include only nearest neighbors of molecules (λ, κ). Then each function $f^2(\vec{r}_\lambda - \vec{R}_i)$ was expanded about its value evaluated at the equilibrium lattice site $\vec{r}_\lambda = \vec{R}_\lambda$, and angle averaged. This procedure was similarly applied to the $f^2(\vec{r}_\kappa - \vec{R}_j)$. The expectation value of the Hamiltonian [Eq. (8)] then reduced to an easily soluble two-dimensional integral. Although the results were fairly promising, it was later established that the expansion of the $f(r)$ about their equilibrium lattice positions converge satisfactorily only for a limited class of pair correlation functions, namely those which reach their asymptotic values for values of $r \lesssim R_0$, where R_0 is the equilibrium nearest-neighbor separation. This limited variational capability was considered unsatisfactory and the procedure was therefore abandoned.

A more direct approach, hereafter called the "static-field" approximation, is to evaluate Eq. (11) exactly but only for a limited number of correlations. In bcc solid helium, for example, only pair correlations between atoms within three nearest-neighbor shells of atom λ have any appreciable effect on the behavior of the λth atom and similarly for the κth atom. All the other $f(r)$ in Eq. (11) can be replaced by unity with the effect of changing predicted ground-state energies by less than 1%. For fcc molecular hydrogen, two nearest-neighbor shells are sufficient to produce equivalent accuracy. The $G(\vec{r}_\lambda, \vec{r}_\kappa)$ resulting from this procedure was substituted into Eq. (8) and the lattice sum was evaluated for all different (λ, κ) pairs up to tenth nearest neighbors. Beyond that, lattice sums were evaluated for a classical static lattice. The error associated with this latter procedure is extremely small, on the order of 0.1%. The six-dimensional integrals in Eq. (8) were evaluated on a 7094 computer. Although the results are reasonably good at low pressures, their agreement with experiment becomes considerably worse as the pressure increases. Another disquieting feature of the calculation is that the minimum energy is obtained at all volumes for a value of the parameter $\beta = 0$. The energy actually varies quite slowly with β for small β. In the cluster expansion, $\beta = 0$ implies that the solid is not stable because the functions $\varphi(r)$ in Eq. (1) are no longer spatially localized. This difficulty does not exist in the static-field approximation because $G(\vec{r}_\lambda, \vec{r}_\kappa)$, rather than being unity as in the cluster expansion, is instead given by Eq. (11). The resulting internal field, acting on (λ, κ) produce the restoring force necessary to localize the atoms about their equilibrium lattice sites $\{R_i\}$. This localization is evident upon calculating the single-particle distribution function $R(r)$, in terms of the atomic displacement from equilibrium, $r = |\vec{r}_i - \vec{R}_i|$. These

data are presented in Sec. III A. Nevertheless, the static-field approximation is, in some sense, internally inconsistent. On one hand the molecular-field atoms are initially fixed on their equilibrium lattice sites by taking the limit $\beta \to \infty$, yet the minimization of the energy gives the result $\beta = 0$ for the test particles (λ, κ).

C. Dynamic-field approximation

It is believed that the lack of good agreement between the static field results and experiment is due primarily to the rigidity of the lattice producing the local molecular field on (λ, κ). As an example, when an excursion of particle λ takes it into close proximity to molecular-field atom j, the molecular-field atom will tend to move out of the way. This cannot happen in the static-field approximation. The motion of (λ, κ) is, therefore, restricted. In order to correct this deficiency in the theory, the motion of nearest neighbors to molecules λ and κ has been incorporated into the calculation of the molecular field. Then

$$G(\vec{r}_\lambda, \vec{r}_\kappa) = \prod_{s \neq nn\lambda}' f^2(r_\lambda - R_s) \prod_{\rho \neq nn\kappa}' f^2(r_\kappa - R_\rho)$$
$$\times \prod_{i=nn\lambda}' M_i(\vec{r}_\lambda) \prod_{j=nn\kappa}' M_j(\vec{r}_\kappa)$$
$$\times \prod_{l=nn\lambda\kappa}' N_l(\vec{r}_\lambda, \vec{r}_\kappa), \qquad (12)$$

where the primes indicate that the product is not to include index λ or κ, $nn\lambda \leftrightarrow$ nearest neighbors to particle λ, $nn\lambda\kappa \leftrightarrow$ nearest neighbors to particles λ and κ.

$$M_j(\vec{r}_\kappa) = \int f^2(r_{\kappa j}) \varphi^2(\vec{r}_j - \vec{R}_j) d\vec{r}_j, \qquad (13)$$

$$N_l(r_\lambda, r_\kappa) = \int f^2(r_{\lambda l}) f^2(r_{\kappa l}) \varphi^2(\vec{r}_l - \vec{R}_l) d\vec{r}_l. \qquad (14)$$

The first two products in Eq. (12) include all atoms which are second- or third-nearest neighbors to λ or κ. These products are simply the static-field terms. As in the static-field approximation, pair correlations beyond third-nearest neighbors are neglected, a procedure which leads to no appreciable error. The third product in Eq. (12) extends over all nearest neighbors to λ except for κ. As an example, consider a bcc lattice with (λ, κ) nearest neighbors. Then there are seven terms in that product. The fourth product in Eq. (12) is, of course, similar to the third. The last product does not exist in this case because there are no nearest neighbors common to both λ and κ when they themselves are nearest neighbors. When λ

and κ are second-nearest neighbors, however, there are four atoms which are nearest neighbors to both λ and κ. Then, the last three products in Eq. (12) each contain four terms. Slightly different results are, of course, obtained for fcc and hcp structures. When λ and κ are third-nearest neighbors or greater we simply return to the static-field approximation, in which case

$$M_j(\vec{r}_\kappa) \simeq f^2(\vec{r}_\kappa - \vec{R}_j),$$
$$N_l(\vec{r}_\lambda, \vec{r}_\kappa) \simeq f^2(\vec{r}_\lambda - \vec{R}_l) f^2(\vec{r}_\kappa - \vec{R}_l). \tag{15}$$

Again, for (λ, κ) separated farther than tenth-nearest neighbors, the lattice sums are simply taken over a static lattice. Clearly, it is the integrals N and M in Eq. (12) which provide the dynamical correlations connecting atoms (λ, κ) to the local field. Although the atoms responsible for the local field couple dynamically to atoms λ and κ, they do not couple dynamically to one another, as evidenced by the separable integrals in Eq. (12). The reason for this fortunate circumstance is, of course, traced to the original approximation, exhibited in Eq. (10). This separability reduced an impossibly complex analysis to that of evaluating a simple nine-dimensional integral on the 7094 computer. The details of this procedure are discussed in the Appendix.

To summarize, the dynamical motion of the molecular-field atoms and the effect of this motion on the various pairs (λ, κ) considered only when λ and κ are either first- or second-nearest neighbors to one another. Then only molecular-field atoms which are nearest neighbors to λ and/or κ are dynamically incorporated into the analysis. All other pair correlations are with a static field. It is clear that the dynamical correlations have been incorporated only into the leading terms in the

lattice sum, that is, for all first- and second-nearest-neighbor pairs. Nevertheless, this is sufficient to dramatically improve the results. Additional dynamical contributions are found to be small.

Within the dynamic-field approximation, the single-particle distribution function $R(r)$ is simply

$$R(|\vec{r}_\lambda - \vec{R}_\lambda|) = \int \varphi^2(\vec{r}_\lambda - \vec{R}_\lambda) \varphi^2(\vec{r}_\kappa - \vec{R}_\kappa) f^2(r_{\lambda\kappa})$$
$$\times G(\vec{r}_\lambda, \vec{r}_\kappa) d\vec{r}_\kappa d\Omega_\lambda, \tag{16}$$

where $d\Omega_\lambda$ is the element of solid angle for the λth particle, $G(\vec{r}_\kappa, \vec{r}_\lambda)$ is given by Eq. (11), and the normalization $R(0) = 1.0$ is used. A similar expression as Eq. (16) exists for the root-mean-square atomic deviation from its equilibrium lattice site $\langle r^2 \rangle^{1/2}$. The pressures and compressibilities are derived by taking appropriate derivatives of the ground-state energy with respect to the volume.

III. RESULTS AND DISCUSSION

A. Static-field approximation

Results for the ground-state energy of solid bcc ^{3}He and ^{4}He are presented on Figs. 1 and 2. We are not concerned with the fact that solid helium also exists in a close-packed lattice phase because the energy difference between different structures are known to be very small. In these figures, the circles represent the experimental data[12] and the dotted line represents the results of the static-field approximation. The triangles represent the Monte Carlo (MC) calculation of Hansen and Levesque[1] and the inverted triangles represent a similar MC calculation by Hansen and Pollock.[2] Although the static-field results compare reason-
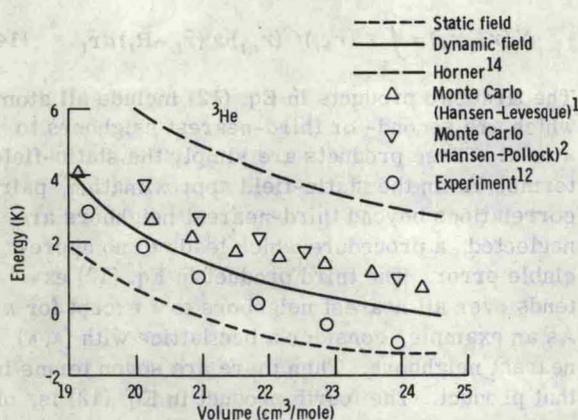

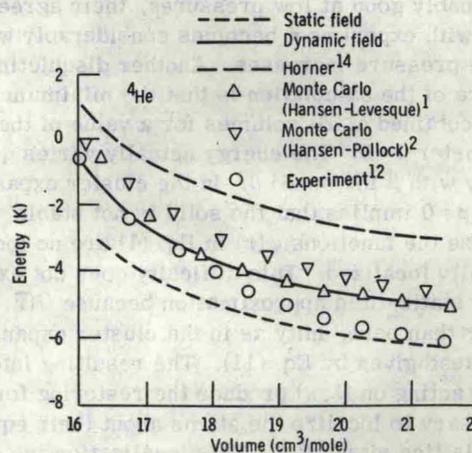FIG. 1. Energy vs volume for solid bcc ^{3}He. A comparison is made with different theoretical and experimental works.

FIG. 2. Energy vs volume for solid ^{4}He. A comparison is made with different theoretical and experimental works.