Approximate Solution of a Finite Many-Particle System with Translational Invariance. I*

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(Received 22 June 1964)

A formal technique is developed to study internal properties of finite many-particle systems possessing translational invariance. The basic objective is to discover a method of calculating, in a modified shell model, average values of operators referred to the center of mass, particularly those which have to do with the surface of the system, such as the density of particles. The formalism is based on the method of redundant variables, in which the shell-model wave function describes the internal degrees of freedom of the system, while a superfluous variable is introduced to satisfy the conservation law and to handle the collective motion. The spurious degeneracy which results from the introduction of the extra variable is removed by suitable subsidiary conditions. With the aid of these restricted solutions, it is shown that the density with respect to the center of mass can be calculated in terms of a one-body operator. The dynamics of the system is then formulated in terms of density matrices suitably defined from these restricted solutions. Within the context of the modified shell model, the density matrices consist of the Dirac density matrices of the shell model plus correction terms which depend nonlinearly on these Dirac matrices and matrix elements of the coordinate X. The single-particle states of the shell model are finally chosen to minimize the expectation of the Hamiltonian. The resulting variational equation contains a homogeneous part which has the structure of the conventional Hartree-Fock equation together with an inhomogeneous term depending nonlinearly on the single-particle states. The solution of this equation is finally expanded about the nontranslationally invariant Hartree-Fock solution to first order in perturbation theory.

I. INTRODUCTION

IT is a well-established law that total linear momentum is conserved for dynamical systems which are isolated from external influences. The law emerges quantum mechanically as a consequence of the invariance of the Hamiltonian function H with respect to arbitrary translations of the origin of coordinates. More precisely, the total linear momentum $\mathbf{P}_c$ commutes with H, and the eigenfunctions of H may be chosen as simultaneous eigenfunctions of $\mathbf{P}_c$, i.e.,

$$\psi_{\mathbf{k},n}=e^{i\mathbf{k}\cdot\mathbf{R}_c}\varphi_{0,n}, \tag{1.1}$$

where $\mathbf{R}_c$ is the coordinate describing the center of mass and $\varphi_{0,n}$ is a zero-momentum eigenfunction satisfying $\mathbf{P}_c\varphi_{0,n}=0$. Except for a phase factor, the eigenstates of H are therefore translationally invariant. Although in any practical situation one is seldom so fortunate as to obtain exact eigenfunctions of H, one believes that any reasonable description of the system should be consistent with this conservation law.

In recent years the connection between long-range correlations involving many particles and the conservation law for the associated collective variable has been widely studied.[1,2] The role of center-of-mass correlations in particular has for a long time demanded attention in nuclear physics. The center-of-mass problem in many-particle systems has three inherent difficulties:

First, if one attempts to calculate the density of particles as the expectation value in the state (1.1) of the one-body operator

$$\sum_{i=1}^{N}\delta(\mathbf{x}-\mathbf{x}_i)=\sum_{i=1}^{N}e^{-i\mathbf{x}\cdot\mathbf{p}_i/\hbar}\delta(\mathbf{x}_i)e^{i\mathbf{x}\cdot\mathbf{p}_i/\hbar}$$

$$=\sum_{i=1}^{N}e^{-i\mathbf{x}\cdot\mathbf{P}_c/\hbar}\delta(\mathbf{x}_i)e^{i\mathbf{x}\cdot\mathbf{P}_c/\hbar}, \tag{1.2}$$

where

$$\mathbf{P}_c=\sum_{i=1}^{N}\mathbf{p}_i,$$

one obtains a constant, since (1.1) is an eigenfunction of $\mathbf{P}_c$, and the expectation value of

$$\sum_{i=1}^{N}\delta(\mathbf{x}_i)$$

is a constant. It is well known, however, that a many-particle system in a bound state has a well-defined distribution of particles about its center of mass. The fact that the calculated density is constant means that the true distribution is being averaged over all positions of the center of mass. To study surface effects, for example, or other effects which depend on the center of

* Jointly supported by Advanced Research Projects Agency through the U. S. Office Naval Research Contract Nonr-285(49), and the U. S. Army Research Office-Durham through Grant No. DA-ARO-(D)-31-124-G276.

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[1] H. Lipkin, Ann. Phys. (N. Y.) 12, 452 (1961).

[2] H. Lipkin, Ann. Phys. (N. Y.) 9, 272 (1959).

mass, one must refer all operators to the center of mass. This is unpleasant because these operators are of the N-particle type.

Secondly, if one separates the center-of-mass motion for a system of N particles, one cannot rewrite the Hamiltonian describing the internal dynamics in a symmetric way, since the $N-1$ vector coordinates which remain do not treat the particles symmetrically. It becomes very difficult, therefore, to impose the Pauli principle on the internal wave function.

The third difficulty has to do with the degree to which the independent particle picture has dominated our thinking. If one contemplates a shell model, one encounters the following dilemma. Since the conservation of linear momentum means that any change in the momentum of one particle correlates with changes of momenta of all other particles, the one-particle states of a shell model wave function must be plane waves. However, plane wave states cannot describe a bound system, since in order to form a bound complex the particles must be localized relative to each other either by being localized to some preferred origin or by being correlated in motion. These alternatives are, unfortunately, inconsistent with the conservation of momentum, on the one hand, and the shell model picture on the other.

There are two classes of investigations which have been proposed to describe aspects of translationally invariant finite systems. The first, which predates the second, adopts the point of view that total linear momentum is a collective variable having little to do with certain internal aspects of the system, and that it is pointless to sacrifice the flexibility of the independent particle picture and the Hartree-Fock method in an attempt to conserve momentum. These result in errors of the order of $1/N$ in the calculation of level spectra, electric and magnetic moments, binding energies, and transition rates when approximate wave functions ignoring the motion of the center of mass are used. These corrections are of course important for nuclei of small mass number, and must be included if the accuracy of the calculated quantities is also of order $1/N$.

The second approach[3] attempts to formulate, by means of wave functions which violate momentum conservation, a theory which is consistent with the conservation law. Among the most typical of these are the following. In the method of generator coordinates,[4,5] Griffin and Wheeler develop a variational principle with the aid of wave functions which are translational averages of independent particle functions. In the method of redundant variables,[6–9] superfluous degrees of freedom are introduced to allow for the possibility of simultaneously satisfying the conservation of momentum while describing the internal properties of the system in terms of shell-model wave functions. The method of Gartenhaus and Schwartz[10] explicitly exhibits a unitary operator which enables one to project from a many-particle function its translationally invariant part. Klein and Kerman[11] formulate a generalized Hartree-Fock scheme in which the single-particle states to be determined self-consistently are labeled both by the particle variables and the quantum numbers of the collective motion. In somewhat similar spirit, Bolsterli[12] presents a technique for solving the N-particle problem in terms of N- to $(N+1)$-particle amplitudes which are invariant under translations in both configuration and velocity space. These methods have been applied with reasonable success to the calculation of the $1/N$ corrections to measurable quantities. However, little attention has been given to discovering a density of particles which displays surface structure.

In the present work we seek to achieve two objectives. First, we show that within the framework of the method of redundant variables, it is possible to define the density of particles referred to the center of mass in terms of a one-body operator, and to introduce density matrices in terms of which properties depending on the surface of the system may be calculated. In the method of redundant variables, the actual dynamical system is embedded in an enlarged system S, whose degrees of freedom are increased by a superfluous coordinate $\mathbf{R}$. By this means, one introduces a spurious degeneracy of eigenstates of the system, since the wave functions in the enlarged space are products of the eigenstates of the actual Hamiltonian with an arbitrary function $u(\mathbf{R})$. A canonical transformation is then invented to an image space S', defined by intrinsic variables which are in one-to-one correspondence with the actual particle coordinates. The solutions of the enlarged system S, which are equivalent to the solutions of the original system, are those satisfying suitable subsidiary restrictions. We shall demonstrate that the choice of the subsidiary condition

$$|u(\mathbf{R})|^2=\delta(\mathbf{R})$$

has the virtue that a conventional calculation in the image space S' of the density via a one-body operator of the form (1.2) has the meaning of a density referred to the center of mass in the actual system. We then introduce in the image space a sequence of density

[3] H. Lipkin, Phys. Rev. **110**, 1395 (1958).
[4] J. Griffin and J. Wheeler, Phys. Rev. **108**, 311 (1957).
[5] R. Peierls and J. Yoccoz, Proc. Phys. Soc. (London) **A70**, 381 (1957).
[6] H. Lipkin, A. de-Shalit, and I. Talmi, Nuovo Cimento **2**, 773 (1955).
[7] T. Tamura, Nuovo Cimento **4**, 713 (1956).
[8] R. Skinner, Can. J. Phys. **34**, 901 (1956).
[9] F. Villars, Ann. Rev. Nucl. Sci. **7**, 185 (1957).
[10] S. Gartenhaus and C. Schwartz, Phys. Rev. **108**, 482 (1957).
[11] A. Klein and A. Kerman, Phys. Rev. **132**, 1326 (1963).
[12] M. Bolsterli, Phys. Rev. **129**, 2830 (1963).

matrices which are equivalent to, but have more direct physical meaning than, the wave function.

The second objective is to formulate a technique in which the wave function only approximately satisfies the remaining subsidiary restriction. In general, the exact eigenfunction of H in the enlarged space S is $u(\mathbf{R})\psi_n(\mathbf{r}_i)$, where $\mathbf{P}\psi_n=0$ and $\mathbf{P}$ is the momentum conjugate to $\mathbf{R}$. We will relax the condition on ψ_n to admit approximate solutions of the form $u(\mathbf{R})\psi_n(\mathbf{r}_i,\mathbf{R})$ so that, when transformed to the image space S', the function $\psi_n(\mathbf{r}_i(\mathbf{r}_i',\mathbf{R}'),\mathbf{R}(\mathbf{r}_i'))$ may be of the determinantal form $\det(\varphi_i(\mathbf{r}_j'))$. In terms of this approximate wave function, the density matrices are then expressible as the usual Dirac density matrices plus correction terms which are themselves nonlinear combinations of Dirac matrices and matrix elements of the coordinate x between pairs of one-body states φ_i. The correction terms are of course peculiar to the choice of a δ function for the function $u(\mathbf{R})$. The single-particle states φ_i are finally chosen to minimize the energy. The resulting variational equation has the structure of the usual Hartree-Fock equation plus an inhomogeneous term which depends nonlinearly on the states φ_i. The form of this equation strongly suggests the possibility of expanding φ_i in a perturbation series about the translationally invariant solution of the Hartree-Fock equation. This procedure is outlined to first order in perturbation theory. Although it was not possible to show directly for general pair potentials the order of neglected contributions to the energy when only the Hartree-Fock solutions are used, it is reasonably straightforward to do so in any specific case, and one suspects that such corrections are at most of order $1/N^2$. However, it is certain that one must go beyond the Hartree-Fock solutions when calculating matrix elements of other quantities.

In Sec. II we investigate in a first-quantized picture the meaning of a density with respect to the center of mass. We review the essential features of the method of redundant variables, and offer an explicit proof that the expectation value of the operator (1.2) calculated in the image space S' is the appropriate prescription. Section III is devoted to the dynamical description of the system within the modified shell model. We derive the formulas linking the density matrices for the problem with the Dirac density matrices using a functional approach. The variational equation for the single-particle states of the model is obtained, and the perturbative expansion of these states about the translationally invariant Hartree-Fock solutions is generated.

II. THE DENSITY FUNCTION

In a first quantized theory, the probability density for finding a particle in the neighborhood of a point $\mathbf{x}$ is the expectation value of the operator

$$\sum_{i=1}^{N}\delta(\mathbf{x}-\mathbf{r}_i) \tag{2.1}$$

with respect to the exact ground state of the N-particle system. The generalization to a distribution referred to the center of mass introduces at once the difficulty of computing matrix elements of N-body operator

$$\sum_{i=1}^{N}\delta\left\{\mathbf{x}-\left(\mathbf{r}_i-\frac{1}{N}\sum_{j=1}^{N}\mathbf{r}_j\right)\right\}. \tag{2.2}$$

In a density matrix formalism, this would require a knowledge of the N-particle matrix, and hence the solution of the first N equations of the hierarchy, which is of course highly impractical. This difficulty may conceivably be circumvented by isolating the center-of-mass motion by means of a canonical transformation to center-of-mass and relative variables. However, due to the linear dependence of the intrinsic variables, a one-to-one correspondence cannot be made between the N particle coordinates of the actual system and the $(N-1)$ independent intrinsic vector variables. Thus an identification of the new variables as particle coordinates is not possible, and the meaning of an independent particle model becomes obscure.

The method of redundant variables,[8–10] as we shall demonstrate in the following, has the advantage of preserving the meaning of particle coordinates while allowing the prescription of the density function in terms of a one-body operator. Consider a system of N fermions described by the translationally invariant Hamiltonian

$$H(\mathbf{x},\mathbf{p})=\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}+\tfrac{1}{2}\sum_{i\neq j}v(\mathbf{r}_i-\mathbf{r}_j) \tag{2.3}$$

on the domain $(\mathbf{x},\mathbf{p})$. If one performs the separation

$$H(\mathbf{x},\mathbf{p})=H_r(\mathbf{x},\mathbf{p})+H_{\text{c.m.}}, \tag{2.4}$$

where

$$H_r(\mathbf{x},\mathbf{p})=\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}-\frac{1}{2mN}\Big(\sum_{j=1}^{N}\mathbf{p}_j\Big)^2+\tfrac{1}{2}\sum_{i\neq j}v(\mathbf{r}_i-\mathbf{r}_j)$$

$$=\frac{1}{4mN}\sum_{i,j=1}^{N}(\mathbf{p}_i-\mathbf{p}_j)^2+\tfrac{1}{2}\sum_{i\neq j}v(\mathbf{r}_i-\mathbf{r}_j) \tag{2.5}$$

and

$$H_{\text{c.m.}}=\frac{1}{2mN}\Big(\sum_{j=1}^{N}\mathbf{p}_j\Big)^2. \tag{2.6}$$

It is readily seen that the eigenfunctions of H are products of the form

$$\psi_n(\mathbf{x})=\exp\{i\mathbf{k}\cdot\sum_{i=1}^{N}\mathbf{r}_i\}\,\varphi_{0n}(\cdots\mathbf{r}_k-\mathbf{r}_l\cdots) \tag{2.7}$$

with

$$\mathbf{P}'\varphi_{0n}=0, \quad \mathbf{P}'=\sum_{i=1}^{N}\mathbf{p}_i.$$

Thus, associated with each intrinsic state φ_{0n} defined by the eigenvalue equation

$$H_r\varphi_{0n}=E_n\varphi_{0n},$$

there is a continuous spectrum of center-of-mass motion.

We next insert our dynamical system in an enlarged system by augmenting the coordinate domain with the redundant variable $\mathbf{R}$ and its conjugate momentum $\mathbf{P}$, and by simultaneously extending the definition of the Hamiltonian to read

$$\hat{H}(\mathbf{x},\mathbf{p};\mathbf{R},\mathbf{P})\equiv H(\mathbf{x},\mathbf{p}). \tag{2.8}$$

Since $\hat{H}$ is independent of $\mathbf{P}$, $\hat{H}$ clearly commutes with $\mathbf{R}$, and therefore this embedding process has the sole consequence of introducing an infinite degeneracy into the eigenstates of H. The eigenfunctions of $\hat{H}$ are given by

$$\hat{\psi}_n(\mathbf{x},\mathbf{R})=\psi_n(\mathbf{x})u(\mathbf{R}), \tag{2.9}$$

$u(\mathbf{R})$ being any normalizable function of $\mathbf{R}$. The enlarged system is equivalent to the actual dynamical system in the sense that the expectation value of physical operators, namely, those defined in terms of $\mathbf{x}$ and $\mathbf{p}$, may be calculated equally well in either system.

With this extension of domain, we are now in a position to introduce a canonical transformation to new variables $(\mathbf{x}',\mathbf{p}';\mathbf{R}',\mathbf{P}')$ which are in one-to-one correspondence with the set $(\mathbf{x},\mathbf{p};\mathbf{R},\mathbf{P})$. The one-to-one character of the transformation preserves the meaning of the particle coordinates, while the demand that the transformation be canonical guarantees the invariance of the commutation relations between coordinates and their conjugate momenta and the existence of a Heisenberg equation in the image space. The transformation equations are as follows:

$$\begin{aligned}\mathbf{r}_i&=\mathbf{r}_i'-\frac{1}{N}\sum_{j=1}^{N}\mathbf{r}_j'+\mathbf{R}'; \quad \mathbf{R}=\frac{1}{N}\sum_{i=1}^{N}\mathbf{r}_i',\\ \mathbf{p}_i&=\mathbf{p}_i'-\frac{1}{N}\sum_{j=1}^{N}\mathbf{p}_j'+\mathbf{P}'; \quad \mathbf{P}=\sum_{i=1}^{N}\mathbf{p}_i'.\end{aligned} \tag{2.10}$$

The fact that the inverse of the transformation (2.10) is obtained simply by the replacements

$$\begin{aligned}&\mathbf{r}_i\rightleftarrows\mathbf{r}_i'; \quad \mathbf{R}\rightleftarrows\mathbf{R}'\\ &\mathbf{p}_i\rightleftarrows\mathbf{p}_i'; \quad \mathbf{P}\rightleftarrows\mathbf{P}'\end{aligned}$$

reflects the remarkable symmetry of the defining equations.

The mathematical consequences of (2.10) are immediately apparent from Eqs. (2.4)–(2.9), once one observes that the difference coordinates and momenta are invariant, i.e.,

$$\mathbf{r}_i-\mathbf{r}_j\rightarrow\mathbf{r}_i'-\mathbf{r}_j'; \quad \mathbf{p}_i-\mathbf{p}_j\rightarrow\mathbf{p}_i'-\mathbf{p}_j'.$$

The Hamiltonian $\hat{H}(\mathbf{x},\mathbf{p};\mathbf{R},\mathbf{P})$ transforms into

$$H'(\mathbf{x}',\mathbf{p}';\mathbf{R}',\mathbf{P}')=\frac{1}{4mN}\sum_{i,j=1}^{N}(\mathbf{p}_i'-\mathbf{p}_j')^2+\tfrac{1}{2}\sum_{i\neq j}v(\mathbf{r}_i'-\mathbf{r}_j')+\frac{\mathbf{P}'^2}{2mN} \tag{2.11}$$

with the associated eigenfunction

$$\Psi_n'(\mathbf{x}',\mathbf{R}')=\varphi_{0n}(\cdots\mathbf{r}_k'-\mathbf{r}_l'\cdots)e^{i\mathbf{k}\cdot\mathbf{R}'}u\left(\frac{1}{N}\sum_{i=1}^{N}\mathbf{r}_i'\right). \tag{2.12}$$

The dependence of (2.12) on the quantity

$$\frac{1}{N}\sum_{i=1}^{N}\mathbf{r}_i'$$

is especially convenient since, as can be verified directly, the associated operator commutes with H'.

We now append the subsidiary conditions which are necessary to extract the required subset of solutions of the enlarged system. In order to relieve us of the necessity of carrying the dependence of H' on the variable $\mathbf{P}'$, we demand that the eigenvalue k be zero. Secondly, we restrict the arbitrariness of the function u in a way which leads to a definition of a density with respect to the center of mass. Since both the operators

$$\frac{1}{N}\sum_{i=1}^{N}\mathbf{r}_i' \quad \text{and} \quad \sum_{i=1}^{N}\mathbf{p}_i'$$

commute with H', the function u may in general be chosen to be the eigenfunction of any reasonable function of these operators. In particular, the choice of u as an eigenfunction of

$$\sum_{i=1}\mathbf{p}_i'$$

reduces the wave function (2.12) trivially to the translationally invariant function (2.7), and the only departure from the original $\mathbf{x}$-space analysis is the requirement to use the intrinsic Hamiltonian in calculating the energy. As we shall show in the following, the appropriate choice of u for our purpose is

$$|u|^2=\delta(\sum_{i=1}^{N}\mathbf{r}_i'),$$

i.e., u is required to be an eigenfunction of

$$\sum_{i=1}^{N}\mathbf{r}_i'.$$

It now remains to be demonstrated explicitly that

the density function calculated in the $\mathbf{x}'-\mathbf{R}'$ space from the one-body operator

$$\sum_{i=1}^{N}\delta(\mathbf{z}-\mathbf{r}_i')$$

($\mathbf{z}$ is some point in $\mathbf{x}'$ space) does indeed reduce to the density referred to the center of mass in the actual system. To show this, it is more convenient to utilize an alternate form for this operator, viz.,

$$\sum_{i=1}^{N}e^{-i\mathbf{z}\cdot\mathbf{p}_i'/\hbar}\delta(\mathbf{r}_i')e^{i\mathbf{z}\cdot\mathbf{p}_i'/\hbar}. \tag{2.13}$$

In the $\mathbf{x}'-\mathbf{R}'$ space, the density function is defined to be the matrix element

$$n(\mathbf{z})=\sum_{i=1}^{N}\int d\mathbf{R}'\prod_{j=1}^{N}d\mathbf{r}_j'\,\varphi^*(\cdots\mathbf{r}_k'-\mathbf{r}_l'\cdots)\delta\left(\frac{1}{N}\sum_{m=1}^{N}\mathbf{r}_m'\right)e^{-i\mathbf{z}\cdot\mathbf{p}_i'/\hbar}\delta(\mathbf{r}_i')e^{i\mathbf{z}\cdot\mathbf{p}_i'/\hbar}\varphi(\cdots\mathbf{r}_k'-\mathbf{r}_l'\cdots).$$

We now employ the relation

$$\sum_{j=1}^{N}\mathbf{p}_j'\varphi(\cdots\mathbf{r}_k'-\mathbf{r}_l'\cdots)=0 \tag{2.14}$$

and the properties of the translation operator to rewrite the expression for $n(\mathbf{z})$ as follows:

$$\begin{aligned}n(\mathbf{z})=\sum_{i=1}^{N}\int d\mathbf{R}'\prod_{j=1}^{N}d\mathbf{r}_j'\,\varphi^*(\cdots\mathbf{r}_k'-\mathbf{r}_l'\cdots)\delta\left(\frac{1}{N}\sum_{m=1}^{N}\mathbf{r}_m'\right)\exp\left\{-\frac{i\mathbf{z}}{\hbar N}\cdot\sum_{n=1}^{N}\mathbf{p}_n'\right\}\\ \times\exp\left\{-\frac{i\mathbf{z}}{\hbar}\cdot\left(\mathbf{p}_i'-\frac{1}{N}\sum_{n=1}^{N}\mathbf{p}_n'\right)\right\}\delta(\mathbf{r}_i')\exp\left\{\frac{i\mathbf{z}}{\hbar}\cdot\left(\mathbf{p}_i'-\frac{1}{N}\sum_{n=1}^{N}\mathbf{p}_n'\right)\right\}\varphi(\cdots\mathbf{r}_k'-\mathbf{r}_l'\cdots)\\ =\sum_{i=1}^{N}\int d\mathbf{R}'\prod_{j=1}^{N}d\mathbf{r}_j'\,\varphi^*(\cdots\mathbf{r}_k'-\mathbf{r}_l'\cdots)\delta\left(\frac{\mathbf{z}}{N}+\frac{1}{N}\sum_{m=1}^{N}\mathbf{r}_m'\right)\exp\left\{-\frac{i\mathbf{z}}{\hbar}\cdot\left(\mathbf{p}_i'-\frac{1}{N}\sum_{n=1}^{N}\mathbf{p}_n'\right)\right\}\delta(\mathbf{r}_i')\\ \times\exp\left\{\frac{i\mathbf{z}}{\hbar}\cdot\left(\mathbf{p}_i'-\frac{1}{N}\sum_{n=1}^{N}\mathbf{p}_n'\right)\right\}\varphi(\cdots\mathbf{r}_k'-\mathbf{r}_l'\cdots).\end{aligned}$$

Transforming to the $\mathbf{x}-\mathbf{R}$ space by means of the Eqs. (2.10), we obtain

$$\begin{aligned}n(\mathbf{z})=\sum_{i=1}^{N}\int d\mathbf{R}\prod_{j=1}^{N}d\mathbf{r}_j\varphi^*(\cdots\mathbf{r}_k-\mathbf{r}_l\cdots)\delta\left(\frac{\mathbf{z}}{N}+\mathbf{R}\right)\exp\left\{-\frac{i\mathbf{z}}{\hbar}\cdot\left(\mathbf{p}_i-\frac{1}{N}\sum_{n=1}^{N}\mathbf{p}_n\right)\right\}\delta\left(\mathbf{r}_i-\frac{1}{N}\sum_{m=1}^{N}\mathbf{r}_m+\mathbf{R}\right)\\ \times\exp\left\{\frac{i\mathbf{z}}{\hbar}\cdot\left(\mathbf{p}_i-\frac{1}{N}\sum_{n=1}^{N}\mathbf{p}_n\right)\right\}\varphi(\cdots\mathbf{r}_k-\mathbf{r}_l\cdots).\end{aligned}$$

If the relation (2.7) is now used to eliminate terms involving the total momentum, we have, upon performing the $\mathbf{R}$ integration,

$$\begin{aligned}n(\mathbf{z})&=\sum_{i=1}^{N}\int\prod_{j=1}^{N}d\mathbf{r}_j\varphi^*(\cdots\mathbf{r}_k-\mathbf{r}_l\cdots)\exp\left[-\frac{i\mathbf{z}}{\hbar}\cdot\mathbf{p}_i\right]\delta\left(\mathbf{r}_i-\frac{1}{N}\sum_{m=1}^{N}\mathbf{r}_m-\frac{\mathbf{z}}{N}\right)\exp\left[\frac{i\mathbf{z}}{\hbar}\cdot\mathbf{p}_i\right]\varphi(\cdots\mathbf{r}_k-\mathbf{r}_l\cdots)\\ &=\sum_{i=1}^{N}\int\prod_{j=1}^{N}d\mathbf{r}_j|\,\varphi(\cdots\mathbf{r}_k-\mathbf{r}_l\cdots)|^2\delta\left(\mathbf{r}_i-\frac{1}{N}\sum_{m=1}^{N}\mathbf{r}_m-z\right),\end{aligned}$$

which is by definition the density referred to the center of mass.

We have shown in the preceding that we may study internal aspects of the actual system by the conventional techniques of computing expectation values of one- and two-body operators, provided we work in the $\mathbf{x}'-\mathbf{R}'$ space with the modified Hamiltonian

$$H=\sum_{i=1}^{N}\frac{\mathbf{p}_i'^2}{2m}-\frac{(\sum_{i=1}\mathbf{p}_i')^2}{2mN}+\tfrac{1}{2}\sum_{i\neq j}v(\mathbf{r}_i'-\mathbf{r}_j') \tag{2.15}$$

together with the eigenfunction

$$\Psi' = \varphi_{0n}(\cdots \mathbf{r}_k' - \mathbf{r}_l' \cdots)\delta^{1/2}(\sum_{i=1}^{N} \mathbf{r}_i'). \quad (2.16)$$

In particular, the density with respect to the center of mass in the actual system is the expectation in the state (2.16) of the one-body operator

$$\sum_{i=1}^{N} \delta(\mathbf{x} - \mathbf{r}_i').$$

III. THE INTRINSIC INDEPENDENT-PARTICLE MODEL

In order to develop an approximation scheme, it is most convenient first to transcribe the foregoing into a density matrix formalism. Accordingly, we introduce the class of averages

$$\langle \mathbf{x}_1' \cdots \mathbf{x}_n' | \Gamma^{(n)} | \mathbf{x}_1 \cdots \mathbf{x}_n \rangle = \langle NE\mathbf{R} | \psi^\dagger(\mathbf{x}_1) \cdots \psi^\dagger(\mathbf{x}_n)\psi(\mathbf{x}_n') \cdots \psi(\mathbf{x}_1') | NE\mathbf{R} \rangle \quad (3.1)$$

where the operators $\psi^\dagger(\mathbf{x})$ and $\psi(\mathbf{x})$ are Fermion creation and annihilation operators, and the matrix elements of interest are to be taken with respect to the exact ground state of the system consistent with fixed particle number N, energy E, and position of the center of mass $\mathbf{R}$. The role of the quantity $\mathbf{R}$ in the above definition is seen most clearly by determining what restrictions are imposed on the density matrices by the subsidiary condition, and discovering what ansatz for the ground state is consistent with these restrictions.

The subsidiary condition demands that the operator

$$\mathbf{X} = \int d\mathbf{x} \psi^\dagger(\mathbf{x}) \mathbf{x} \psi(\mathbf{x}), \quad (3.2)$$

the second quantized equivalent of the symmetric one-body operator

$$\sum_{m=1}^{N} \mathbf{r}_m',$$

annihilate the state function $|NE\mathbf{R}\rangle$, or equivalently, that $\mathbf{X}$ commute with the density matrices. Since the commutator of $\mathbf{X}$ with the product

$$\psi^\dagger(\mathbf{x}_1) \cdots \psi^\dagger(\mathbf{x}_n)\psi(\mathbf{x}_n') \cdots \psi(\mathbf{x}_1')$$

merely multiplies the latter by a factor

$$\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{x}_i'),$$

it is clear that

$$\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{x}_i') \langle \mathbf{x}_1' \cdots \mathbf{x}_n' | \Gamma^{(n)} | \mathbf{x}_1 \cdots \mathbf{x}_n \rangle = 0, \quad (3.3)$$

which is the requirement that the n-body density matrix contain a factor

$$\delta(\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{x}_i')).$$

It is now readily verified that if the representation in configuration space of $|NE\rangle$ is the amplitude

$$\langle \mathbf{x}_1 \cdots \mathbf{x}_N | NE \rangle = \langle 0 | \psi(\mathbf{x}_1) \cdots \psi(\mathbf{x}_N) | NE \rangle = \phi_{0n},$$

in (2.16), then the ansatz for $|NE\mathbf{R}\rangle$ is

$$|NE\mathbf{R}\rangle = \int d\mathbf{s} e^{i\mathbf{s}\cdot\mathbf{X}} |NE\rangle.$$

A straightforward application of the relation

$$e^{i\mathbf{s}\cdot\mathbf{X}} \psi^\dagger(\mathbf{x}) e^{-i\mathbf{s}\cdot\mathbf{X}} = e^{i\mathbf{s}\cdot\mathbf{x}} \psi^\dagger(\mathbf{x})$$

to the definition $\bar{\Psi}' = \langle \mathbf{x}_1 \cdots \mathbf{x}_n | NE\mathbf{R} \rangle$ yields the expression (2.16), while the definition (3.1) reduces to

$$\langle \mathbf{x}_1' \cdots \mathbf{x}_n' | \Gamma^{(n)} | \mathbf{x}_1 \cdots \mathbf{x}_n \rangle = \delta(\sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{x}_i')) \langle \mathbf{x}_1' \cdots \mathbf{x}_n' | \bar{\Gamma}^{(n)} | \mathbf{x}_1 \cdots \mathbf{x}_n \rangle$$

where the reduced matrix

$$\langle \mathbf{x}_1' \cdots \mathbf{x}_n' | \bar{\Gamma}^{(n)} | \mathbf{x}_1 \cdots \mathbf{x}_n \rangle = \int d\boldsymbol{\lambda} \langle NE | e^{i\boldsymbol{\lambda}\cdot\mathbf{X}} \psi^\dagger(\mathbf{x}_1) \cdots \psi(\mathbf{x}_1') | NE \rangle. \quad (3.4)$$

The exact description of a system in terms of density matrices requires in principle the simultaneous solution of the set of hierarchy equations. However, in any practical situation, nontrivial solutions can only be obtained by truncating this hierarchy at low order, since the equations of motion couple density matrices of various orders. In order to indicate the direction to be followed in making such an approximation, we return temporarily to the line of reasoning in Sec. II. We demonstrated that the wave function appropriate to the definition of a density with respect to the center of mass is

$$\Psi' = \varphi_{0n}(\cdots \mathbf{r}_k' - \mathbf{r}_l' \cdots)\delta^{1/2}(\sum_{i=1}^{N} \mathbf{r}_i'),$$

where φ_{0n} is a zero momentum wave function, and hence cannot be expressed in determinantal form except for the case of plane waves. In order to generate an approximation which is manageable, we shall relax the condition

$$\sum_{i=1}^{N} \mathbf{p}_i' \varphi_{0n} = 0$$

by considering approximate solutions of the form

$$\delta^{1/2}(\sum_{i=1}^{N} \mathbf{r}_i') \hat{\varphi}(\mathbf{r}_i', \sum_{k=1}^{N} \mathbf{r}_k'), \quad (3.5)$$

where $\hat{\varphi}$ is of determinantal form; the single-particle states so introduced are no longer required to be translationally invariant. We shall see that there are some similarities of form to the Hartree-Fock method. This approximate description might be expected to be reasonable if the forces are slowly varying and long range, and to include the most essential features of the correlations associated with the collective motion.

The independent-particle characteristics of non-translationally invariant systems find their expression traditionally in the Hartree-Fock equation, where the one-particle states collectively define a self-consistent one-particle potential. The essential ingredient from our standpoint is the prescription of a product state which minimizes the energy. In somewhat the same spirit, we introduce what we shall call an intrinsic independent-particle model by defining

$$|NE\rangle=\prod_{i=1}^{N} a_i^\dagger|0\rangle$$

$$=\prod_{i=1}^{N}\int d\mathbf{x}u_i(\mathbf{x})\psi^\dagger(\mathbf{x})|0\rangle,$$

in which the connection between the operators $\psi(\mathbf{x})$ and a_i is via the familiar superposition in terms of orthonormal one-particle states $u_i(\mathbf{x})$, i.e.,

$$\psi(\mathbf{x})=\sum_{i=1}^{\infty} u_i(\mathbf{x})a_i, \quad a_i|0\rangle=0.$$

Our ultimate objective is to obtain relations between the density matrices $\langle|\bar{\Gamma}|\rangle$ which may be conveniently handled, and for this purpose we employ a functional approach. To begin with, we derive a generating functional F from which the matrices of interest can be recovered by functional differentiation.

Let us consider the quantity

$$Z_M=\langle ME|e^{i\boldsymbol{\lambda}\cdot\mathbf{X}}|ME\rangle$$

$$=\left\langle 0\left|\prod_{i=1}^{M}\left(\int d\mathbf{y}u_i^*(\mathbf{y})e^{i\boldsymbol{\lambda}\cdot\mathbf{y}}\psi(\mathbf{y})\right)\right.\right.$$

$$\left.\left.\times\prod_{j=1}^{M}\left(\int d\mathbf{x}u_j(\mathbf{x})\psi^\dagger(\mathbf{x})\right)\right|0\right\rangle. \quad (3.6)$$

We may rewrite Z_M in the more suggestive form

$$Z_M=\frac{1}{M!}\left\langle 0\left|:\left(\int d\mathbf{x}d\mathbf{y}\rho(\mathbf{y},\mathbf{x};\boldsymbol{\lambda})\psi(\mathbf{y})\psi^\dagger(\mathbf{x})\right)^M:\right|0\right\rangle, \quad (3.7)$$

where

$$\rho(\mathbf{y},\mathbf{x};\boldsymbol{\lambda})=e^{i\boldsymbol{\lambda}\cdot\mathbf{y}}\sum_{i=1}^{M}u_i^*(\mathbf{y})u_i(\mathbf{x}),$$

and the dots represent an ordering of operators in which the creation operators appear to the right of the destruction operators. This expression may be verified by a simple application of the binomial theorem as follows:

$$\left(\int d\mathbf{x}d\mathbf{y}\,\rho(\mathbf{y},\mathbf{x};\boldsymbol{\lambda})\psi(\mathbf{y})\psi^\dagger(\mathbf{x})\right)^M=\sum_{n_1+n_2+\cdots+n_M=M} M!\prod_{i=1}^{M}\frac{1}{n_i!}\left(\int d\mathbf{x}d\mathbf{y}e^{i\boldsymbol{\lambda}\cdot\mathbf{y}}u_i^*(\mathbf{y})u_i(\mathbf{x})\psi(\mathbf{y})\psi^\dagger(\mathbf{x})\right)^{n_i}.$$

Since the exclusion principle requires that it be impossible to create two fermions at the same space-time point, i.e., $\psi^2=0$, the numbers $n_i=1$, and the ordering operation then reduces the above to the identity (3.6).

The generating functional we seek is defined by the power series expansion

$$F[\rho]=\sum_{M=0}^{\infty} z^M\int Z_M d\boldsymbol{\lambda}$$

$$=\int d\boldsymbol{\lambda}\left\langle 0\left|:\exp\left(z\int d\mathbf{x}d\mathbf{y}\rho(\mathbf{y},\mathbf{x};\boldsymbol{\lambda})\psi(\mathbf{y})\psi^\dagger(\mathbf{x})\right):\right|0\right\rangle. \quad (3.8)$$

We now transform to a representation in which the exponent in (3.8) is diagonal because there the vacuum expectation value may be easily evaluated, viz.,

$$F[\rho]=\int d\boldsymbol{\lambda}\left\langle 0\left|:\exp\left(z\int d\mathbf{x}\rho(\mathbf{x};\mathbf{x};\boldsymbol{\lambda})\chi(\mathbf{x})\chi^\dagger(\mathbf{x})\right):\right|0\right\rangle$$

$$=\int d\boldsymbol{\lambda}\prod_{\mathbf{x}}(1+z\rho(\mathbf{x};\mathbf{x};\boldsymbol{\lambda})).$$

The nature of the operators $\chi(\mathbf{x})$ is of special interest only insofar as they reflect the uncertainty principle ($\chi^2=0$), since F reduces to the exponential of a trace, and the trace is invariant under similarity transformations. In fact, since $\chi^2=0$, only the first two terms in the expansion of the exponential survive, and the resulting continuous

product is recognized as a continuous determinant. By means of the identity

$$\det A = \exp \operatorname{tr} \ln A ,$$

we may rewrite F in the very useful form

$$F[\rho] = \int d\lambda e^{\operatorname{tr} \ln[1+z\rho(\lambda)]} = \int d\lambda e^{\Phi(\lambda)} \tag{3.9}$$

where $\rho(\lambda)$ is an operator whose matrix element

$$\langle \mathbf{y} | \rho(\lambda) | \mathbf{x} \rangle = \rho(\mathbf{y},\mathbf{x};\lambda) .$$

We shall now characterize the density matrices $\langle | \bar{\Gamma} | \rangle$ in terms of the generating function F by explicitly demonstrating that

$$\lim_{z\to\infty} z^{-n} F[\rho]^{-1} \frac{\delta^n F}{\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)\cdots\delta\rho(\mathbf{x}_n',\mathbf{x}_n;\lambda)}\bigg|_{\rho=\bar{\rho}} = \int d\lambda \langle NE | e^{i\lambda\cdot\mathbf{x}} \psi(\mathbf{x}_1')\cdots\psi(\mathbf{x}_n')\psi^\dagger(\mathbf{x}_n)\cdots\psi^\dagger(\mathbf{x}_1) | NE \rangle , \tag{3.10}$$

where $\langle \mathbf{y} | \bar{\rho}(\lambda) | \mathbf{x} \rangle$ consists of N orbitals, and the state $|NE\rangle$ is the product state of our model. (In the future we shall refer to the above expectation value as $\langle \psi\cdots\psi^\dagger \rangle$.) The right-hand side of (3.10) is directly related to $\langle | \bar{\Gamma}^{(n)} | \rangle$ by the commutation relations for Fermi fields, and in practice it is immediately apparent what portion of the left hand side defines $\langle | \bar{\Gamma}^{(n)} | \rangle$ directly. In order to verify this relation, we need the following lemma:

$$Z_M[\rho]|_{\rho=\bar{\rho}} = 0 \quad \text{for} \quad M > N \quad \text{if} \quad \langle \mathbf{y} | \bar{\rho} | \mathbf{x} \rangle \tag{3.11}$$

consists of N orbitals. The proof of this lemma closely parallels the line of reasoning followed in establishing the connection between Eqs. (3.7) and (3.6). One expands $Z_{N+i}[\bar{\rho}]$, $i \geq 1$, in a binomial series, and need only observe that the requirement

$$\sum_{j=1}^{N} n_j = N+i$$

implies that at least one of the numbers n_j be greater than one. The statistics then forces $Z_{N+i}[\bar{\rho}]$ to be zero. There is an immediate corollary:

$$\frac{\delta^n Z_M}{\delta\rho\cdots\delta\rho}\bigg|_{\rho=\bar{\rho}} = 0 \quad \text{for} \quad M > N+n. \tag{3.12}$$

That this is true follows from the observation that, apart from unessential factors, the nth functional derivative of Z_M is Z_{m-n}, which vanishes according to lemma (3.11) when $\rho=\bar{\rho}$ and $M-n>N$.

With these results, the functionals $F[\bar{\rho}]$ and $(\delta^n F/\delta\rho\cdots\delta\rho)|_{\rho=\bar{\rho}}$ are expressible as finite series in the parameter z, viz.,

$$\lim_{z\to\infty} z^{-n} F[\rho]^{-1} \frac{\delta^n F}{\delta\rho\cdots\delta\rho}\bigg|_{\rho=\bar{\rho}} = \lim_{z\to\infty} z^{-n} \sum_{m=0}^{\infty} z^m \int d\lambda \frac{\delta^n Z_m}{\delta\rho\cdots\delta\rho} \Big/ \sum_{q=0}^{\infty} z^q \int d\lambda Z_q \bigg|_{\rho=\bar{\rho}}$$

$$= \lim_{z\to\infty} z^{-n} \sum_{m=0}^{N+n} z^m \int d\lambda \frac{\delta^n Z_m}{\delta\rho\cdots\delta\rho} \Big/ \sum_{q=0}^{N} z^q \int d\lambda Z_q \bigg|_{\rho=\bar{\rho}} .$$

Dividing numerator and denominator by z^{N+n}, the above achieves the form

$$\lim_{z\to\infty} \int d\lambda \left[\frac{\delta^n Z_{N+n}}{\delta\rho\cdots\delta\rho} + O\left(\frac{1}{z}\right) \right] \Big/ \int d\lambda \left[Z_N + O\left(\frac{1}{z}\right) \right] \bigg|_{\rho=\bar{\rho}} = \bar{Z}_N^{-1}[\bar{\rho}] \int \frac{\delta^n Z_{N+n}}{\delta\rho\cdots\delta\rho}\bigg|_{\rho=\bar{\rho}} d\lambda .$$

Now the quantity $\bar{Z}_N[\bar{\rho}]$ is just the normalization of the state function, assumed to be 1, and from the expression (3.7) the nth derivative of Z_{N+n} yields

$$\frac{1}{N!} \int d\lambda \left\langle 0 \middle| : \left(\int d\mathbf{x} d\mathbf{y}\, \bar{\rho}(\mathbf{y},\mathbf{x};\lambda)\psi(\mathbf{y})\psi^\dagger(\mathbf{x}) \right)^N \psi(\mathbf{x}_1')\cdots\psi(\mathbf{x}_n')\psi^\dagger(\mathbf{x}_n)\cdots\psi^\dagger(\mathbf{x}_1) : \middle| 0 \right\rangle$$

$$= \int d\lambda \langle NE | e^{i\lambda\cdot\mathbf{x}} \psi(\mathbf{x}_1')\cdots\psi^\dagger(\mathbf{x}_1) | NE \rangle$$

which establishes the required relation. Finally, the above property of $\bar{Z}_N[\bar{\rho}]$ and lemma (3.11) may be used to eliminate the dependence of (3.10) on $F^{-1}[\rho]$, and to realize the more convenient form:

$$\lim_{z\to\infty}\frac{1}{z^{N+n}}\frac{\delta^n F}{\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)\cdots\delta\rho(\mathbf{x}_n',\mathbf{x}_n;\lambda)}\bigg|_{\rho=\bar{\rho}}=\int d\lambda\langle NE|e^{i\lambda\cdot\mathbf{x}}\psi(\mathbf{x}_1')\cdots\psi(\mathbf{x}_n')\psi^\dagger(\mathbf{x}_n)\cdots\psi^\dagger(\mathbf{x}_1)|NE\rangle. \quad (3.13)$$

Anticipating the possibility of establishing relations between the density matrices of various orders, we now proceed to express the matrices $\langle|\bar{\Gamma}^{(n)}|\rangle$ explicitly in terms of derivatives of F. We illustrate the procedure for the one- and two-particle matrices, and indicate the extension to the case of the n-particle matrix. From the definition of F in Eq. (3.9) we obtain

$$\frac{\delta F}{\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)}=\int d\lambda e^{\Phi(\lambda)}\frac{\delta\Phi}{\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)} \quad (3.14)$$

where

$$\frac{\delta\Phi}{\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)}=z\left(\frac{1}{1+z\rho(\lambda)}\right)_{(\mathbf{x}_1,\mathbf{x}_1')}.$$

The definition (3.13) and the commutation relations for Fermi fields combine with (3.14) to determine the one-particle density matrix indirectly in terms of $\bar{\rho}$ as follows:

$$\begin{aligned}\langle\psi(\mathbf{x}_1')\psi^\dagger(\mathbf{x}_1)\rangle&=\delta(\mathbf{x}_1-\mathbf{x}_1')-\langle\mathbf{x}_1'|\bar{\Gamma}^{(1)}|\mathbf{x}_1\rangle\\&=\lim_{z\to\infty}\frac{1}{z^N}\int d\lambda e^{\Phi(\lambda)}\left[\delta(\mathbf{x}_1-\mathbf{x}_1')-z\left(\frac{\bar{\rho}(\lambda)}{1+z\bar{\rho}(\lambda)}\right)_{(\mathbf{x}_1,\mathbf{x}_1')}\right].\end{aligned}$$

We have, therefore, the explicit connection

$$\langle\mathbf{x}_1'|\bar{\Gamma}^{(1)}|\mathbf{x}_1\rangle=\lim_{z\to\infty}\frac{1}{z^N}\int d\lambda e^{\Phi(\lambda)}\langle\mathbf{x}_1|\gamma(\lambda;z)|\mathbf{x}_1'\rangle \quad (3.15)$$

where the operator γ is defined to be

$$\gamma(\lambda,z)=\frac{z\bar{\rho}(\lambda)}{1+z\bar{\rho}(\lambda)}=\frac{z\exp(i\lambda\cdot\hat{x})\rho_0}{1+z\exp(i\lambda\cdot\hat{x})\rho_0} \quad (3.16)$$

and

$$\begin{aligned}\langle\mathbf{y}|\bar{\rho}|\mathbf{x}\rangle&=e^{i\lambda\cdot\mathbf{y}}\sum_{n=1}^{N}u_n^*(\mathbf{y})u_n(\mathbf{x})\\&=e^{i\lambda\cdot\mathbf{y}}\langle\mathbf{y}|\rho_0|\mathbf{x}\rangle.\end{aligned}$$

In order to discover the structure of the two-body density matrix, we first write the second derivative of F in terms of first derivatives of Φ. For this purpose we observe that the second derivative of Φ

$$\begin{aligned}&\frac{\delta^2\Phi}{\delta\rho(\mathbf{x}_2',\mathbf{x}_2;\lambda)\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)}\\&=\frac{\delta}{\delta\rho(\mathbf{x}_2',\mathbf{x}_2;\lambda)}\left(\frac{z}{1+z\rho(\lambda)}\right)_{(\mathbf{x}_1,\mathbf{x}_1')}\\&=-z^2\left(\frac{1}{1+z\rho(\lambda)}\frac{\delta\rho}{\delta\rho(\mathbf{x}_2',\mathbf{x}_2;\lambda)}\frac{1}{1+z\rho(\lambda)}\right)_{(\mathbf{x}_1,\mathbf{x}_1')}\\&=-z^2\left(\frac{1}{1+z\rho(\lambda)}\right)_{(\mathbf{x}_1,\mathbf{x}_2')}\left(\frac{1}{1+z\rho(\lambda)}\right)_{(\mathbf{x}_2,\mathbf{x}_1')}\end{aligned}$$

is a product of first derivatives of Φ. As a consequence, the second derivative of F is seen to involve a determinant of first derivatives of Φ, viz.:

$$\begin{aligned}&\frac{\delta_z F}{\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)\delta\rho(\mathbf{x}_2',\mathbf{x}_2;\lambda)}\\&=\int d\lambda e^{\Phi(\lambda)}\left[\frac{\delta\Phi}{\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)}\frac{\delta\Phi}{\delta\rho(\mathbf{x}_2',\mathbf{x}_2;\lambda)}+\frac{\delta^2\Phi}{\delta\rho(\mathbf{x}_2',\mathbf{x}_2;\lambda)\delta\rho(\mathbf{x}_1',\mathbf{x}_1;\lambda)}\right]\\&=\int d\lambda e^{\Phi(\lambda)}\det{}^{(2)}\left(\frac{\delta\Phi}{\delta\rho(\mathbf{x}_i',\mathbf{x}_j;\lambda)}\right). \quad (3.17)\end{aligned}$$

Now a straightforward calculation using the commutation relation shows that

$$\begin{aligned}\langle\mathbf{x}_1',\mathbf{x}_2'|\bar{\Gamma}^{(2)}|\mathbf{x}_1\mathbf{x}_2\rangle&=\langle\psi^\dagger(\mathbf{x}_1)\psi^\dagger(\mathbf{x}_2)\psi(\mathbf{x}_2')\psi(\mathbf{x}_1')\rangle\\&=\langle\psi(\mathbf{x}_1')\psi(\mathbf{x}_2')\psi^\dagger(\mathbf{x}_2)\psi^\dagger(\mathbf{x}_1)\rangle\\&\quad-\delta(\mathbf{x}_2-\mathbf{x}_2')\langle\psi(\mathbf{x}_1')\psi^\dagger(\mathbf{x}_1)\rangle\\&\quad+\delta(\mathbf{x}_1'-\mathbf{x}_2)\langle\psi(\mathbf{x}_2')\psi^\dagger(\mathbf{x}_1)\rangle\\&\quad-\delta(\mathbf{x}_1'-\mathbf{x}_1)\langle\psi(\mathbf{x}_2')\psi^\dagger(\mathbf{x}_2)\rangle\\&\quad+\delta(\mathbf{x}_1-\mathbf{x}_2')\langle\psi(\mathbf{x}_1')\psi^\dagger(\mathbf{x}_2)\rangle\\&\quad+\delta(\mathbf{x}_1-\mathbf{x}_1')\delta(\mathbf{x}_2-\mathbf{x}_2')\\&\quad-\delta(\mathbf{x}_1-\mathbf{x}_2')\delta(\mathbf{x}_2-\mathbf{x}_1').\end{aligned}$$

This identity, together with the definition (3.13) and relations (3.14) and (3.17), allows one to rewrite $\langle|\bar{\Gamma}^{(2)}|\rangle$ completely as a function of derivatives of Φ by

$$\begin{aligned}\langle\mathbf{x}_1'\mathbf{x}_2'|\bar{\Gamma}^{(2)}|\mathbf{x}_1\mathbf{x}_2\rangle&=\lim_{z\to\infty}\frac{1}{z^N}\int d\lambda e^{\Phi(\lambda)}\\&\times\det{}^{(2)}\left(\delta(\mathbf{x}_i'-\mathbf{x}_j)-\frac{\delta\Phi}{\delta\rho(\mathbf{x}_i',\mathbf{x}_j;\lambda)}\right)_{\rho=\bar{\rho}}, \quad (3.18)\end{aligned}$$

where $\langle \mathbf{y}|\bar{\rho}|\mathbf{x}\rangle$ consists of N orbitals. This immediately leads to the following factorization in terms of γ:

$$\langle \mathbf{x}_1'\mathbf{x}_2'|\bar{\Gamma}^{(2)}|\mathbf{x}_1\mathbf{x}_2\rangle = \lim_{z\to\infty}\frac{1}{z^N}\int d\lambda e^{\Phi(\lambda)} \times \det{}^{(2)}(\langle \mathbf{x}_j|\gamma(\lambda,z)\mathbf{x}_i'\rangle). \quad (3.19)$$

For the sake of completeness, we remark that the foregoing may be extrapolated to the case of higher order density matrices. In fact, one can show that the nth derivative of F retains the same structure as (3.19), where in this case an nth order determinant appears. The connection between the n-body density matrix and the nth derivative of F via the commutation relations will then yield

$$\langle \mathbf{x}_1'\cdots\mathbf{x}_n'|\bar{\Gamma}^{(n)}|\mathbf{x}_1\cdots\mathbf{x}_n\rangle = \lim_{z\to\infty}\frac{1}{z^N}\int d\lambda e^{\Phi(\lambda)} \times \det{}^{(n)}(\langle \mathbf{x}_j|\gamma(\lambda;z)|\mathbf{x}_i'\rangle). \quad (3.20)$$

In the preceding analysis we have succeeded in writing the density matrices defined in the intrinsic independent particle model as λ averages over a certain distribution function $e^{\Phi(\lambda)}$ of determinants of the generalized one-body matrix $\langle \mathbf{x}|\gamma|\mathbf{y}\rangle$. Although this λ-averaging can at least in principle be done exactly, we shall for mathematical simplicity perform the integration in Eq. (3.20) by the method of steepest descent, which we hope will include the most significant correlative effects of the motion of the center of mass. The distribution function is structurally an exponential whose argument has a vanishing gradient at the point $\lambda=0$ if we assume that the one-particle states of the model have definite parity. To see this, we insert into the expression for the gradient of $\Phi(\lambda)$ the condition that ρ_0 is idempotent, i.e., $\rho_0^2=\rho_0$, which is the operator equivalent of the statement that the one-body states are orthonormal.

$$\nabla_\lambda\Phi(\lambda)|_{\lambda=0} = \nabla_\lambda \operatorname{tr}\ln(1+z\exp(i\lambda\cdot\hat{x})\rho_0)|_{\lambda=0}$$
$$= -iz\operatorname{tr}\left(\hat{x}\frac{\rho_0}{1+z\rho_0}\right)$$
$$= -i\left(\frac{z}{1+z}\right)\operatorname{tr}(\hat{x}\rho_0)=0. \quad (3.21)$$

Similarly, the condition $\rho_0^2=\rho_0$ implies that

$$\Phi(0)=\operatorname{tr}\ln(1+z\rho_0)=N\ln(1+z).$$

We therefore assume that to a reasonable approximation the function $\Phi(\lambda)$ is

$$\Phi(\lambda)\cong N\ln(1+z)-\lambda\cdot Q\cdot\lambda, \quad (3.22)$$

where the matrix Q in the dyadic is positive-definite. The elements of Q are second derivatives of Φ with respect to λ, viz.,

$$2Q_{ij} = -\partial_{\lambda_i\lambda_j}{}^2 \operatorname{tr}\ln(1+z\exp(i\lambda\cdot\hat{x})\rho_0)|_{\lambda=0}$$
$$= \partial_{\lambda_i}\operatorname{tr}(i\hat{x}_j\gamma)_{\lambda=0}$$
$$= \operatorname{tr}\hat{x}_j(1-\gamma)\hat{x}_i\gamma|_{\lambda=0}$$
$$= \left(\frac{z}{1+z}\right)\operatorname{tr}\hat{x}_j\left(1-\frac{z}{1+z}\rho_0\right)\hat{x}_i\rho_0.$$

Since a limit $z\to\infty$ is to be taken finally, we concern ourselves only with

$$2Q_{ij}=\operatorname{tr}\hat{x}_j(1-\rho_0)\hat{x}_i\rho_0. \quad (3.23)$$

It is easily verified that for one-dimensional systems Q is positive-definite, for then

$$2Q=\operatorname{tr}\hat{x}(1-\rho_0)\hat{x}\rho_0$$
$$=\sum_{n=1}^{N}\sum_{m=N+1}^{\infty}|\langle n|\hat{x}|m\rangle|^2. \quad (3.24)$$

For two- and three-dimensional systems, the positive-definiteness of Q may be guaranteed by suitable restrictions on the rotational properties of the system. With these simplifications, the integrals in the expression (3.20) may be performed in the following manner:

$$\langle \mathbf{x}_1'\cdots\mathbf{x}_n'|\bar{\Gamma}^{(n)}|\mathbf{x}_1\cdots\mathbf{x}_n\rangle$$
$$=\lim_{z\to\infty}\frac{e^{\Phi(0)}}{z^N}\int d\lambda e^{-\lambda\cdot Q\cdot\lambda}\det{}^{(n)}(\langle \mathbf{x}_j|\gamma|\mathbf{x}_i'\rangle)$$
$$=\lim_{z\to\infty}\int d\lambda\exp-(\lambda\cdot Q\cdot\lambda-\lambda\cdot\tilde{\nabla}_\lambda) \times\det{}^{(n)}(\langle \mathbf{x}_j|\gamma(0;z)|\mathbf{x}_i'\rangle).$$

The notation $\tilde{\nabla}_\lambda$ means that all differential operators stand to the right of the quantities λ. Since $\tilde{\nabla}_\lambda$ commutes with Q, Q being independent of λ, one may formally complete the square in the exponent to read

$$\lambda\cdot Q\cdot\lambda-\lambda\cdot\tilde{\nabla}_\lambda=(\lambda-\tfrac{1}{2}Q^{-1}\tilde{\nabla}_\lambda)\cdot Q\cdot(\lambda-\tfrac{1}{2}Q^{-1}\tilde{\nabla}_\lambda) -\tfrac{1}{4}\nabla_\lambda\cdot Q^{-1}\cdot\nabla_\lambda. \quad (3.25)$$

The integration may then be completed to give

$$\langle \mathbf{x}_1'\cdots\mathbf{x}_n'|\bar{\Gamma}^{(n)}|\mathbf{x}_1\cdots\mathbf{x}_n\rangle=\lim_{z\to\infty}\exp[\tfrac{1}{4}\nabla_\lambda\cdot Q^{-1}\cdot\nabla_\lambda] \times\det{}^{(n)}(\langle \mathbf{x}_j|\gamma(\lambda,z)|\mathbf{x}_i'\rangle)|_{\lambda=0}, \quad (3.26)$$

where Q^{-1} is the inverse of the matrix (3.23).

The truncation formula (3.26) is a generalization of the Hartree-Fock factorization in the following sense. If the operator ρ_0, which is the projection operator for states within the ground-state configuration in an independent particle description, is known, all the density matrices defined in the intrinsic independent particle model may be calculated directly by means of

(3.26). In fact, the zeroth-order contribution to the n-particle density matrix is just the familiar Hartree-Fock factorization, and the matrix element $\langle \mathbf{y}|\rho_0|\mathbf{x}\rangle$ is the Dirac density matrix defined with respect to single-particle states yet to be fully prescribed.

We shall now demand that the one-particle states be chosen to minimize the energy. In the following we shall carry out the required variational principle for the one-dimension situation; the 3-dimensional problem is a straightforward extension of these results. Further, because of the inherent complexity of the calculations, we shall only treat the two leading terms of the expansion (3.26). The expectation value of the Hamiltonian (2.15)

$$\langle \Psi'|H|\Psi'\rangle \equiv E[\varphi] = -\frac{\hbar^2}{2m}\left(\frac{N-1}{N}\right)\int dx \partial_x{}^2 \langle x'|\bar{\Gamma}^{(1)}|x\rangle|_{x'=x} + \int dxdy \bar{v}(x,y)\langle x'y'|\bar{\Gamma}^{(2)}|x,y\rangle|_{x'=x,y'=y}, \quad (3.27)$$

where

$$\bar{v}(x,y) = \frac{\hbar^2}{2mN}\partial_x\partial_y + \tfrac{1}{2}v(x-y).$$

Using the identity

$$\partial_\lambda \gamma(\lambda) = i(1-\gamma)\hat{x}\gamma$$

derived from (3.16) and the fact that ρ_0 is idempotent, it is easily verified that

$$\langle x'|\bar{\Gamma}^{(1)}|x\rangle = \exp\left[\frac{1}{4Q}d_\lambda{}^2\right]\langle x|\gamma(\lambda,z)|x'\rangle|_{\lambda=0,z\to\infty} = \langle x|\rho_0|x'\rangle + \frac{1}{4Q}\langle|\Lambda|x'x\rangle + \cdots \quad (3.28)$$

and

$$\langle x'y'|\bar{\Gamma}^{(2)}|xy\rangle = \begin{vmatrix}\langle x|\rho_0|x'\rangle & \langle y|\rho_0|x'\rangle \\ \langle x|\rho_0|y'\rangle & \langle y|\rho_0|y'\rangle\end{vmatrix} + \frac{1}{4Q}\left\{\begin{vmatrix}\langle x|\Lambda|x'\rangle & \langle y|\rho_0|x'\rangle \\ \langle x|\Lambda|y'\rangle & \langle y|\rho_0|y'\rangle\end{vmatrix} + \begin{vmatrix}\langle x|\rho_0|x'\rangle & \langle y|\Lambda|x'\rangle \\ \langle x|\rho_0|y'\rangle & \langle y|\Lambda|y'\rangle\end{vmatrix} - 2\begin{vmatrix}\langle x|\Pi|x'\rangle & \langle y|\Pi|x'\rangle \\ \langle x|\Pi|y'\rangle & \langle y|\Pi|y'\rangle\end{vmatrix}\right\} + \cdots, \quad (3.29)$$

where

$$\Lambda = -(1-\rho_0)\hat{x}(1-2\rho_0)\hat{x}\rho_0 \quad \text{and} \quad \Pi = (1-\rho_0)\hat{x}\rho_0. \quad (3.30)$$

We may therefore rewrite $E[\varphi]$ in the more suggestive form

$$E[\varphi] = \epsilon(\rho_0) + \frac{1}{4Q}[\epsilon_1(\Lambda) - \epsilon_2(\Pi)], \quad (3.31)$$

first observing that the direct terms associated with $(\hbar^2/2m)\partial_{xy}{}^2$ which are contributed by the first three determinants in (3.29) vanish because of assumed definite parity of the single-particle states, and secondly, that the first two terms of (3.29) give identical contributions if the potential $\bar{v}(x,y)$ is assumed to be symmetric. The quantity

$$\epsilon(\rho_0) = -\frac{\hbar^2}{2m}\left(\frac{N-1}{N}\right)\int dxdx'\delta(x-x')\partial_x{}^2\langle x|\rho_0|x'\rangle - \frac{\hbar^2}{2mN}\int dxdydx'dy'\delta(x-x')\delta(y-y')\partial_{xy}{}^2\langle x|\rho_0|y'\rangle\langle y|\rho_0|x'\rangle + \frac{1}{2}\int dxdy v(x-y)[\langle x|\rho_0|x\rangle\langle y|\rho_0|y\rangle - \langle x|\rho_0|y\rangle\langle y|\rho_0|x\rangle] \quad (3.32)$$

has the usual Hartree-Fock structure, while

$$\epsilon_1(\Lambda) = -\frac{\hbar^2}{2m}\left(\frac{N-1}{N}\right)\int dxdx'\delta(x-x')\partial_x{}^2\langle x|\Lambda|x'\rangle - \frac{\hbar^2}{mN}\int dxdydx'dy'\delta(x-x')\delta(y-y')\partial_{xy}{}^2\langle x|\Lambda|y'\rangle\langle y|\rho_0|x'\rangle + \int dxdy v(x-y)[\langle x|\Lambda|x\rangle\langle y|\rho_0|y\rangle - \langle x|\Lambda|y\rangle\langle y|\rho_0|x\rangle] \quad (3.33)$$

and

$$\epsilon_2(\Pi) = \int dxdydx'dy'\delta(x-x')\delta(y-y')\left(\frac{\hbar^2}{mN}\partial_{xy}{}^2 + v(x-y)\right)[\langle x|\Pi|x'\rangle\langle y|\Pi|y'\rangle - \langle x|\Pi|y'\rangle\langle y|\Pi|x'\rangle]. \quad (3.34)$$

We must now vary $E[\varphi]$ with respect to the single-particle states $u_l(z)$, subject to the normalization condition

$$\mathrm{tr}\bar{\Gamma}^{(1)} = N.$$

This restriction is the same as the condition $\mathrm{tr}\rho_0=N$, since all correction terms to ρ_0 in the expression for $\bar{\Gamma}^{(1)}$ are of the form $(1-\rho_0)0\rho_0$, and therefore have vanishing traces, ρ_0 being idempotent. Introducing the above condition by means of a Lagrange parameters λ_l, we obtain the variational equation

$$\frac{\delta\epsilon(\rho_0)}{\delta u_l(z)}+\lambda_l\frac{\delta}{\delta u_l(z)}\mathrm{tr}\rho_0=-\frac{\delta}{\delta u_l(z)}\left[\frac{1}{4Q}(\epsilon_1(\Lambda)-\epsilon_2(\Pi))\right]. \tag{3.35}$$

In order to obtain explicit expressions for the various terms in this equation, we need the following derivatives:

$$\frac{\delta}{\delta u_l(z)}\langle x|\rho_0|x'\rangle=\frac{\delta}{\delta u_l(z)}\sum_{l'}u_{l'}{}^*(x)u_{l'}(x')$$
$$=u_l{}^*(x)\delta(x'-z). \tag{3.36}$$

$$\frac{\delta}{\delta u_l(z)}\langle x|\Lambda|x'\rangle=-\frac{\delta}{\delta u_l(z)}\langle x|(1-\rho_0)\hat{x}(1-2\rho_0)\hat{x}\rho_0|x'\rangle$$
$$=-\frac{\delta}{\delta u_l(z)}\int dqdq'\langle x|(1-\rho_0)|q\rangle q\langle q|(1-2\rho_0)|q'\rangle q'\langle q'|\rho_0|x'\rangle$$
$$=zu_l{}^*(x)\langle z|(1-2\rho_0)\hat{x}\rho_0|x'\rangle+2z\langle z|\rho_0|x'\rangle\int dq\langle x|(1-\rho_0)\hat{x}|q\rangle u_l{}^*(q)$$
$$-\delta(x'-z)\int dq\langle x|(1-\rho_0)\hat{x}(1-2\rho_0)\hat{x}|q\rangle u_l{}^*(q) \tag{3.37}$$

and

$$\frac{\delta}{\delta u_l(z)}\langle x|\Pi|x'\rangle=\frac{\delta}{\delta u_l(z)}\langle x|(1-\rho_0)\hat{x}\rho_0|x'\rangle$$
$$=-z\langle z|\rho_0|x'\rangle u_l{}^*(x)+\delta(x'-z)\int dq\langle x|(1-\rho_0)\hat{x}|q\rangle u_l{}^*(q) \tag{3.38}$$

and

$$\frac{\delta}{\delta u_l(z)}Q=\frac{1}{2}\frac{\delta}{\delta u_l(z)}\mathrm{tr}\hat{x}(1-\rho_0)\hat{x}\rho_0$$
$$=\frac{z}{2}\int dq\langle z|(1-2\rho_0)\hat{x}|q\rangle u_l{}^*(q). \tag{3.39}$$

It is easily verified, using these relations, that the left-hand side of the variational equations (3.35) becomes

$$\int dx\,H(z,x)u_l{}^*(x)+\lambda_l u_l{}^*(z),$$

where

$$H(z,x)=-\frac{\hbar^2}{2m}\left(\frac{N-1}{N}\right)\delta(x-z)\partial_x{}^2-\frac{\hbar^2}{mN}\partial_z\langle z|\rho_0|x\rangle\partial_x+\delta(x-z)\int dyv(z-y)\langle y|\rho_0|y\rangle-v(x-z)\langle z|\rho_0|x\rangle \tag{3.40}$$

is the Hartree-Fock self-consistent Hamiltonian defined for the exact Hamiltonian (2.15). The variational equation (3.35) now reads

$$\int dxH(z,x)u_l{}^*(x)+\lambda_l u_l{}^*(z)=V[u], \tag{3.41}$$

the inhomogeneous term being defined explicitly in terms of the single-particle states by the relations (3.33) through (3.39).

It is to be expected that an exact solution of (3.41) can be found only in a comparatively small number of simple cases. In general, one can take advantage of the structure of the equation to obtain corrections to the solutions of the homogeneous equation (the Hartree-Fock solution) to first order in perturbation theory as follows: consider the solutions u_l of

$$(H+\lambda_l)u_l=V[u], \tag{3.42}$$

and denote by $u_l{}^{(0)}$ the solution of the homogeneous equation $(H+\lambda_l{}^{(0)})u_l{}^{(0)}=0$. We then substitute the

expansion

$$u_l = u_l^{(0)} + \sum_{m \neq l} c_{ml} u_m^{(0)} \tag{3.43}$$

into Eq. (3.42) to obtain

$$(\lambda_l - \lambda_l^{(0)}) u_l^{(0)} + \sum_{m \neq l} c_{ml} (\lambda_l - \lambda_m^{(0)}) u_m^{(0)} = V[u^{(0)}].$$

To determine the constants, we take the scalar product of both sides with $u_k^{(0)}$ and employ the orthogonality relations:

$$c_{ml} = \frac{\langle u_m^{(0)}, V[u^{(0)}] \rangle}{\lambda_l - \lambda_m^{(0)}} \tag{3.44}$$

with $\lambda_l = \lambda_l^{(0)} + \langle u_l^{(0)}, V[u^{(0)}] \rangle$. The expression for $V[u^{(0)}]$ may be simplified if one observes that in terms of the self-consistent Hamiltonian of (3.40) the quantity

$$\epsilon_1(\Lambda) = \mathrm{tr}(H\Lambda).$$

Now the Hartree-Fock equation $(H + \lambda_l^{(0)}) u_l^{(0)} = 0$ for the single-particle states is equivalent to the statement

$$H\rho_0 = \rho_0 H$$

for the density matrix ρ_0. Consequently, when evaluated for the states $u_k^{(0)}$, ϵ_1 vanishes because ρ_0 is idempotent; in fact,

$$\begin{aligned} \epsilon_1(\Lambda)\,|_{u_k^{(0)}} &= -\mathrm{tr}(H(1-\rho_0)\hat{x}(1-2\rho_0)\hat{x}\rho_0) \\ &= -\mathrm{tr}(\rho_0 H(1-\rho_0)\hat{x}(1-2\rho_0)\hat{x}), \end{aligned}$$

using the cyclic property of the trace. Commuting ρ_0 with H and observing that $\rho_0(1-\rho_0) = 0$, we obtain $\epsilon_1(\Lambda)\,|_{u_k^{(0)}} = 0$. The solution of (3.41) which is required is therefore

$$u_l = u_l^{(0)} + \sum_{m \neq l} \frac{\langle u_m^{(0)}, V[u^{(0)}] \rangle}{\lambda_l - \lambda_m^{(0)}} u_m^{(0)} \tag{3.45}$$

where

$$\lambda_l = \lambda_l^{(0)} + \langle u_l^{(0)}, V[u^{(0)}] \rangle$$

and

$$V[u^{(0)}] = -\frac{1}{4Q^2}\epsilon_2(\Pi)\frac{\delta Q}{\delta u_l(z)}\Big|_{u^{(0)}} - \frac{1}{4Q}\frac{\delta}{\delta u_l(z)}(\epsilon_1(\Lambda) - \epsilon_2(\Pi))\,|_{u^{(0)}}.$$

We conclude from the above discussion that, within the framework of the intrinsic independent-particle model, the density matrices are obtained by first determining the nontranslationally invariant solutions of the Hartree-Fock problem defined by the Hamiltonian describing the internal dynamics of the system, and then generating corrections from the relations (3.45), (3.28), and (3.29). In general, one might hope that the Hartree-Fock single-particle states might be adequate to calculate the energy to order $1/N^2$, although for other operators the corrections (3.45) will certainly be important. Unfortunately, it is not possible to make a general statement about the order of the corrections,

$$-\frac{1}{4Q}\epsilon_2(\Pi)\,|_{u^{(0)}},$$

to the Hartree-Fock energy. However, it is certainly of interest to discover what corrections to Hartree-Fock calculations ignoring the center of mass arise from the inclusion of correction terms to the density matrices in (3.28) and (3.29). A case in point is the calculation by Aviles and Jastrow[13] of the binding energy of He^4 using Yukawa pair forces.

IV. SUMMARY

Within the framework of the method of redundant variables, we have presented in a modified independent particle picture an approximate description of translationally invariant systems consisting of a finite number of fermions. We have demonstrated in what sense a Hartree-Fock scheme, ignoring the conservation of total linear momentum, is a reasonable starting point for higher corrections. The method offers two types of corrections: first, those which generalize the customary Dirac density matrices into the form (3.26), and reflect to some degree the correlations associated with the center of mass.

Corrections of the second type, (3.45), modify the Hartree-Fock single-particle states, and are a direct consequence of the appearance in the variational equations of an inhomogeneous term in addition to the usual Hartree-Fock terms.

Since the requirement of nontranslational invariance of the Hartree-Fock solution is somewhat usual, it is of interest to re-examine the self-consistency method in this context. Because of the inherent complexity of this method, one must, to be practical, resort to the less accurate but simpler semiclassical approach of Thomas and Fermi. We shall discuss in a forthcoming study the formulation of the Thomas-Fermi problem for the case of attractive Coulomb and Yukawa pair interactions. The latter system is certainly relevant to nuclear problems, especially as it relates to the density of particles.

[13] J. Aviles and R. Jastrow, Bull. Am. Phys. Soc. **2**, 25 (1957).