Method of Correlated Basis Functions*

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The method of correlated basis functions provides a means of systematically exploiting our intuitive understanding of real physical systems. Here we seek especially to develop a formalism for describing systems of strongly interacting fermions, for example, nuclei and liquid He^3, using a complete set of correlated functions $\Psi_m = F\Phi_m/(\Phi_m, F^2\Phi_m)^{1/2}$. F is taken as a product of two-body factors, $\Pi_{i<j} f(r_{ij})$, the $f(r_{ij})$ embodying at least the correlations arising from strong short-range repulsions; and $\{\Phi_m\}$, a set of independent-particle-model functions which might serve as a basis in the absence of highly singular interactions. The matrix elements $\mathfrak{H}_{mn}$, $\mathfrak{N}_{mn}$ of the Hamiltonian and identity operators with respect to the correlated basis $\{\Psi_m\}$ are evaluated by generalization of cluster-expansion techniques developed originally for the calculation of the partition function of a classical imperfect gas and adapted to the quantum-mechanical many-body problem by Iwamoto and Yamada. Contributions to our expansions for the $\mathfrak{H}_{mn}$ are classified according to order of magnitude in the quantity $\rho\omega$, where $\omega = \int (f^2(r)-1)d\mathbf{r}$ is a "correlation parameter" and ρ the average particle density. To the extent that $|\rho\omega|$ is small, it provides a true expansion parameter. A detailed technical discussion of the cluster expansions is given, with special emphasis on their symmetry properties upon truncation. Although the many-body problem is soluble by simultaneous diagonalization of the matrices $(\mathfrak{H}_{mn})$ and $(\mathfrak{N}_{mn})$, it is preferable first to transform to an orthonormal basis of "unperturbed" correlated functions $\{\Theta_m\}$ with respect to which the Hamiltonian and identity operators have the matrix representations (H_{mn}) and $(N_{mn}) = (\delta_{mn})$, and then to attempt the separate diagonalization of (H_{mn}). In general, such a transformation is expedited by the Löwdin procedure carried out to the desired order in $\rho\omega$. However, a Schmidt orthogonalization scheme might prove more advantageous in specific cases. Field-theoretic techniques (of both perturbative and nonperturbative nature) may be brought to bear in the diagonalization of (H_{mn}). The inverse of the unitary transformation which takes the basis $\{\Phi_m\}$ into the basis $\{\Theta_m\}$, applied to the given singular Hamiltonian, leads—for any F in the class considered—to a nonsingular "effective Hamiltonian." Following this formal cue, we set out to construct explicitly a second-quantized effective Hamiltonian which generates the same matrix elements, to prescribed order in $\rho\omega$, when operating between independent-particle kets of the model occupation-number representation, as does the given Hamiltonian in the configuration-space representation, between the corresponding correlated functions of the Löwdin basis. The quasiparticles described by this effective Hamiltonian interact via well-behaved two-body, three-body, $\cdots$, Q-body, $\cdots$ potentials, in contrast to the highly singular two-body interactions of the real particles. For small $|\rho\omega|$, the effective two-body forces predominate. An avenue to deeper understanding of the applicability of the nuclear-shell model and the dressed-quasiparticle theory of liquid He^3 has been opened. This article treats only the formalism for a uniform extended medium. Numerical calculations, as well as the extension of the method to finite systems, will follow.

I. INTRODUCTION

LET us consider[1] a collection of N identical nonrelativistic particles in interaction, the states of the system being determined by a Hamiltonian with the configuration-space form

$$H = -\sum_{i=1}^{N} \frac{\hbar^2}{2M}\Delta_i + \sum_{i<j} v(ij), \qquad \text{(I.1)}$$

where $v(ij)$ is some given two-body potential. In this paper we concentrate on a uniform, infinitely extended Fermi system, characterized by a strong, short-range, two-particle potential of gross behavior in coordinate space as shown in Fig. 1. Prime examples of physical interest are nuclear matter and liquid He^3. Any straightforward attempt to describe such a system in a basis $\{\Phi_m\}$ of independent-particle functions is of course doomed at the outset, since all matrix elements of H in this representation are positively infinite.

Brueckner and others[2] have developed one method of circumventing the difficulties resulting from the singu-

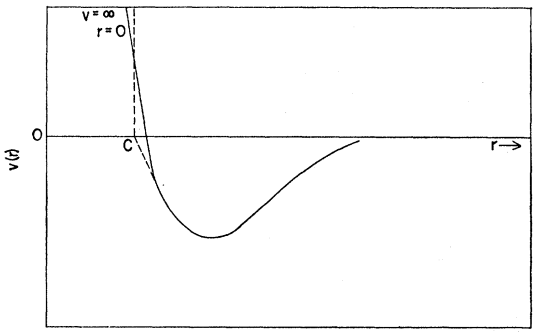

FIG. 1. Highly singular potential $v(r)$ typical of the interaction of two nucleons or two helium atoms, consisting of a short-range repulsion (increasing faster than $1/r$ as $r \to 0$) followed by an attraction of somewhat longer range. r=interparticle separation. C="radius" of an effective hard core.

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[1] This introduction was written with the nonspecialist or the casual reader in mind: We present here the physical motivation for the method of correlated basis functions and a comprehensive outline of its development. All technical details which would tend to obscure the essential simplicity of the underlying ideas are put aside for later sections.

[2] K. A. Brueckner, in *The Many Body Problem: Lecture Notes of the Les Houches Summer School*, edited by C. Dewitt (Dunod Cie., Paris, 1959), pp. 47–255.

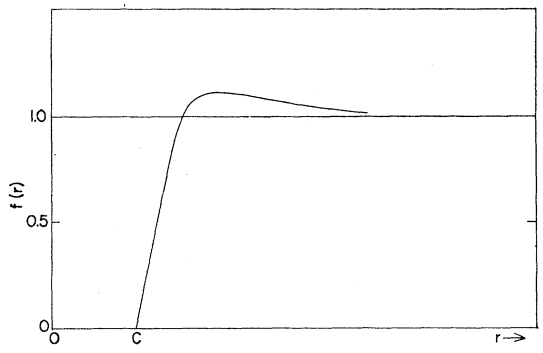

FIG. 2. Qualitative behavior required of a reasonable two-body correlation factor, the strong repulsive component of $v(r)$ having been replaced by a hard core of radius C. $f(r)$ should be essentially unity outside the range of the attraction.

larity in v. The starting point is the linked (Rayleigh-Schrödinger) perturbation expansion for the energy in terms of the independent-particle basis, an expansion involving *divergent* v-matrix elements. A rearrangement is performed, generating an expansion involving only reaction or t-matrix elements, the reaction matrix being obtained by a solution of the two-particle problem *in the medium*. This rearrangement is accomplished by execution of the most vital partial summations on the perturbation expansion. In spite of considerable semiquantitative success,[2,3] the detailed application of the method requires approximations whose merit is difficult to judge, not to mention the fact that great care must be exercised in giving precise definition to the basic ingredients of the theory.[4] Further, the extension to finite systems is not at all easy.

Thus, while the exploration and application of Brueckner's method has led to a very significant enhancement of our understanding of strongly interacting many-body systems, there is clearly room for an alternative approach. The method of correlated basis functions (CBF) offers another resolution of the strong-interaction difficulty which is at least as flexible and interesting as Brueckner's and which provides a convenient framework for the construction of weakly interacting-quasiparticle pictures of such systems as nuclei and liquid He^3. The basic ideas of this method are so elementary that its full development might well have come much earlier.

First of all, we consider the behavior of the many-particle wave function in the presence of repulsive cores. For ease of speaking, the strong repulsion in Fig. 1 may be replaced by a suitable hard core of radius C. Then the system wave function must certainly vanish for configurations in which any two particles are closer than C. This suggests that trial functions of the form

$$\Psi = F\Phi, \tag{I.2}$$

where F is a real, non-negative, *correlation factor* symmetric in the particle coordinates and Φ is a *model function* embodying the statistics and symmetry properties of the system under study, might be especially valuable. The statement "F is a correlation factor" means that F is characterized by

$$\begin{aligned} &F=0, \quad \text{any} \quad r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|\leqslant C, \\ &F\to 1, \quad \text{all} \quad r_{ij}\gg C. \qquad (i,j=1,\cdots,N) \end{aligned} \tag{I.3}$$

We say nothing specific yet about the second factor except that (as indicated by the term "model function") it may at least in first approximation be taken as a function of the type commonly used for the description of the system in the absence of strong, short-range interactions.

The primary quantity of interest is the expectation value of the energy for the proposed trial function,

$$E[\Psi]=(\Psi,H\Psi)/(\Psi,\Psi). \tag{I.4}$$

Two practical choices for F are being investigated:

(1) $F=\prod_{i<j} f(r_{ij})$,

(Bijl-Dingle-Jastrow (BDJ) form)

$$\begin{aligned} &f(r_{ij})=0, \quad r_{ij}\leqslant C, \\ &f(r_{ij})\to 1, \quad r_{ij}\gg C. \end{aligned} \tag{I.5}$$

The detailed choice of the two-body correlation factor f is a story in itself. An appropriate qualitative behavior is indicated in Fig. 2, and general criteria for the determination of f are discussed in Sec. V. In the greater part of the paper, however, we shall suppose f^2-1 is always negative; this is merely to enable us to avoid certain semantic difficulties.

(2) $F=\Psi_0{}^B$ (Bose form),

$$\begin{aligned} &H_{SI}\Psi_0{}^B=E_0{}^B\Psi_0{}^B, \\ &H=H_{SI}+H_{SD}. \end{aligned} \tag{I.6}$$

Here the correlation factor is taken as the (symmetrical, positive semidefinite) ground-state solution of the *Bose* problem corresponding to the spin-independent Hamiltonian H_{SI}, for some separation of H into spin-

[3] K. A. Brueckner and K. S. Masterson, Jr., Phys. Rev. **128**, 2267 (1962); K. A. Brueckner, J. L. Gammel, and H. Weitzner, *ibid.* **110**, 431 (1958); K. A. Brueckner and D. T. Goldman, *ibid.* **116**, 424 (1959); **117**, 207 (1960); K. A. Brueckner, A. M. Lockett, and M. Rotenberg, *ibid.* **121**, 255 (1961); K. S. Masterson, Jr., and A. M. Lockett, *ibid.* **129**, 776 (1963). Cf. also S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) **11**, 65 (1960); Nucl. Phys. **29**, 665 (1962), B. L. Scott and S. A. Moszkowski, Ann. Phys. (N. Y.) **14**, 107 (1961); H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. **129**, 225 (1963); M. Razavy, *ibid.* **130**, 1091 (1963); B. H. Brandow, Phys. Letters **4**, 8 (1963).

[4] We refer here specifically to troubles introduced by t-matrix singularities, off-the-energy-shell propagation, and three-body correlations. Critical discussions of these and other fine points of the Brueckner theory are to be found in papers by: J. S. Bell and E. J. Squires, Advan. Phys. **10**, 211 (1961); R. L. Becker, Phys. Rev. **127**, 1328 (1962); G. A. Baker, Jr., *ibid.* **131**, 1869 (1963); G. A. Baker, Jr., J. L. Gammel, and B. J. Hill, *ibid.* **132**, 1373 (1963); G. A. Baker, Jr., B. J. Hill, and Robert J. McKee, Jr., *ibid.* **135**, A922 (1964); H. A. Bethe, B. H. Brandow, and A. G. Petschek (see Ref. 3); G. E. Brown, G. T. Schappert, and C. W. Wong, Nucl. Phys. **56**, 199 (1964); H. A. Bethe, Phys. Rev. **138**, B804 (1965).

independent and spin-dependent parts.[5] There is now a good approximation method for solving this hypothetical problem,[6,7] based on techniques borrowed from the theory of classical fluids [specifically the Kirkwood superposition approximation and the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) integral equation for the radial distribution function[8]], a method that has been applied with success by Massey[9] to liquid He^4. All the matrix elements in the Fermi problem can then be reduced, again using the Kirkwood superposition approximation, to expressions involving the (calculable) Bose liquid-structure factor $S(k)$—the potential having been, as such, eliminated from the matrix elements at the outset.[5,10] In practice a BDJ form is assumed for the Bose solution, so we can to this extent regard the present choice of F as a special case of (1); some flexibility is lost, but there is a *great* gain in facility of calculation.

We shall develop here the formalism of the CBF method based on the *BDJ choice.* In large measure our work will parallel and reinforce that of Feenberg and Woo[10] (FW) for the Bose correlation factor. At the present time, our path would seem to point more directly to a theory of nuclei; theirs, to an understanding of the properties of liquid He^3. (This "divergence" is of course due to the *detailed* differences in the potentials that act in the two cases. Recall, for example, that the two-nucleon interaction is highly spin- and isospin-dependent.)

Throughout this paper, we shall attempt to frame the development in such a way that the modifications necessary for adapting our method to finite systems are easily visible, and adhere to notation convenient even when the transition is made. Most of the statements made in the present section apply as well to finite as to infinite systems.

The techniques to be introduced for the evaluation of the matrix elements that enter will be useful if the volume $|N\omega|$, with

$$\omega=\int[f^2(r)-1]d\mathbf{r}, \tag{I.7}$$

is small compared to the volume Ω of the system. The quantity ω serves as a measure of the strength of dynamical correlations incorporated into F. We shall see that, in many respects, $|N\omega/\Omega|$ plays the role of an expansion parameter in our method.

The proposal (I.2) for the wave function, in its simplest trial form (Bijl-Dingle-Jastrow F, independent-particle Φ) has a long history,[11–25,6] yet its greater potentialities have been recognized only in recent years by Feenberg and his students.[5,7,9,10,26–30] The central idea is that the set $\{\Psi_m|\Psi_m\equiv F\Phi_m/(\Phi_m,F^2\Phi_m)^{1/2}\}$ serves to define matrix elements of the Hamiltonian and identity operators

$$\begin{aligned}\mathfrak{H}_{mn}&=(\Psi_m,H\Psi_n),\\ \mathfrak{N}_{mn}&=(\Psi_m,\Psi_n),\end{aligned} \tag{I.8}$$

with $\mathfrak{H}_{mn}$ finite, even when the two-particle interaction is singular [e.g., when $v(ij)$ contains a hard core]. All calculations are to be based on these matrix elements. As indicated above, for $\{\Phi_m\}$ we may take a complete orthonormal set of independent-particle functions, or a restricted set of them, not complete but still orthonormal, which would be useful for treating the most important properties of the system if the strong interactions were not present. (More generally, we could let the $\{\Phi_m\}$ contain some dynamical correlations, as proper, for example, to a weakly interacting but "superconducting" system.[31] This possibility, however, will not be exploited here.)

Writing the trial wave function as a linear combination of the Ψ_m,

$$\Psi=\textstyle\sum_m c_m\Psi_m, \tag{I.9}$$

there results the following expression for the expectation value (I.4) in terms of $\mathfrak{H}_{mn}$, $\mathfrak{N}_{mn}$:

$$E=\textstyle\sum_{mn} c_m^*c_n\mathfrak{H}_{mn}/\sum_{pq} c_p^*c_q\mathfrak{N}_{pq}. \tag{I.10}$$

Whatever state we are trying to describe, the best value that can be obtained for its energy using the class of

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trial functions $\Psi=\sum_m c_m\Psi_m$ is some value stationary relative to the c_m, or equivalently, the c_m^*. The extremum conditions

$$\partial E/\partial c_m^*=0, \quad \text{all } \mathbf{m}, \tag{I.11}$$

yield the relations

$$\sum_n c_n[\mathfrak{H}_{mn}-E\mathfrak{N}_{mn}]=0, \quad \text{all } \mathbf{m}, \tag{I.12}$$

which, in turn, imply the well-known secular equation,

$$\det(\mathfrak{H}_{mn}-E\mathfrak{N}_{mn})=0. \tag{I.13}$$

The set of equations (I.12), (I.13) provides a very general framework within which to launch attacks on the many-body problem. In particular, if the set $\{\Phi_m\}$ is complete, the set $\{\Psi_m\}$ is also complete; then the solutions of (I.13) are the *exact* energy eigenvalues and the corresponding solutions of (I.12) produce, via (I.9), the associated exact wave functions.

One systematic technique of simultaneous diagonalization of the matrices $(\mathfrak{H}_{mn})$, $(\mathfrak{N}_{mn})$, leads in a natural way to various perturbation theories, of the Feenberg-Feshbach,[32] Brillouin-Wigner,[33] and Rayleigh-Schrödinger[34] types, which of course in detail display more complicated structure than ordinarily encountered.[35] Nevertheless, it is expedient—both for mathematical convenience and for purposes of physical interpretation—to transform from our *nonorthogonal* set of correlated functions to an *orthonormal* one before attempting to calculate energy eigenvalues.

Thus three problems must be faced: (1) evaluation of the matrix elements $\mathfrak{H}_{mn}$, $\mathfrak{N}_{mn}$ of the Hamiltonian and identity operators with respect to the set of correlated functions $\{\Psi_m\}$; (2) transformation from the set $\{\Psi_m\}$ to set $\{\Theta_m\}$ with respect to which these operators have the corresponding matrix elements H_{mn}, $N_{mn}=\delta_{mn}$; (3) diagonalization of the matrix (H_{mn}). (Needless to say, the H_{mn} may be expressed entirely in terms of the $\mathfrak{H}_{pq}$, $\mathfrak{N}_{pq}$.)

Problem (1) has been essentially solved by generalization of cluster-expansion techniques designed for calculation of the partition function of a classical imperfect gas.[36] It turns out, as described in Sec. II, that one can set up a method for the evaluation of the $\mathfrak{N}_{mm}$ which may be readily extended to generate the $\mathfrak{H}_{mm}$ and, by simple tricks, the nondiagonal matrix elements as well. We go on to present detailed calculations of the $\mathfrak{N}_{mn}$ and the $\mathfrak{H}_{mn}$ accurate respectively to second order and to first order in cluster expansions whose terms are classified according to their order of magnitude in the correlation parameter ω, for Φ_m, Φ_n differing in any number of orbitals. Our treatment leans heavily on the earlier work of Iwamoto and Yamada (IY).[15] (In an Appendix we investigate in what measure the cluster expansions obtained as in Ref. 10 or Sec. II satisfy obvious symmetry requirements, upon truncation according to the prescriptions of FW and the present paper. Our classification of contributions by order in ω is found to be superior—in this regard, at least—to the FW classification by number of distinct indices. Forthcoming papers by the authors and D. Chakkalakal will treat in more detail the formal properties of the cluster expansions.)

A procedure put forth by Löwdin[37] appears, in general, well suited to the accomplishment of (2), and its consequences are explored in Sec. III, where the matrix elements H_{mn} are evaluated, again to first order in the corresponding cluster expansions. However, in specific cases a Schmidt orthogonalization procedure may be more advantageous and thus is also exhibited in this section. To be definite, the symbols $\{\Theta_m\}$, (H_{mn}) will be reserved for the Löwdin set and corresponding matrix representation of H.

Having the matrix elements H_{mn}, to prescribed cluster order, we are ready for an assault on problem (3), the diagonalization of (H_{mn}). In the new representation, our problem takes more conventional form, and hence is more susceptible to conventional approaches.[38] Indeed, if the set $\{\Theta_m\}$ is complete, a very natural restatement of the information contained in the matrix elements H_{mn} will enable us to take advantage of the great arsenal of field-theoretic techniques—both perturbative and nonperturbative—that have recently been developed for attacking many-body problems involving well-behaved potentials.[39] First note that since $N_{mn}=\delta_{mn}$ (this is in fact true order by order in ω), the transformation taking the basis $\{\Phi_m\}$ into the basis $\{\Theta_m\}$ is unitary. The corresponding unitary operator is of course just the product $\hat{L}\hat{F}$ of the operator $\hat{F}$ corresponding to the factor $F/(\Phi_m,F^2\Phi_m)^{1/2}$ and the operator $\hat{L}$ corresponding to the Löwdin transformation. A rotation of axes in the Hilbert space of the system has been performed. But a different interpretation of what we have accomplished is more convenient: the operator $(\hat{L}\hat{F})^\dagger$ defines a canonical transformation of the given *singular* Hamiltonian which yields a *nonsingular* "effective

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[38] If the set $\{\Phi_m\}$ is finite one may also envision the possibility of diagonalizing the resulting energy matrix (H_{mn}) by numerical techniques employing a computer. For example, shell-model configuration-mixing calculations could be extended to allow use of the "real" two-nucleon potential rather than some *ad hoc* substitute.

[39] *The Many-Body Problem*, edited by D. Pines (W. A. Benjamin, Inc., New York, 1961); A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice Hall, Inc., Englewood Cliffs, New Jersey, 1963); P. Nozières, *Theory of Interacting Fermi Systems* (W. A. Benjamin, Inc., New York, 1964); T. D. Schultz, *Quantum Field Theory and the Many-Body Problem* (Gordon and Breach Science Publishers, Inc., New York, 1964).

Hamiltonian." [The foregoing statements are obviously quite general and not limited to any specific choice of F within the class satisfying (I.5).] Thus, in Sec. IV an effective, second-quantized Hamiltonian is devised which has the same matrix elements with respect to independent-particle kets of the model occupation number space as does the given Hamiltonian between the Löwdin correlated basis functions, to the cluster order previously considered. This effective Hamiltonian may be looked upon as describing a system of quasiparticles having intrinsic properties associated with the orbitals of the model functions and interacting through well-behaved two-body, three-body, four-body,$\cdots$potentials. If $|N\omega/\Omega|$ is small, the many (>2)-body potentials are, however, of little importance. (In practical calculations on the physical systems of interest, it is expected that the two-body forces of the lowest cluster order will indeed predominate, but that the two-, three-, and four-body forces arising in the next cluster order will be appreciable and will lead to important effects.)

The immediate utility of our second-quantized effective Hamiltonian is illustrated in Sec. IV: we set up a scheme for the self-consistent determination of the one-body potential $V(i)$ of the input independent-particle model.

In summary, we would like to emphasize that, given a system of strongly interacting fermions and a preferred independent-particle model, our method consists in replacement of the physical problem in which the real particles interact via singular two-body potentials, by a fictitious problem in which quasiparticles corresponding to the model interact via well-behaved, two-body, three-body, four-body,$\cdots$potentials. A detailed prescription is furnished for the construction of these effective or residual potentials. Further canonical transformations will, in general, be required to reduce the problem to one of essentially independent quasiparticles. The CBF method, as pursued here and in the paper of FW, thus lays the way for an exploration of the domain of validity of the shell model of the nucleus and the dressed quasiparticle theory of liquid He^3, through practical calculations on these systems.

Section V is devoted to remarks on the implementation of the formalism we have built up. We focus on the flexibility in the choice of the correlation factor f and in the choice of the potential V of the input model. Clearly, our reformulation of the many-particle problem is a useful one if (but not necessarily only if) the dynamical correlations of the real system are well represented by an F (with $f^2-1<0$) corresponding to small $|N\omega/\Omega|$, for then the matrix (H_{mn}) is not far from diagonal and a low-cluster-order calculation suffices for the evaluation of its elements. In this respect, the physical situation appears more favorable to success for nuclear matter than for liquid He^3. An extensive program of nuclear applications has been initiated.

The method of correlated basis functions is of course much more general than we might have implied by concentrating on the many-fermion problem with short-range forces: As examples of its application to a wide range of Fermi and Bose problems we may cite all prior work based on BDJ wave functions,[11–25] together with the more general approaches of Tagami,[40] Nakamura,[31] and Fujita,[41] but single out for closer attention the studies of liquid He^4,[27,28,7,9] liquid He^3,[5,10] and the (hypothetical) charged Bose gas[30] by Feenberg and collaborators. The underlying philosophy of the CBF method may be summed up by saying that it is aimed primarily at calculation of the properties of actual physical systems, starting from a "zeroth-order" description that is rich enough, close enough to physical reality, that there is some hope of attaining this goal.

II. EVALUATION OF MATRIX ELEMENTS FOR BDJ CORRELATION FACTOR

By suitable adaptation of cluster expansion techniques developed for diagonal elements by Iwamoto and Yamada (IY),[15] we shall be able to achieve a systematic evaluation of all the matrix elements, $\mathfrak{N}_{\mathrm{mn}}$, $\mathfrak{H}_{\mathrm{mn}}$. Attention is now centered on an infinitely extended, *uniform* system, whose description will involve, as usual, the ultimate limiting process $N, \Omega\to\infty$, $N/\Omega=\rho$ = constant. A correlation factor F of BDJ form (I.5) is assumed. For each model function Φ_{m} we take a (normalized) Slater determinant of single-particle orbitals φ_{m_i}, $i=1,\cdots,N$ (i=row index); for the φ_{m_i}, the natural choice of plane waves,[42] supplemented by the right spin, isospin factors, normalized to unity and satisfying periodic boundary conditions in a large cube of side length L, $L^3=\Omega$. To avoid confusion of the multitude of superscripts and subscripts that will arise, the following conventions are to be adopted: Let italic Latin letters up to l $(\cdots,i,j,k,l(\doteq 1,\cdots,N))$ be, as appropriate, particle or "place" indices. By "place" we mean the number of the row occupied by a given orbital in a Slater determinant. Reserve boldface Latin characters beginning with $\mathbf{m}$ $(\mathbf{m},\mathbf{n},\mathbf{p},\mathbf{q},\cdots)$ to distinguish independent-particle states. Thus, $\mathbf{m}$ is specified by the sequence of orbital labels $m_1, m_2,\cdots, m_i,\cdots, m_N$. Each m_i signifies a distinct collection of single-particle quantum numbers. We presume further that for the particular pair of states $\mathbf{m}$, $\mathbf{n}$ with which we deal, the place subscripts are so chosen that $m_i=n_{i'}$ only if $i=i'$ and that the $d(\doteq 0,1,\cdots,N)$ orbitals in which $\mathbf{m}$ and $\mathbf{n}$ differ have the first d place indices. [This requirement is eventually relaxed (Sec. IV), with the result that some of the matrix elements $\mathfrak{N}_{\mathrm{mn}}$, $\mathfrak{H}_{\mathrm{mn}}$ for a given set $\{\Psi_{\mathrm{m}}\}$ may differ in sign from those we calculate here.] Finally, in functional arguments, the space, spin, and isospin

[40] T. Tagami, Progr. Theoret. Phys. (Kyoto) **21**, 533 (1959).
[41] J. Fujita, Nucl. Phys. **14**, 648 (1960).
[42] Plane waves are one solution of the Hartree-Fock self-consistency equations for an infinite medium. Whether they are the optimum single-particle orbitals with regard to minimizing the expectation value of a well-behaved Hamiltonian is a topic of current interest. Cf. C. Warke, Phys. Rev. **139**, B17 (1965).

coordinates x_i of particle i are often indicated by i alone.

Given that the Hamiltonian of the system is a sum of one-body and two-body operators only [Eq. (I.1)], all the information we need may be extracted from the behavior of the *generalized normalization integral*

$$I^{\mathrm{mn}}(\beta,\alpha_1\cdots\alpha_N)=(N!)^{1/2}\int\prod_b dx_b\Phi_{\mathrm{m}}^*\times\{\prod_{i<j<k}\exp\beta H_3(ijk)\}\{\prod_{i<j}f^2(r_{ij})\exp\beta H_2(ij)\}\times\{\prod_i\exp\beta H_1(i)\exp(\alpha_i\varphi_{n_i}(i)/\varphi_{m_i}(i))\varphi_{m_i}(i)\}\quad\text{(II.1)}$$

for values of the parameters β, $\alpha_1\cdots\alpha_N$ near zero. The symbol $\int\prod_b dx_b$ implies integration over the space variables and summation over the spin variables of all particles. Here H_1, H_2, and H_3 are properly defined one-particle, two-particle, and three-particle operators, respectively. For example, we shall take

$$H_1(i)=-(\hbar^2/2M)\Delta_i+V(i),$$

$$H_2(ij)=-\frac{\hbar^2}{M}\left\{\frac{\Delta_i f(r_{ij})}{f(r_{ij})}+\frac{\nabla_i f(r_{ij})\cdot\nabla_i+\nabla_j f(r_{ij})\cdot\nabla_j}{f(r_{ij})}\right\}+v(ij)-\frac{1}{N-1}[V(i)+V(j)],\quad\text{(II.2)}$$

$$H_3(ijk)=-\frac{\hbar^2}{M}\sum_{\substack{ijk\\ \text{cyclic}}}\frac{\nabla_j f(r_{ij})\cdot\nabla_j f(r_{jk})}{f(r_{ij})f(r_{jk})},$$

where $V(i)$ is an arbitrary one-body potential (which may later be determined self-consistently). The central role of $I^{\mathrm{mn}}(\beta,\alpha_1\cdots\alpha_N)$ then emerges from the readily verified properties

$$\mathfrak{n}_{\mathrm{mn}}=\int\prod_b dx_b\Phi_{\mathrm{m}}^*F^2\Phi_{\mathrm{n}}=\frac{\partial dI^{\mathrm{mn}}(0,\alpha_1\cdots\alpha_N)}{\partial\alpha_1\cdots\partial\alpha_d}\bigg|_{\alpha_1=\cdots=\alpha_N=0},$$

$$\mathfrak{h}_{\mathrm{mn}}=\int\prod_b dx_b\Phi_{\mathrm{m}}^*FHF\Phi_{\mathrm{n}}=\frac{\partial}{\partial\beta}\frac{\partial^d I^{\mathrm{mn}}(\beta,\alpha_1\cdots\alpha_N)}{\partial\alpha_1\cdots\partial\alpha_d}\bigg|_{\alpha_1=\cdots=\alpha_N=\beta=0}.\quad\text{(II.3)}$$

These are the matrix elements of the identity and Hamiltonian with respect to the set of unnormalized correlated functions $\{F\Phi_{\mathrm{m}}\}$. Clearly contributions to I^{mn} quadratic in any of the parameters β, $\alpha_1\cdots\alpha_N$ may be ignored; also the order of differentiation is immaterial. The reason for the name *generalized normalization integral* is that, so far as the cluster analysis of IY is concerned, I^{mn} looks in all essentials like a diagonal matrix element of the identity, viz., like $\mathfrak{n}_{\mathrm{mm}}$. Our ability to evaluate the $\mathfrak{N}_{\mathrm{mn}}$, $\mathfrak{H}_{\mathrm{mn}}$ thus rests on the great flexibility of the IY formalism. [One may note that $I(\beta)$ of IY is the same as the above $I^{\mathrm{mn}}(\beta,0,\cdots 0)$, to first order in β.]

Let us now begin the necessary enrichment of the scheme as presented in the first IY paper, by defining subnormalization integrals involving lesser numbers of orbitals (suppress superscripts for the moment):

$$I_i=(1!)^{1/2}\int dx_1\varphi_{m_i}^*(1)\exp\beta H_1(1)\exp[\alpha_i\varphi_{n_i}(1)/\varphi_{m_i}(1)]\varphi_{m_i}(1),$$

$$I_{ij}=(2!)^{1/2}\int dx_1dx_2\Phi_{m_im_j}^*(12)f^2(r_{12})\exp\beta H_2(12)\exp\beta[H_1(1)+H_1(2)]\times\exp[\alpha_i\varphi_{n_i}(1)/\varphi_{m_i}(1)]\exp[\alpha_j\varphi_{n_j}(2)/\varphi_{m_j}(2)]\varphi_{m_i}(1)\varphi_{m_j}(2),\quad\text{(II.4)}$$

$$I_{ijk}=(3!)^{1/2}\int dx_1dx_2dx_3\Phi_{m_im_jm_k}^*(123)\exp\beta H_3(123)f^2(r_{12})f^2(r_{23})f^2(r_{31})\exp\beta[H_2(12)+H_2(23)+H_2(31)]\times\exp[\alpha_i\varphi_{n_i}(1)/\varphi_{m_i}(1)]\exp[\alpha_j\varphi_{n_j}(2)/\varphi_{m_j}(2)]\exp[\alpha_k\varphi_{n_k}(3)/\varphi_{m_k}(3)]\varphi_{m_i}(1)\varphi_{m_j}(2)\varphi_{m_k}(3),$$

$$\vdots$$

$$I_{12\ldots N}=I(\beta,\alpha_1\cdots\alpha_N),$$

and, in terms of these, cluster integrals X_i, X_{ij}, $X_{ijk},\cdots$

$$\begin{aligned}I_i&=X_i,\\ I_{ij}&=X_iX_j+X_{ij},\\ I_{ijk}&=X_iX_jX_k+X_iX_{jk}+X_jX_{ki}+X_kX_{ij}+X_{ijk},\\ &\vdots\\ I=I_{12\ldots N}&=\sum_{\substack{\text{all partitions}\\ b+\cdots+c=N}}X_{i_1\cdots i_b}\cdots X_{j_1\cdots j_c}b,\ \cdots,\ c\text{ positive integers}.\end{aligned}\quad\text{(II.5)}$$

[In the definition of $I_{i\cdots l}$, $\Phi_{m_i\cdots m_l}$ is a (normalized) Slater determinant involving the orbitals $\varphi_{m_i},\cdots,\varphi_{m_l}$, a function of as many sets of particle coordinates.] Indices occurring on an $I\ldots$ or an $X\ldots$ are always supposed to be distinct.[43] Clearly neither the $I\ldots$ nor the $X\ldots$ depend on the order of their indices.

In order to classify the successive contributions to I^{mn}, we introduce a parameter ω whose magnitude measures the effective volume in which—as depicted by the correlation factor f—a particle's correlations with a second fixed particle are very strong: Decomposing the correlation factor $f^2(r_{ij})=1+\eta(r_{ij})$, we now set

$$\omega=\int[f^2(r_{ij})-1]d\mathbf{r}_{ij}=\int\eta(r_{ij})d\mathbf{r}_{ij}\,, \tag{I.7}$$

though it may be better to take ω as a suitable average of antisymmetric two-body matrix elements of η.[15] (If the total $|N\omega|$ of all such volumes, taking each particle in turn as the fixed particle, is "sufficiently small" compared to the normalization volume Ω, then the expansions we shall ultimately obtain for the $\mathfrak{N}_{\mathrm{mn}}$ and $\mathfrak{H}_{\mathrm{mn}}$ will converge rapidly.) To assign an order of magnitude in the *correlation parameter* ω to any integral involving some number of η's, consider the η's as Dirac delta functions on the separations r_{ij}, etc., contained in their arguments and count the number of *independent* delta functions that result.

Certain useful but not essential simplifications emerge if $V(i)$ is chosen such that the φ_{p_j}'s are eigenfunctions of H_1:

$$H_1(i)\varphi_{p_j}(i)=\epsilon_{p_j}\varphi_{p_j}(i)\,. \tag{II.6}$$

Solving for the first few X's, we obtain

$$\begin{aligned}
&X_i=I_{i=0}\;O(1)\,,\\
&X_{ij}=(m_im_j|\,h_2(12)\,|m_im_j)_{a=0}\;O(\omega/\Omega)\,,\\
&X_{ijk}=(m_im_jm_k|\,h_2(12)h_2(23)+h_2(23)h_2(31)+h_2(31)h_2(12)\\
&\qquad\qquad+h_2(12)h_2(23)h_2(31)+g_2(12)g_2(23)g_2(31)h_3(123)\,|\,m_im_jm_k)_{a=0}\;O((\omega/\Omega)^2)\,,\\
&X_{ijkl}'=(m_im_jm_km_l|\,h_2(12)h_2(34)+h_2(13)h_2(24)+h_2(14)h_2(23)\,|\,m_im_jm_km_l)_a\\
&\qquad\qquad-X_{ij}X_{kl}-X_{ik}X_{jl}-X_{il}X_{jk=0}\;O((\omega/\Omega)^2)\,,
\end{aligned} \tag{II.7}$$

with $g_2(12)=f^2(r_{12})\exp\beta H_2(12)$, $h_2(12)=g_2(12)-1$, etc., $g_3(123)=\exp\beta H_3(123)$, $h_3(123)=g_3(123)-1$, and the notation

$$\begin{aligned}
(m_i\cdots m_l|\,\mathcal{O}(1\cdots k)\,|m_i\cdots m_l)_a=(k!)^{1/2}\int dx_1\cdots dx_k\Phi_{m_i\ldots m_l}{}^*\mathcal{O}(1\cdots k)\exp\beta[H_1(1)+\cdots+H_1(k)]\\
\times\exp[\alpha_i\varphi_{n_i}(1)/\varphi_{m_i}(1)]\cdots\exp[\alpha_l\varphi_{n_l}(k)/\varphi_{m_l}(k)]\varphi_{m_i}(1)\cdots\varphi_{m_l}(k)
\end{aligned} \tag{II.8}$$

(the subscript a stands for "antisymmetrized"). The order-of-magnitude assignments in ω and Ω, given at the right in the above expressions, are appropriate to zero values of all the parameters β, $\alpha_1\cdots\alpha_N$. In this sense, we have given explicitly *all* X's of second or lower order in the correlation parameter. (It should be remarked that X_{ijkl}' is only that part of X_{ijkl} in which two separate h_2's are connected by exchange.) For the one-index cluster integral, we have the properties

$$\begin{aligned}
&X_i^{\mathrm{mn}}|_{\beta=\alpha_i=0}=1\,, \qquad \frac{\partial X_i^{\mathrm{mn}}}{\partial\alpha_i}\bigg|_{\beta=\alpha_i=0}=\delta_{m_in_i}\,,\\
&\frac{\partial X_i^{\mathrm{mn}}}{\partial\beta}\bigg|_{\beta=\alpha_i=0}=\epsilon_{m_i}\,, \qquad \frac{\partial}{\partial\beta}\frac{\partial X_i^{\mathrm{mn}}}{\partial\alpha_i}\bigg|_{\beta=\alpha_i=0}=\epsilon_{m_i}\delta_{m_in_i}\,,
\end{aligned} \tag{II.9}$$

the last two being consequences of the choice of $V(i)$ implied by (II.6). For the cluster integrals with more than one index, differentiation with respect to β (with respect to an α) reduces by one (leaves unchanged) the order in ω of a given cluster integral as shown in (II.7) and of course cannot affect its order in Ω. [This statement is clear for the term in X_{ijk} involving $H_3(123)$ only after an integration by parts.]

Asymptotically ($N,\Omega\to\infty$, $\rho=$const) the last equation of (II.5) does not provide a useful expansion for I^{mn}, since the successive groups of terms in the explicit series increase as higher and higher powers of N. The transformation of I from the last of (II.5) to the asymptotically valid exponential or Ursell[36] form

$$\begin{aligned}
&I^{\mathrm{mn}}(\beta,\alpha_1\cdots\alpha_N)=\prod_{i=1}^{N}X_i(\beta,\alpha_i)\exp NG^{\mathrm{mn}}(\beta,\alpha_1\cdots\alpha_N)\,,\\
&\qquad\qquad N,\Omega\to\infty\,,\quad \rho=\mathrm{const}\,,\\
&G^{\mathrm{mn}}=O(N\omega/\Omega)
\end{aligned} \tag{II.10}$$

goes through exactly as described for $I(\beta)$ by IY, with modifications indicated by Iwamoto.[44] These authors utilize in particular the feature that there are no duplications or omissions of place indices in the last of (II.5), to develop a set of partial differential equations for $G^{\mathrm{mn}}(\beta,0\cdots0)$ which may be solved by successive approximations. A more satisfying justification of the transformation [and concomitant generation of

[43] Note that an $I\ldots$ with two equal indices would vanish by antisymmetry of the $\Phi\ldots{}^*$ in its integrand.

[44] F. Iwamoto (private communication to F. Y. Wu and E. Feenberg).

$G^{mn}(\beta,0\cdots0)$ expansion] has been offered by Wu and Feenberg,[5] and analyzed with great care by Wu.[29] The result of both procedures, *applicable to our more general I*, is

$$G=\frac{1}{N}\sum_{i<j}x_{ij}-\frac{1}{2N}\sum_{i<j}x_{ij}^2-\frac{1}{2N}\sum_{i,j,k}x_{ij}x_{jk}$$
$$+\frac{1}{N}\sum_{i<j<k}x_{ijk}+\frac{1}{N}\sum_{i<j<k<l}x_{ijkl}'+O((N\omega/\Omega)^3), \quad \text{(II.11)}$$

where the (small) x's are so-called normalized cluster integrals,

$$x_{i\cdots l}=X_{i\cdots l}/X_i\cdots X_l. \quad \text{(II.12)}$$

The first term is $O(N\omega/\Omega)$, the second, $O(N^{-1}(N\omega/\Omega)^2)$ and hence asymptotically negligible, and the next three, $O((N\omega/\Omega)^2)$. The analysis of the four-index term is a bit tricky. For a full explanation the reader is referred to IY; we will, however, take time to point out, in our explicit results, the unusual features which arise from this term.

Using (II.3) together with (II.10), (II.11), and the properties (II.9), we arrive at the following working formulas for the computation of the matrix elements $\mathfrak{N}_{mn}$, $\mathfrak{H}_{mn}$ with respect to our set of normalized correlated functions:

$$\mathfrak{N}_{mn}=\mathfrak{n}_{mn}/(\mathfrak{n}_{mm}\mathfrak{n}_{nn})^{1/2}=\mathcal{P}_{mn}(0),$$
$$\mathfrak{H}_{mn}=\mathfrak{h}_{mn}/(\mathfrak{n}_{mm}\mathfrak{n}_{nn})^{1/2} \quad \text{(II.13)}$$
$$=\mathcal{E}_m\mathcal{P}_{mn}(0)+\frac{\partial}{\partial\beta}\mathcal{P}_{mn}(\beta)\,|_{\beta=0},$$

where

$$\mathcal{E}_m\equiv\sum_i\epsilon_{m_i},$$
$$\mathcal{P}_{mn}(\beta)\equiv\frac{\partial^d}{\partial\alpha_1\cdots\partial\alpha_d}\exp NG^{mn}(\beta,\alpha_1\cdots\alpha_N)\,|_{\alpha_1=\cdots=\alpha_N=0}$$
$$\times\exp[-\tfrac{1}{2}N(G^{mm}(0,0\cdots0)+G^{nn}(0,0\cdots0))]. \quad \text{(II.14)}$$

In a calculation accurate to second order in ω for $\mathfrak{N}_{mn}$ and to first order for $\mathfrak{H}_{mn}$, we need only consider the following (five) cases:

Diagonal Elements: $m_i=n_i$, $i=1,\cdots,N$.

$$\mathfrak{N}_{mm}=\mathcal{P}_m=1,$$
$$\mathfrak{H}_{mm}=\mathcal{E}_m+\mathcal{P}_{m,\beta}=\mathcal{E}_m+NG_{,\beta}^{m}$$
$$=\mathcal{E}_m+\underset{O(N)}{\sum_{i<j}}X_{ij,\beta}^{m}-\underset{O(N\omega)}{\sum_{i<j}}X_{ij}^{m}(\epsilon_{m_i}+\epsilon_{m_j})$$
$$-\underset{O(N\omega)}{\sum_{i,j,k}}X_{ij,\beta}^{m}X_{ik}^{m}+\underset{O(N\omega)}{\sum_{i<j<k}}X_{ijk,\beta}^{m} \quad \text{(II.15)}$$
$$+\underset{O(N\omega)}{\sum_{i<j<k<l}}X_{ijkl,\beta}'^{m}+O(N\omega^2).$$

Here we have initiated certain helpful practices: (i) Order of magnitude assignments are placed under the explicit terms; in these the average density $\rho=N/\Omega$ is taken unity to simplify writing. (ii) A repeated model-state label on a given symbol is often omitted. (ii) Differentiation is indicated with a comma followed by the variable with respect to which the differentiation is carried out, it being henceforth understood that the parameters $\beta,\alpha_1\cdots\alpha_N$ are set zero finally in *all* expressions.

It should be remarked that the addend involving a sum over four place indices, instead of being $O(N^2\omega)$ as one might at first suspect, is indeed of the order indicated, since, as detailed examination of the structure of $X_{ijkl,\beta}'^{m}$ will reveal, the indices i,j,k,l associated with nonvanishing contributions are not independent but are connected, because of our periodic plane-wave choice of single-particle functions, by one of three relations of linear dependence among the corresponding wave vectors[15]:

$$\mathbf{k}_{m_i}+\mathbf{k}_{m_j}=\mathbf{k}_{m_k}+\mathbf{k}_{m_l},$$
$$\mathbf{k}_{m_i}+\mathbf{k}_{m_k}=\mathbf{k}_{m_j}+\mathbf{k}_{m_l}, \quad \text{(II.16)}$$
$$\mathbf{k}_{m_i}+\mathbf{k}_{m_l}=\mathbf{k}_{m_j}+\mathbf{k}_{m_k}.$$

Nondiagonal Elements

One Orbital Different: $m_1\neq n_1$, $m_i=n_i$, $i>1$.

Our choice of single-particle orbitals leads to a *momentum conservation theorem*, $\mathfrak{H}_{mn}=0$, $\mathfrak{N}_{mn}=0$ unless $\sum_i\mathbf{k}_{m_i}=\sum_i\mathbf{k}_{n_i}$. Since model-function momentum cannot be conserved in the present case, the required matrix elements are zero. One should note at this juncture the collateral vanishing of integrals X_{ij,α_i}, $X_{ij,\alpha_i\beta}$, X_{ijk,α_i}, $X_{ijk,\alpha_i\beta},\cdots$; hence, the vanishing of $NG_{,\alpha_i}$, $NG_{,\alpha_i\beta}$, for $i=1,\cdots,d$, again—as we say—due to momentum conservation in the extended medium. These relations allow simplification of calculation in subsequent cases. All future order of magnitude assignments are made on the supposition that the momentum of model state **n** is *equal* to the momentum of model state **m**.

The above *momentum* conservation theorem holds strictly for our uniform extended medium. However, two model states **m**, **n** might differ just in the spin (isospin) quantum number of the 1st orbital. If so, and the particles interact via a two-body potential which conserves the total spin (isospin), $\mathfrak{N}_{mn}$ and $\mathfrak{H}_{mn}$ still vanish, but in the presence of a two-body potential which is able to alter the total spin (isospin), $\mathfrak{H}_{mn}$ (for such a one-orbital difference) may survive. The generalizations required to treat the latter kinds of potential, not profound, will be developed as needed in future applications.

Two Orbitals Different: $m_1\neq n_1$, $m_2\neq n_2$, $m_i=n_i$, $i>2$.

$$\mathcal{P}_{\mathbf{mn}}=NG_{,\alpha_1\alpha_2}{}^{\mathbf{mn}}\exp\tfrac{1}{2}N(G^{\mathbf{m}}-G^{\mathbf{n}}),$$

$$\mathcal{P}_{\mathbf{mn},\beta}=(NG_{,\alpha_1\alpha_2\beta}{}^{\mathbf{mn}}+NG_{,\alpha_1\alpha_2}{}^{\mathbf{mn}}NG_{,\beta}{}^{\mathbf{m}})\exp\tfrac{1}{2}N(G^{\mathbf{m}}-G^{\mathbf{n}}),$$

$$NG_{,\alpha_1\alpha_2}{}^{\mathbf{mn}}=\underset{O(\omega/N)}{X_{12,\alpha_1\alpha_2}{}^{\mathbf{mn}}}-\underset{O(\omega^2/N)}{X_{12,\alpha_1\alpha_2}{}^{\mathbf{mn}}\sum_i(X_{1i}{}^{\mathbf{m}}+X_{2i}{}^{\mathbf{m}})}+\underset{O(\omega^2/N)}{\sum_i X_{12i,\alpha_1\alpha_2}{}^{\mathbf{mn}}}+\underset{O(\omega^2/N)}{\sum_{i<j}X_{12ij,\alpha_1\alpha_2}{}'^{\mathbf{mn}}}+O(\omega^3/N),$$

$$NG_{,\alpha_1\alpha_2\beta}{}^{\mathbf{mn}}=\underset{O(1/N)}{X_{12,\alpha_1\alpha_2\beta}{}^{\mathbf{mn}}}-\underset{O(\omega/N)}{X_{12,\alpha_1\alpha_2}{}^{\mathbf{mn}}(\epsilon_{m_1}+\epsilon_{m_2})}-\underset{O(\omega/N)}{X_{12,\alpha_1\alpha_2\beta}{}^{\mathbf{mn}}\sum_i(X_{1i}{}^{\mathbf{m}}+X_{2i}{}^{\mathbf{m}})}$$

$$-\underset{O(\omega/N)}{X_{12,\alpha_1\alpha_2}{}^{\mathbf{mn}}\sum_i(X_{1i,\beta}{}^{\mathbf{m}}+X_{2i,\beta}{}^{\mathbf{m}})}+\underset{O(\omega/N)}{\sum_i X_{12i,\alpha_1\alpha_2\beta}{}^{\mathbf{mn}}}+\underset{O(\omega/N)}{\sum_{i<j}X_{12ij,\alpha_1\alpha_2\beta}{}'^{\mathbf{mn}}}+O(\omega^2/N).$$

In the $\sum_{i<j}$ above, only one of i,j is independent, as will be seen by inspecting again the fourth member of (II.7), or better, (II.29), (II.30).

An expansion of the exponential factor in $\mathcal{P}_{\mathbf{mn},\beta}$ is permissible.

$$\exp\tfrac{1}{2}N(G^{\mathbf{m}}-G^{\mathbf{n}})=\exp[\tfrac{1}{4}\sum_{i,j}(X_{ij}{}^{\mathbf{m}}-X_{ij}{}^{\mathbf{n}})+O(\omega^2)]$$

$$=1+\underset{O(\omega)}{\tfrac{1}{2}\sum_i(X_{1i}{}^{\mathbf{m}}+X_{2i}{}^{\mathbf{m}}-X_{1i}{}^{\mathbf{n}}-X_{2i}{}^{\mathbf{n}})}+O(\omega^2).$$

Thus, we obtain finally

$$\mathfrak{N}_{\mathbf{mn}}=\underset{O(\omega/N)}{X_{12,\alpha_1\alpha_2}{}^{\mathbf{mn}}}-\underset{O(\omega^2/N)}{\tfrac{1}{2}X_{12,\alpha_1\alpha_2}{}^{\mathbf{mn}}\sum_i(X_{1i}{}^{\mathbf{m}}+X_{2i}{}^{\mathbf{m}}+X_{1i}{}^{\mathbf{n}}+X_{2i}{}^{\mathbf{n}})}+\underset{O(\omega^2/N)}{\sum_i X_{12i,\alpha_1\alpha_2}{}^{\mathbf{mn}}}+\underset{O(\omega^2/N)}{\sum_{i<j}X_{12ij,\alpha_1\alpha_2}{}'^{\mathbf{mn}}}+O(\omega^3/N),$$

$$\mathfrak{H}_{\mathbf{mn}}=\underset{O(1/N)}{X_{12,\alpha_1\alpha_2\beta}{}^{\mathbf{mn}}}-\underset{O(\omega/N)}{\tfrac{1}{2}X_{12,\alpha_1\alpha_2}{}^{\mathbf{mn}}(\epsilon_{m_1}+\epsilon_{m_2}+\epsilon_{n_1}+\epsilon_{n_2})}-\underset{O(\omega/N)}{\tfrac{1}{2}X_{12,\alpha_1\alpha_2\beta}{}^{\mathbf{mn}}\sum_i(X_{1i}{}^{\mathbf{m}}+X_{2i}{}^{\mathbf{m}}+X_{1i}{}^{\mathbf{n}}+X_{2i}{}^{\mathbf{n}})}$$

$$-\underset{O(\omega/N)}{\tfrac{1}{2}X_{12,\alpha_1\alpha_2}{}^{\mathbf{mn}}\sum_i(X_{1i,\beta}{}^{\mathbf{m}}+X_{2i,\beta}{}^{\mathbf{m}}+X_{1i,\beta}{}^{\mathbf{n}}+X_{2i,\beta}{}^{\mathbf{n}})}+\underset{O(\omega/N)}{\sum_i X_{12i,\alpha_1\alpha_2\beta}{}^{\mathbf{mn}}}+\underset{O(\omega/N)}{\sum_{i<j}X_{12ij,\alpha_1\alpha_2\beta}{}'^{\mathbf{mn}}}$$

$$+\underset{O(\omega)}{\tfrac{1}{2}\mathfrak{N}_{\mathbf{mn}}(\mathfrak{H}_{\mathbf{mm}}+\mathfrak{H}_{\mathbf{nn}})}+O(\omega^2/N). \quad \text{(II.17)}$$

The occurrence in $\mathfrak{H}_{\mathbf{mn}}$ of a contribution $O(\omega)$, which would seem to dominate all the others, might be a bit disturbing at this point. There is nothing amiss, however, since the nondiagonal $\mathfrak{H}_{\mathbf{mn}}$ only enter into many-body calculations in forms like $\mathfrak{H}_{\mathbf{mn}}-\mathfrak{H}_{\mathbf{ss}}\mathfrak{N}_{\mathbf{mn}}$, **s** differing from **m**,**n** in numbers of orbitals small compared to N, so that terms $O(\omega)$ do not survive.

Three Orbitals Different: $m_1\neq n_1$, $m_2\neq n_2$, $m_3\neq n_3$, $m_i=n_i$, $i>3$.

$$\mathcal{P}_{\mathbf{mn}}=NG_{,\alpha_1\alpha_2\alpha_3}{}^{\mathbf{mn}}\exp\tfrac{1}{2}N(G^{\mathbf{m}}-G^{\mathbf{n}}),$$

$$\mathcal{P}_{\mathbf{mn},\beta}=(NG_{,\alpha_1\alpha_2\alpha_3\beta}{}^{\mathbf{mn}}+NG_{,\alpha_1\alpha_2\alpha_3}{}^{\mathbf{mn}}NG_{,\beta}{}^{\mathbf{m}})\exp\tfrac{1}{2}N(G^{\mathbf{m}}-G^{\mathbf{n}}),$$

$$NG_{,\alpha_1\alpha_2\alpha_3}{}^{\mathbf{mn}}=\underset{O(\omega^2/N^2)}{X_{123,\alpha_1\alpha_2\alpha_3}{}^{\mathbf{mn}}}+\underset{O(\omega^2/N^2)}{\sum_i X_{123i,\alpha_1\alpha_2\alpha_3}{}'^{\mathbf{mn}}}+O(\omega^3/N^2),$$

$$NG_{,\alpha_1\alpha_2\alpha_3\beta}{}^{\mathbf{mn}}=\underset{O(\omega/N^2)}{X_{123,\alpha_1\alpha_2\alpha_3\beta}{}^{\mathbf{mn}}}+\underset{O(\omega/N^2)}{\sum_i X_{123i,\alpha_1\alpha_2\alpha_3\beta}{}'^{\mathbf{mn}}}+O(\omega^2/N^2).$$

Take note here that the index i appearing in the sum terms is restricted to only a few possibilities by the relations of linear dependence of the type (II.16) which one must always associate with the primed part of the four-index cluster integral.

Expanding the exponential,

$$\exp\tfrac{1}{2}N(G^{m}-G^{n})=1+\tfrac{1}{2}\sum_{i}(X_{1i}{}^{m}+X_{2i}{}^{m}+X_{3i}{}^{m}-X_{1i}{}^{n}-X_{2i}{}^{n}-X_{3i}{}^{n})+O(\omega^{2}).$$

$O(\omega)$

Thus, to the cluster orders of interest, we have quite simply

$$\begin{aligned}\mathfrak{N}_{mn}&=X_{123,\alpha_1\alpha_2\alpha_3}{}^{mn}+\sum_{i}X_{123i,\alpha_1\alpha_2\alpha_3}{}'^{mn}+O(\omega^{3}/N^{2}),\\ &\quad O(\omega^{2}/N^{2}) \qquad\qquad O(\omega^{2}/N^{2})\\ \mathfrak{H}_{mn}&=X_{123,\alpha_1\alpha_2\alpha_3\beta}{}^{mn}+\sum_{i}X_{123i,\alpha_1\alpha_2\alpha_3\beta}{}'^{mn}+\tfrac{1}{2}\mathfrak{N}_{mn}(\mathfrak{H}_{mm}+\mathfrak{H}_{nn})+O(\omega^{2}/N^{2}).\\ &\quad O(\omega/N^{2}) \qquad\qquad O(\omega/N^{2}) \qquad\qquad O(\omega^{2}/N)\end{aligned} \tag{II.18}$$

For the same reason as before, the term $O(\omega^2/N)$ presents no difficulties. If we elect to retain, in $\mathfrak{H}_{mn}$, nothing of higher than first order in ω, we are (formally) justified in omitting this term completely; it has been kept explicit only to emphasize a general feature. Similar statements apply to the next case.

Four Orbitals Different: $m_1\neq n_1$, $m_2\neq n_2$, $m_3\neq n_3$, $m_4\neq n_4$, $m_i=n_i$, $i>4$.

$$\mathcal{P}_{mn}=(NG_{,\alpha_1\alpha_2\alpha_3\alpha_4}{}^{mn}+NG_{,\alpha_1\alpha_2}{}^{mn}NG_{,\alpha_3\alpha_4}{}^{mn}+NG_{,\alpha_1\alpha_3}{}^{mn}NG_{,\alpha_2\alpha_4}{}^{mn}+NG_{,\alpha_1\alpha_4}{}^{mn}NG_{,\alpha_2\alpha_3}{}^{mn})\exp\tfrac{1}{2}N(G^{m}-G^{n}),$$

$$\begin{aligned}\mathcal{P}_{mn,\beta}=[&NG_{,\alpha_1\alpha_2\alpha_3\alpha_4\beta}{}^{mn}+NG_{,\alpha_1\alpha_2\beta}{}^{mn}NG_{,\alpha_3\alpha_4}{}^{mn}+NG_{,\alpha_1\alpha_2}{}^{mn}NG_{,\alpha_3\alpha_4\beta}{}^{mn}+\cdots\\ &+NG_{,\alpha_1\alpha_4}{}^{mn}NG_{,\alpha_2\alpha_3\beta}{}^{mn}+(NG_{,\alpha_1\alpha_2\alpha_3\alpha_4}{}^{mn}+\cdots+NG_{,\alpha_1\alpha_4}{}^{mn}NG_{,\alpha_2\alpha_3}{}^{mn})NG_{,\beta}{}^{m}]\exp\tfrac{1}{2}N(G^{m}-G^{n}).\end{aligned}$$

Additional complexity enters suddenly at this stage, since it is possible to have products of α derivatives of G without violating the momentum conservation theorem. This complexity is only illusory here, however. The extra terms actually *simplify* the structure of the final results:

$$\begin{aligned}\mathfrak{N}_{mn}&=\bar{X}_{1234,\alpha_1\alpha_2\alpha_3\alpha_4}{}'^{mn}+O(\omega^{3}/N^{2}),\\ &\quad O(\omega^{2}/N^{2})\\ \mathfrak{H}_{mn}&=\bar{X}_{1234,\alpha_1\alpha_2\alpha_3\alpha_4\beta}{}'^{mn}+\tfrac{1}{2}\mathfrak{N}_{mn}(\mathfrak{H}_{mm}+\mathfrak{H}_{nn})+O(\omega^{2}/N^{2}),\\ &\quad O(\omega/N^{2}) \qquad\qquad O(\omega^{2}/N)\end{aligned} \tag{II.19}$$

where $\bar{X}_{ijkl}{}'^{mn}(\beta,\alpha_i\cdots\alpha_l)$ is $X_{ijkl}{}'$ of (II.7) *with the last three terms omitted.* As usual, we should comment on the peculiarities associated with the four-index contributions. In this case, though, the situation is a bit different than before, because of the difference between $\bar{X}_{ijkl}{}'^{mn}(\beta,\alpha_i\cdots\alpha_l)$ and $X_{ijkl}{}'^{mn}(\beta,\alpha_i\cdots\alpha_l)$. Nevertheless, there are *still* restrictions on the wave vectors corresponding to the single-particle states m_i, n_i, $i=1,\cdots,4$. The explicit terms in $\mathfrak{N}_{mn}$, $\mathfrak{H}_{mn}$ above do not enter the picture unless the wave vectors involved satisfy one of

$$\begin{aligned}&\mathbf{k}_{m_1}+\mathbf{k}_{m_2}=\mathbf{k}_{n_1}+\mathbf{k}_{n_2},\\ &\mathbf{k}_{m_1}+\mathbf{k}_{m_3}=\mathbf{k}_{n_1}+\mathbf{k}_{n_3},\\ &\mathbf{k}_{m_1}+\mathbf{k}_{m_4}=\mathbf{k}_{n_1}+\mathbf{k}_{n_4},\\ &\mathbf{k}_{m_1}+\mathbf{k}_{m_2}=\mathbf{k}_{n_3}+\mathbf{k}_{n_4},\\ &\mathbf{k}_{m_1}+\mathbf{k}_{m_3}=\mathbf{k}_{n_2}+\mathbf{k}_{n_4},\\ &\mathbf{k}_{m_1}+\mathbf{k}_{m_4}=\mathbf{k}_{n_2}+\mathbf{k}_{n_3}\end{aligned} \tag{II.20}$$

(in addition, of course, to the presumed over-all momentum conservation condition $\mathbf{k}_{m_1}+\mathbf{k}_{m_2}+\mathbf{k}_{m_3}+\mathbf{k}_{m_4}=\mathbf{k}_{n_1}+\mathbf{k}_{n_2}+\mathbf{k}_{n_3}+\mathbf{k}_{n_4}$).

To the cluster order considered, the matrix elements vanish for five or more orbitals different.

We cite for future use the following *general* formula for the matrix elements of the Hamiltonian:

$$\begin{aligned}\mathfrak{H}_{mn}=(&\sum_{\substack{\text{all partitions}\\ a+b+\cdots+c=d\\ a,\,b,\,\cdots,c\geq 2}} NG_{,\alpha_{i(1)}\cdots\alpha_{i(a)}}\cdots NG_{,\alpha_{j(1)}\cdots\alpha_{j(b)}}\\ &\cdot NG_{,\alpha_{k(1)}\cdots\alpha_{k(c)}\beta})\exp\tfrac{1}{2}N(G^{m}-G^{n})\\ &+\tfrac{1}{2}\mathfrak{N}_{mn}(\mathfrak{H}_{mm}-\mathfrak{H}_{nn})+\tfrac{1}{2}\mathfrak{N}_{mn}(\mathfrak{H}_{mm}+\mathfrak{H}_{nn}).\end{aligned} \tag{II.21}$$

Let us examine some of the X's in detail to gain familiarity with the structure of the matrix elements we have treated. Consider the (most important) nondiagonal case of two orbitals different. We need in particular

$$X_{12,\alpha_1\alpha_2}{}^{mn}=(m_1m_2|\,\eta(12)\,|n_1n_2)_a \tag{II.22}$$

and

$$\begin{aligned}X_{12,\alpha_1\alpha_2\beta}{}^{mn}&=(m_1m_2|\,f^{2}(12)H_2(12)+\eta(12)[H_1(1)+H_1(2)]\,|n_1n_2)_a\\ &=(2!)^{1/2}\int dx_1dx_2f(12)\Phi_{m_1m_2}{}^{*}\Big\{-\frac{\hbar^{2}}{2M}(\Delta_1+\Delta_2)+V(1)+V(2)\\ &\qquad+\Big[v(12)-\frac{1}{N-1}[V(1)+V(2)]\Big]\Big\}f(12)\varphi_{n_1}(1)\varphi_{n_2}(2),\end{aligned} \tag{II.23}$$

the matrix element of a (manifestly Hermitian) two-particle Hamiltonian between two-particle correlated functions. [Here $\eta(12)=h_2(12)\,|_{\beta=0}$ and $)_a=\}_a|_{\alpha_1=\cdots=\alpha_N=\beta=0.}$] A more convenient form for the latter cluster integral is

$$X_{12,\alpha_1\alpha_2\beta}{}^{\mathrm{mn}}=\tfrac{1}{2}[X_{12,\alpha_1\alpha_2\beta}{}^{\mathrm{mn}}+(X_{12,\alpha_1\alpha_2\beta}{}^{\mathrm{nm}})^*]$$
$$=\underset{O(1/N)}{(m_1m_2|\tilde{w}_2(12)|n_1n_2)_a}+\tfrac{1}{2}\underset{O(\omega/N)}{(m_1m_2|f^2(12)-1|n_1n_2)_a}(\epsilon_{m_1}+\epsilon_{m_2}+\epsilon_{n_1}+\epsilon_{n_2}), \tag{II.24}$$

where

$$\tilde{w}_2(12)=\frac{\hbar^2}{M}(\nabla f(12))^2+f^2(12)v(12)-\frac{1}{N-1}f^2(12)[V(1)+V(2)] \tag{II.25}$$

is an *effective two-body interaction*. Observe that the second term in this expression for $X_{12,\alpha_1\alpha_2\beta}{}^{\mathrm{mn}}$, $O(\omega/N)$, exactly cancels the second term in $\mathfrak{H}_{\mathrm{mn}}$. It is thus advantageous to consider the first two terms in $\mathfrak{H}_{\mathrm{mn}}$ as a unit.

Proceeding to more complicated cluster integrals, we find

$$X_{12i,\alpha_1\alpha_2}{}^{\mathrm{mn}}=(m_1m_2m_i|\sum_{\substack{123\\ \text{cyclic}}}[\eta(12)\eta(23)]+\eta(12)\eta(23)\eta(31)|n_1n_2m_i)_a, \tag{II.26}$$

$$X_{12i,\alpha_1\alpha_2\beta}{}^{\mathrm{mn}}=(m_1m_2m_i|\sum_{\substack{123\\ \text{cyclic}}}[\eta(12)f^2(23)H_2(23)+\eta(23)f^2(12)H_2(12)$$
$$+\eta(31)\eta(12)f^2(23)H_2(23)]+\underset{O(\omega/N^2)}{f^2(12)f^2(23)f^2(31)H_3(123)|n_1n_2m_i)_a}$$
$$+(m_1m_2m_i|\sum_{\substack{123\\ \text{cyclic}}}[\eta(12)\eta(23)]+\eta(12)\eta(23)\eta(31)|n_1n_2m_i)_a(\epsilon_{n_1}+\epsilon_{n_2}+\epsilon_{m_i}) \tag{II.27}$$
$$=\underset{O(\omega/N^2)}{(m_1m_2m_i|\tilde{w}_3(123)|n_1n_2m_i)_a}+O(\omega^2/N^2),$$

where

$$\tilde{w}_3(123)=\sum_{\substack{123\\ \text{cyclic}}}[\eta(12)\tilde{w}_2(23)+\eta(23)\tilde{w}_2(12)+\eta(31)\eta(12)\tilde{w}_2(23)]+f^2(12)f^2(23)f^2(31)H_3(123) \tag{II.28}$$

is an *effective three-body interaction*. Finally,

$$X_{12ij,\alpha_1\alpha_2}{}'^{\mathrm{mn}}=(m_1m_2|\eta(12)|m_im_j)_a(m_im_j|\eta(34)|n_1n_2)_a$$
$$+(m_1m_i|\eta(12)|n_2m_j)_a(m_2m_j|\eta(34)|n_1m_i)_a+(m_1m_j|\eta(12)|m_in_2)_a(m_im_2|\eta(34)|n_1m_j)_a, \tag{II.29}$$

$$X_{12ij,\alpha_1\alpha_2\beta}{}'^{\mathrm{mn}}=6\underset{O(\omega/N^2)}{(m_1m_2m_im_j|\eta(12)f^2(34)H_2(34)|n_1n_2m_im_j)'_a{}'}+O(\omega^2/N^2)$$
$$=6\underset{O(\omega/N^2)}{(m_1m_2m_im_j|\eta(12)\tilde{w}_2(34)|n_1n_2m_im_j)'_a{}'}+O(\omega^2/N^2), \tag{II.30}$$

where the quotes on the a mean that in the antisymmetrization one should omit terms resulting from permutations 1, (m_1m_2), (m_im_j), $(m_1m_2)\cdot(m_im_j)$.

Reduction of the X's to explicit forms in terms of f^2, η, $\tilde{w}_2$, $\tilde{w}_3$ may also be carried through for the other cases, by trivial modification of the above.[45] To bring out a general feature, note in particular that for the diagonal Hamiltonian matrix elements,

$$X_{ij,\beta}{}^{\mathrm{m}}-X_{ij}{}^{\mathrm{m}}(\epsilon_{m_i}+\epsilon_{m_j})=(m_im_j|\tilde{w}_2(12)|m_im_j)_a. \tag{II.31}$$

This provides the prototype for combinations that may be made in all orders of our $\mathfrak{H}_{\mathrm{mm}}$ expansion to eliminate the single-particle energies that appear in one order higher, at the same time replacing all two- or more-index cluster integrals $X\ldots$ by their corresponding matrix elements in terms of $\tilde{w}_2$. We have not displayed the terms $O(N\omega^2)$ which are needed to make this recombination and rewrite (II.15) in $\tilde{w}_2$ language, but they are evidently present. Similar recombinations may be made in all orders of expansion for the nondiagonal matrix elements; again there is a cancellation of terms containing single-particle energies and $\tilde{w}_2$ takes over a basic role. Thus a general theorem may be proved: The cluster expansions for the matrix elements $\mathfrak{H}_{\mathrm{mn}}$ may be rearranged so that single-particle energies enter only in the form $\frac{1}{2}\sum_i(\epsilon_{m_i}+\epsilon_{n_i})\mathfrak{N}_{\mathrm{mn}}$ [cf. the last term in (II.21)]. This gives a more satisfying justification of our revision of the explicit forms in (II.15), (II.17), (II.18), (II.19) than the mere fact that all differences are of higher order than we choose to consider.

The effective interaction operators $\tilde{w}_2$, $\tilde{w}_3$ that occur in the preceding formulas are *local* apart from non-

[45] The contributions to the diagonal elements $\mathfrak{H}_{\mathrm{mm}}$ have been subjected to considerable manipulation by previous authors. See Refs. 16, 18, 20, 26, and 28.

locality introduced by $v(ij)$ itself, or the V's. Upon omission of the V's the tildes are to be removed. We shall at times make use of the further decomposition:

$$(m_i m_j|\tilde{w}_2(12)|n_i n_j)_a = (m_i m_j|w_2(12)-(N-1)^{-1}[V(1)+V(2)]|n_i n_j)_a - (N-1)^{-1}(m_i m_j|\underset{O(\omega/N)}{\eta(12)}[V(1)+V(2)]|n_i n_j)_a . \tag{II.32}$$

III. LÖWDIN TRANSFORMATION TO AN ORTHONORMAL BASIS

As they stand, our correlated functions, being nonorthogonal, do not yield to direct interpretation as a set of "unperturbed" state functions. Furthermore, there persists the rather uncomfortable feature that the Hamiltonian matrix elements $\mathfrak{H}_{mn}$ contain contributions which would appear to swamp by a factor N the vital terms carrying all the physical information. While neither of these defects causes any serious difficulty, it is certainly clear that considerable formal advantages are to be gained by transforming from our original set $\{\Psi_m\}$ to an *orthonormal set of correlated functions* $\{\Theta_m\}$. This may be effected by means of the Löwdin transformation,[37] leading to a systematic orthogonalization scheme which fits neatly into the framework of our basic cluster-expansion procedure for approximate evaluation of the required matrix elements.

The transformation law for going to the new set is compactly stated if we interpret $\{\Psi_m\}$, $\{\Theta_m\}$ as row matrices $\boldsymbol{\Psi}$, $\boldsymbol{\Theta}$, respectively, and denote the matrix of $\mathfrak{N}_{mn}$ by $\mathfrak{N}$:

$$\boldsymbol{\Theta}=\boldsymbol{\Psi}\mathfrak{N}^{-1/2}. \tag{III.1}$$

One can check that, for $\mathfrak{N}^{-1/2}$ Hermitian, $(\Theta_m,\Theta_n)=\delta_{mn}$. Defining $\mathbf{H}$ as the matrix of elements $H_{mn}=(\Theta_m,H\Theta_n)$, we have then

$$\mathbf{H}=\mathfrak{N}^{-1/2}\mathfrak{H}\mathfrak{N}^{-1/2}, \tag{III.2}$$

where, of course, $\mathfrak{H}=(\mathfrak{H}_{mn})$. Let $\mathfrak{I}$ be the deviation of $\mathfrak{N}$ from the unit matrix $\mathbf{I}$, and suppose it is small in the sense that the matrix binomial expansion provides a *meaningful definition* of $\mathfrak{N}^{-1/2}$:

$$\mathfrak{N}^{-1/2}=(\mathbf{I}+\mathfrak{I})^{-1/2}\equiv\mathbf{I}-\tfrac{1}{2}\mathfrak{I}+\tfrac{3}{8}\mathfrak{I}^2-\tfrac{5}{16}\mathfrak{I}^3+\cdots. \tag{III.3}$$

[Now $\mathfrak{N}^{-1/2}$ is manifestly Hermitian, and one can further verify that $(\Theta_m,\Theta_n)=\delta_{mn}$ is fulfilled order by order in $\mathfrak{I}$.] For the calculation of the H_{mn} we thus propose the (Löwdin) expansion

$$\mathbf{H}=\mathfrak{H}-\tfrac{1}{2}[\mathfrak{I}\mathfrak{H}+\mathfrak{H}\mathfrak{I}]+\tfrac{3}{8}[\mathfrak{I}^2\mathfrak{H}+\mathfrak{H}\mathfrak{I}^2]+\tfrac{1}{4}\mathfrak{I}\mathfrak{H}\mathfrak{I}-\tfrac{5}{16}[\mathfrak{I}^3\mathfrak{H}+\mathfrak{H}\mathfrak{I}^3]-\tfrac{3}{16}[\mathfrak{I}^2\mathfrak{H}\mathfrak{I}+\mathfrak{I}\mathfrak{H}\mathfrak{I}^2]+\cdots. \tag{III.4}$$

The expansions (III.3), (III.4) are qualitatively of the same nature as the cluster expansions for $\mathfrak{N}$, $\mathfrak{H}$, in the sense that convergence should be rapid if the deviation of F from 1 (which is, indeed, responsible for the deviation of the set $\{\Psi_m\}$ from orthogonality) occurs over a small enough region of configuration space, which will be true in our work if the function $\eta(r)=f^2(r)-1$ has short enough range. Thus the Löwdin expansion seems quite appropriate to our over-all attack.

Note further that

$$\mathfrak{I}_{mm}=0, \qquad \mathfrak{I}_{mn}=\mathfrak{N}_{mn}, \quad \mathbf{m}\neq\mathbf{n}, \tag{III.5}$$

so, from the general formula (II.21),

$$H_{mn}=\mathfrak{H}_{mn}-\tfrac{1}{2}\sum_p[\mathfrak{I}_{mp}\mathfrak{H}_{pn}+\mathfrak{H}_{mp}\mathfrak{I}_{pn}]+\cdots = NG_{,\alpha_1\cdots\alpha_d\beta}{}^{mn}\exp\tfrac{1}{2}N(G^m-G^n)+\cdots +\tfrac{1}{2}\mathfrak{N}_{mn}(\mathfrak{H}_{mm}-\mathfrak{H}_{nn}) -\tfrac{1}{2}\sum_{p\neq m,n}[\mathfrak{I}_{mp}\mathfrak{H}_{pn}+\mathfrak{H}_{mp}\mathfrak{I}_{pn}]+\cdots. \tag{III.6}$$

The contribution $\frac{1}{2}\mathfrak{N}_{mn}(\mathfrak{H}_{mm}+\mathfrak{H}_{nn})$ with disconcerting N dependence is cancelled completely. The last addend shown explicitly contains $\mathfrak{H}$-matrix elements and hence again unphysical terms; however, these terms may be shown to cancel against further contributions from the Löwdin expansion, so that one may obtain, finally, an expansion for the matrix element in which every term has the expected dependence on the particle number. [It is far from obvious that the Löwdin expansion for a given matrix element, H_{mn}, contains *no* contributions with catastrophic N dependence. This assertion has, however, been checked for low ω orders by Woo. Even if we are satisfied that the "improper" parts of the $\mathfrak{H}_{mn}$ create no difficulty, the surface appearance of the expansions is discouraging due to the presence of unlinked terms analogous to those of the usual Rayleigh-Schrödinger perturbation theory, but the absence of terms analogous to the renormalization corrections responsible, in that case, for the complete cancellation of unphysical contributions. Analogy fails; here the cancellation is accomplished by terms, arising from the $\mathfrak{H}_{mn}$, $\mathfrak{I}_{mn}$ cluster expansions, which contain *barred* four-index X's. (The unusual features of the $\bar{X}_{ijkl}{}'^{mn}$ have been noted previously.) A thorough treatment of this problem will be presented elsewhere. Care must be exercised beginning with the corrections of second order in ω for the off-diagonal elements of $\mathfrak{H}$, and with third-order corrections for the diagonal elements.]

More to the point, if we ask only for accuracy to first order in ω, terms of order $\mathfrak{I}^2$ or higher in (III.4), which produce at most contributions to the H_{mn} of one order higher in ω than needed, may be discarded. Any nondiagonal H_{mn} that enters then may be obtained from the corresponding $\mathfrak{H}_{mn}$ of Sec. II simply by dropping the term $\frac{1}{2}\mathfrak{N}_{mn}(\mathfrak{H}_{mm}+\mathfrak{H}_{nn})$ and attaching an "orthogonality

correction," which has the form

$$-\tfrac{1}{2}\sum_{\substack{p_1<p_2\\ p_1,\,p_2\notin\{m_i\},\,\{n_i\}}}[(m_1m_2|\eta(12)|p_1p_2)_a(p_1p_2|\tilde{w}_2(12)|n_1n_2)_a$$

$$+(m_1m_2|\tilde{w}_2(12)|p_1p_2)_a(p_1p_2|\eta(12)|n_1n_2)_a] \quad \text{(III.7)}$$

in the case of two orbitals different and is easily deduced in the other two cases. As for the diagonal elements, one just adds an orthogonality correction term

$$-\tfrac{1}{2}\sum_{m_1<m_2}\sum_{\substack{p_1<p_2\\ p_1,\,p_2\notin\{m_i\}}}[(m_1m_2|\eta(12)|p_1p_2)_a$$

$$\times(p_1p_2|\tilde{w}_2(12)|m_1m_2)_a+\text{c.c.}]. \quad \text{(III.8)}$$

We have, of course, neglected contributions of second and higher order in ω contained in the last explicit addend of (III.6).

The occurrence of the term (III.8) in all the $H_{\mathbf{mn}}$ raises an interesting problem. Since the $\Theta_{\mathbf{m}}$ are orthogonal, the $H_{\mathbf{mm}}$ provide upper bounds for the first K states of the system, K being the number of members in the set $\{\Psi_{\mathbf{m}}\}$. For the class of F's we have discussed, the ground-state energy will be approximated by $H_{\mathbf{00}}$, where $\Phi_{\mathbf{0}}$ is the Slater determinant built from the φ's with the N lowest single-particle energies (describing in our case a completely filled Fermi sphere); the energy of the first excited state by $H_{\mathbf{11}}$ where $\Phi_{\mathbf{1}}$ is the[46] Slater determinant built by replacing the φ in $\Phi_{\mathbf{0}}$ with the Nth lowest energy by that with the $(N+1)$th lowest energy (describing the lowest particle-hole state relative to the filled Fermi sphere); and so on. Now suppose, for the sake of argument, that the Löwdin expansion is rapidly convergent, and the second term in the expansion (III.4) applied to the $H_{\mathbf{mm}}$ well approximated by (III.8). Suppose further that (III.8) is positive. Then a better value of the ground-state energy is obtained with $\Psi_{\mathbf{0}}$ than with $\Theta_{\mathbf{0}}$.

Feenberg and Woo[47] indicate that their analog of (III.8) is indeed positive, and thus propose the replacement of the set $\{\Theta_{\mathbf{m}}\}$ by what they consider an energetically more advantageous one, $\{\Theta_{\mathbf{m}}'\}$, giving the ground state a special role by exempting $\Psi_{\mathbf{0}}$ from the Löwdin procedure. The new set to be orthogonalized by Löwdin's process is

$$\Psi_{\mathbf{m}}'=(\Psi_{\mathbf{m}}-\mathfrak{N}_{\mathbf{0m}}\Psi_{\mathbf{0}})/(1-|\mathfrak{N}_{\mathbf{0m}}|^2)^{1/2},\quad \mathbf{m}\neq\mathbf{0}, \quad \text{(III.9)}$$

all members being manifestly orthogonal to $\Psi_{\mathbf{0}}\equiv\Theta_{\mathbf{0}}'$.

Keeping only asymptotically significant contributions, we find easily, for the Hamiltonian matrix in the representation defined by the new orthonormal set $\{\Theta_{\mathbf{m}}'\}$, the following relations which are correct to first order in the correlation parameter:

$$H_{\mathbf{00}}'=\mathfrak{H}_{\mathbf{00}},$$

$$H_{\mathbf{m0}}'=H_{\mathbf{m0}}+\tfrac{1}{2}\mathfrak{N}_{\mathbf{m0}}(\mathfrak{H}_{\mathbf{mm}}-\mathfrak{H}_{\mathbf{00}}),\quad \mathbf{m}\neq\mathbf{0},$$

$$H_{\mathbf{0m}}'=H_{\mathbf{0m}}+\tfrac{1}{2}\mathfrak{N}_{\mathbf{0m}}(\mathfrak{H}_{\mathbf{mm}}-\mathfrak{H}_{\mathbf{00}}),\quad \mathbf{m}\neq\mathbf{0},$$

$$H_{\mathbf{mm}}'=\mathfrak{H}_{\mathbf{mm}}-\tfrac{1}{2}\sum_{\mathbf{p}\neq\mathbf{m}}[\mathfrak{N}_{\mathbf{mp}}\mathfrak{H}_{\mathbf{pm}}+\mathfrak{H}_{\mathbf{mp}}\mathfrak{N}_{\mathbf{pm}}] \quad \text{(III.10)}$$

$$=H_{\mathbf{mm}},\quad \mathbf{m}\neq\mathbf{0},$$

$$H_{\mathbf{mn}}'=H_{\mathbf{mn}}-\mathfrak{N}_{\mathbf{m0}}\mathfrak{H}_{\mathbf{0n}}-\mathfrak{H}_{\mathbf{m0}}\mathfrak{N}_{\mathbf{0n}},$$

$$\mathbf{m}\neq\mathbf{n},\quad \mathbf{m},\mathbf{n}\neq\mathbf{0}.$$

(It should be noted that, to the order in ω prescribed, the second term in $H_{\mathbf{m0}}'$, $\mathbf{m}\neq\mathbf{0}$, is present only for the case of two orbitals different, and the last two terms in $H_{\mathbf{mn}}'$, $\mathbf{m}\neq\mathbf{n}$, $\mathbf{m}$, $\mathbf{n}\neq\mathbf{0}$, only if both $\mathbf{m}$ and $\mathbf{n}$ differ from $\mathbf{0}$ in just two orbitals, while $\mathbf{m}$ differs from $\mathbf{n}$ in exactly three or four.) In view of these relations, it is clear that the above reformulation is never appropriate to a normal system (though it *may* be useful for a system displaying superfluid properties). For if the "extra" term (III.8) in $H_{\mathbf{00}}$ *is* positive, there will be introduced into the new spectrum of bounds, $H_{\mathbf{mm}}'$ versus $\mathbf{m}$, a gap which must be removed by subsequent approximations. On the other hand, if the extra term is negative, the temptation to go to the modified orthonormal set does not arise, the ground-state upper bound being lowered by the original orthogonalization process.

The Schmidt orthogonalization procedure may, on the other hand, provide a useful substitute for the set $\{\Theta_{\mathbf{m}}\}$ in the case that (III.8) is positive and the system is normal. A set $\{\Upsilon_{\mathbf{m}}\}$ of orthonormal correlated functions is given by the well-known formula

$$b_{\mathbf{m}}\Upsilon_{\mathbf{m}}=\Psi_{\mathbf{m}}-\sum_{\mathbf{p}=\mathbf{0}}^{\mathbf{m}-\mathbf{1}}\Upsilon_{\mathbf{p}}(\Upsilon_{\mathbf{p}},\Psi_{\mathbf{m}}), \quad \text{(III.11)}$$

where the $b_{\mathbf{m}}$ are to be chosen such that $(\Upsilon_{\mathbf{m}},\Upsilon_{\mathbf{m}})=1$, and the energy ordering sketched above has been adopted for the labels $\mathbf{m}$. Retaining only contributions of first or lower order in ω, this collapses simply to

$$\Upsilon_{\mathbf{m}}=\Psi_{\mathbf{m}}-\sum_{\mathbf{p}=\mathbf{0}}^{\mathbf{m}-\mathbf{1}}\Psi_{\mathbf{p}}\mathfrak{N}_{\mathbf{pm}}. \quad \text{(III.12)}$$

(All terms containing products of nondiagonal matrix elements $\mathfrak{N}_{\mathbf{qr}}$ may be discarded, and all $b_{\mathbf{m}}$ set equal to unity.) Thus we obtain, for the matrix elements $\mathfrak{K}_{\mathbf{mn}}=(\Upsilon_{\mathbf{m}},H\Upsilon_{\mathbf{n}})$ of the Hamiltonian in the representation defined by this Schmidt set,

$$\mathfrak{K}_{\mathbf{mn}}=\mathfrak{H}_{\mathbf{mn}}-\sum_{\mathbf{p}=\mathbf{0}}^{\mathbf{n}-\mathbf{1}}\mathfrak{H}_{\mathbf{mp}}\mathfrak{N}_{\mathbf{pn}}-\sum_{\mathbf{p}=\mathbf{0}}^{\mathbf{m}-\mathbf{1}}\mathfrak{N}_{\mathbf{mp}}\mathfrak{H}_{\mathbf{pn}}+\cdots, \quad \text{(III.13)}$$

the terms neglected (dots) being, as usual, of second order in the correlation parameter. The spectrum of

[46] Of course there will in general be degeneracy, but this is more or less irrelevant here.

[47] E. Feenberg and C. W. Woo (private communication).

bounds,

$$\mathcal{K}_{\mathbf{mm}}=\mathfrak{H}_{\mathbf{mm}}-\sum_{\mathbf{p}=\mathbf{0}}^{\mathbf{m}-\mathbf{1}}[\mathfrak{H}_{\mathbf{mp}}\mathfrak{N}_{\mathbf{pm}}+\text{c.c.}], \quad \text{(III.14)}$$

displays no gap, because the summation in the new correction term now extends only up to the state label *preceding* **m**. For $\mathbf{m}\neq\mathbf{n}$, say $\mathbf{m}>\mathbf{n}$,

$$\mathcal{K}_{\mathbf{mn}}=\mathfrak{H}_{\mathbf{mn}}-\sum_{\mathbf{p}=\mathbf{0}}^{\mathbf{n}-\mathbf{1}}\mathfrak{H}_{\mathbf{mp}}\mathfrak{N}_{\mathbf{pn}}-\sum_{\substack{\mathbf{p}=\mathbf{0}\\ \mathbf{p}\neq\mathbf{n}}}^{\mathbf{m}-\mathbf{1}}\mathfrak{N}_{\mathbf{mp}}\mathfrak{H}_{\mathbf{pn}}-\mathfrak{N}_{\mathbf{mn}}\mathfrak{H}_{\mathbf{nn}}, \quad \text{(III.15)}$$

and the last term suffices to cancel the unphysical component of $\mathfrak{H}_{\mathbf{mn}}$, leaving, just as in the case of the Löwdin procedure, a matrix element having the correct asymptotic dependence on the particle number. Notice, however, that the sums over states involved here will certainly be more difficult to evaluate than those of the Löwdin prescription, the ordering of the state labels now playing an essential role.

IV. CONSTRUCTION OF A QUASIPARTICLE HAMILTONIAN

In the last few years, the application of field-theoretic methods to many-body problems involving nonsingular, well-behaved two-particle interactions—i.e., two-particle interactions with Fourier transforms—has reached an advanced stage of development.[39] In order to make direct use of these techniques, we now phrase our results for the matrix elements $H_{\mathbf{mn}}$ in field-theoretic language, by constructing a second-quantized effective Hamiltonian H^{eff} which has the same matrix elements with respect to the independent-particle basis kets $|\Phi_{\mathbf{m}}\rangle$ of the model occupation number representation as we have found for the given first-quantized Hamiltonian H of (I.1) with respect to the corresponding correlated wave functions $\Theta_{\mathbf{m}}$.[48,49] Contrary to H rewritten immediately as a second-quantized operator, H^{eff} is certainly well behaved in the sense that the coefficients of all combinations of creation and destruction operators that appear are finite. For this we must make a sacrifice: our effective Hamiltonian will contain many-body potentials. These are, of course, artifacts of the method, not of fundamental origin, but some of them must be included, or at least estimated, in any accurate calculation to be based on the dynamically uncorrelated states of the given model (i.e., on the $|\Phi_{\mathbf{m}}\rangle$).

To see most simply how such many-body potentials arise, look at

$$\mathfrak{h}_{\mathbf{mn}}=\int\prod_b dx_b F\Phi_{\mathbf{m}}^* HF\Phi_{\mathbf{n}}=\int\prod_b dx_b\Phi_{\mathbf{m}}^*\{\prod_{i<j}f(r_{ij})H\prod_{k<l}f(r_{kl})\}\Phi_{\mathbf{n}}.$$

If this is regarded as a matrix element with respect to independent-particle wave functions, the (configuration space) operator that is sandwiched is a truly many-body operator: though H itself is a sum of one-body operators plus a sum of two-body operators, the operator in curly brackets can couple independent-particle functions differing in as many as N orbitals.

The same point may be brought out in more useful fashion by consideration of the results of our cluster evaluation of the $H_{\mathbf{mn}}$—we not only see explicitly that each $H_{\mathbf{mn}}$ may be written as a sum of contributions from one-body, two-body, three-body,$\cdots$, Q-body,$\cdots$ operators, taken between the independent-particle state vectors signalled by **m** and **n**, but also notice that, to the extent that $|N\omega/\Omega|$ is small, the importance of the Q-body operators will decrease rapidly (though not necessarily monotonically) with Q, independent-particle states labeled **m** and **n** being only very weakly connected if **m** differs from **n** in a large number of orbitals. In particular, if we are satisfied with stopping at first order in ω—and preliminary work indicates that at least for nuclear matter this should still permit an adequate description of most properties—, then H^{eff} will contain only two-body, three-body, and four-body potentials, whose precise forms we now derive.

Going over to a more appropriate labeling scheme than employed in Sec. II, we designate the complete set of single-particle orbitals by $\{\varphi_\kappa\}$, with $\kappa=1,2,\cdots,\infty$. (The label κ may, for instance, denote the energy order of the orbital φ_κ, $\epsilon_1\leqslant\epsilon_2\leqslant\cdots\leqslant\epsilon_\kappa\leqslant\cdots$, a convenient ordering prescription for degenerate single-particle states having been adopted. Each m_i of Sec. II is now supposed to be a certain one of these κ.)

Define operators $c_\kappa^\dagger$, c_κ, obeying the usual fermion anticommutation relations, which respectively create and destroy a (quasi)particle in orbital φ_κ. Then to first order in the correlation parameter, H^{eff} assumes the form

$$H^{\text{eff}}=\sum_\kappa\epsilon_\kappa a_\kappa^\dagger a_\kappa+\frac{1}{2!}\sum_{\kappa\lambda,\kappa'\lambda'}(\kappa\lambda|U_2|\kappa'\lambda')a_\kappa^\dagger a_\lambda^\dagger a_{\lambda'}a_{\kappa'}+\frac{1}{3!}\sum_{\kappa\lambda\mu,\kappa'\lambda'\mu'}(\kappa\lambda\mu|U_3|\kappa'\lambda'\mu')a_\kappa^\dagger a_\lambda^\dagger a_\mu^\dagger a_{\mu'}a_{\lambda'}a_{\kappa'}+\frac{1}{4!}\sum_{\kappa\lambda\mu\nu,\kappa'\lambda'\mu'\nu'}(\kappa\lambda\mu\nu|U_4|\kappa'\lambda'\mu'\nu')a_\kappa^\dagger a_\lambda^\dagger a_\mu^\dagger a_\nu^\dagger a_{\nu'}a_{\mu'}a_{\lambda'}a_{\kappa'}, \quad \text{(IV.1)}$$

[48] We suppose in this section that the set $\{\Theta_{\mathbf{m}}\}$ is complete, hence provides a basis.

[49] The construction of such an effective Hamiltonian in configuration space has been envisaged by Fujita, Ref. 41.

where $a_\kappa=(-)^{\Sigma_\sigma<\kappa N_\sigma}, N_\sigma=c_\sigma^\dagger c_\sigma$, and the U matrices are to be determined from the requirement

$$\langle\Phi_\mathrm{m}|H^\mathrm{eff}|\Phi_\mathrm{n}\rangle=H_\mathrm{mn}, \quad \text{all } \mathbf{m},\mathbf{n}. \tag{IV.2}$$

After detailed study of both sides of (IV.2), the U matrices which emerge are:

$$\begin{aligned}
&(\kappa_1\cdots\kappa_Q|U_Q|\kappa_1'\cdots\kappa_Q')=(\kappa_1\cdots\kappa_Q|U_{Q(Q)}|\kappa_1'\cdots\kappa_Q')+(\kappa_1\cdots\kappa_Q|U_{Q(\mathrm{orth})}|\kappa_1'\cdots\kappa_Q'), \quad Q=1,\cdots,4,\\
&(\kappa\lambda|U_{2(2)}|\kappa'\lambda')=(\kappa\lambda|\tilde w_2|\kappa'\lambda'),\\
&(\kappa\lambda|U_{2(\mathrm{orth})}|\kappa'\lambda')=-\tfrac14\textstyle\sum_{\mu\mu'}[(\kappa\lambda|\eta|\mu\mu')(\mu\mu'|\tilde w_2|\kappa'\lambda')_a\\
&\qquad\qquad+(\kappa\lambda|\tilde w_2|\mu\mu')(\mu\mu'|\eta|\kappa'\lambda')_a](1-\delta_{\{\mu,\mu'\},\{\kappa,\lambda\}})(1-\delta_{\{\mu,\mu'\},\{\kappa',\lambda'\}}),\\
&(\kappa\lambda\mu|U_{3(3)}|\kappa'\lambda'\mu')=(\kappa\lambda\mu|U_{3(3),2}|\kappa'\lambda'\mu')+(\kappa\lambda\mu|U_{3(3),3}|\kappa'\lambda'\mu'),\\
&(\kappa\lambda\mu|U_{3(3),2}|\kappa'\lambda'\mu')=3!\{-(\kappa\lambda|\tilde w_2|\kappa'\lambda')(\kappa\mu|\eta|\kappa\mu')_a\,\delta_{\{\kappa,\lambda\},\{\kappa',\lambda'\}}-\tfrac14\{(\kappa\lambda|\eta|\kappa'\lambda')[(\kappa\mu|\tilde w_2|\kappa\mu')_a+(\lambda\mu|\tilde w_2|\lambda\mu')_a\\
&\qquad+(\kappa'\mu|\tilde w_2|\kappa'\mu')_a+(\lambda'\mu|\tilde w_2|\lambda'\mu')_a]+(\kappa\lambda|\tilde w_2|\kappa'\lambda')[(\kappa\mu|\eta|\kappa\mu')_a+(\lambda\mu|\eta|\lambda\mu')_a\\
&\qquad+(\kappa'\mu|\eta|\kappa'\mu')_a+(\lambda'\mu|\eta|\lambda'\mu')_a]\}\delta_{\mu\mu'}(1-\delta_{\{\kappa,\lambda\},\{\kappa',\lambda'\}})\},\\
&(\kappa\lambda\mu|U_{3(3),3}|\kappa'\lambda'\mu')=(\kappa\lambda\mu|\tilde w_3|\kappa'\lambda'\mu'),\\
&(\kappa\lambda\mu|U_{3(\mathrm{orth})}|\kappa'\lambda'\mu')=-\tfrac34\textstyle\sum_\nu[(\kappa\lambda|\eta|\kappa'\nu)_a(\mu\nu|\tilde w_2|\mu'\lambda')_a(1-\delta_{\{\kappa,\lambda\},\{\kappa',\nu\}})(1-\delta_{\{\mu,\nu\},\{\mu',\lambda'\}})\\
&\qquad+(\kappa\nu|\eta|\kappa'\lambda')_a(\mu\lambda|\tilde w_2|\mu'\nu)_a(1-\delta_{\{\kappa,\nu\},\{\kappa',\lambda'\}})(1-\delta_{\{\mu,\lambda\}\{\mu',\nu\}})],\\
&(\kappa\lambda\mu\nu|U_{4(4)}|\kappa'\lambda'\mu'\nu')=(\kappa\lambda|\eta|\kappa'\lambda')(\mu\nu|\tilde w_2|\mu'\nu')[\mathcal{Q}\delta_{\{\kappa,\lambda,\mu,\nu\},\{\kappa',\lambda',\mu',\nu'\}}+(1-\delta_{\{\kappa,\lambda,\mu,\nu\},\{\kappa',\lambda',\mu',\nu'\}})],\\
&(\kappa\lambda\mu\nu|U_{4(\mathrm{orth})}|\kappa'\lambda'\mu'\nu')=-6(\kappa\lambda|\eta|\kappa'\lambda')(\mu\nu|\tilde w_2|\mu'\nu')(1-\delta_{\{\kappa,\lambda\},\{\kappa',\lambda'\}})(1-\delta_{\{\mu,\nu\},\{\mu',\nu'\}}).
\end{aligned} \tag{IV.3}$$

In these expressions $\{\kappa,\lambda,\cdots\}$ stands for the set of indices κ, $\lambda,\cdots$ and

$$\begin{aligned}
\delta_{\{\kappa,\lambda,\ldots\},\{\kappa',\lambda',\ldots\}}&=1, \quad \{\kappa,\lambda,\cdots\}=\{\kappa',\lambda',\cdots\},\\
&=0, \quad \text{otherwise}.
\end{aligned} \tag{IV.4}$$

Also,

$$\begin{aligned}
\mathcal{Q}(\kappa\lambda\mu\nu,\kappa'\lambda'\mu'\nu')&=1, \quad [\mu\neq\mu',\nu';\ \nu\neq\mu',\nu';\ \kappa\neq\kappa',\lambda';\ \lambda\neq\kappa',\lambda'] \quad \text{all satisfied},\\
&=0, \quad \text{otherwise}.
\end{aligned} \tag{IV.5}$$

Those terms containing (orth) subscripts arise from the orthogonality corrections derived in Sec. III. The second-quantized operator generating these corrections was obtained as follows. In the notation of Sec. III, let the matrix $\mathfrak{K}=\mathfrak{H}-\mathfrak{H}_\mathrm{diag}$, $\mathfrak{H}_\mathrm{diag}=(\mathfrak{H}_\mathrm{mm}\delta_\mathrm{mn})$. To $\mathfrak{J}$ and $\mathfrak{K}$ there correspond second-quantized operators $\mathfrak{J}^\mathrm{eff}$ and $\mathfrak{K}^\mathrm{eff}$ such that

$$\begin{aligned}
\langle\Phi_\mathrm{m}|\mathfrak{J}^\mathrm{eff}|\Phi_\mathrm{n}\rangle&=\mathfrak{J}_\mathrm{mn},\\
\langle\Phi_\mathrm{m}|\mathfrak{K}^\mathrm{eff}|\Phi_\mathrm{n}\rangle&=\mathfrak{H}_\mathrm{mn}-\mathfrak{H}_\mathrm{mm}\delta_\mathrm{mn}.
\end{aligned} \tag{IV.6}$$

Then, since $\{|\Phi_\mathrm{m}\rangle\}$ is a complete orthonormal set,

$$\begin{aligned}
\tfrac12\sum_{\mathrm{p}\neq\mathrm{m},\mathrm{n}}[\mathfrak{J}_\mathrm{mp}\mathfrak{H}_\mathrm{pn}+\mathfrak{H}_\mathrm{mp}\mathfrak{J}_\mathrm{pn}]&=\tfrac12\sum_\mathrm{p}[\langle\Phi_\mathrm{m}|\mathfrak{J}^\mathrm{eff}|\Phi_\mathrm{p}\rangle\langle\Phi_\mathrm{p}|\mathfrak{K}^\mathrm{eff}|\Phi_\mathrm{n}\rangle+\langle\Phi_\mathrm{m}|\mathfrak{K}^\mathrm{eff}|\Phi_\mathrm{p}\rangle\langle\Phi_\mathrm{p}|\mathfrak{J}^\mathrm{eff}|\Phi_\mathrm{n}\rangle]\\
&=\tfrac12\langle\Phi_\mathrm{m}|\mathfrak{J}^\mathrm{eff}\mathfrak{K}^\mathrm{eff}+\mathfrak{K}^\mathrm{eff}\mathfrak{J}^\mathrm{eff}|\Phi_\mathrm{n}\rangle.
\end{aligned} \tag{IV.7}$$

Thus $\mathfrak{J}^\mathrm{eff}\mathfrak{K}^\mathrm{eff}+\mathfrak{K}^\mathrm{eff}\mathfrak{J}^\mathrm{eff}$ is the required operator. Evidently, in lowest nonvanishing ω orders,

$$\begin{aligned}
\mathfrak{J}^\mathrm{eff}&=\tfrac12\sum_{\kappa\lambda\kappa'\lambda'}(\kappa\lambda|\eta|\kappa'\lambda')(1-\delta_{\{\kappa,\lambda\},\{\kappa',\lambda'\}})a_\kappa^\dagger a_\lambda^\dagger a_{\lambda'}a_{\kappa'},\\
\mathfrak{K}^\mathrm{eff}&=\tfrac12\sum_{\mu\nu\mu'\nu'}(\mu\nu|\tilde w_2|\mu'\nu')(1-\delta_{\{\mu,\nu\},\{\mu',\nu'\}})a_\mu^\dagger a_\nu^\dagger a_{\nu'}a_{\mu'}.
\end{aligned} \tag{IV.8}$$

The resulting symmetrized product, accurate (as needed) to first order in ω, was then split up into two-, three-, and four-particle operators by reduction of the products of eight creation and destruction operators to normal form.

The notation for the other addend of each U_Q matrix should be obvious: $U_{Q(b)}$ is the part of U_Q arising from b index terms in $\mathfrak{H}_\mathrm{mn}$.

The appearance of the step function $\mathcal{Q}$ in the $U_{4(4)}$ matrix is a consequence of the omission of contributions from certain permutations in the construction of the four-index terms entering into the diagonal elements $\mathfrak{H}_\mathrm{mm}$; the step function $1-\delta_{\{\kappa,\lambda,\mu,\nu\},\{\kappa',\lambda',\mu',\nu'\}}$ guarantees that this restriction is not applied in the case of off-diagonal matrix elements. [See the last of (II.7) together with the discussion surrounding (A4) in the Appendix.]

Notice that although the term

$$U_{3(3),2}{}^{\text{eff}} \equiv \sum_{\kappa\lambda\mu,\kappa'\lambda'\mu'} (\kappa\lambda\mu|\, U_{3(3),2}\,|\kappa'\lambda'\mu') \times a_\kappa{}^\dagger a_\lambda{}^\dagger a_\mu{}^\dagger a_{\mu'} a_{\lambda'} a_{\kappa'}$$

in the effective Hamiltonian is bicubic in the creation and destruction operators, it is unable to couple independent-particle kets differing in three occupation numbers and in this sense acts like a sum of two-particle operators rather than a sum of three-particle operators. Thus we are naturally led to ask under what circumstances this term can be approximated by a biquadratic form. Now the contributions of $U_{3(3),2}{}^{\text{eff}}$ to the $H_{\mathbf{mn}}$ [see the second $O(N\omega)$ term in (II.15) and the third and fourth $O(\omega/N)$ terms in (II.17)] contain sums over all single-particle states involved in *both* **m** and **n**. If N is very large, and if the only important matrix elements are those in which **m**, **n** differ from **0** in just a few orbitals (for $N=10^{23}$, a few could be 10^{21}), we make negligible error—essentially of order unity compared to N—by replacing these sums by sums $\sum^<$ over the single-particle states occupied in $|\Phi_0\rangle$. Then it is permissible to replace $U_{3(3),2}{}^{\text{eff}}$ by

$$U_{2(3)}{}^{\text{eff}} = \sum_{\kappa\lambda,\kappa'\lambda'} (\kappa\lambda|\, U_{2(3)}\,|\kappa'\lambda') a_\kappa{}^\dagger a_\lambda{}^\dagger a_{\lambda'} a_{\kappa'},$$

where

$$(\kappa\lambda|\, U_{2(3)}\,|\kappa'\lambda') = \{-\tfrac{1}{2}(\kappa\lambda|\,\eta\,|\kappa'\lambda')\textstyle\sum_\mu{}^< [(\kappa\mu|\,\tilde{w}_2\,|\kappa\mu)_a + (\lambda\mu|\,\tilde{w}_2\,|\lambda\mu)_a + (\kappa'\mu|\,\tilde{w}_2\,|\kappa'\mu)_a + (\lambda'\mu|\,\tilde{w}_2\,|\lambda'\mu)_a]$$
$$-\tfrac{1}{2}(\kappa\lambda|\,\tilde{w}_2\,|\kappa'\lambda')\textstyle\sum_\mu{}^< [(\kappa\mu|\,\eta\,|\kappa\mu)_a + (\lambda\mu|\,\eta\,|\lambda\mu)_a + (\kappa'\mu|\,\eta\,|\kappa'\mu)_a + (\lambda'\mu|\,\eta\,|\lambda'\mu)_a]\}(1-\tfrac{1}{2}\delta_{\{\kappa,\lambda\},\{\kappa',\lambda'\}}). \quad \text{(IV.9)}$$

Under the same circumstances, the sums in the orthogonality correction terms such as (III.7), (III.8) may be replaced by sums $\sum^>$ over the single-particle states not occupied in $|\Phi_0\rangle$. Such modifications of the effective Hamiltonian and its matrix elements are of obvious computational advantage; they are an essential feature of the work of FW. The underlying assumption—loosely speaking, that there exists a "macroscopically occupied condensate"—is already widely made in many-particle theory.

Clearly the matrix elements of $U_{2(2)}$ are of zeroth order in the correlation parameter; those of all the other explicit U's, of first order.

One more technical remark is necessary: The signs of corresponding matrix elements $\langle\Phi_{\mathbf{m}}|\,H^{\text{eff}}\,|\Phi_{\mathbf{n}}\rangle$, $H_{\mathbf{mn}}$ will agree in general if and only if the same ordering has been adopted for the single-particle states in both occupation number and configuration-space representations. To be definite, we may impose the aforementioned ordering according to energy, i.e., choose the $\kappa(=1, 2, \cdots, \infty)$ such that $\epsilon_1 \leqslant \epsilon_2 \leqslant \cdots$ (with suitable prescription for degeneracy), hence requiring for all **m** the ordering of the $m_i(\doteq 1, 2, \cdots, \infty, i=1, \cdots, N)$ such that $\epsilon_{m_1} \leqslant \epsilon_{m_2} \leqslant \cdots \leqslant \epsilon_{m_N}$ (with the same prescription for degeneracy). Thus, upon computing $\langle\Phi_{\mathbf{m}}|\,H^{\text{eff}}\,|\Phi_{\mathbf{n}}\rangle$ using (IV.1), (IV.3) we must attach a sign $(-)$ raised to a power equal to the combined number of interchanges required to go from the ordering adopted in Sec. II for the single-particle states in the Slater determinants $\Phi_{\mathbf{m}}$, $\Phi_{\mathbf{n}}$ to this energy ordering.

Our result for H^{eff} has an elegant and useful interpretation in terms of quasiparticles. The first term, diagonal in the orbital occupation number operators $a_\kappa{}^\dagger a_\kappa$,[50] is the Hamiltonian for a system of noninteracting Fermi quasiparticles, moving in a one-body field $V(i)$, carrying spin $\frac{1}{2}$ and (for our extended system) momentum $\hbar\mathbf{k}_\kappa$. These quasiparticles, though having free properties [set $V(i)=0$] identical with those of the real particles, interact not through a *singular* two-body potential but instead via *well-behaved* two-body, three-body, and four-body potentials given by the remaining terms in H^{eff}. (The dominant interaction between the quasiparticles is of two-body nature, arising from $U_{2(2)}$.) We thus arrive at a Hamiltonian susceptible to a powerful array of field-theoretic methods, including linearization of equations of motion,[51] canonical transformation,[52] the Green's function formalism,[53] etc.

The lowest cluster order result (zeroth order in ω) is quite interesting—and, at least in the nuclear case where, as we shall see, simple f's give $|N\omega/\Omega| \approx \frac{1}{8}$, should contain most of the physics. To this order no many-body forces appear, and the effective Hamiltonian in configuration space has the same form as the Hamiltonian H from which we started, with the replacement of the highly singular potential $v(ij)$ by the well-behaved *two-body* potential $w_2(ij) = (\hbar^2/M)[\nabla f(ij)]^2 + f^2(ij)v(ij)$. For an f of the general type we consider—i.e., one for which the cluster expansions are sensibly convergent—not only the repulsive but also the attractive component of $w_2(ij)$ may be considerably reduced from that of $v(ij)$: qualitatively, the singular repulsion goes into a repulsive edge at or a repulsive bump near the equivalent hard-core radius and the depth of the attraction is diminished, while the long-

[50] Following Feenberg and Woo, one may extract from the U terms additional contributions which are quadratic, cubic, and quartic functions of the quasiparticle number operators $a_\kappa{}^\dagger a_\kappa$, and thus split H^{eff} into diagonal and nondiagonal components. This is possibly the best way to proceed in practice. However, we find the form as given in (IV.1) more suitable for preliminary discussion in terms of conventional field-theoretic techniques.

[51] K. Sawada, K. A. Brueckner, N. Fukuda, and R. Brout, Phys. Rev. **108**, 507 (1957); H. Suhl and N. H. Werthamer, *ibid.* **122**, 359 (1961); K. Sawada and N. Fukuda, Progr. Theoret. Phys. (Kyoto) **25**, 653 (1961).

[52] N. Bogoliubov, Zh. Eksperim. i Teor. Fiz. **34**, 58 (1958) [English transl.: Soviet Phys.—JETP **7**, 41 (1958)]; J. G. Valatin, Nuovo Cimento **7**, 843 (1958).

[53] V. Galitskii and A. Migdal, Zh. Eksperim. i Teor. Fiz. **34**, 139 (1958) [English transl.: Soviet Phys.—JETP **7**, 96 (1958)]; A. Klein and R. Prange, Phys. Rev. **112**, 994 (1958). The very extensive literature on the three classes of field-theoretic methods just cited is indexed in the bibliographies of Ref. 39.

range behavior is left unaffected. (See the next section for an example.) So, for such an f and suitably chosen V, the interactions of the quasiparticles as described by (IV.1) may indeed be weak enough that it is not a bad first approximation to regard these entities as independent.

Nonetheless, the residual two-body interactions must be expected to be crucial for a variety of system properties. Their inclusion by Goldstone-Hugenholtz perturbation theory[54] (if applicable) proceeds as usual. And the available field-theoretic techniques for nonperturbative approximate diagonalization of a second-quantized Hamiltonian are of *immediate* utility: specifically, we may appeal to the random-phase approximation[51] to treat long-range collective effects (as exist in an electron gas) and the Bogoliubov-Valatin transformation[52] to treat pairing effects (as exist in a superconductor). Both these methods are in wide use as means of dressing the quasiparticles of the shell model in nuclear physics,[55] and the question of a possible superfluid transition (due to strong pairing correlations) in liquid He^3 is still open.[56] A large measure of the uncertainty in this work lies in ignorance as to the effective or residual interactions that should be inserted, an ignorance we hope to eliminate.

We have derived here definite rules for generating suitable two-body, three-body, four-body,$\cdots$residual interactions for use in a quasiparticle or model calculation accurate to given cluster expansion order.[57] The inclusion of the three-body, four-body,$\cdots$interactions in the quasiparticle Hamiltonian leads to complications beyond those normally encountered, which may spur development of new techniques, associated with new facets of the many-body problem.

For those accustomed to the Brueckner method, and, in particular, to the double-counting difficulties which plague the use of an effective Hamiltonian in which the t matrix replaces the v matrix, our advocation of carefree treatment of the above H^{eff} as a true Hamiltonian might require more explicit justification. Recall that the orthonormality of each of the bases $\{|\Phi_m\rangle\},\{|\Theta_m\rangle\}$ implies the existence of a unitary operator which transforms one into the other. Our effective "many-body" Hamiltonian, then, may be regarded as the result of a similarity transformation upon the original, singular "two-body" Hamiltonian via this unitary operator. Viewed in this way, the CBF method allows us to inject our physical intuition into the choice of a *canonical* transformation[57] of the original many-body problem to another many-body problem which is presumably easier to solve.

Let us present a simple example of the use of H^{eff}, for the self-consistent determination of $V(i)$. It will be imagined for generality that our system is *finite*, yet explicit results will be stated only for the specific form of H^{eff} that we have derived, a form which has strict validity just for a uniform, extended medium. The independent-(quasi)particle ket

$$|\Phi\rangle=\prod_{\kappa=1}^{N} a_\kappa^\dagger|0\rangle, \quad |0\rangle=\text{vacuum ket}, \tag{IV.10}$$

renders the expectation value $E=\langle H^{\text{eff}}\rangle$ stationary (we desire a minimum) if and only if

$$\langle\delta\Phi|H^{\text{eff}}-E|\Phi\rangle=0. \tag{IV.11}$$

A sufficiently arbitrary first-order change $|\delta\Phi\rangle$ in $|\Phi\rangle$ is given by

$$|\delta\Phi\rangle=\zeta a_{\kappa'}^\dagger a_\kappa|\Phi\rangle, \quad \kappa=1,\cdots,N, \quad \kappa'>N, \tag{IV.12}$$

where ζ is a first-order infinitesimal. Thus, obviously, $\langle\delta\Phi|E|\Phi\rangle=0$, and using the anticommutation relations of the a's and $a^\dagger$'s our stationary condition becomes

$$0+\sum_{\lambda=1}^{N}(\kappa'\lambda|U_2|\kappa\lambda)_a+\frac{1}{2!}\sum_{\lambda,\mu=1}^{N}(\kappa'\lambda\mu|U_3|\kappa\lambda\mu)_a$$
$$+\frac{1}{3!}\sum_{\lambda,\mu,\nu=1}^{N}(\kappa'\lambda\mu\nu|U_4|\kappa\lambda\mu\nu)_a+\cdots=0. \tag{IV.13}$$

Note that all the U-matrix elements involve V through $\tilde{w}_2$.

For a Hamiltonian of the usual sort with only two-body interaction terms (as considered by Thouless,[58] whose procedure we have adapted), the determination of $V(i)$ is trivial; ignoring $U_{2(\text{orth})}$, U_3, and U_4, in fact, all contributions of first or higher order in ω, we readily achieve a solution of the same type. Recalling the defini-

[54] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957); N. M. Hugenholtz, Physica **23**, 481 (1957).

[55] M. Baranger, in *1962 Cargèse Lectures in Theoretical Physics*, edited by M. Levy (W. A. Benjamin, Inc., New York, 1963), Chap. 5; A. M. Lane, *Nuclear Theory* (W. A. Benjamin, Inc., New York, 1964).

[56] A. M. Sessler, in *Proceedings of the International School of Physics "Enrico Fermi," Course XXI, Liquid Helium*, edited by G. Careri (Academic Press Inc., New York, 1963), pp. 188–292; V. J. Emery, Ann. Phys. (N. Y.) **28**, 1 (1964). It should be mentioned that the experimental work of V. Peshkov, reported at the Ninth International Conference on Low Temperature Physics, held at Ohio State University-Battelle Institute, 1964 (unpublished), points to a second-order phase transition at very low temperature.

[57] Interesting comparisons may be made with the program of F. Tabakin, Ann. Phys. (N. Y.) **30**, 51 (1964) and J. Da Providencia and C. M. Shakin, *ibid.* **30**, 95 (1964), based on a suggestion by Villars: a model Hamiltonian with given smooth two-body residual interactions may be reproduced, apart from effective many-body terms, by a canonical transformation applied to the realistic Hamiltonian. The correlation factor F of our method is replaced by a unitary model operator. See also J. S. Bell, in the *Many-Body Problem, Lecture Notes of the First Bergen International School of Physics—1961* (W. A. Benjamin, Inc., New York, 1962), pp. 214–222; F. Villars, in *Proceedings of the International School of Physics "Enrico Fermi," Course XXIII, Nuclear Physics*, edited by V. Weisskopf (Academic Press Inc., New York, 1963), pp. 24–28.

[58] D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic Press Inc., New York, 1961), Chap. III.

tions of $\tilde{w}_2$ and w_2, and noting

$$-\frac{1}{N-1}\sum_{\lambda=1}^{N}(\kappa'\lambda|f^2(12)[V(1)+V(2)]|\kappa\lambda)_a$$
$$=-\frac{1}{N-1}\sum_{\lambda=1}^{N}(\kappa'\lambda|[V(1)+V(2)]|\kappa\lambda)_a-\frac{1}{N-1}\sum_{\lambda=1}^{N}(\kappa'\lambda|(f^2(12)-1)[V(1)+V(2)]|\kappa\lambda)_a$$
$$=-(\kappa'|V(1)|\kappa)-\frac{1}{N-1}\sum_{\lambda=1}^{N}(\kappa'\lambda|\eta(12)[V(1)+V(2)]|\kappa\lambda)_a, \quad \text{(IV.14)}$$

(IV.13) yields as a zeroth approximation

$$(\kappa'|V^{[0]}|\kappa)^{[0]}=\sum_{\lambda=1}^{N}(\kappa'\lambda|w_2|\kappa\lambda)_a^{[0]},$$
$$\kappa=1,\cdots,N,\quad \kappa'>N. \quad \text{(IV.15)}$$

The superscript [0] outside the matrix elements indicates that correspondingly approximate φ's, $\varphi^{[0]}$'s obeying (II.6) with $V\to V^{[0]}$ and hence *self-consistent* with $V^{[0]}$, are to be inserted. [Remember that our explicit results depend on the satisfaction of (II.6).] However, we do not as yet have an unambiguous prescription for the $\varphi^{[0]}$'s and $V^{[0]}$, since (IV.15) restricts only a subset of matrix elements of $V^{[0]}$. Generalizing (IV.15), we define a self-consistent Hamiltonian,

$$H_{SC}^{[0]}=\sum_{\lambda\mu}\left[\left(\lambda\left|-\frac{\hbar^2}{2M}\Delta_1\right|\mu\right)^{[0]}+(\lambda|V^{[0]}|\mu)^{[0]}\right]a_\lambda^\dagger a_\mu, \quad \text{(IV.16)}$$

where

$$(\lambda|V^{[0]}|\mu)^{[0]}=\sum_{\nu}{}^{<}(\lambda\nu|w_2|\mu\nu)_a^{[0]} \quad \text{(IV.17)}$$

without restriction on λ, μ. Consider the operation of this Hamiltonian in a one-body space. We are certainly free to suppose, within the framework of our variational criterion (IV.13), that the $|\varphi\rangle$'s are in zeroth-approximation eigenkets of $H_{SC}^{[0]}$,[59] i.e., we are free to choose a single-(quasi)particle representation based on $|\varphi_\lambda^{[0]}\rangle$ which *diagonalize* $H_{SC}^{[0]}$. [In other words, we may take (IV.16), (IV.17) as defining H_1 in (II.6).] This "Hartree-Fock" self-consistent choice of orbitals provides, with (IV.17), a *complete* self-consistent determination of $V^{[0]}$.

The inclusion of the effect of the higher terms in ω on V is straightforward but tedious. In particular, self-consistency to first order in ω is achieved as follows: Replace V by $V^{[0]}$ and the φ's by the $\varphi^{[0]}$'s, in all terms of (IV.13) except that providing the first term on the right in (IV.14). In the resulting expression, discard all contributions of second and higher order in ω, to obtain

$$(\kappa'|V^{[1]}|\kappa)^{[1]}=(\kappa'|V^{[0]}|\kappa)^{[0]}+(\kappa'|R^{(1)}|\kappa)^{[0]},$$
$$\kappa=1,\cdots,N,\quad \kappa'>N, \quad \text{(IV.18)}$$

where $(\kappa'|R^{(1)}|\kappa)^{[0]}$ stands for the sum of (first-order) terms arising from the initially neglected second term of (IV.14) and from $U_{2(\text{orth})}$, U_3, and U_4. Finally, extend (IV.18) to all matrix elements $(\lambda|V^{[1]}|\mu)^{[1]}$, define therewith a self-consistent Hamiltonian $H_{SC}^{[1]}$, and diagonalize this Hamiltonian in the one-body space to obtain the self-consistent orbitals $\varphi^{[1]}$. Self-consistency order by order in ω is accomplished by an obvious generalization of this iteration scheme. To any order P in ω, the $\epsilon_\lambda^{[P]}-\epsilon_\mu^{[P]}$ obtained upon diagonalizing the corresponding $H_{SC}^{[P]}$ may be interpreted in the usual way as approximate excitation energies for the system (associated with quasiparticle-quasihole excitations).

For the infinite medium, one set[42] of Hartree-Fock single-(quasi)particle functions is supplied by our choice of plane waves supplemented by appropriate spin factors: With these orbitals the momentum conservation theorem of Sec. II implies that all matrix elements on the left in (IV.13) vanish, so that $(\kappa'|V|\kappa)=0$, meaning H_{SC} [defined as in (IV.16) but with the [0] removed] is diagonalized. The triviality of this result—which is often stated as an immediate consequence of translational invariance—is alleviated by the fact that (IV.15) or any higher iterate (here the [0]'s on the φ's may be omitted, the orbitals being the same in all orders), generalized in form to diagonal matrix elements, determines a correspondingly approximate "self-consistent" dispersion law for the motion of our quasiparticles in the quasiparticle medium. However, as is the case of the ordinary Hartree-Fock method, it is only in application to finite systems that the full advantages of the procedure outlined will be realized.

V. PRELIMINARY REMARKS ON APPLICATIONS

Having completed our exposition of the formalism of the CBF approach, we now turn to some problems that must be faced in actual execution of the method. In this section, rather than belabor details that are better deferred until the proposed calculations have been carried out, we want to emphasize one salient point: There is considerable flexibility in the choice of the factor F in the decomposition of the exact wave function according to $\Psi=F\Phi$; nevertheless it is essential to strike a compromise between the inclusion of correlation effects in F versus their inclusion in the model

[59] This follows from invariance of the trace. See Ref. 58 or A. Messiah, *Quantum Mechanics* (North-Holland Publishing Company, Amsterdam, 1963), Vol. II, pp. 776–778, for a complete discussion.

function Φ. The degree of correlation incorporated into F must not be so great that the cluster expansions that arise fail to converge with sufficient rapidity, yet great enough that Φ is only weakly correlated in the sense that simple methods are still apt for the diagonalization of H_{mn}.

Can one realize an expedient compromise for the two systems, nuclear matter and liquid He^3, whose description is of most concern to us? A satisfactory answer to this question can only be given after extensive computational exploration. We have, however, found the following qualitative considerations useful in motivating our program of applications.

In practical calculations we must at present exclude from consideration all choices of f leading to cluster expansions for the H_{mn} that may not be truncated after terms of *first* order in the correlation parameter. When the strong repulsion in $v(ij)$ is replacable by a hard core of some radius C, the *simplest* possible choice of two-body correlation factor is just a step function,

$$\begin{aligned} f(r)&=0, \quad r\leqslant C, \\ &=1, \quad r>C. \end{aligned} \tag{V.1}$$

This is assuredly not a "realistic" choice in the sense that the Φ required to reproduce in $\Psi=F\Phi$ the exact wave function contains minimal dynamical correlation, but within the class of f's such that $\eta<0$, it gives the smallest values for the parameter $|N\omega/\Omega|$. For nuclear matter, the core radius C is 0.5 F or less and the radius r_0 of the specific volume is about 1 F, so we find, to our satisfaction,

$$|N\omega/\Omega|\approx\tfrac{1}{8}, \tag{V.2}$$

while for liquid He^3, the effective C is essentially the *same* as r_0, i.e., 2.43 Å, yielding the disturbing answer

$$|N\omega/\Omega|\approx 1. \tag{V.3}$$

The former result should not, however, be viewed with too much enthusiasm, nor the latter with too much alarm; such estimates as (V.2) and (V.3) can hardly provide the last word on the utility of the CBF approach. As we should have emphasized before, it is safe to regard $|N\omega/\Omega|$ as a true expansion parameter *provided* it is so small that η may be treated as a delta function and thus all many-body integrals factored. On the other hand, for $|N\omega/\Omega|\approx 1$, this quantity is of questionable relevancy as a measure of the rate of convergence of the cluster expansions.[60] In any event, one may anticipate appreciable cancellation among terms classified in the same order.[16,18,40] Further, if we relax the restriction $\eta<0$, as for example in Fig. 2, it seems plausible that regions of positive and negative correlation will, to some extent, compensate one another, insofar as their effect on the size of the first and higher cluster corrections is concerned. (This is certainly true if η has very short range compared to the other characteristic lengths of the problem, viz., r_0 and the potential range.) These remarks prompt the search for an "optimum" f, one which produces, so far as one can tell, the most rapid convergence for the cluster expansion of some quantity of central interest, say the ground-state energy. It then remains to be determined whether or not f's we would consider "realistic" are near enough to "optimum." For the nuclear-matter problem, there is enough evidence, especially from the work of Brueckner and Gammel[61] and Gomes, Walecka, and Weisskopf,[62] to support some degree of confidence in the claim that they are. The correlation factors one extracts from these independent-pair theories have essentially the behavior shown in Fig. 2, with a region of small positive correlation (meaning f exceeds unity), and lead to quite manageable first-order cluster corrections.[40] In the case of liquid He^3, there is, on the other hand, no definite reason for optimism. With this in mind, we have decided to explore first the more promising nuclear applications of our method. A parallel study of liquid He^3 is being carried out by Feenberg and Woo, following an alternate path of the general CBF method more appropriate to this system (described in Sec. I).

There exists of course another source of flexibility which we have not mentioned in the above discussion: The one-body potential V of the input independent-particle model is at our disposal. For instance, we are free to choose V so as to greatly suppress the cluster contributions to the ground-state energy of first order in ω. This can, however, be accomplished only at the sacrifice of self-consistency; i.e., for such a V, (IV.13) will not be met.

Perturbation calculations of the gross properties of nuclear matter (binding energy per particle, equilibrium spacing, compressibility, symmetry energy) for realistic two-nucleon potentials[63–65] are projected. An appropriate (Rayleigh-Schrödinger) form of perturbation theory arises out of stepwise solution of the set of linear equations

$$\textstyle\sum_n c_n'(H_{mn}-E\delta_{mn})=0, \tag{V.4}$$

where $\Psi=\sum_m c_m'\Theta_m$, according to the procedure of Feshbach.[66,35] The Rayleigh-Schrödinger expansions for the coefficients c_m' and energy E corresponding to a given state, say the ground state, to which we shall

[60] Nevertheless, our classification of contributions according to the ω prescription remains a highly valuable one, for the reasons detailed in the Appendix.

[61] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958).

[62] L. C. Gomes, J. D. Walecka, and V. F. Weisskopf, Ann. Phys. (N. Y.) **3**, 241 (1958).

[63] J. L. Gammel and R. M. Thaler, in *Progress in Cosmic Ray Physics*, edited by J. G. Wilson and S. A. Wouthuysen (North-Holland Publishing Company, Amsterdam, 1960), Vol. V, Chap. II.

[64] T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 383 (1962).

[65] K. E. Lasilla, M. H. Hull, Jr., H. M. Ruppel, F. A. McDonald, and G. Breit, Phys. Rev. **126**, 881 (1962).

[66] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Part II, Sec. 9.1.

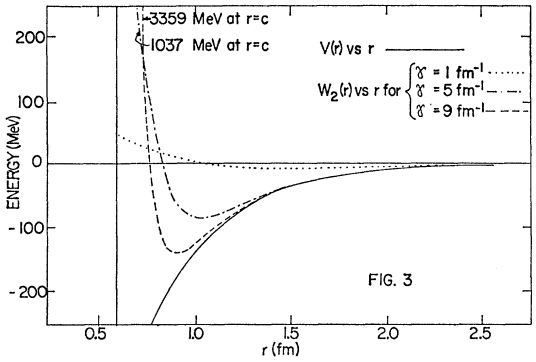

FIG. 3. Effective two-body potential $w_2(r)$ for the Iwamoto-Yamada choice (V.7) of two-body correlation factor and the Ohmura-Morita-Yamada two-nucleon potential (V.6) (singlet-even states).

specialize, consist of series of terms of increasing order in some finite perturbative parameter μ, associated with off-diagonal elements of H. Each of these terms must be evaluated by cluster expansion. To lowest cluster order, one obtains perturbative expansions for the c_m', E which are identical in all save two respects with those of the usual theory based on an independent-particle resolution of the Hamiltonian, i.e., a resolution

$$H=H^0+H^I, \quad H^0=\sum_i[-(\hbar^2/2M)\Delta_i+V(i)],$$

$$H^I=\sum_{i<j}\tilde{v}(ij), \quad \tilde{v}(ij)=v(ij)-(N-1)^{-1}(V(i)+V(j)).$$

The two required modifications of the standard theory are:

(1) $\tilde{v}(ij)\rightarrow\tilde{w}_2(ij)$

everywhere, and

(2) $\epsilon_\lambda\rightarrow\epsilon_\lambda+\sum_\nu{}^<(\lambda\nu|\tilde{w}_2|\lambda\nu)_a$

in all energy denominators.[67] [Clearly, the same lowest cluster-order expansions are obtained if we instead apply the Feshbach procedure to the determination of c_m, E in

$$\sum_n c_n(\mathfrak{H}_{mn}-E\mathfrak{N}_{mn})=0, \qquad (V.5)$$

where $\Psi=\sum_m c_m\Psi_m$, since all orthogonalization effects are of first order in the correlation parameter.] Higher order corrections $c_m'^{(P,P')}$, $E^{(P,P')}$ of Pth order in ω and P'th order in μ ($P, P'\geqslant 1$) are easy enough to generate formally. However, only the contributions labeled (0,0), (1,0), and (0,1) appear immediately susceptible to practical evaluation.[68]

Lowest cluster-order perturbative calculations provide an illuminating example of the sort of compromise that must be achieved. Certainly f must be near enough to "optimum." But it must also be such that w_2 is relatively weak; otherwise we will have to go to high order in the perturbative expansion to obtain meaningful results. To make this statement more concrete, we present, in Fig. 3, plots of $w_2(ij)$ for the following simple choices of $v(ij)$ and f, corresponding to the cluster-method study of nuclear matter by Iwamoto and Yamada[16]:

$$\begin{aligned} v(r)&=\infty, && r\leqslant C,\\ &=-Ae^{-\alpha(r-C)}, && r>C, \end{aligned} \qquad (V.6)$$

$A=397.3$ MeV, $\alpha=2.627$ F^{-1}, $C=0.6$ F (Ohmura-Morita-Yamada[69] singlet parameters, for Serber force)

$$\begin{aligned} f(r)&=0, && r\leqslant C,\\ &=1-e^{-\gamma(r-C)}, && r>C, \end{aligned} \qquad (V.7)$$

with γ in turn 1.0, 5.0, 9.0 F^{-1}. We see that the reduction in strength of w_2 from v decreases as we go from longer to shorter range for $f^2-1=\eta$ (hence from larger to smaller $|N\omega/\Omega|$).[70] IY found 5.0 F^{-1} as the most advantageous value for γ by minimizing the (new) first-order perturbation expression for the energy (which of course is an expectation value), ignoring, however, the cluster contributions of first and higher order in ω. Estimates of these first-order cluster corrections showed them to be appreciable, but sufficiently small that their neglect does not spoil the semiquantitative nature of the results. In this case of $\gamma=5.0$ F^{-1}, comparison with the work of Euler,[71] Huby,[72] Swiatecki,[73] Bethe,[74] Thouless,[75] and Brueckner[2] indicates that the effective reduction in strength of the potential should be enough that a second-order perturbation calculation is adequate. For much smaller γ, the cluster expansions may converge too slowly; for much larger γ, on the other hand, the per-

[67] The second difference has the consequence that, in contrast to the situation in the usual Rayleigh-Schrödinger theory, the Feshbach procedure leads to energy denominators which automatically incorporate a dispersion effect. It is interesting to note that, for the infinite medium, the self-consistent choice (IV.17) and the choice $V(i)=0$ give identical results. In the extension to finite systems, V will be more instrumental in hastening convergence of the perturbation expansion: For the self-consistent choice all diagrams corresponding to single-quasiparticle excitations—absent from the outset for the infinite medium because of "momentum conservation"—are cancelled, so that self-consistent and vanishing V's no longer give equivalent results term by term.

[68] Of course, rearrangements of the type discussed by Brueckner in Ref. 2 may be applied to the ω^0 expansion. In particular, large classes of terms may be summed to all orders in the new (finite) perturbative parameter by the introduction of an appropriate reaction operator, defined in the same way as Brueckner's except that w_2 replaces v. Further, important three-body effects may be included by summing out three-quasihole diagrams as described by H. A. Bethe (Ref. 4). However, the necessity of such refinements would in large measure destroy the utility of our method.

[69] T. Ohmura, M. Morita, and M. Yamada, Prog. Theoret. Phys. (Kyoto) **15**, 222 (1956).

[70] Also note that the limiting case $\gamma\rightarrow\infty$ is inadmissible, because it leads us back to a singular potential in the sense that $\int w_2(r)r^2dr$ diverges. This limiting case is just the step function used for estimates of ω. It is what we might be led to call the optimum correlation factor within the class (V.7), since it produces smallest $|\omega|$, but it is energetically so unfavorable in a variational calculation that we must exclude it as quite unrealistic (cf. Ref. 13).

[71] H. Euler, Z. Physik **105**, 553 (1937).

[72] R. Huby, Proc. Phys. Soc. (London) **A62**, 62 (1949).

[73] W. J. Swiatecki, Phys. Rev. **103**, 265 (1956).

[74] H. A. Bethe, Phys. Rev. **103**, 1353 (1956).

[75] D. J. Thouless, Phys. Rev. **107**, 559 (1957).

turbation expansion may become useless.[67] Numerical evidence in favor of sensible convergence, for the value $\gamma=5.0$ F^{-1}, of both perturbative and cluster expansions has emerged from recent photonuclear calculations based on the CBF method and realistic two-nucleon potentials.[76]

A more favorable situation is to be expected with a more flexible f than (V.7), one displaying some restricted amount of positive correlation. (There is quite a lore connected with the choice of the correlation factor f.[77] In particular, one must avoid the "Emery difficulty."[19]) Ultimately, we might envisage the determination of f and V from *coupled* Euler-Lagrange equations, these derived by extremizing the energy expectation value, to given cluster approximation, subject to such constraints as are required to suppress the magnitude of higher cluster corrections. It is likely, though, that this will be more of a luxury than a necessity, i.e., that intuitively motivated analytic trial forms for f will suffice. We reserve thorough analysis of this problem for a later paper.

With an understanding of the gross or "normal" properties of nuclear matter, the next interesting questions are:

(1) Is nuclear matter a "superfluid"; more specifically, does it possess a ground state with strong pairing correlations of the type existing in a superconductor?

(2) If so, as is now believed,[78] what is the magnitude of the energy gap in the excitation spectrum?

These are indeed delicate questions. The methods used to deal with them previously have not been very satisfactory because they lean *too directly* on a formalism designed for nonsingular potentials.[79]

For a well-behaved potential $v(r)$ which allows no bound state (or at most one of zero energy), a *sufficient* condition for an energy gap is[80]

$$(v)_{k_f}=\int_0^\infty \sin^2 k_f r v(r) dr \leqslant 0. \qquad \text{(V.8)}$$

The leading terms in our effective Hamiltonian yield formally the same problem, even when v is singular, except that w_2 must be used everywhere in place of v. Therefore a sufficient condition for a gap, in the situation that cluster corrections of first order in the correlation parameter exert negligible effect, is $(w_2)_{k_f}\leqslant 0$, provided of course the effective potential w_2 does not bind.[81] The quantity $(w_2)_{k_f}$ has been evaluated for three choices of the singlet-even two-nucleon potential (Ohmura-Morita-Yamada,[69,16] Brueckner-Gammel-Thaler,[61] and Hamada-Johnston[64]) and the simple correlation factor (V.7), over a range of γ's. Results are cited in Table I, and should be looked upon as only a tentative indication of the physical situation. [It might be noted that the value $\gamma=5.0$ F^{-1} seems to play a special role. A calculation like that of IY was carried out using the singlet-even Brueckner-Gammel-Thaler potential, and again this value was found to be the most advantageous energetically.[82] A similar result ($\gamma=6.0$ F^{-1}) was obtained by Temkin[22] for his spin-dependent Serber potential, using a modified cluster expansion method but the same class of trial f's.] In order to arrive at definitive answers to questions (1) and (2), a detailed investigation employing the Bogoliubov canonical transformation method (as described by Bell,[79] for example) is being carried out by Chakkalakal.

TABLE I. Results for $(w_2)_{k_f}$ (in MeV-F) at various k_f and γ (both in F^{-1}), for the Iwamoto-Yamada choice of correlation factor and three different two-nucleon potentials (singlet-even states): Ohmura-Morita-Yamada (A), Brueckner-Gammel-Thaler (B), and Hamada-Johnston (C). Under the assumptions of the text, negative values signal an energy gap in the excitation spectrum of nuclear matter. Equilibrium density is usually taken to correspond to $k_f\approx 1.4$ F^{-1}.

Potential	k_f \ γ	1	3	5	7	9
A	1.0	−1.05	−13.8	−15.3	−10.4	−2.36
	1.4	3.07	1.50	6.64	18.3	33.8
	1.8	5.87	19.4	36.1	57.1	81.3
B	1.0	−2.85	−17.0	−20.6	−19.6	−16.4
	1.4	0.545	−8.47	−10.3	−6.52	0.169
	1.8	3.29	4.77	8.94	17.7	29.4
C	1.0	0.099	−13.9	−20.3	−21.3	−19.2
	1.4	2.15	−7.61	−13.1	−12.1	−6.78
	1.8	3.93	3.88	4.53	10.5	20.9

Once f and V are selected, $\tilde{w}_2$ and $\tilde{w}_3$ are fixed and thus H^{eff} completely determined. An important question remains to be answered: Is the H^{eff} resulting from a choice of f, V appropriate to accurate practical calculation of the *ground-state energy* in the framework of the new perturbation theory conducive to accurate practical calculation of the *energy spectrum of low-lying excited states*? One may well be driven to criteria other than or in addition to those we have suggested, in making the "best" choice of f and V for treating a given aspect of the many-body problem. This *general* statement

[76] T. P. Wang and J. W. Clark (to be published).

[77] J. S. Bell and E. J. Squires (see Ref. 4).

[78] L. N. Cooper, R. L. Mills, and A. M. Sessler, Phys. Rev. **114**, 1377 (1959); R. L. Mills, A. M. Sessler, S. A. Moszkowski, and D. G. Shankland, Phys. Rev. Letters **3**, 381 (1959); V. J. Emery and A. M. Sessler, Phys. Rev. **119**, 248 (1960); K. A. Brueckner, T. Soda, P. W. Anderson, and P. Morel, *ibid.* **118**, 1442 (1960); E. M. Henley and L. Wilets, *ibid.* **133**, B1131 (1964).

[79] However, cf. E. M. Henley and L. Wilets, Phys. Rev. **133**, B1118 (1964). Comprehensive reviews of work done before 1961 are given by Bell and Squires in Ref. 4 and by J. S. Bell, in *The Many-Body Problem, Lecture Notes of the First Bergen International School of Physics—1961* (W. A. Benjamin, Inc., New York, 1962), pp. 197–213.

[80] V. J. Emery, Nucl. Phys. **12**, 69 (1959); **19**, 154 (1960).

[81] One would hardly expect w_2 to bind for realistic f, if v does not. However, this possibility is still open for the f's we have used, and is being examined.

[82] One must refrain, however, from taking very seriously, for the actual nuclear-matter problem, the saturation properties that come out of preliminary calculations of this sort—certainly the tensor component of the force plays too important a role to be ignored; also we should be more clever in our selection of the class of f's.

applies, *in particular*, to the aforementioned energy-gap calculation.

In extending our formalism to finite nuclei, complications will arise most obviously from the fact that terms of order $1/N$ can no longer be neglected.[83] And since plane waves do not provide appropriate orbitals for a system which has a surface, momentum conservation cannot be invoked to discard large classes of matrix elements as we have done. Sums over states become more difficult. Nonetheless the formal work is quite straightforward and is now in progress. For the φ_i we may take either self-consistent single-particle wave functions, or, more practically, suitable shell-model orbitals. Configuration-mixing calculations, according to the procedures of Ref. 35, and studies of pairing and collective effects on the basis of an effective second-quantized Hamiltonian, using field-theoretic methods as described in Sec. IV, are definite possibilities. All work begins with a "second-principles" potential, which fits a selected collection of two-particle data.

We close with a remark about three-body nuclear forces. If one does, say, a very elaborate configuration-mixing shell-model calculation for a number of nuclear states, for a number of nuclei, with an adjustable weak two-body potential (the same for all cases) and finds that the data can be fitted well only with the inclusion of a three-body potential, one is of course not justified in citing this result as evidence for the presence of a fundamental three-nucleon potential of appreciable strength (which could, if we knew how, be derived from meson theory). Such a result, as we have seen, may very well be an *artifact* of the model that has been adopted—one can certainly replace the problem of interaction of the real particles via strong two-body potentials by an equivalent problem of interaction of quasiparticles via weak two-body potentials, plus additional three-body, four-body,$\cdots$potentials.[84] On the other hand, the fact that the sophisticated shell model works so well without introduction of many-body potentials is good evidence for the applicability of our method and the rapid convergence of the cluster expansions for suitably chosen f, V.

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APPENDIX: SYMMETRIES OF TRUNCATED CLUSTER EXPANSIONS

Here we direct attention to certain symmetries of the matrix elements of the identity and Hamiltonian operators, and examine to what extent these symmetries survive in truncated cluster expansion formulas for the matrix elements.

Certainly $\mathfrak{N}_{mn}$, $\mathfrak{H}_{mn}$ are

(1) Hermitian,

(2) if diagonal, symmetric in any two orbitals m_i, m_j; if nondiagonal, with $m_i \neq n_i$, $i \leqslant d$, $m_i = n_i$, $i > d$, antisymmetric in m_i, m_j and in n_i, n_j, i, $j \leqslant d$, and symmetric in m_i, m_j, i, $j > d$,

(3) invariant under a unitary transformation of the single-particle orbitals used to construct the model functions Φ_m, Φ_n.

Two prescriptions for truncation of the cluster expansions have been proposed. One, that of keeping all terms of say Pth order or lower in the correlation parameter and discarding those of higher order, has been inherent to our development. The other is that of Feenberg and Woo (FW), who instead define a Pth-order calculation as one including all contributions arising from terms in G involving no more than P distinct indices. Consideration of symmetries (1), (2), (3) leads to a preference for our classification of orders of approximation. [However, it should be kept in mind that the failure of successive approximations in a given computational method to satisfy symmetry properties of the quantity to be calculated is not sufficient reason for rejecting this method; for example, failure of the invariance (3) implies the existence of some optimum choice of single-particle orbitals for which the corresponding successive truncated approximants converge most rapidly.[10] We await detailed calculations to throw additional light on the merits of the proposed classification procedures.]

A meaningful comparison with the work of FW is possible only after we are convinced that the "linear combination method" used by them to extract nondiagonal matrix elements from diagonal ones is equivalent—within the framework of the present discussion—to the "α-parameterization scheme" we have adopted, i.e.,

[83] For one thing, the assumption of a "macroscopically occupied condensate" is no longer meaningful.

[84] See also J. Dabrowski (Ref. 18) and *Proceedings of the Rutherford Jubilee International Conference, Manchester, 1961*, edited by J. B. Birks (Heywood and Company, Ltd., London, 1961), pp. 739–748, as well as Ref. 57.

we want to be sure that any differences in the degree to which (1), (2), (3) are met by the truncated expansions of FW and ourselves are indeed due to the different prescriptions for truncation. Their procedure is the following: In $\mathfrak{n}_{\mathbf{mm}}$, $\mathfrak{h}_{\mathbf{mm}}$ replace $\mathbf{m}$ by $\mathbf{m}^\star$, i.e.,

$$\begin{aligned}&\varphi_{m_i}\rightarrow\varphi_{m_i}{}^\star,\\&\varphi_{m_i}{}^\star=a_{m_i}\varphi_{m_i}+b_{n_i}\varphi_{n_i},\quad i=1,\cdots,d,\\&\varphi_{m_i}{}^\star=\varphi_{m_i},\quad i>d,\end{aligned}\tag{A1}$$

where a_{m_i}, b_{n_i} are arbitrary coefficients, and do this also in the cluster expansions for these matrix elements. The required nondiagonal matrix elements $\mathfrak{n}_{\mathbf{mn}}$, $\mathfrak{h}_{\mathbf{mn}}$ are then obtained by matching coefficients of $a_{m_1}{}^*\cdots a_{m_d}{}^* b_{n_1}\cdots b_{n_d}$ in the "generating functions" $\mathfrak{n}_{\mathbf{m}^\star\mathbf{m}^\star}$, $\mathfrak{h}_{\mathbf{m}^\star\mathbf{m}^\star}$ and their cluster expansion representations. In practice the magnitudes of a_{m_i}, b_{n_i}, $i\leqslant d$, are set equal to $\sqrt{\frac{1}{2}}$, the remaining (arbitrary) phases being used to separate the various contributions that enter. The role played by this choice in the formalism is not yet clear—but surely any deviations from the results for some other recipe for reducing the "excess arbitrariness" can only come about due to a truncation of the cluster expansions which is, to this extent, inappropriate.

Our α-parametrization procedure can be phrased in the same language. Note that for α_i near zero

$$\exp(\alpha_i\varphi_{n_i}/\varphi_{m_i})\varphi_{m_i}\sim\varphi_{m_i}+\alpha_i\varphi_{n_i},\tag{A2}$$

so that we also replace φ_{m_i} (but only in the right-hand wave function) in $\mathfrak{n}_{\mathbf{mm}}$, $\mathfrak{h}_{\mathbf{mm}}$ by a linear combination of φ_{m_i} and φ_{n_i} and—by the artifice of differentiating with respect to $\alpha_1,\cdots,\alpha_d$ and setting all the α's zero—seek the coefficients of $\alpha_1\cdots\alpha_d$ in the resulting cluster expansions. The primary difference, then, between the FW procedure and ours is in the reduction in excess arbitrariness of the coefficients in the linear combinations (A1): We suppose $a_{m_i}=1$ and b_{n_i} is small but otherwise arbitrary. [It is worth remarking that the β-parametrization procedure, the much-used device for drawing matrix elements $\mathfrak{h}_{\mathbf{mm}}$ of the Hamiltonian from a generalized normalization integral resembling $\mathfrak{n}_{\mathbf{mm}}$, is really in the same spirit. For small β, we have, for example,

$$(\exp\beta H_1)\varphi_{m_i}\sim\varphi_{m_i}+\beta H_1\varphi_{m_i}.\tag{A3}$$

Again, in effect, φ_{m_i} in the right-hand wave function is replaced by a linear combination (this time involving, in general, *all* the single-particle orbitals) and the coefficient of β in the resulting cluster expansion is sought.] The fact that only the right-hand wave function in $\mathfrak{n}_{\mathbf{mm}}$, $\mathfrak{h}_{\mathbf{mm}}$ is replaced deserves mention in connection with symmetry property (1). This feature has the consequence that our $I^{\mathbf{mn}}$, in contrast to $I^{\mathbf{mm}}(\mathbf{m}\rightarrow\mathbf{m}^\star)$ of FW, is *not* Hermitian, i.e., while $I^{\mathbf{mm}}(\mathbf{m}\rightarrow\mathbf{m}^\star)$ goes to $(I^{\mathbf{mm}}(\mathbf{m}\rightarrow\mathbf{m}^\star))^*$ upon interchange of the roles of m_i and n_i, $i=1,\cdots,d$, our $I^{\mathbf{mn}}\neq(I^{\mathbf{nm}})^*$. However, all that is actually required is Hermiticity of the *derivatives*,

$$\begin{aligned}&\partial^d I^{\mathbf{mn}}/\partial\alpha_1\cdots\partial\alpha_d\,|_{\alpha_1=\cdots=\alpha_N=\beta=0}=\mathfrak{n}_{\mathbf{mn}},\\&\partial^{d+1}I^{\mathbf{mn}}/\partial\beta\partial\alpha_1\cdots\partial\alpha_d\,|_{\alpha_1=\cdots=\alpha_N=\beta=0}=\mathfrak{h}_{\mathbf{mn}},\end{aligned}$$

and this requirement *is* fulfilled for our definition of $I^{\mathbf{mn}}$, with the choice (II.2) of H_1, H_2, H_3. Further, the final results of Sec. II are Hermitian order by order in ω, in fact, term by term.

Our calculations of $\mathfrak{N}_{\mathbf{mn}}$, $\mathfrak{H}_{\mathbf{mn}}$ of Sec. II were repeated, using the Feenberg-Woo linear combination method. The results are in fact identical to those we came by earlier, *provided* all terms of second or lower order in ω for $\mathfrak{N}_{\mathbf{mn}}$ and of first or lower order in ω for $\mathfrak{H}_{\mathbf{mn}}$, and only those terms, are retained; so the techniques in question are equivalent, to the approximation considered in this paper. Furthermore, the results obtained are formally identical with those of FW, if, as they, we keep the contributions from all terms in G with no more than three distinct indices; the choice of BDJ versus Bose correlation factor, though leading to detailed differences in the explicit forms for the cluster integrals, is essentially immaterial to the present discussion. With this latter truncation there arise certain embarassing terms which violate the antisymmetry requirement in (2). These terms, besides being weakened due to internal cancellation (they involve differences of cluster integrals which are the same apart from the particular orbitals that appear), are all of *third order* in ω for the $\mathfrak{N}_{\mathbf{mn}}$ and of *second order* for the $\mathfrak{H}_{\mathbf{mn}}$ in our classification scheme, hence only need be considered in a higher order calculation than we have given, where they are presumably compensated by other terms also failing of antisymmetry. To reiterate: excluding these terms, i.e., replacing (in FW's notation) all $\cosh\frac{1}{2}(\delta\mathcal{G}_{(1')}-\delta\mathcal{G}_{(1)})$, $\cosh\frac{1}{2}(\delta\mathcal{G}_{(2')}-\delta\mathcal{G}_{(2)})\cdots$ factors by unity and omitting all $\delta E(1,1')$, $\delta E(2,2'),\cdots$ contributions, then adding the proper contributions from the $x_{ijkl'}$ term in G, we obtain exact agreement with our results of Sec. II. One might speculate that differences caused by different assumptions for magnitudes or phases in the linear combinations (A1) (which still allow, though, sufficient arbitrariness to separate the various contributions) will appear, in calculations otherwise following that of FW, only in these "small" terms.

A consistent ω-classification scheme is not easily devised for the final explicit cluster integrals given by FW for the Bose correlation factor, since no η's appear, but it is clear from formal analogy to our work just which contributions should be kept to given order in the relevant correlation parameter.

Testing the final results of Sec. II according to (2), we find, order by order in ω and term by term, an entirely satisfactory situation. The only source of difficulty might be the four-index contributions. For the diagonal elements there is certainly no difficulty—these contributions are indeed symmetrical under interchange of any

two orbitals. For the nondiagonal elements, we must look at [cf. the last member of (II.7)]

$$-(m_im_j|h_2|n_in_j)_a(m_km_l|h_2|n_kn_l)_a - (m_im_k|h_2|n_in_k)_a(m_jm_l|h_2|n_jn_l)_a - (m_im_l|h_2|n_in_l)_a(m_jm_k|h_2|n_jn_k)_a. \quad \text{(A4)}$$

Interchanging m_i, m_j (we may suppose $m_i \neq n_i$, $m_j \neq n_j$), this becomes

$$+(m_im_j|h_2|n_in_j)_a(m_km_l|h_2|n_kn_l)_a - (m_jm_k|h_2|n_in_k)_a(m_im_l|h_2|n_jn_l)_a - (m_jm_l|h_2|n_in_l)_a(m_im_k|h_2|n_jn_k)_a. \quad \text{(A5)}$$

If either $m_k=n_k$ or $m_l=n_l$, the last two terms (whose presence would imply a deviation of our approximations for $\mathfrak{N}_{mn}$, $\mathfrak{H}_{mn}$ from antisymmetry in m_i, m_j) vanish in the limit of a uniform, infinite medium by momentum conservation. In the remaining case of four-orbital excitation, (A4) is irrelevant, for then it is the *barred* four-index cluster integrals which enter, and these are clearly antisymmetric with respect to interchange of any two "left" orbitals or any two "right" orbitals with indices $\leqslant d$.

Feenberg and Woo also noticed that their truncated forms (derived on the basis of the IY cluster formalism) do not display invariance under a unitary transformation of the single-particle basis functions. The terms which fail of invariance arise from contributions to G involving a repeated index, as $\sum_{ijk} x_{ij}x_{jk}$. An invariant cluster formulation, in which all FW approximants manifestly do meet the symmetry requirement (3), may be devised by defining subnormalization integrals $I_{(b)}$, $b=1,\cdots,N$, which are averages over those of the IY formalism, and, in terms of these, cluster integrals $X_{(b)}$:

$$\begin{aligned} I_{(1)} &= \frac{1}{N}\sum_i I_i = X_{(1)}, \\ I_{(2)} &= \frac{1}{N(N-1)}\sum_{ij} I_{ij} = X_{(1)}^2 + X_{(2)}, \\ I_{(3)} &= \frac{1}{N(N-1)(N-2)}\sum_{ijk} I_{ijk} = X_{(1)}^3 + 3X_{(1)}X_{(2)} + X_{(3)}, \\ &\vdots \\ I_{(N)} = I &= \sum_{\substack{\text{all partitions} \\ \sum_{b=1}^{N} b\nu_b = N}} \frac{N! X_{(1)}\cdots X_{(b)}\cdots X_{(N)}}{\prod_b (b!)^{\nu_b}\nu_b!}. \end{aligned} \quad \text{(A6)}$$

The last expression is to be compared with the last of (II.5). It leads to an exponential formula,

$$\begin{aligned} I_{(N)} &= I_{(1)}{}^N \exp N G_{\mathrm{AHT}}, \\ G_{\mathrm{AHT}} &= \tfrac{1}{2}Nx_{(2)} + \tfrac{1}{6}N^2(x_{(3)} - 3x_{(2)}{}^2) \\ &\quad + (1/24)N^3 x_{(4)} + \cdots, \quad x_{(b)} = X_{(b)}/X_{(1)}{}^b, \end{aligned} \quad \text{(A7)}$$

analogous to (II.10), (II.11), (II.12) (**m**, **n** labels are again omitted). The AHT on G serves to indicate that this form of the cluster expansion theory is the same as that investigated by Aviles and by Hartogh and Tolhoek. The calculations of Sec. II were repeated in the framework of this formalism [using the α-parametrization scheme and our truncation prescription, but the above basic formulas (A6), (A7)]. At first the results for $\mathfrak{N}_{mn}$, $\mathfrak{H}_{mn}$ appear to fail of (1), Hermiticity. For example, in the case of two orbitals different,

$$\mathfrak{N}_{mn} = \underset{O(\omega/N)}{\tfrac{1}{2}N^2 X_{(2),\alpha_1\alpha_2}{}^{mn}} + \underset{O(\omega^2/N)}{\tfrac{1}{8}N^4 X_{(2),\alpha_1\alpha_2}{}^{mn}(X_{(2)}{}^m - X_{(2)}{}^n)} - \underset{O(\omega^2/N)}{N^3 X_{(2),\alpha_1\alpha_2}{}^{mn} X_{(2)}{}^m} + \underset{O(\omega^2/N)}{\tfrac{1}{6}N^3 X_{(3),\alpha_1\alpha_2}{}^{mn}} + \underset{O(\omega^2/N)}{(1/24)N^4 X_{(4),\alpha_1\alpha_2}{}'^{mn}} + O(\omega^3/N), \quad \text{(A8)}$$

$$\begin{aligned} \mathfrak{H}_{mn} &= \underset{O(1/N)}{\tfrac{1}{2}N^2 X_{(2),\alpha_1\alpha_2\beta}{}^{mn}} - \underset{O(\omega/N)}{N X_{(2),\alpha_1\alpha_2}{}^{mn}\mathcal{E}_m} + \underset{O(\omega/N)}{\tfrac{1}{4}N^2 X_{(2),\alpha_1\alpha_2}{}^{mn}(\mathcal{E}_m - \mathcal{E}_n)} \\ &\quad - \underset{O(\omega/N)}{N^3 X_{(2),\alpha_1\alpha_2\beta}{}^{mn} X_{(2)}{}^m} + \underset{O(\omega/N)}{\tfrac{1}{8}N^4 X_{(2),\alpha_1\alpha_2\beta}{}^{mn}(X_{(2)}{}^m - X_{(2)}{}^n)} - \underset{O(\omega/N)}{N^3 X_{(2),\alpha_1\alpha_2}{}^{mn} X_{(2),\beta}{}^m} \\ &\quad + \underset{O(\omega/N)}{\tfrac{1}{8}N^4 X_{(2),\alpha_1\alpha_2}{}^{mn}(X_{(2),\beta}{}^m - X_{(2),\beta}{}^n)} + \underset{O(\omega/N)}{\tfrac{1}{6}N^3 X_{(3),\alpha_1\alpha_2\beta}{}^{mn}} + \underset{O(\omega/N)}{(1/24)N^3 X_{(4),\alpha_1\alpha_2\beta}{}'^{mn}} + O(\omega^2/N). \end{aligned} \quad \text{(A9)}$$

The unsymmetrical appearance of the results is, however, illusory: In fact they may be seen to reproduce exactly those of Sec. II (which are certainly Hermitian), upon application of various α, β derivatives of the identities

$$\begin{aligned} (1/24)N^4 X_{(4)} &= \sum_{i<j<k<l} X_{ijkl} + \tfrac{1}{2}N^3 X_{(2)}{}^2 - \sum_{i<j<k} [X_{ij}X_{jk} + X_{jk}X_{ki} + X_{ki}X_{ij}], \\ x_{(2),\beta} &= \frac{1}{N(N-1)}\sum_{i,j} x_{ij,\beta} - \frac{1}{N(N-1)}\sum_{i,j} X_{ij}(2X_{(1),\beta} - X_{i,\beta} - X_{j,\beta}). \end{aligned} \quad \text{(A10)}$$

(The first of these was given by FW. Both relations are easy to check from the basic definitions.) The importance of this finding, with regard to the invariance property (3), is to be emphasized. Because of the *equivalence* of the IY and AHT formalisms to second order in ω for the $\mathfrak{N}_{mn}$ and to first order in ω for the $\mathfrak{H}_{mn}$, our IY results of Sec. II *must* be invariant under a unitary transformation of the single-particle basis. Again one might at first be deceived: The presence of terms in (II.15), for example, with overlapping indices is not at all reassuring; however, any apparent lack of invariance melts away upon recognition of the subtle differences between the AHT cluster integrals and averages of the IY cluster integrals, as displayed in (A10), these differences compensating the noninvariant terms. It is also clear, from the first of (A10), why the truncated cluster expansions of FW, based on the IY formalism, violate (3)—the four-index X_{ijkl} terms have an important role in restoring invariance. The FW truncation prescription produces different results for IY and AHT formalisms in given "order." In contrast, it is quite reasonable to conjecture that IY and AHT formalisms will continue to be equivalent order by order when, instead, our ω classification is used.

At any rate, our final results for the IY formalism satisfy symmetry (1) term by term as well as order by order in ω and (3) only order by order; our final results for the AHT formalism satisfy (1) only order by order and (3) term by term as well as order by order.

It must be admitted that $N\omega/\Omega$ is not a genuine expansion parameter; ω factors cannot in general be extracted rigorously from a cluster integral with three or more indices because the integrations over r_{12}, r_{23},$\cdots$ are just not separable. Nevertheless, *the ω classification of cluster integrals is unambiguous and leads*, as has become clear in this Appendix, *to truncated cluster expansions with all the desired symmetry properties*—in these respects our expansions do indeed behave like power series in $N\omega/\Omega$.

To avoid a possible misunderstanding, perhaps we should point out that the (asymptotic) cluster expansions we have derived are not power series in the density ρ. This is obvious from the presence of sums over single-particle states coupled with the fact that the system obeys Fermi statistics. But also, if any parameters in f are determined variationally, as proposed, these parameters become (generally, nonanalytic) function of the density, implying a corresponding ρ dependence of each cluster contribution with more than one index.