FIG. 10. Single-particle distribution function $R(r)$ vs particle displacement from equilibrium for solid ^{4}He at various volumes.

this result illustrates the importance of pair correlations at all pressures but it is worth emphasizing that approximate approaches such as the Heitler-London method and the Domb-Salter approximation also properly account for these correlations at high pressures. With increasing density, the dependence of the energy upon the parameter β becomes increasingly weak. That is, the energy minimum with respect to β forms a very shallow well. Hydrogen, for example, has an energy minimum at 9 cm^3/mole for $\beta \approx 150$. However, for $\beta = 100$, the energy is less than 1% greater than the minimum value. The physical implications of this result are not fully understood. Because of this relatively weak dependence of the energy on β, the minimizing values of β listed in the tables are not very accurate at the higher pressures.

An important approximation in the dynamic-field method is the cutoff of products of two-body-correlation functions $f(r_{ij})$. The products retained in

$G(\vec{r}_\lambda, \vec{r}_\kappa)$ are the correlations of molecules λ and κ to their first-, second-, and third-nearest neighbors. The functions f outside this range are replaced by unity. Some idea of the effect of this approximation can be seen in Table VI where $\langle T \rangle$, $\langle V \rangle$, and E_0 are presented for a typical ^{4}He calculation of 21.6 cm^3/mole. These results are displayed as a function of the number of nearest-neighbor shells contained in the product of pair-correlation functions $f(r_{ij})$. As can be seen from the table, these results converge quickly even though the $f(r)$ used in this study are fairly long ranged. Most of the results for H$_2$ were obtained with a second-nearest-neighbor cutoff in products of $f(r)$, a procedure which resulted in negligible error.

As mentioned earlier, the integrals in the lattice sum of Eq. (8) were calculated exactly only for the first ten nearest-neighbor shells. The contributions from remaining shells are evaluated for a static lattice. It was found that over the range of densities studied, the energy could be determined to within 0.5 K if only the contributions from the first four nearest-neighbor shells were calculated exactly, with the other shells being evaluated for a static lattice. This approximation is made in most Monte Carlo studies.[1-3] The use of static lattice sums after ten nearest-neighbor shells leads to negligible error. Some idea of the magnitude of contributions to the energy from different nearest-neighbor shells can be seen in Table VII. This table contains contributions to $\langle T \rangle$, $\langle V \rangle$, and E_0 from different groups of nearest-neighbor shells for ^{4}He at 21.6 and 10.25 cm^3/mole. As can be seen from this table, the contributions from the first two nearest-neighbor shells are very large at low density. The contributions from other shells become increasingly important with higher densities. However, the contributions from the first four or five shells dominate the total energy even at these high densities.

TABLE IV. $R(r)$ data for He^4

| Volume (cm^3/mole)	Particle displacement from equilibrium $r(\sigma)$										
	0.0	0.05	0.10	0.15	0.20	0.30	0.40	0.50	0.60	0.70	0.80
10.25	1.00	0.916	0.681	0.417	0.207	0.027	0.0012				
11.82	1.00	0.922	0.730	0.495	0.292	0.064	0.0070				
13.75	1.00	0.955	0.809		0.412	0.133	0.026	0.0028			
15.50	1.00		0.829		0.484	0.217	0.068	0.019	0.0022	0.0019	
17.50	1.00		0.862		0.587	0.319	0.137	0.045	0.011	0.011	0.0028
21.60	1.00		0.901		0.675	0.424	0.227	0.102	0.038		
					Static-field approximation						
10.25	1.00	0.885	0.610	0.323	0.130	0.0084	0.00015				
21.60	1.00	0.975	0.902		0.657	0.380	0.168	0.054	0.013	0.0022	0.00032
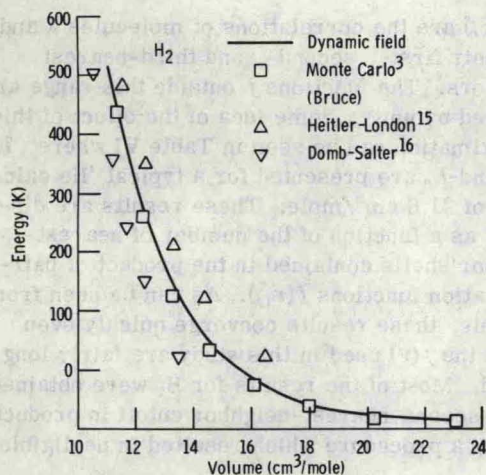
FIG. 11. Energy vs volume for solid fcc H_2 over the volume range $10 \leq V \leq 22.65$ cm^3/mole. A comparison is made with other theoretical work.

Figure 15 contains a comparison of the single-particle distribution function and $e^{-\beta r^2}$ for ^{4}He at two specific volumes. The quantity $e^{-\beta r^2}$ would be the single-particle distribution function if the wave function did not contain pair correlations. This figure, therefore, gives some indication of how much the pair correlations contribute to localizing the individual molecules about their equilibrium lattice sites. Note that the pair-correlation functions are responsible for a substantial portion of
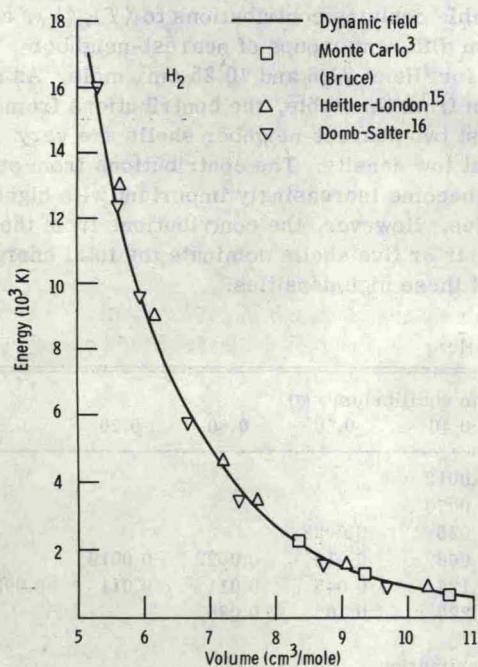

FIG. 12. Energy vs volume for solid fcc H_2 over the volume range $5 \leq V \leq 11$ cm^3/mole. A comparison is made with other theoretical work.
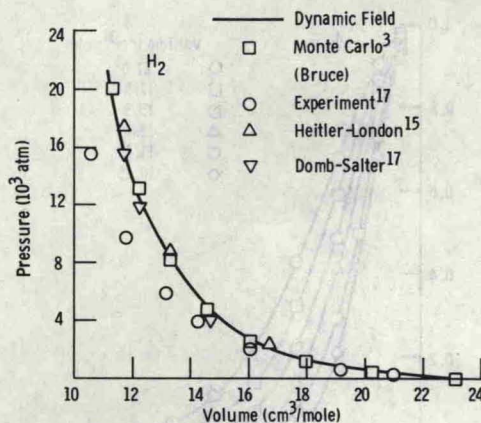

FIG. 13. Pressure vs volume for solid fcc H_2 over the volume range $10 \leq V \leq 22.65$ cm^3/mole. A comparison is made with other theoretical work and experiment.

the localization at both volumes tested.

To recapitulate, the principal approximation of this calculation is the decoupling of pair correlations between different molecular-field atoms, as exhibited by Eq. (10). This approximation together with the others already discussed earlier in this section, have lead to a theoretical description of solid ^{3}He, ^{4}He, and H_2 which is essentially in very close agreement with the results of Monte Carlo calculations. The agreement with experiment is also excellent, except at high pressures, where, for both helium and hydrogen, the poor comparisons are attributed to an inadequate representation of the pair potential.

Several major advantages over the Monte Carlo work accrue to this method of calculation. In addition to the considerably less computational effort required and the physical insight afforded by the the successful approximation techniques,
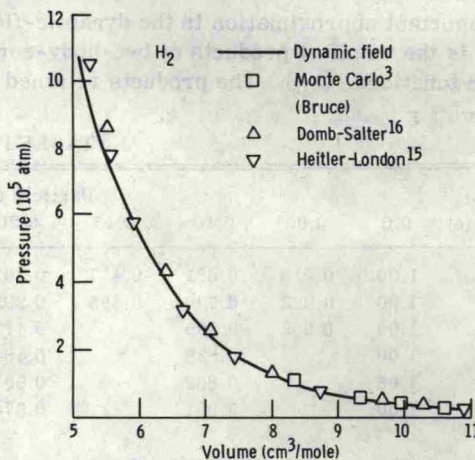

FIG. 14. Pressure vs volume for solid fcc H_2 over the volume range $5 \leq V \leq 11$ cm^3/mole. A comparison with other theoretical work is made.