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Critique of the Saunders Theory of Solid ^{3}He at 0°K†

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An examination is made of the theory of the ground state of solid ^{3}He proposed by Saunders (EMS) and modified by Garwin and Landesman (GL). We find the theory is inconsistent or wrong in the following respects: Unphysical single-particle functions result from a misapplication of the Pluvinage method of generating a wave function; the heuristic derivation of an expression for the exchange integral J is inconsistent with this wave function; a correct solution for the integral equation for the single-particle probability density has not been given; the heuristic expression used for the cohesive energy is inconsistent with the Pluvinage method. The use of the Pluvinage method and the single-particle probability density in the theory are analyzed in detail. The numerical results given in EMS and GL, such as for the exchange integral, are shown to be in doubt because of the errors. We discuss a possible modification of the method, which is not subject to these criticisms, and which gives results similar to those of Nosanow's cluster-expansion theory.

I. INTRODUCTION

SEVERAL years ago, Saunders proposed a theoretical analysis[1] of the ground-state properties of solid ^{3}He. Despite the fact that some workers[2–5] noted that EMS contains numerous errors and some approximations which are difficult to justify, the results of the theory have frequently been quoted and compared with experiment. Recently, Garwin and Landesman[3] corrected some major numerical errors and slightly generalized some of the procedures of the method. One of their contributions, was to give the correct solution of the EMS differential equation for the correlation function $\chi(r)$. However, they did not question the basic equations of the theory, since their main intent was to give an example of what is required to calculate the ^{3}He exchange integral once one has an adequate theory.

The purpose of this paper is to examine the validity of the basic assumptions made in EMS. We find that there are more difficulties with the theory than just the numerical errors corrected in GL; many of the basic procedures of the theory are incorrect as we will show. Garwin and Landesman felt that the EMS theory merited reexamination and correction because the predicted value of the exchange integral is in reasonable agreement with experiment.[2,3] However, our work indicates that this agreement with experiment apparently is fortuitous. In EMS a heuristic derivation is given of an expression for the exchange integral which agrees in general form with the results of other derivations.[6,7] This expression may give a correct order of magnitude to the exchange integral if a helium atom is confined with approximately the correct distribution in its Wigner-Seitz cell. However, we will show that because of a poor approximation neither the distribution used in EMS nor the one used in GL is the one actually predicted by the theory and that the theory's agreement with exchange experiments is now in doubt.

In addition to poor approximations, a serious fault of the theory is its lack of consistency or rigor in its derivation of expressions for the most fundamental quantities, such as the cohesive energy and the exchange integral. Indeed, we show that a treatment of these two quantities consistent with the basic assumptions of the theory would lead to far different expressions, and in the case of the exchange integral, to a physically unreasonable result.

In Sec. II we list some apparent shortcomings which will make it clear that the Saunders theory is unacceptable in its present form. A detailed examination of the theory is presented in Secs. III and IV. In Sec. III we discuss the use of the Pluvinage method of generating a wave function and in Sec. IV, the method of the single-particle probability density is investigated. The analyses of Secs. III and IV suggest a fundamental modification of the theory based on one approximation of the EMS method, which might lead to a consistent theory of solid helium. This modification is discussed in Sec. V. In an Appendix we discuss some numerical methods used.

II. SOME SERIOUS DIFFICULTIES WITH THE EMS THEORY

There are several aspects of the EMS treatment which make the theory suspect and which immediately suggest that deeper analysis should be made:

(1) The first of the difficulties concerns the character

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[1] E. M. Saunders, Phys. Rev. **126**, 1724 (1962). We refer to this paper as EMS.

[2] R. L. Garwin and A. Landesman, Phys. Rev. **133**, A1503 (1964).

[3] R. L. Garwin and A. Landesman, Physics **2**, 107 (1965). We refer to this paper as GL.

[4] L. H. Nosanow and G. L. Shaw, Phys. Rev. **128**, 546 (1962).

[5] L. H. Nosanow, Phys. Rev. **146**, 120 (1966).

[6] N. Bernardes and H. Primakoff, Phys. Rev. **119**, 968 (1960).

[7] L. H. Nosanow and W. J. Mullin, Phys. Rev. Letters **14**, 133 (1965).

of the solid-state wave function given, which is

$$\psi=\prod_{i<j} \chi(r_{ij})\Big[\sum_{\nu}(-1)^{p_\nu}P_\nu \prod_{k} \phi_k(\mathbf{r}_k)\eta_k\Big], \tag{2.1}$$

where the χ_{ij} are correlation functions which vanish at small r_{ij} and to go unity at large r_{ij}; the η_k are spin functions; and the ϕ_k turn out to be *free* single-particle functions which are given crystal-lattice boundary conditions. The function ψ is made antisymmetric by summing over all permutations ν of $\prod\phi_k$, with P_ν a permutation operator and p_ν the parity of the permutation. We question the presence of these nonlocalized free-particle functions in ψ, which is meant to describe a solid. Clearly, if the ϕ_k were localized, (2.1) would describe a solid. It is also possible[8] to construct a (trial) wave function for a solid which contains, as a factor, a Slater determinant of Bloch functions (each of which is a linear combination of localized single-particle functions); but one would expect these functions to be far different from *free*-particle functions. Further, in such a function one does not associate spin with the Bloch state. It is even possible[9] to describe a crystal by a function simply of the form $\psi=\prod \chi_{ij}$. But we are unable to see any physical reason for the presence of the free-particle ϕ_i used in EMS.

(2) Because $\prod \chi_{ij}$ is completely symmetric, the Fermion properties of the wave function are carried entirely by the antisymmetrized product of the $\phi_i(\mathbf{r}_i)$. We can show by a simple argument that this property would lead to unreasonable results for the exchange properties of solid ^{3}He, if the calculations of EMS had actually been carried out in a manner consistent with the wave function. If we define

$$\phi_0=\prod_{i} \phi_i, \tag{2.2}$$

and note that the permutation operator can be written as a product of a spacial part $P_{\nu0}$ and a spin part $P_{\nu s}$,

$$P_\nu=P_{\nu0}P_{\nu s}, \tag{2.3}$$

then the energy expectation value is

$$E=\frac{\sum_{\nu}(-1)^{p_\nu}\int(\prod_{i<j} \chi_{ij}\phi_0^*)H(\prod_{i<j} \chi_{ij}P_{\nu0}\phi_0)d\tau\langle P_{\nu s}\rangle}{\sum_{\nu}(-1)^{p_\nu}\int \prod_{i<j} \chi_{ij}^2\phi_0^*P_{\nu0}\phi_0 d\tau\langle P_{\nu s}\rangle}. \tag{2.4}$$

In (2.4) H is the Hamiltonian of the system; $d\tau$ is the many-body volume element $d\mathbf{r}_1 d\mathbf{r}_2\cdots d\mathbf{r}_N$; and $\langle P_{\nu s}\rangle$ is the spin-space expectation value of the spin-permutation operator. If we write E as a sum of a "direct" energy and an "exchange" energy (plus multiparticle exchange terms), the direct energy will contain the terms which have $P_{\nu0}=1$, and the (pair) exchange energy will contain terms for which $(-1)^{p_\nu}P_{\nu0}\phi_0\langle P_{\nu s}\rangle$ is of the form[10]

$$(-1)\phi_k(\mathbf{r}_l)\phi_l(\mathbf{r}_k) \prod_{i\neq k,l} \phi_i(\mathbf{r}_i)\langle(P_{lk}{}^{kl})_s\rangle. \tag{2.5}$$

Thus the exchange energy E_{ex} will be like a Heisenberg Hamiltonian

$$E_{\text{ex}}=-\sum_{k<l} J_{kl}\langle(P_{lk}{}^{kl})_s\rangle \tag{2.6}$$

with an "exchange integral" of the form[10]

$$J_{kl}=\frac{1}{D}\int(\prod_{i<j} \chi_{ij}\phi_0^*)A \times\Big[\prod_{i<j} \chi_{ij}\phi_k(\mathbf{r}_l)\phi_l(\mathbf{r}_k) \prod_{i\neq k,l} \phi_i(\mathbf{r}_i)\Big]d\tau, \tag{2.7}$$

where A is an operator and D is a normalization denominator. (E_{ex} is of the Heisenberg form because $(P_{lk}{}^{kl})_s$ contains a term in $\mathbf{S}_l\cdot\mathbf{S}_k$ where $\mathbf{S}_l$ is a spin operator.) In the EMS theory the localization of the particles about lattice sites is provided entirely by the factor $(\prod \chi_{ij})^2$ in the probability density. Suppose we consider an extreme case (large particle mass) for which $\prod \chi_{ij}$ provides almost perfect localization, that is, it is essentially a product of δ functions centered on lattice sites. Then J_{kl} will be of order

$$\phi_l^*(\mathbf{R}_l)\phi_k^*(\mathbf{R}_k)\phi_k(\mathbf{R}_l)\phi_l(R_k), \tag{2.8}$$

where $\mathbf{R}_k$ and $\mathbf{R}_l$ are the positions of lattice sites k and l. Even in this extreme case of localization, for which exchange effects should vanish, J_{kl} depends on overlap of nonlocalized free-particle functions, which is not small. This situation is certainly not improved if we consider less extreme localization as it occurs in solid ^{3}He. Thus it seems that the mechanism of exchange provided by the EMS wave function is entirely unphysical. However, in EMS this difficulty is avoided somewhat by the use of heuristic arguments which lead to an exchange-energy expression of a more reasonable form.

(3) There is another rather general peculiarity concerning the ϕ_i: There is no single numerical result in the EMS theory which depends on the nature of the ϕ_i. For example, as we have just pointed out, the exchange effects are derived on the basis of arguments which have nothing to do with the antisymmetrization of the wave function, and indeed are inconsistent with the nature of the wave function. Further, the evaluation of the direct energy and of the all-important single-particle density are independent of the choice of the ϕ_i. As we will see when we make a more detailed examination of the theory, the ϕ_i are actually a mathematically and physically extraneous feature of the theory. This last fact need not have been so, of course. For example, if the $\phi_i(\mathbf{r}_i)$ had been chosen to be *localized* about lattice

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[8] J. H. Hetherington (private communication).

[9] W. L. McMillan, Phys. Rev. **138**, A442 (1965).

[10] See, for example, W. J. Carr, Phys. Rev. **92**, 28 (1953); W. J. Mullin, *ibid.* **136**, A1126 (1964); or Ref. 7.

sites, then the trial wave function would have been physically reasonable and exchange effects could have received a consistent treatment.

One reason the cohesive energy E does not depend on the ϕ_i is that the derivation of E is a heuristic one which is altogether inconsistent with the energy expression which comes from the Pluvinage method used to generate the wave function of EMS. (See Sec. III for details.)

(4) The central element in the EMS theory, the single-particle probability density, is defined by

$$\Gamma(\mathbf{r}_1)\equiv\int|\psi|^2 d\mathbf{r}_2 d\mathbf{r}_3\cdots d\mathbf{r}_N\,, \tag{2.9}$$

where we assume ψ to be normalized. An integral equation is developed for $\Gamma(\mathbf{r}_1)$ by a derivation which we shall review in Sec. IV. This equation is

$$\Gamma(\mathbf{r}_1)=(\text{const})\prod_{k(\neq 1)}\int\Gamma(\mathbf{r}_k)\chi^2(r_{1k})d\mathbf{r}_k\,. \tag{2.10}$$

For a solid it is expected that

$$\Gamma(\mathbf{r}_i)=\sum_j\gamma(\mathbf{r}_i-\mathbf{R}_j)\,, \tag{2.11}$$

where $\gamma(\mathbf{r}_i-\mathbf{R}_j)$ localizes particle i about the lattice site at $\mathbf{R}_j$. It is assumed that each particle is near a specific lattice site so that

$$\Gamma(\mathbf{r}_i)\approx\gamma(\mathbf{r}_i-\mathbf{R}_i)\,. \tag{2.12}$$

Then Eq. (2.10) becomes

$$\gamma(\mathbf{u}_1)=(\text{const})\prod_{k(\neq 1)}\int\gamma(\mathbf{u}_k)\chi^2(r_{1k})d\mathbf{r}_k\,, \tag{2.13}$$

where $\mathbf{u}_i=\mathbf{r}_i-\mathbf{R}_i$. The EMS method is to assume as a first approximation that $\gamma(\mathbf{u}_k)$, on the right side of (2.13), may be replaced by

$$\gamma^{(1)}(\mathbf{u}_k)=\delta(\mathbf{r}_k-\mathbf{R}_k)\,, \tag{2.14}$$

and then to solve for $\gamma^{(2)}(\mathbf{u}_1)$ on the left. One must, of course, repeat this procedure until the sequence $\gamma^{(n)}(\mathbf{u}_1)$ converges. In EMS it is argued that further iterations yield no change and that

$$\gamma(\mathbf{u}_1)=\gamma^{(2)}(\mathbf{u}_1)=\prod_{k(\neq 1)}\chi^2(|\mathbf{r}_1-\mathbf{R}_k|)\,. \tag{2.15}$$

Further, in GL, Eq. (2.15) is assumed to be adequate and $\gamma^{(2)}(\mathbf{u}_1)$ is found using the GL solution for $\chi(r)$. We have used a reasonable analytic approximation to the $\chi(r)$ of EMS and the exact numerical $\chi(r)$ given in GL and have *iterated* Eq. (2.13) with an approximate numerical procedure. We give some details of this calculation in the Appendix. The results are as follows: For the $\chi(r)$ given in EMS we were unable to find a localized solution of Eq. (2.13). We note that

$$\gamma(\mathbf{u}_i)=\text{const} \tag{2.16}$$

does satisfy Eq. (2.13) since $\int\chi(r_{1k})d\mathbf{r}_k$ is independent of $\mathbf{r}_1$. The sequence of $\gamma^{(n)}(\mathbf{u}_1)$ appeared to be relaxing to the solution (2.16). For the $\chi(r)$ given by GL, which has a large maximum at $r\approx 4$ Å, we found a localized solution; however, it differs considerably from $\gamma^{(2)}(\mathbf{u}_1)$. In Fig. 1 we show plots of $\gamma^{(2)}(\mathbf{u}_1)$ and our solution $\gamma(\mathbf{u}_1)=\gamma^{(\infty)}(\mathbf{u}_1)\cong\gamma^{(6)}(\mathbf{u}_1)$. Clearly, a poor approximation to $\gamma(\mathbf{u})$ is used in EMS and GL. (Note that all of our expressions for $\gamma(\mathbf{u}_i)$ are functions of magnitude $|\mathbf{u}_i|$ only, because of a spherically symmetrizing approximation made for mathematical simplicity. This approximation consists of replacing a lattice sum over vector $\mathbf{R}_{k1}=\mathbf{R}_k-\mathbf{R}_1$ by an average over the angles of $\mathbf{R}_{k1}$, plus a sum over the magnitudes $|\mathbf{R}_{k1}|$. (See the Appendix.)

The use of the correct solution to Eq. (2.13) instead of $\gamma^{(2)}(\mathbf{u}_1)$ would undoubtedly lead to considerably larger values of the exchange integral since it is a much wider function. For reasons discussed in Sec. IV we cannot accurately estimate what value the theory would now predict for the exchange interaction. However, there are some indications that its prediction may now be too large (see Sec. IV).

In this section we have given only a superficial discussion of the difficulties of the EMS theory. In the next two sections we present a much more detailed investigation.

III. SAUNDERS'S USE OF THE PLUVINAGE METHOD

To understand the EMS theory we must first understand the Pluvinage-Walsh-Borowitz (PWB) method[11,12] upon which it is based. Pluvinage[11] noted that, in solving the Schrödinger equation for a two-electron atom, one could take the nucleus-electron distances $r_1=|\mathbf{r}_1|$, $r_2=|\mathbf{r}_2|$, the interelectron distance $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$, and three Euler angles as independent variables. Then the Hamiltonian depends only on r_1, r_2, and r_{12}:

$$H=H_0+H'\,, \tag{3.1}$$

with

$$H_0=-\frac{\hbar^2}{2m}(\nabla_{r_1}{}^2+\nabla_{r_2}{}^2+2\nabla_{r_{12}}{}^2)-\frac{Ze^2}{r_1}\quad\frac{Ze^2}{r_2}\quad\frac{e^2}{r_{12}}\,, \tag{3.2}$$

where

$$\nabla_r{}^2\equiv\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right). \tag{3.3}$$

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[11] P. Pluvinage, Ann. Phys. (Paris) **5**, 145 (1950).

[12] P. Walsh and S. Borowitz, Phys. Rev. **115**, 1206 (1959); **119**, 1274 (1960).

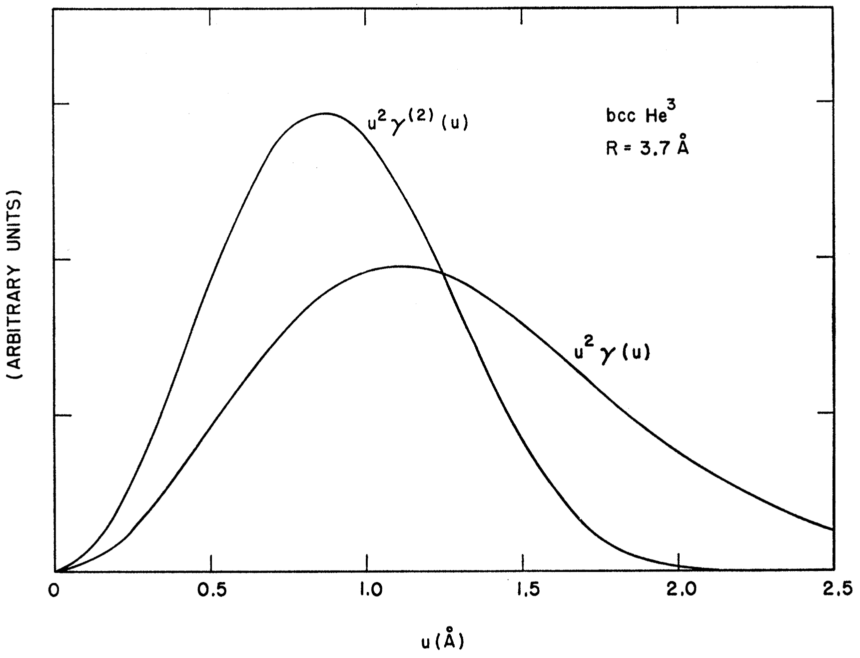

FIG. 1. Plots of $u^2\gamma^{(2)}(u)$ and $u^2\gamma(u)$ for bcc ^{3}He. $\gamma^{(2)}(u)$ is a spherically symmetrized approximation to the function (2.15) assumed, in EMS (Ref. 1) and GL (Ref. 3), to be the solution of the fundamental EMS equation [Eq. (2.13)] for the single-particle probability density. $\gamma(u)$ is the actual solution of (2.13) which we find in the spherical approximation. We have used the GL correlation function $\chi(r)$. The large difference in the two curves illustrates the gross error made in the EMS theory. The curves are normalized to have equal values of $\int_0^\infty u^2\gamma^{(n)}(u)du$.

Also

$$H'=-\frac{\hbar^2}{2m}\left(\frac{r_1{}^2-r_2{}^2+r_{12}{}^2}{r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}}+\frac{r_2{}^2-r_1{}^2+r_{12}{}^2}{r_2r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}}\right). \quad (3.4)$$

The operator H_0 contains all the singularities in H and so H' is taken as perturbation. The unperturbed equation

$$H_0\psi_0=E_0\psi_0$$

separates in the variables r_1, r_2, r_{12} and so ψ_0 has the form

$$\psi_0=\phi(r_1)\phi(r_2)w(r_{12}). \quad (3.5)$$

The $\phi(r_i)$ are hydrogeniclike wave functions while $w(r_{12})$ is an electron-electron scattering function. The ground-state energy is then estimated by using ψ_0 as a trial wave function for the complete Hamiltonian.

This method was extended by Walsh and Borowitz[12] to many-electron systems. They showed that a separation of the unperturbed ψ_0, analogous to Eq. (3.5) was a mathematically rigorous procedure only for atoms with two or three electrons. The reason is that, for an N-electron atom, the electron-nucleus distances, the interelectron distances, and the three Euler angles total $N+\frac{1}{2}N(N-1)+3$ variables. The original number of degrees of freedom is $3N$. Equating these two quantities gives $N=2$ or 3. For $N>3$ "redundant" variables have been introduced, i.e., not all the variables are independent of one another. However, for the sake of easily generating a trial function which behaves properly at all the singularities in the potential, one *assumes* they are all independent in solving the unperturbed Schrödinger equation. If an important aspect of the problem is the nonindependence of these variables then a very poor trial wave function may be generated.

Some simple one-dimensional examples may serve to illustrate the PWB method:

(1) First consider the two-particle harmonic-oscillator problem illustrated in Fig. 2(a). The Hamiltonian,

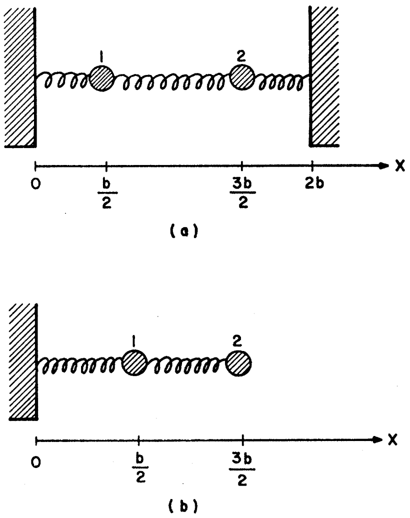

FIG. 2. Two one-dimensional systems used to illustrate the Pluvinage method of generating a trial wave function.

with $\hbar^2/m=1$, is

$$-\frac{1}{2}\left(\frac{d^2}{dq_1^2}+\frac{d^2}{dq_2^2}\right)+\tfrac{1}{2}k[q_1^2+(q_1-q_2)^2+q_2^2], \quad (3.6)$$

where k is the spring constant for all three springs; and $q_1=x_1-\frac{1}{2}b$, $q_2=x_2-\frac{3}{2}b$. As variables we choose q_1, $q_{12}=q_1-q_2$, and q_2. Assuming the wave function will be a function of these variables we write

$$\frac{d}{dq_1}=\frac{\partial}{\partial q_1}+\frac{dq_{12}}{dq_1}\frac{\partial}{\partial q_{12}}=\frac{\partial}{\partial q_1}+\frac{\partial}{\partial q_{12}}. \quad (3.7)$$

Similarly

$$\frac{d}{dq_2}=\frac{\partial}{\partial q_2}-\frac{\partial}{\partial q_{12}}. \quad (3.8)$$

The Hamiltonian becomes

$$H=H_0+H', \quad (3.9)$$

$$H_0=-\frac{1}{2}\left(\frac{\partial^2}{\partial q_1^2}+\frac{\partial^2}{\partial q_2^2}+2\frac{\partial^2}{\partial q_{12}^2}\right)+\tfrac{1}{2}k[q_1^2+q_2^2+q_{12}^2], \quad (3.10)$$

$$H'=-\left(\frac{\partial^2}{\partial q_1\partial q_{12}}-\frac{\partial^2}{\partial q_2\partial q_{12}}\right). \quad (3.11)$$

We drop H' and proceed *as if* q_1, q_2, and q_{12} were all *independent* variables. Two particles in one dimension have only two independent variables, so actually one of these variables is "redundant." The Schrödinger equation then separates, with ground-state solution

$$\psi_0=\phi_1\phi_2\phi_{12}, \quad (3.12)$$

where ϕ_1, for example, satisfies

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial q_1^2}+\tfrac{1}{2}kq_1^2\right)\phi_1=E_1\phi_1. \quad (3.13)$$

Thus,

$$\phi_i=A_1\exp\{-(\tfrac{1}{2}\sqrt{k})q_i^2\}, \quad i=1, 2, \quad (3.14)$$

and, similarly,

$$\phi_{12}=A_{12}\exp\left\{-\frac{\sqrt{k}}{2\sqrt{2}}q_{12}^2\right\}. \quad (3.15)$$

The expectation value of H_0 is the sum of three energies

$$E_0=E_1+E_2+E_{12}=(\sqrt{k})(\tfrac{1}{2}+\tfrac{1}{2}+1/\sqrt{2})=1.71\sqrt{k} \quad (3.16)$$

compared with the exact result

$$E=1.36\sqrt{k}. \quad (3.17)$$

If one uses ψ_0 as a trial wave function with the exact Hamiltonian, that is, one now considers the perturbation H', a much improved energy upper-bound results:

$$E_1+E_2+E_{12}+\langle H'\rangle=(1.71-0.29)\sqrt{k}=1.42\sqrt{k}. \quad (3.18)$$

Without using any variational parameters we have obtained a result containing only 4% error.

We wish to emphasize that the equation $H_0\psi_0=E_0\psi_0$ is not actually separable in q_1, q_2, q_{12}. Treating them as independent is only a *trick* to construct a trial wave function.

(2) As a second example, consider the two-particle oscillator system with one wall and one end spring removed as in Fig. 2(b). This situation will illustrate a difficulty introduced by the redundant variables which helps us to understand certain peculiar aspects of the EMS theory. For this system the PWB method gives

$$H_0=-\frac{1}{2}\left(\frac{\partial^2}{\partial q_1^2}+\frac{\partial^2}{\partial q_2^2}+2\frac{\partial^2}{\partial q_{12}^2}\right)+\tfrac{1}{2}k(q_1^2+q_{12}^2). \quad (3.19)$$

H' is again given by Eq. (3.11).

If we assume that q_1, q_2, and q_{12} are independent as before, we find once more that ϕ_1 and ϕ_{12} are given by Eqs. (3.14) and (3.15), but that ϕ_2 satisfies

$$\left[-\frac{1}{2}\frac{d^2}{dq_2^2}\right]\phi_2(q_2)=E_2\phi_2, \quad (3.20)$$

a free-particle equation. Thus

$$\phi_2=Ae^{+iKq_2}+Be^{-iKq_2}, \quad (3.21)$$

$$E_2=\tfrac{1}{2}K^2. \quad (3.22)$$

Such a ϕ_2 is a physically unreasonable quantity which certainly does not appear in the true wave function. It arises simply because we have considered q_1, q_2, and q_{12} as independent, which implies that q_2 is a free-particle variable; this is certainly incorrect. Nevertheless, we can obtain a reasonable trial function by setting $K=0$. With $\psi_0=\phi_1\phi_2$ as trial function, the energy expectation value is

$$E_0=1.21\sqrt{k}, \quad (3.23)$$

with the perturbation expectation value

$$\langle H'\rangle=0. \quad (3.24)$$

The exact result is

$$E=1.12\sqrt{k}. \quad (3.25)$$

The error is about 8%.

In EMS, free-particle equations similar to Eq. (3.20) are found because of the redundant variable difficulty. However, instead of discarding them, they appear to be used in a fundamental way to provide an antisymmetric wave function.

Saunders splits the many-helium-atom Hamiltonian,

$$H=-\frac{\hbar^2}{2m}\sum_i\nabla_{r_i}^2+\sum_{i<j}V(r_{ij}), \quad (3.26)$$

into H_0 and H' in a way analogous to Eqs. (3.1)–(3.4) so that

$$H_0=-\frac{\hbar^2}{2m}\Big[\sum_i \nabla_{r_i}{}^2+2\sum_{i<j}\nabla_{r_{ij}}{}^2\Big]+\sum_{i<j}V(r_i)_j. \qquad (3.27)$$

The definition of $\nabla_r{}^2$ was given in Eq. (3.3). H', which we will not write down, contains the cross derivatives in analogy to Eq. (3.4). The differential operators of (3.27) have been developed just as in (3.7)–(3.11) on the assumption that the wave function will depend only on r_i and r_{ij}. The EMS method is to proceed as if r_i, r_{ij} were all independent variables (which of course they are not) and to separate the H_0 equation into the equations

$$-\frac{\hbar^2}{2m}\nabla_{r_i}{}^2\phi_i(r_i)=\epsilon_i\phi_i(r_i)\,, \qquad (3.28)$$

$$\left[-\frac{\hbar^2}{2m}\nabla_{r_{ij}}{}^2+\tfrac{1}{2}V(r_{ij})\right]\chi(r_{ij})=\epsilon_{ij}\chi(r_{ij})\,. \qquad (3.29)$$

The final trial wave function is then

$$\psi=\prod_i \phi_i(r_i)\prod_{i<j}\chi(r_{ij}) \qquad (3.30)$$

if we neglect symmetry effects for a moment.

Note that, unlike the many-electron systems studied in Ref. 12, there are no single-particle potentials $V(r_i)$ in this problem. Thus the ϕ_i are *free*-particle functions. We saw in our oscillator problem [Fig. 2(b)] that such a factor is unphysical and is a fault of the invalid assumption that all the r_i and r_{ij} are independent. Hopefully, one can still get a reasonable trial function by setting the $\phi_i=1$ as we did in our simple example. In fact, one can even leave them in the trial function, since the choice of trial wave function is rather free, but there is no reason to believe that they will improve the value of the energy expectation value anyway. Indeed, there is no single result in EMS which depends on the ϕ_i being different from unity. However, the antisymmetrization of the solid ^{3}He wave function and the resulting exchange effects which are computed are made to seem entirely dependent on the ϕ_i. We will discuss the EMS treatment of symmetry effects more completely below.

We now discuss the solution of Eq. (3.29) for the pair functions $\chi(r_{ij})$. In contrast to our harmonic-oscillator examples, Eq. (3.29) does not have a pair bound-state solution if m is the ^{3}He atomic mass, and if $V(r_{ij})$ is the Lennard-Jones potential; there are only scattering solutions. In this case the simplest thing to do is to use the solution for $\epsilon_{ij}=0$. The resulting $\chi(r_{ij})\rightarrow 1$ as $r_{ij}\rightarrow\infty$ and does not oscillate at infinity. Such oscillations certainly have no physical meaning in this problem and should be avoided just as the ϕ_i should have been avoided. On the other hand, the fact that $\chi(r_{ij})\rightarrow 0$ as $r_{ij}\rightarrow 0$, because of the singularity in $V(r_{ij})$, is a very important feature because then the trial wave function $\psi=\prod \chi_{ij}$ behaves properly at all the singularities in the Hamiltonian; the development of such a property of ψ was just the reason the PWB method was invented.

Sometimes other circumstances may prevent the PWB method from giving a reasonable trial function. For example, in the case of ^{4}He, the bound-state (or resonance) eigenvalue occurs very near $\epsilon_{ij}=0$. Thus it is shown in GL that, while $\chi(r)$ does approach unity at large distances, it has an enormous maximum for $r\approx 4$ Å. Such a feature could make ψ an extremely poor choice of trial function. The occurrance of such sticky problems leads us to question the wisdom of using the PWB method at all for generating a trial function for solid helium. After all, one can immediately write down an analytic trial correlation function which has all the necessary properties. McMillan,[9] Nosanow, and coworkers,[5,13] and Levesque *et al.*,[14] have used analytic forms for the correlation function with success. In each case a minimization of the energy was used to determine the best correlation function.

Once the trial function is settled upon then the energy expectation value must be found. From the PWB method the energy is

$$E=\langle H\rangle=\sum_i \epsilon_i+\sum_{i<j}\epsilon_{ij}+\langle H'\rangle=\sum_i \epsilon_i+\langle H'\rangle. \qquad (3.31)$$

The last equality holds since $\epsilon_{ij}=0$. Furthermore, the unphysical single-particle functions should be discarded by setting $\epsilon_i=0$. However, Eq. (3.31) is not the energy estimate used in EMS. There, an involved heuristic argument leads to

$$E\approx-\frac{\hbar^2 N}{2m}\int\gamma^{1/2}(\mathbf{u}_1)(\nabla_{r_1}{}^2/3)\gamma^{1/2}(\mathbf{u}_1)d\mathbf{r}_1+\langle H'\rangle\,, \qquad (3.32)$$

where $\langle H'\rangle$ is neglected without real justification. It is clear that the heuristic argument is incorrect since the first term in Eq. (3.32) bears no relation to $\sum\epsilon_i$ of Eq. (3.31).

Since we have shown that the nonlocalized single-particle ϕ_i's are unphysical and cannot account for the exchange effects in solid ^{3}He, we may ask how symmetry effects should be treated. The trial function $\psi_0=\prod\chi_{ij}$ is completely symmetric and cannot be antisymmetrized without including a single-particle function factor. In fact, however, as we have mentioned before, the single-particle functions are never used in EMS to discuss exchange effects. Exchange is discussed in terms of the overlap of neighboring single-particle densities which are actually dependent on only the properties of $\prod\chi_{ij}$ and not on the ϕ_i. Thus dropping the ϕ_i is of no real consequence. It merely points out that the theory does not derive exchange effects in a consistent way. It injects them at the end in a heuristic way. Given correct

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[13] J. H. Hetherington, W. J. Mullin, and L. H. Nosanow, Phys. Rev. **154**, 175 (1967).

[14] D. Levesque, D. Shiff, T. Khiet, and L. Verlet (unpublished).

single-particle densities this heuristic derivation may very well give a decent order-of-magnitude estimate of the exchange integral J. However, the lack of a consistent derivation always causes some doubt in this problem because J contains much internal cancellation and is very sensitively dependent on the overlap of neighboring single-particle probability density functions.[7]

One consistent way the trial wave function can be changed to allow antisymmetrization is to include, as a factor, a Slater determinant of *localized* single-particle functions.[7] Apparently such functions also lower the energy upper bound as shown in the Monte Carlo work of Levesque *et al.*[14]

IV. EMS SINGLE-PARTICLE PROBABILITY DENSITY

In Sec. II we presented a preliminary discussion of the single-particle density and indicated that it had been inaccurately computed in previous work.[1,3] We would now like to enlarge upon that discussion.

The derivation given in EMS leading to an equation like (2.13) is clear. Nevertheless, the derivation we give here is slightly different. We first drop the exchange in the wave function (2.1) on the basis that such terms lead to small contributions to the energy because overlap factors like $\phi_i^*(1)\phi_j(1)$ are small. Of course, this would be correct for physically reasonable ϕ_i (such as localized ϕ_i) and according to our argument in Sec. II it is incorrect for the ϕ_i used in EMS. However, such a difficulty is of secondary importance to us in this section and we will proceed for awhile as if we had appropriate ϕ_i. If we assume each particle is in a specific single-particle state and the wave function is the unsymmetrized form

$$\psi=\phi_1(\mathbf{r}_1)\cdots\phi_N(\mathbf{r}_N)\prod_{i<j}\chi(r_{ij})\,,$$

then

$$\Gamma(\mathbf{r}_1)=(\text{const})\,|\phi_1(\mathbf{r}_1)|^2\int\prod_{k(\neq1)}|\phi_k(\mathbf{r}_k)|^2\chi^2(r_{1k})\times\prod_{i<j\neq1}\chi^2(r_{ij})d\mathbf{r}_2\cdots d\mathbf{r}_N\,,\qquad(4.1)$$

where we have neglected spin. The basic EMS assumption is that

$$\prod_{k(\neq1)}|\phi_k|^2\prod_{i<j\neq1}\chi^2{}_{ij}\approx\prod_{k(\neq1)}\Gamma(\mathbf{r}_k)\,,\qquad(4.2)$$

so that

$$\Gamma(\mathbf{r}_1)=(\text{const})\,|\phi_1(\mathbf{r}_1)|^2\prod_{k(\neq1)}\int\Gamma(\mathbf{r}_k)\chi^2(r_{1k})d\mathbf{r}_k\,.\qquad(4.3)$$

If we no longer neglect the wave-function symmetrization, so that any distribution of particles among single-particle states is equally probable, then we find

$$\Gamma(\mathbf{r}_1)=(\text{const})\sum_j|\phi_j(\mathbf{r}_1)|^2\prod_{k(\neq1)}\int\Gamma(\mathbf{r}_k)\chi^2(r_{1k})d\mathbf{r}_k\,,\qquad(4.4)$$

where the overlap terms are still neglected. Now in EMS, it is claimed that for the nonlocalized free-particle ϕ_i used,

$$\sum_j\phi_j(r_1)\approx\text{const}\,.\qquad(4.5)$$

With (4.5), Eq. (4.4) reduces to Eq. (2.10). The final EMS form [our Eq. (2.13)] is then derived as shown in Sec. II.

Note that Eq. (2.10) and Eq. (2.13) would result from this derivation if the wave function were simply of the form

$$\psi=\prod_{i<j}\chi(r_{ij})\qquad(4.6)$$

because the ϕ_i no longer appear in the theory. But then Eq. (4.6) leads to

$$\Gamma(\mathbf{r}_1)=\int|\psi|^2d\mathbf{r}_2\cdots d\mathbf{r}_N=\text{const}\,.\qquad(4.7)$$

because the $\chi(r_{ij})$ depend on interparticle distances only. Equation (4.7) expresses the translational invariance of the ψ of (4.6); that is, because the center of mass of the system can be anywhere, each particle also is equally likely to be anywhere. [It is interesting that the wave function of the harmonic crystal can be written in the form[15] $\prod_{i<j}f_{ij}(\mathbf{r}_{ij}-\mathbf{R}_{ij})$ and has the property (4.7).] And, indeed, one solution of Eq. (2.10) is

$$\Gamma(\mathbf{r}_i)=\text{const}\,.\qquad(4.8)$$

However, we do not believe that this discussion invalidates the EMS method. After all, the approximation (4.2) breaks the translational invariance, as long as $\gamma(\mathbf{u}_i)\neq1$, and is really periodic as Eq. (2.11) implies.

A similar problem has been treated by Brout[16] in a discussion of the partition function for a classical solid. In fact, Brout derives an equation for a single-particle function which, in some respects, is similar to the EMS equation. This equation is solved by Brout, Nettel, and Thomas[17] for solid argon. Brout[16] notes that his equation also has the trivial solution corresponding to $\Gamma(\mathbf{r}_1)=\text{const}$. However, a localized solution is found as well, in Ref. 17.

We have noted that our solution for the single-particle density is a broader function than the functions of EMS and GL. This will lead to a larger theoretical value of the exchange integral J. One way we might

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[15] This can be shown by some simple manipulations of configuration space representation of the crystal-wave function as given by T. R. Koehler, Phys. Rev. **144**, 789 (1966).

[16] R. Brout, Physica **29**, 1041 (1963).

[17] R. Brout, S. Nettel, and H. Thomas, Phys. Rev. Letters **13**, 474 (1964).

estimate this value is by fitting our solution with a Gaussian and using the EMS expression for J. In EMS this curve fitting was done in the neighborhood of the origin, $\mathbf{u}=0$. When such a procedure was followed in GL, an exchange integral several orders of magnitude too large was found. This occurs for a least two reasons: First, even our spherically symmetric approximation to $\gamma^{(2)}(\mathbf{u}_i)$ falls off faster than a Gaussian so that a Gaussian approximation results in an overestimate of J. Second, a nonspherically symmetric $\gamma^{(2)}(\mathbf{u}_i)$, such as that computed in GL, will fall off faster in the directions of the neighboring particles than in the intermediate directions. Thus a spherical average (such as the Gaussian) also will lead to an overestimate of J.

An estimate of J using our spherically symmetric approximation to the correct solution, $\gamma(\mathbf{u}_i)$, would be subject to the second cause of overestimation. However, the first does not hold. Our $\gamma(\mathbf{u}_i)$ falls off *more slowly* than a Gaussian, so a Gaussian approximation tends to give an underestimate of J. We get a Gaussian approximation by normalizing $\gamma(\mathbf{u})$ to unity at $\mathbf{u}=0$ and then determining a Gaussian parameter δ by taking

$$\gamma(\mathbf{r}_0)=\exp\{-\delta^2\mathbf{r}_0^2\} \tag{4.9}$$

for $|\mathbf{r}_0|=1$ Å, rather than near the origin. This gives a slightly more realistic fit because near $u=1$ Å, $u^2\gamma(\mathbf{u})$ has a maximum. If the resulting δ's are used in the EMS expression for J, we get J's that are two to three orders of magnitude too large. Of course, for the reasons given above, we do not know how reliable such an estimate is. To achieve a realistic estimate one would need to iterate Eq. (2.13) without making any spherically symmetrizing approximation and then compute J as in GL. Such a computation is quite difficult and we believe that there are so many objections to the theory in its present form that such a computation is not warranted.

For the sake of some comparisons we list in Table I the δ^2 values gotten in EMS, and here, and also some equivalent Gaussian parameters from other theories of bcc ^{3}He. We see that the present results for δ^2 are not much different from those of the Bernardes-Primakoff theory[6]; the Gaussian parameters of that theory are now thought to be too small.[18]

We have carried out an analysis, similar to the one described above for hcp ^{4}He using the GL $\chi(r)$. Although the solution we find for $\gamma(\mathbf{u})$ is a bit wider than $\gamma^{(2)}(\mathbf{u})$ it still seems too narrow a function to provide a reasonable description of ^{4}He, in agreement with the GL conclusion. For $R=3.7$ Å we find, as above, $\delta^2=2.3$ Å^{-2} whereas, for example, the equivalent parameter in the Nosanow theory[5] is $\delta^2=1.80$ Å^{-2}. (We should note that the GL conclusion was that the theory led to "ridiculous" results for ^{4}He. While our results seem poor for ^{4}He, they are not ridiculously far off.)

TABLE I. Values of the Gaussian parameter δ^2 for bcc ^{3}He from our calculations (see text) with the GL solution for $\chi(r)$; from EMS (Ref. 1); from the Bernardes and Primakoff theory (Ref. 6); and from the Nosanow theory (Ref. 5). R is the nearest-neighbor distance in Å for bcc ^{3}He. The units of δ^2 are Å^{-2}.

R (Å) \ Source of δ^2	This work $\gamma^{(2)}$, GL-χ	This work $\gamma^{(\infty)}$, GL-χ	EMS $\gamma^{(2)}$, EMS-χ	Bernardes-Primakoff	Nosanow
3.5	1.8	1.1	2.38	0.84	1.60
3.6	1.5	0.9	1.92	0.83	1.48
3.7	1.3	0.85	1.56	0.82	1.36

We wish to emphasize that any detailed conclusions concerning the usefulness or accuracy of $\gamma(\mathbf{u})$ based on our numerical calculations are clearly tentative because we have made certain simplifying approximations. Nevertheless our basic point concerning $\gamma(\mathbf{u})$ has been made: The calculations of Refs. 1 and 3 are incorrect because they have used $\gamma^{(2)}(\mathbf{u})$ instead of the fully iterated solution $\gamma(\mathbf{u})$. Any future calculations based on the EMS method must avoid this error.

In the analysis of this section we have not questioned one basic assumption of the Saunders theory, our Eq. (4.2), indeed, we find this approximation rather appealing although we have no way of testing it. In an attempt in the next section to make the Saunders theory into a more consistent treatment of solid helium we will retain this approximation.

V. DISCUSSION OF A POSSIBLE MODIFICATION OF THE EMS THEORY

We would like to suggest some improvements in the EMS method, which make use of the basic approximation (4.2) but which are not subject to the objections we have raised. The introduction of localized single-particle functions results in some simplifications. Further, it seems valuable to choose an *analytic* form for $\chi(r)$ and to minimize the energy expectation value with respect to parameters contained in it, rather than choosing a fixed form *a priori*.

If we neglect symmetry effects for a moment and use

$$\psi=\prod_k \phi(\mathbf{r}_k-\mathbf{R}_k)\prod_{i<j} \chi_{ij}\,, \tag{5.1}$$

with real ϕ_k and χ_{ij}, and if we use the identity

$$\int \psi\nabla_i^2\psi d\mathbf{r}_1\cdots d\mathbf{r}=\frac{1}{2}\int \psi^2\nabla_i^2 \ln\psi d\mathbf{r}_1\cdots d\mathbf{r}_N\,, \tag{5.2}$$

we find

$$E=\langle H\rangle=\left\{-\frac{\hbar^2}{4m}\sum_i \int (\nabla_i^2 \ln\phi_i)\psi^2 d\mathbf{r}_1\cdots d\mathbf{r}_N \right.$$

$$\left. +\sum_{i<i} \tilde{V}_{ij}\psi^2 d\mathbf{r}_1\cdots d\mathbf{r}_N\right\} \Bigg/ \int \psi^2 d\mathbf{r}_1\cdots d\mathbf{r}_N\,, \tag{5.3}$$

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[18] L. H. Nosanow, Phys. Rev. Letters 13, 270 (1964).

where

$$\tilde{V}(r_{ij}) = V(r_{ij}) - \frac{\hbar^2}{2m}\nabla_i^2 \ln\chi_{ij}. \tag{5.4}$$

Using the single-particle density $\gamma(\mathbf{u}_i)$ and introducing the two-particle probability density

$$p(\mathbf{r}_1,\mathbf{r}_2) \equiv \int \psi^2 d\mathbf{r}_3\cdots d\mathbf{r}_N \Big/ \int \psi^2 d\mathbf{r}_1\cdots d\mathbf{r}_N, \tag{5.5}$$

we are led to

$$E = -\frac{\hbar^2}{2m}\frac{1}{2}\sum_i \int (\nabla_i^2 \ln\phi_i)\gamma(\mathbf{u}_i)d\mathbf{r}_i + \sum_{i<j}\int \tilde{V}(r_{ij})p(\mathbf{r}_i,\mathbf{r}_j)d\mathbf{r}_i d\mathbf{r}_j. \tag{5.6}$$

With localized single-particle functions Saunders's derivation for $\gamma(\mathbf{u}_i)$ is altered. Now Eq. (4.5) no longer holds and Eq. (2.13) is replaced by

$$\gamma(\mathbf{u}_1) = (\text{const})\phi^2(\mathbf{u}_1)\prod_{k(\neq 1)}\int \gamma(\mathbf{u}_k)\chi^2(r_{1k})d\mathbf{r}_k. \tag{5.7}$$

In this form the degree of localization of $\gamma(\mathbf{u}_1)$ will depend crucially on that of $\phi^2(\mathbf{u}_1)$ which can contain variational parameters. An appropriate iteration procedure for solving this equation is to substitute $\phi^2(\mathbf{u}_k)$ for $\gamma(\mathbf{u}_k)$ on the right side of (4.9) and then solve for $\gamma(\mathbf{u}_1)$, etc. For *some* (not all) types of trial χ_{1k} it turns out that

$$\gamma(\mathbf{u}_1) \approx (\text{const.})\phi^2(\mathbf{u}_1) \tag{5.8}$$

since

$$\prod_{k(\neq 1)}\int \gamma(\mathbf{u}_k)\chi^2(r_{1k})d\mathbf{r}_k \approx \text{const}. \tag{5.9}$$

for the important values of $\mathbf{r}_1$ within the Wigner-Seitz cell around $\mathbf{R}_1$. We have verified this result for the correlation function and Gaussian single-particle function used by Nosanow.[5,13] Figure 3 illustrates that Eq. (5.8) is not too bad an approximation in this case. Note that the fact that the left side of Eq. (5.9) is a very broad function, almost constant throughout the cell, is now an advantage rather than a difficulty as it would be in the EMS theory.

A similar approximation scheme can be set up for the two-particle density. Write

$$p(\mathbf{r}_1,\mathbf{r}_2) = (\text{const})\phi^2(\mathbf{u}_1)\phi^2(\mathbf{u}_2)\chi^2(r_{12}) \times \int \prod_{k(\neq 1,2)} \chi^2(r_{1k})\chi^2(r_{2k}) \times[\text{remaining factors}]d\mathbf{r}_3\cdots d\mathbf{r}_N. \tag{5.10}$$

In the spirit of Eq. (4.2) we assume

$$[\text{remaining factors}] = \prod_{k(\neq 1,2)} \gamma(\mathbf{r}_k), \tag{5.11}$$

so that

$$p(\mathbf{r}_1,\mathbf{r}_2) = (\text{const.})\phi^2(\mathbf{u}_1)\phi^2(\mathbf{u}_2)\chi^2(r_{12}) \times\left[\prod_{k(\neq 1,2)}\int \chi^2(r_{1k})\chi^2(r_{2k})\gamma(\mathbf{r}_k)d\mathbf{r}_k\right]. \tag{5.12}$$

Now if Eq. (5.9) holds, it is reasonable to presume that the quantity in square brackets in (5.12) is near unity for all important values of $\mathbf{r}_1$, $\mathbf{r}_2$. Then

$$p(\mathbf{r}_1,\mathbf{r}_2) \cong \phi^2(\mathbf{u}_1)\phi^2(\mathbf{u}_2)\chi^2(r_{12}) \Big/ \int \phi_1^2\phi_2^2\chi_{12}^2 d\mathbf{r}_1 d\mathbf{r}_2,$$

where we have included the normalization constant.

With all these approximations, E reduces to

$$E = -\frac{\hbar^2}{4m}\sum_i \int \phi_i^2\nabla_i^2 \ln\phi_i d\mathbf{r}_i + \sum_{i<j}\frac{\int \phi_i^2\phi_j^2\chi_{ij}^2 \tilde{V}_{ij} d\mathbf{r}_i d\mathbf{r}_j}{\int \phi_i^2\phi_j^2\chi_{ij}^2 d\mathbf{r}_i d\mathbf{r}_j} \tag{5.13}$$

if we assume ϕ_i to be normalized. This quantity can be minimized as a function of the variational parameters. Equation (5.13) is just the approximation to the energy studied in Refs. 5 and 13, on the basis of a cluster-expansion procedure. One advantage of the cluster-expansion procedure is that it gives the correction terms to (5.13). Here we have correction factors in Eqs. (5.7) and (5.11) (and Fig. 3 indicates that these factors are sufficiently different from a constant that a serious theory along these lines would have to consider them); however, there are also the approximations of Eqs. (4.2) and (5.10) and we have no way of estimating the errors of those approximations. We note that the criterion found for convergence of the cluster expansion[13] is somewhat similar to the condition of Eq. (5.9).

There is a certain consistency in the approximations made in this section. The functions $\gamma(\mathbf{u}_1)$ and $p(\mathbf{r}_1,\mathbf{r}_2)$ obey a sequential equation because of their definitions in terms of the wave function, i.e.,

$$\gamma(\mathbf{u}_1) = \int p(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_2. \tag{5.14}$$

With our approximations this requires

$$\phi^2(\mathbf{u}_1) = \phi^2(\mathbf{u}_1)\left[\frac{\int \phi^2(\mathbf{u}_2)\chi^2(r_{12})d\mathbf{r}_2}{\int \phi_1^2\phi_2^2\chi_{12}^2 d\mathbf{r}_1 d\mathbf{r}_2}\right] \tag{5.15}$$

which holds approximately by virtue of (5.9).

With the localized $\phi(\mathbf{u}_i)$ it is possible to treat exchange effects in a consistent manner within the ap-

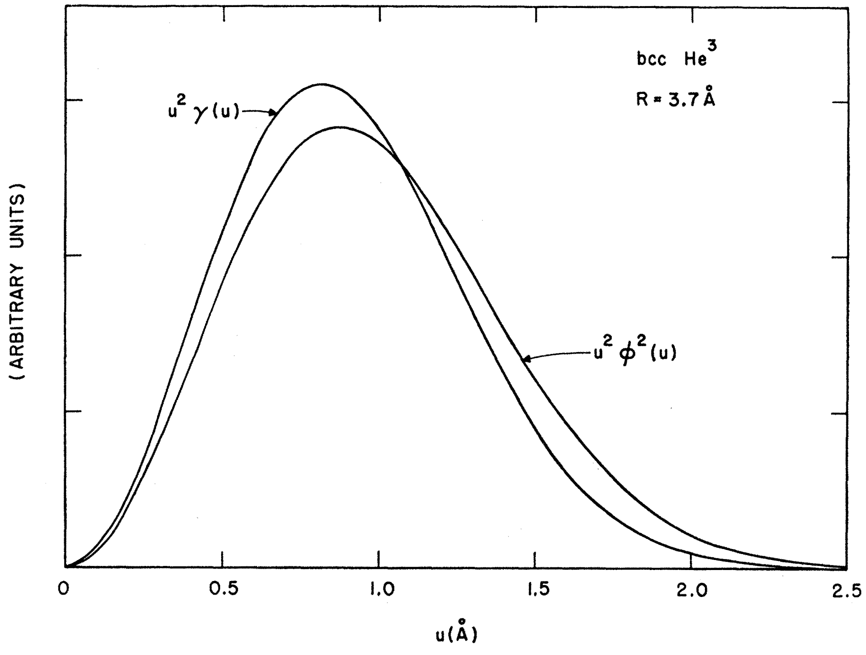

FIG. 3. An illustration of the accuracy of approximation (5.8) to the solution of Eq. (5.7). The function $\phi^2(u)$ is the approximate solution and $\gamma(u)$ is the exact solution. The curves are normalized to enclose equal areas as in Fig. 1.

proximations of this section. One simply antisymmetrizes the factor $\prod\phi(\mathbf{u}_i)$ in (5.1). The addition of antisymmetrization does not change the properties of $\phi(\mathbf{u}_i)$ (such as its localization) since exchange effects are only about 10^{-4} of the direct effects.[7] Thus our neglect of antisymmetrization in this section is a very good approximation. We shall not go into further details concerning exchange here, however.

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We wish to thank Paul Steinback for his help in the numerical work.

APPENDIX

Approximations have been used in our calculations of the single-particle probability density $\gamma(\mathbf{u}_i)$ and we discuss them here. Write Eq. (2.13) in the form

$$\gamma(\mathbf{u}_1)=\alpha\exp\left\{-\sum_{k(\neq 1)}\ln\left[\int\gamma(\mathbf{u}_k)\chi^2(r_{1k})d\mathbf{r}_k\right]\right\}. \quad \text{(A1)}$$

One approximation is to make $\gamma(\mathbf{u}_1)$ a spherically symmetric function of $u_1=|\mathbf{u}_1|$ only, by replacing the lattice sum over $\mathbf{R}_{k1}$ by an angular average over the directions of vector $\mathbf{R}_{k1}$ and a sum over magnitudes $R_{k1}=|\mathbf{R}_{k1}|$. That is,

$$\sum_{k(\neq 1)}=\sum_{\mathbf{R}_{k1}(\neq 0)}=\sum_{R_{k1}(\neq 0)}\frac{n(R_{k1})}{4\pi}\int d\Omega_{\mathbf{R}_{k1}}, \quad \text{(A2)}$$

where $n(R_{k1})$ is the number of particles in the shell at distance R_{k1}. Some simple integrations then give the result

$$\gamma(u_1)=\alpha\exp\left\{\sum_{R_{k1}(\neq 0)}\frac{n(R_{k1})}{2u_1R_{k1}}\times\int_{|u_1-R_{k1}|}^{u_1+R_{k1}}dt\,t\ln\left[\int_0^\infty dx\,x\gamma(x)F(x,t)\right]\right\}, \quad \text{(A3)}$$

with

$$F(x,t)\equiv\frac{1}{t}\int_{|x-t|}^{x+t}dy\,y\chi^2(y). \quad \text{(A4)}$$

The integrations are performed numerically. Sufficient accuracy results for our purpose, if we sum over only the first thirteen shells of particles for bcc ^{3}He.