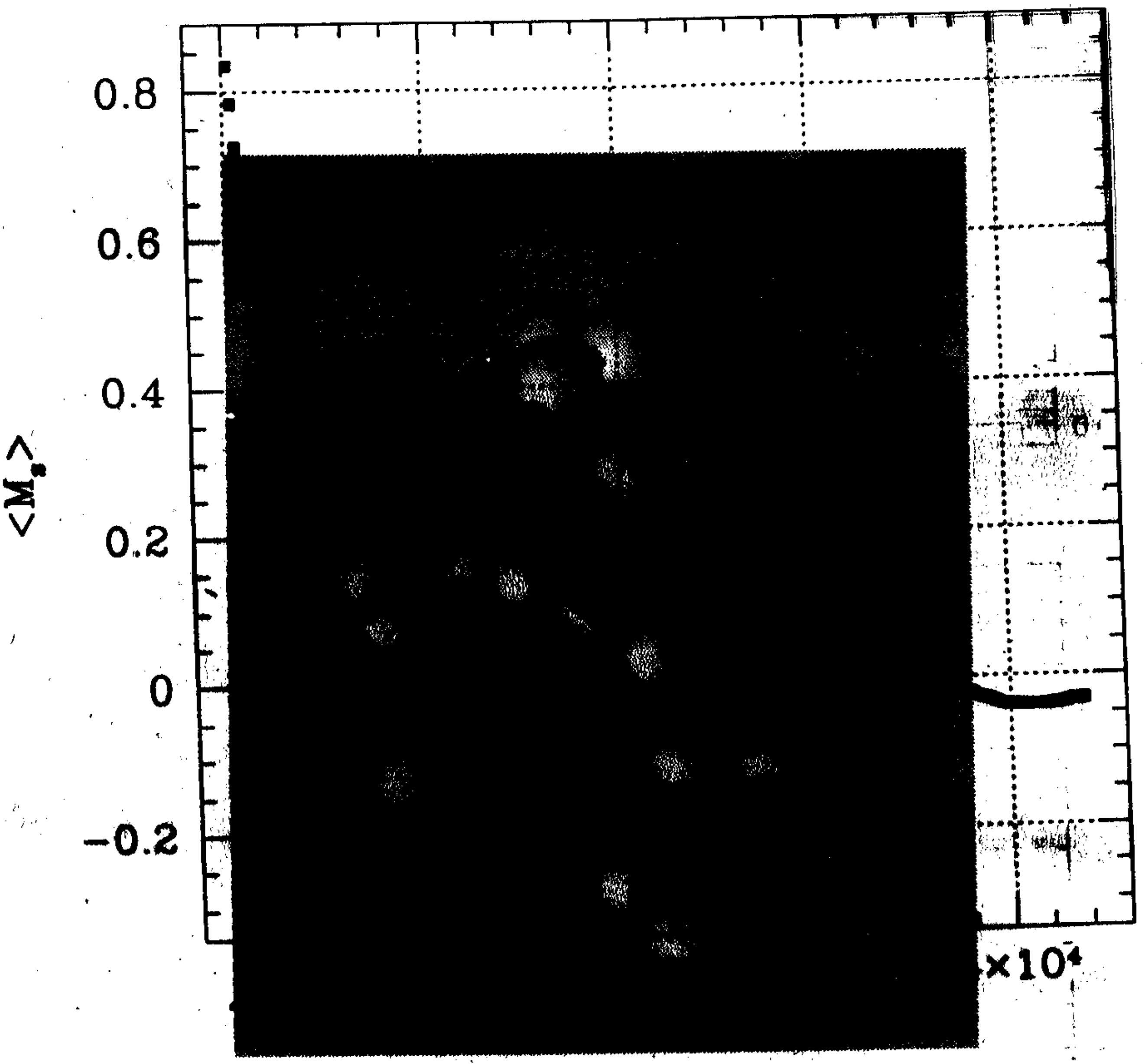
The atoms have different spin assignment and are chosen at random

The acceptance rate of e.m. is about 10%.

PAIR DISTRIBUTION FUNCTION

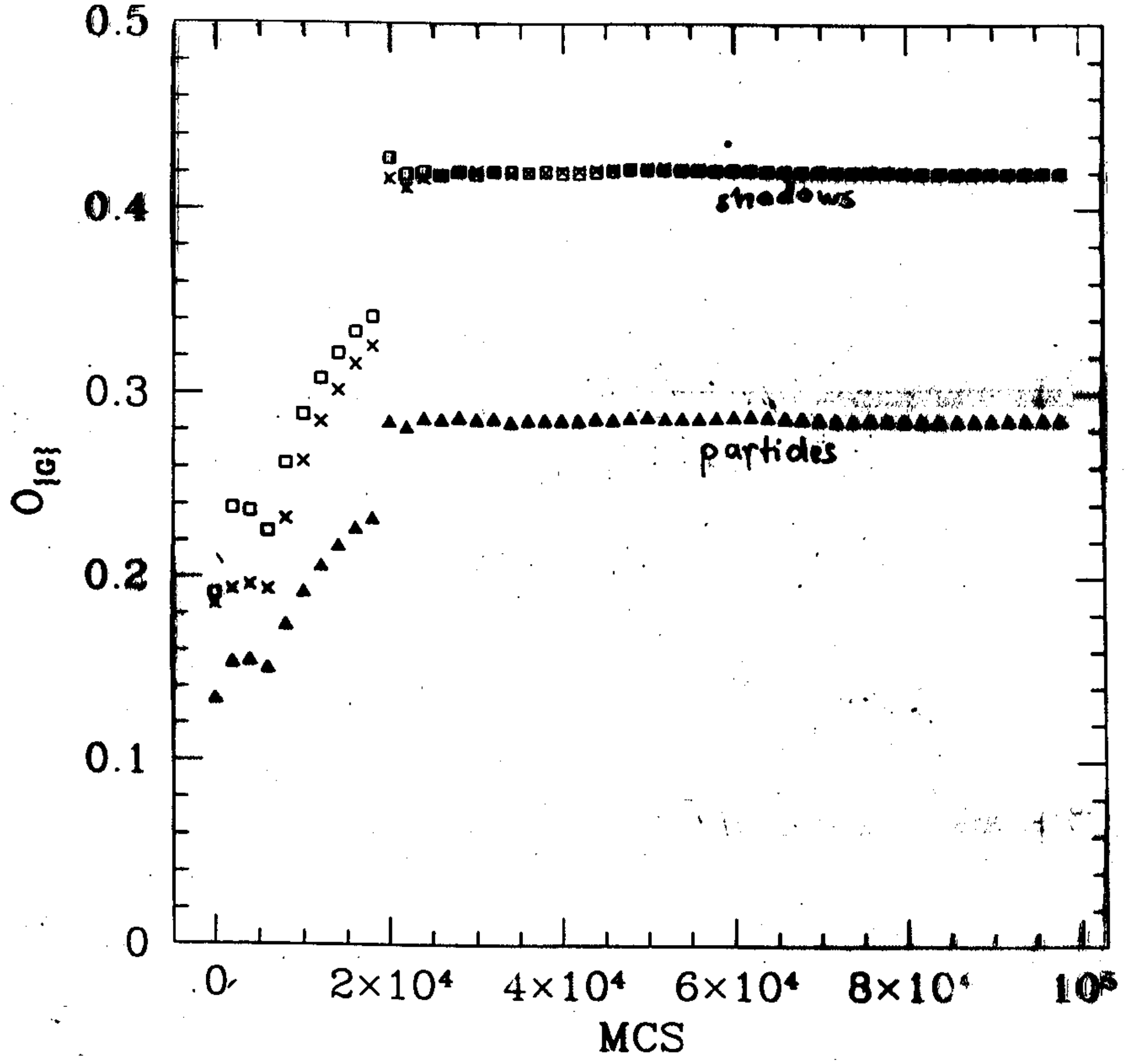


STAGGERED MAGNETIZATION



RYSTALLIZATION

54 particles, density $\rho\sigma^3 = 0.427$



$$O_{\{\vec{G}\}} = \frac{1}{m_{\{\vec{G}\}} N} \left\langle \sum_m \sum_{i=1}^{N} \left| e^{i \vec{G}_m \cdot \hat{r}_i} \right| \right\rangle$$

$$O_{\{\vec{G}\}} = \begin{cases} \sim 1/\sqrt{N} & \text{in the fluid} \\ \gg 1/\sqrt{N} & \text{in the solid} \end{cases}$$

SHADOW · SLATER · BACKFLOW WF

GOOD NEWS:

- PROVIDES A REASONABLE DESCRIPTION OF THE FLUID PHASE
- STABLE b.c.c. ORDER AT HIGH DENSITY

BAD NEWS:

- ENERGY / PARTICLE IN THE SOLID PHASE is TOO HIGH
- ENERGY FOR DIFFERENT MAGNETIC STATES (e.g NAF, PARAMAGNET) TOO DIFFERENT: transitions occur at temperatures of the order of mK

Remark: the nodal structure does not change with the phase, i.e. we have the same nodes in the liquid and in the solid. This is clearly a drawback.

FERMIONIC SHADOW WAVE FUNCTION

M.H. Kalos, L. Reatto 1995

The FSWF can be written as:

$$\psi(R) = \prod_{i<j} f(r_{ij}) \int dS \prod_{\ell} e^{-C(\vec{r}_\ell - \vec{s}_\ell)^2} \times$$

$$\times \prod_{m<n} f_{sh}(s_{mn}) \;\det\left(e^{i\vec{k}_\alpha \cdot \vec{s}_\beta}\right)$$

where the $\vec{k}_\alpha$ vectors are filling the Fermi sea. In the case of an unpolarized fluid the determinant is replaced with the product of two determinants, one per spin orientation.

SOME FACTS: [Demonstrations in : M.H. Kalos, L. Reatto in "Progress in comp. phys. of matter", ed. by L. Reatto and F. Manghi, World Scientific 1995]

- The FSWF has the correct antisymmetry properties for the real degrees of freedom

- Backflow effects are implicitely introduced at any order

- In the case of localization of the particles the nodal structure changes into that of a determinant of gaussians

- FSWF can be justified in terms of projecting the g.s. out of a SS wave function

AVERAGES OF OPERATORS WITH FSWF

As in the case of SWF for bosons, the average of a local operator becomes an integral over three sets of variables, R, S, S'

$$\langle O \rangle = \frac{\int dR\, dS\, dS'\, \Pi(R,S,S')\, O(R)}{\int \Pi(R,S,S')\, dR\, dS\, dS'}$$

where:

$$\Pi(R,S,S') = \left[\prod_{i<j} f(r_{ij})\right]^2 \prod_{\ell} e^{-C(\vec{r}_\ell - \vec{s}_\ell)^2 - C(\vec{r}_\ell - \vec{s}\,'_\ell)^2} \times$$

$$\times \prod_{m<n} f_{sh}(S_{mn}) \prod_{m'<n'} f_{sh}(S'_{m'n'}) \det\left(\underline{e}^{i\vec{k}_\alpha\cdot\vec{s}_\beta}\right) \det\left(\underline{e}^{i\vec{k}_\alpha\cdot\vec{s}\,'_\beta}\right)$$

WE CANNOT USE $\Pi(R,S,S') / \int dR\, dS\, dS'\, \Pi(R,S,S')$ AS PROBABILITY DISTRIBUTION TO SAMPLE BECAUSE <u>IT IS NOT POSITIVE DEFINITE</u>

ONE CAN ALWAYS USE $|\Pi(R,S,S')|$ GIVING THEN A POSITIVE OR NEGATIVE WEIGHT TO THE EVALUATED ESTIMATOR

$$\langle O \rangle = \frac{\sum_i w_i O_i}{\sum_i w_i} \qquad w_i = \pm 1$$

Although we must have $\sum_i w_i > 0$ (because $|\psi|^2 > 0$) the plus and minus signs come out to be nearly equally probable in the sampling, at least in the fluid phase.

$$\Downarrow$$

EXTREMELY LOW SIGNAL/NOISE RATIO

The difficulty of the problem depends on the number of particles:

- 14-body problem [fluid] : FEASIBLE
- 38-body problem [fluid] : HARD BUT SOLVED
- 54-body problem :
  - [fluid] : NOT FEASIBLE YET
  - [solid] : FEASIBLE
- N-body problem : ?

In order to improve the signal-to-noise ratio better and better sampling techniques are needed.

THE FSWF HAS BEEN PROVED TO BE SUPERIOR TO STANDARD VARIATIONAL FUNCTIONS:

LIQUID: (equilibrium density)

FSWF (38 body)	E/N = −2.05 ± 0.07
JS	−1.08 ± 0.03
JS + T + B	−1.91 ± 0.03
OJBTB	−2.09 ± 0.01
ShSB	−1.81 ± 0.01

NO OPTIMIZATION WAS POSSIBLE: IN ORDER TO OBTAIN THE ERROR QUOTED WE NEEDED A RUN OF > 10^8 MCS, ABOUT 1000 CPU hours on THE CTC IBM-SP2

SOLID: ($\rho\sigma^3 = 0.427$, close to melting)

bcc. NAF phase:

	E/N
FSWF	0.72 ± 0.01
ShSB	0.95 ± 0.03

For non NAF configurations preliminary indications are for a reduced difference in energy with FSWF with respect to ShSB.

b.cc. non-NAF phase:

	E/N
FSWF	0.873 ± 0.10
ShSB	2.057 ± 0.04

SUM OVER PERMUTATIONS

M.H. Kalos, F.P. 1995

PERMUTATION OF SHADOWS LEAVE THE WAVE FUNCTION UNCHANGED BUT FOR THE SIGN.

OBSERVATION:

THE SUM OVER ALL POSSIBLE PERMUTATIONS OF SHADOWS HAS AS: LEADING TERMS CONTRIBUTIONS WITH APPROXIMATELY THE SAME MAGNITUDE, BUT OPPOSITE SIGN. IF WE PERFORM ANALITICALLY THIS SUM WE CAN DECREASE THE NOISE

The original observation was made analyzing a simple one dimensional problem.

THE ANALITYC SUM OVER PERMUTATIONS CAN BE WRITTEN IN TERMS OF AN ADDITIONAL DETERMINANT FOR THE PARTICLE-SHADOW TERM

$$\psi(R) = \prod_{i<j} f(r_{ij}) \int dS \, \det\left(e^{-C(\vec{r}_\alpha - \vec{s}_\beta)^2}\right) \times$$

$$\times \prod_{m,n} f_{sh}(s_{mn}) \det\left(e^{-i\vec{k}_\alpha \cdot \vec{s}_\beta}\right)$$

ONE CAN DEMONSTRATE THAT THIS TERM IS EQUIVALENT TO THE ORIGINAL ONE

NOTES:

- Antisymmetry in the real degrees of freedom appears explicitely
- For the unpolarized system we need to compute 8 Slater determinants at each move
- For the same number of steps the error halves ⇒ gains a factor 4 in speed.

COMPARISON WITH EXPERIMENTS

FACT 1: All the theories for ^{3}He (both liquid and solid are approximate.
Nevertheless variational theories seem to work better in the fluid phase. Moreover DMC-TE evaluations of the binding energy starting from optimized wf. are very close to the experimental value.

In the solid we have only variational estimates. The discrepancy with the experimental value is huge (> 1.5 K) (at least in the b.c.c. phase).

FACT 2: An estimate with DMC of the binding energy for MASS 3 BOSONS (i.e. a lower bound) gives a number which is still about 1k HIGHER THAN THE EXP. VALUE IN bcc PHASE.

THIS IS AN OPEN PROBLEM:
APPARENTLY, WE HAVE NO RELIABLE MICROSCOPIC THEORIES FOR bcc ^{3}He

Several hypoteses can be done, but we have no definite answers yet. (WORK IS IN PROGRESS)

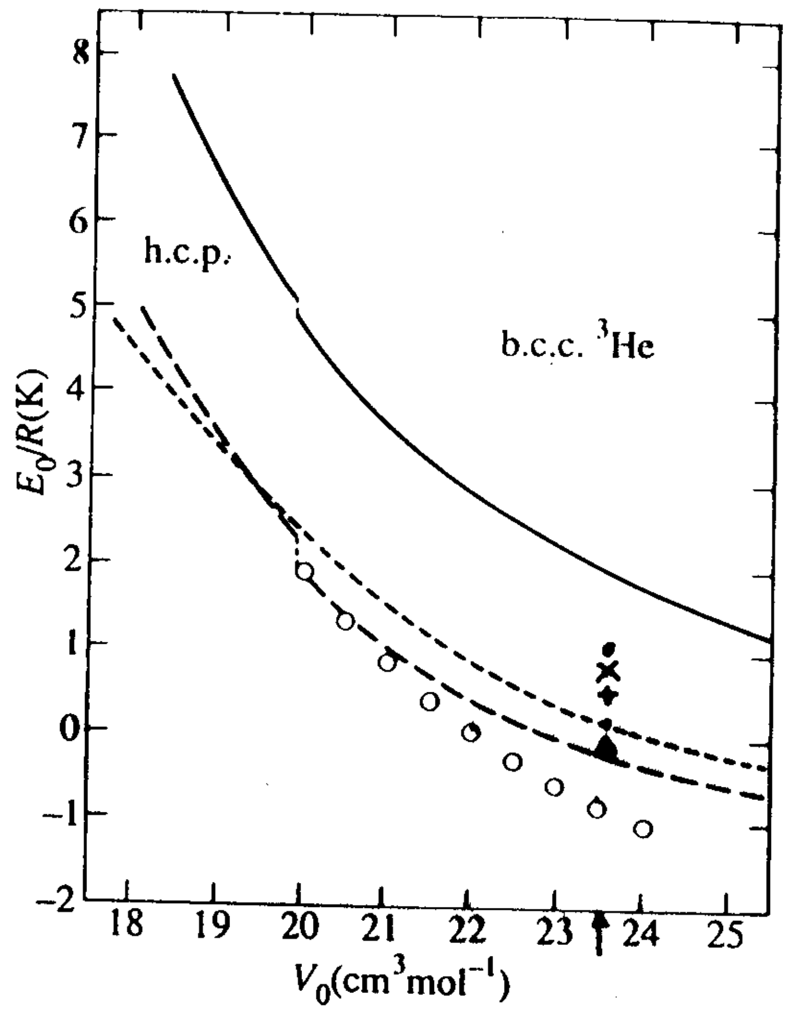


Fig. 3.10 Ground-state energy of b.c.c. ^{3}He: experimental data are Pandorf and Edwards (1968) compared with the LOCV calculations of Svorstøl and Østgaard (1986), using the ESMMSV (solid line) and FDD1 (broken line) potentials, and the Gaussian model (dotted line) of Locke (1984) with a Lennard-Jones (12, 6) potential. The LOCV calculations also show the phase transition to h.c.p. (see Fig. 2.3).

● Jastrow-Nosanow Optimized

× ShSB

+ FSWF

▲ DMC (mass 3 bosons)

CONCLUSIONS (?)

- SHADOW WAVE FUNCTIONS CAN BE SUCCESSFULLY APPLIED ALSO FOR FERMIONIC SYSTEMS
- ShSB PROVIDES A STABLE SOLID PHASE WITH bcc ORDER
- FSWF IS SUPERIOR TO PREVIOUS VARIATIONAL ANSATZS. BINDING ENERGY IMPROVES WITH RESPECT TO ShSB
- COMPARISON WITH EXPERIMENTS IS STILL POOR. APPARENTLY, WE MISS SOME IMPORTANT ASPECT WHICH CANNOT BE DESCRIBED BY THE USUAL THEORIES