Simplified Treatment for Strong Short-Range Repulsions in N-Particle Systems. I. General Theory*

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A new variational approach is developed for studying the properties of systems of particles interacting through singular short-range repulsions that give rise to strong two-particle correlations. The correlated trial function $\Psi_\gamma = e^S\Phi_\gamma$ (state γ) results, with proper choice of S, in a simple form for the energy expectation value $\langle H\rangle$—as well as for other matrix elements of interest—which is devoid of all reference to the strong repulsions except through e^{2S} factors and hence is particularly suited to calculation. In many cases an independent-particle type Φ_γ seems appropriate. The cluster evaluation of this form for $\langle H\rangle$ is discussed, both in the few-particle and many-particle cases. Using the techniques of Iwamoto and Yamada, simplified convergent cluster expansions for the energy expectation value are derived for many-fermion and many-boson systems. A program for application of this method to nuclear problems is being initiated.

1. INTRODUCTION

THE goal of this paper is the development of a simple variational procedure for determining the wave function and energy of an N-particle system in which short-range repulsions produce marked two-particle correlations. The essence of the method is the choice of a trial wave function of the form $\Psi = e^S\Phi$, with the correlation function e^S so chosen that, when Ψ is inserted in the energy expectation value $\langle H\rangle$, terms are generated which cancel out the short range repulsive potentials. For the physical systems considered here, the resulting expression for $\langle H\rangle$ may be brought into a particularly simple form. The subsequent prescription for evaluating $\langle H\rangle$ always involves a cluster expansion.

A similar approach of less specific nature has been developed, and applied to systems with short-range hard-core interactions, by several authors, notably Dingle,[1] Jastrow,[2] Iwamoto and Yamada,[3,4] Iwamoto,[5] Dabrowski,[6,7] and Emery[8]: in place of the factor e^S a product of two-particle correlation functions is assumed; its parameters are determined by a variational procedure. Emery,[8] in particular, has discussed the general restrictions on the choice of such a trial function. The cluster expansion technique for the evaluation of the resultant expression for $\langle H\rangle$ was first introduced by Jastrow,[2] a more systematic treatment of the cluster method being given later by Iwamoto and Yamada.[3]

In Sec. 2 an equation for S is derived. The vital criterion to be satisfied is the following: the transformation $\Psi_\gamma = e^S\Phi_\gamma$ should produce a form for the matrix element of the Hamiltonian between stationary states represented by Ψ_β, Ψ_α in which the short-range repulsion term in the interaction no longer appears. S is further chosen so that this expression for $(\Psi_\beta, H\Psi_\alpha)$ has an appealingly simple structure. Next (Sec. 3) the correlation factor e^S is specialized permanently to a product of two-particle correlation functions $e^{S_{ij}}$, $(i,j=1,\cdots,N)$. Suggestions are offered for dealing with certain three-particle terms which then arise in the relation previously derived for S. A rough estimate of their size is given in Appendix A. The gross character of the S_{ij} is found to be such that the wave function Ψ_γ vanishes very rapidly when two particles in the system come close together—as it should. In Sec. 4 we set $\alpha=\beta$ and look into the physical meaning of the resulting energy expectation value; the forms assumed by other matrix elements of physical interest, when we insert $\Psi_\gamma = e^S\Phi_\gamma$, are also investigated. In Sec. 5 the choice of the "model function" Φ_γ is discussed. An independent-particle type Φ_γ should be quite satisfactory for many problems. Section 6 presents a cluster method for evaluating $\langle H\rangle$ (hence Ψ) for systems in which N is small. If N is small enough, say four or less, it is possible to include, without excessive labor, the contributions of all the clusters. Here our interest focuses on the very light nuclei H^3, He^3, and He^4. Explicit formulas are given for $N=3$. In Sec. 7 we follow the lead of Iwamoto and Yamada[3] to set up a convergent cluster development of $\langle H\rangle$ for both many-fermion and many-boson systems, with our special choice of two-particle correlation function. The expansions obtained are considerably more manageable than those of Iwamoto and Yamada, and should be especially useful in nuclear problems.

In Appendix B an alternative approach is pursued, starting from the many-particle Schrödinger equation with $e^S\Phi$ substituted for the wave function Ψ. The result is a Schrödinger-type wave equation for Φ with a non-Hermitian correction term. Some preliminary calculations indicate that this approach has only limited usefulness.

Utilizing just the results of Sec. 1, we exhibit in Appendix C the beginnings of a perturbation method

* Supported in part by the Office of Scientific Research.
[1] R. B. Dingle, Phil. Mag. **40**, 573 (1949).
[2] R. Jastrow, Phys. Rev. **98**, 1479 (1955).
[3] F. Iwamoto and M. Yamada, Progr. Theoret. Phys. Japan **17**, 543 (1957).
[4] F. Iwamoto and M. Yamada, Progr. Theoret. Phys. Japan **18**, 345 (1957).
[5] F. Iwamoto, Progr. Theoret. Phys. Japan **19**, 595 (1958).
[6] J. Dabrowski, Proc. Phys. Soc. (London) **A71**, 658 (1958).
[7] J. Dabrowski (to be published).
[8] V. J. Emery, Nuclear Phys. **6**, 585 (1958).

(to general order) valid for interactions including strong short-range repulsions. The matrix elements that appear differ from those of ordinary perturbation theory only in the presence of e^{2S} factors.

Our discussion has developed from a study of nuclear problems, but actually the variational treatment sketched above has a much wider field of application. Thus the terminology is kept as general as practicable.

2. FORMAL DEVELOPMENT OF THE METHOD

Consider a system of N identical nonrelativistic particles of mass M, the coordinates (space, spin, and isospin) of the kth particle being denoted collectively by x_k. We write the Hamiltonian for the system in the general form

$$H=K+V, \tag{1}$$

with K the sum of the free-particle Hamiltonians,

$$K=-\frac{\hbar^2}{2M}\sum_k \Delta_k, \tag{2}$$

and V the interaction term (*not* necessarily a sum of two-body interactions alone.) Then V is decomposed into

$$V=V_A+V_R, \tag{3}$$

such that V_R contains *all* the strong[9] short-range interparticle repulsions that may be present, but is otherwise unspecified for the moment.

For our work we take the wave function of the system, in any stationary state γ, to have the structure

$$\Psi_\gamma=e^S\Phi_\gamma, \tag{4}$$

where S is a real function of the particle space coordinates $\mathbf{r}_k$, $(k=1, \cdots, N)$, chosen, when possible, to eliminate V_R from all matrix elements $(\Psi_\beta,H\Psi_\alpha)$. In the calculations, the "model wave function" Φ_γ will be treated as a trial function, and will, most often, be taken to resemble the wave function for the system in the absence of V_R.

The next step is to derive an appropriate differential equation for S. From (1), (2), and (3), we have

$$(\Psi_\beta,H\Psi_\alpha)=\int\Psi_\beta^*\left\{-\frac{\hbar^2}{2M}\sum_k\Delta_k+V_A+V_R\right\}\Psi_\alpha, \tag{5}$$

where the

$$\int\equiv\int\prod_{n=1}^N dx_n$$

implies an integration over the position variables $\mathbf{r}_n$ and summations over spin and isospin variables m_n, t_n, for each particle of the system $(n=1, \cdots, N)$. Integrating by parts and then inserting (4), we see

$$-\int\Psi_\beta^*\Delta_k\Psi_\alpha=\int\nabla_k\Psi_\beta^*\cdot\nabla_k\Psi_\alpha$$

$$=\int e^{2S}[(\nabla_kS)^2\Phi_\beta^*\Phi_\alpha+\nabla_k\Phi_\beta^*\cdot\nabla_k\Phi_\alpha+\nabla_kS\cdot\nabla_k(\Phi_\beta^*\Phi_\alpha)].$$

Another integration by parts converts the last term to

$$\int e^{2S}\nabla_kS\cdot\nabla_k(\Phi_\beta^*\Phi_\alpha)=-\int e^{2S}[(\Delta_kS)+2(\nabla_kS)^2]\Phi_\beta^*\Phi_\alpha.$$

Now we assume V_R may be chosen such that

$$\frac{\hbar^2}{2M}\sum_k[(\nabla_kS)^2+(\Delta_kS)]=V_R \tag{6}$$

is soluble for S,[10] in which case our matrix element reduces to

$$(\Psi_\beta,H\Psi_\alpha)=\int\left\{e^{2S}\frac{\hbar^2}{2M}\sum_k\nabla_k\Phi_\beta^*\cdot\nabla_k\Phi_\alpha+e^S\Phi_\beta^*V_Ae^S\Phi_\alpha\right\}. \tag{7}$$

So if V_A commutes with S,[11] the transition matrix element (state α to state β) assumes a particularly simple form,

$$\langle H\rangle_{\beta\alpha}\equiv(\Psi_\beta,H\Psi_\alpha)/(\Psi_\beta,\Psi_\beta)^{\frac{1}{2}}(\Psi_\alpha,\Psi_\alpha)^{\frac{1}{2}}$$

$$=\frac{\int e^{2S}\left\{\frac{\hbar^2}{2M}\sum_k\nabla_k\Phi_\beta^*\cdot\nabla_k\Phi_\alpha+\Phi_\beta^*V_A\Phi_\alpha\right\}}{\left(\int e^{2S}\Phi_\beta^*\Phi_\beta\right)^{\frac{1}{2}}\left(\int e^{2S}\Phi_\alpha^*\Phi_\alpha\right)^{\frac{1}{2}}}, \tag{8}$$

[9] The interparticle repulsive potential is called strong if the probability of finding two particles close together is greatly reduced by the presence of the repulsive potential. If the repulsive potential is not strong in this sense, the energy shift generated by it can be evaluated by techniques which are adequate for the attractive long-range component, in particular the first and second order Hassé, Brillouin-Wigner, or Schrödinger procedures or suitable refinements on these procedures (including calculation of third-order contributions and uniform displacement of the zeroth-order spectrum). In this connection see, for example, A. M. Feingold, Phys. Rev. **101**, 258 (1956); P. Goldhammer and E. Feenberg, Phys. Rev. **101**, 1233 (1956); M. Bolsterli and E. Feenberg, Phys. Rev. **101**, 1349 (1956); and W. J. Swiatecki, Phys. Rev. **103**, 265 (1956).

[10] This assumption is tenable for a wide range of problems. See Sec. 3.

Note added in proof.—A more flexible procedure results from replacing V_R in Eq. (6) by μV_R, the parameter μ then entering into the calculation of the energy as a variational parameter. Since e^SV_R vanishes when two particles come together the presence of a term $(1-\mu)V_R$ in the transformed matrix element of H is not objectionable. This change can be incorporated in the formalism simply by substituting $V_A'=V_A+(1-\mu)V_R$ for V_A and μV_R for V_R in all equations after Eq. (6). Calculations in progress on the ground-state properties of liquid He^4 confirm the usefulness of the more flexible procedure. Especially simple relations are found using the Lennard-Jones 10–6 potential.

[11] In Sec. 4 we shall study the matrix elements of some operators that do not commute with S.

a form well suited for calculations, as we shall see. Note V_R has been completely removed—the short-range repulsions manifest themselves only in the "weight factor" e^{2S} multiplying each volume element $\prod_n d\mathbf{r}_n$. In fact we may obtain this result from the matrix element in terms of Ψ, written as

$$\langle H\rangle_{\beta\alpha}=\int\left\{\frac{\hbar^2}{2M}\sum_k \nabla_k\Psi_\beta^*\cdot\nabla_k\Psi_\alpha+\Psi_\beta^* V\Psi_\alpha\right\}\Big/\left[\left(\int\Psi_\beta^*\Psi_\beta\right)^{\frac{1}{2}}\left(\int\Psi_\alpha^*\Psi_\alpha\right)^{\frac{1}{2}}\right], \quad (9)$$

merely by replacing Ψ or Φ, V by V_A, and $\prod_n d\mathbf{r}_n$ by $e^{2S}\prod_n d\mathbf{r}_n$, or, equivalently, from the form assumed by (9) when the short-range repulsions are absent ($\Psi\equiv\Phi$, $V\equiv V_A$) by $\prod_n d\mathbf{r}_n\rightarrow e^{2S}\prod_n d\mathbf{r}_n$ alone.

We emphasize that this development, as it stands, does not apply to strong short-range repulsions that are state-dependent, because S is assumed to depend only on the $\mathbf{r}_k$, and hence, by (6), so must V_R. If we do permit state dependence in S, a simple form for $\langle H\rangle_{\beta\alpha}$ like (8) (except with the e^{2S} factors applied to one of the Φ's) may be realized, for S a solution of (6), but only if

$$[e^S,\nabla_i S]=[e^S,\Delta_i S]=0, \quad (i=1,\cdots,N). \quad (10)$$

and consequently only if V_R, as well as V_A, commutes with S. However, for the most useful state-dependent S, namely

$$S=\sum_{i<j}[S_{ij}^{(1)}(r_{ij})+S_{ij}^{(2)}(r_{ij})\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j], \quad r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|,$$

the requirement (10) is not met, so instead a very complicated expression for $\langle H\rangle_{\beta\alpha}$ involving the nonzero commutators $[e^S,\nabla_i S]$ and $[e^S,\Delta_i S]$ results. In any case the greater flexibility in V_R allowed by a state-dependent S does not seem to justify the added complications—and we shall rely on a simple *state-independent* S in all subsequent discussions.

3. REMOVAL OF STRONG SHORT-RANGE TWO-PARTICLE REPULSIONS

In the presence of strong short-range *two-particle* repulsions—this is the case of vital physical importance—we choose

$$S=\sum_{(i,j)} S_{ij}, \quad (i,j=1,\cdots,N), \quad (11)$$

with S_{ij} a function only of the separation r_{ij} of particles i and j. S_{ii} is defined to vanish. (Here, and in the future, we adopt the summation notation of Iwamoto and Yamada: $\sum_{(i_1,\cdots,i_n)}$ means sum over all combinations, $\sum_{i_1,\cdots,i_n}$, sum over all arrangements, of the N possibilities $1,\cdots,N$ for the n indices $i_1,\cdots,i_n$. An analogous notation is to be used for products.) Then, by virtue of the symmetry of S_{ij} in i and j, it is easy to reduce (6) to

$$V_R=\frac{\hbar^2}{M}\sum_{(i,j)}[(\nabla_i S_{ij})^2+(\Delta_i S_{ij})+\sum_k(\nabla_k S_{ik}\cdot\nabla_k S_{kj})]. \quad (12)$$

For later reference, observe at this point that

$$\sum_{(i,j)}\sum_k(\nabla_k S_{ik}\cdot\nabla_k S_{kj})=\sum_{(i,j,k)}[(\nabla_k S_{ik}\cdot\nabla_k S_{kj})+(\nabla_i S_{ji}\cdot\nabla_i S_{ik})+(\nabla_j S_{kj}\cdot\nabla_j S_{ji})]. \quad (13)$$

Next, writing

$$V_R=\sum_{(i,j)} V_{ij}^R, \quad (14)$$

where V_{ij}^R is the corresponding interaction potential of particles i and j *inside the system*, we make the identification

$$\frac{\hbar^2}{M}[(\nabla_i S_{ij})^2+(\Delta_i S_{ij})+\sum_k(\nabla_k S_{ik}\cdot\nabla_k S_{kj})]=V_{ij}^R. \quad (15)$$

The presence of the three-particle terms $(\nabla_k S_{ik}\cdot\nabla_k S_{kj})$ should in many cases cause no discomfort; this is borne out by the estimate of their importance given in Appendix A. In some problems, however—in particular, in those problems in which the contribution to $\langle H\rangle_{\beta\alpha}$ of these three-body terms outweighs the effect of any such interactions known to be present—it would be advisable to redefine S_{ij} and V_{ij}^R so that no three-body terms appear in the differential equation relating them:

$$\frac{\hbar^2}{M}[(\nabla_i S_{ij})^2+(\Delta_i S_{ij})]=V_{ij}^R. \quad (16)$$

Then, of course, such terms (now *not* associated with the interactions of the system particles) would turn up instead in the transition matrix element. Unless otherwise indicated, though, we shall adhere to definition (15). We expect it to be quite satisfactory in nuclear problems (see Appendix A). For $N=2$ both choices give the same result:

$$\frac{\hbar^2}{M}[(\nabla_i S_{ij})^2+(\Delta_i S_{ij})]=v_{ij}^R. \quad (17)$$

[When the pair i,j is isolated, we denote V_{ij}^R by v_{ij}^R. The assumption that many-body forces are absent from V_R is equivalent to setting $V_{ij}^R=v_{ij}^R$ for all N. Obviously, then, $V_{ij}^R=v_{ij}^R$ in (16).]

In performing calculations, we are faced with two alternatives, the choice between them depending on the extent and detail of our phenomenological knowledge of the system at hand:

(1) If the form of the core[12] is considered known, as

[12] By "core" we mean that portion of the overall two-particle potential v_{ij} (isolated i,j) which becomes positively infinite very rapidly as $r_{ij}\rightarrow 0$. (We shall not be interested in cases for which

in the case of a collection of He^3 or He^4 atoms, (17) must actually be solved for S_{ij}. It is here that we use whatever flexibility remains in V_R, to render (17) as easily soluble as possible.

(2) If the shape of the core is ambiguous, as in the nuclear problem, a satisfactory recourse is to choose S_{ij} so that $v_{ij}{}^R$, as given by (17), is very singular, and positive, for $\mathbf{r}_i=\mathbf{r}_j$, but goes to zero rather quickly as i and j separate. This is easily done: for example

$$S_{ij}=-B_R\frac{e^{-r/\alpha_R}}{r},\quad B_R>0,\quad r\equiv r_{ij},$$

leads to

$$v_{ij}{}^R=\frac{\hbar^2}{M}\left[B_R{}^2\left(\frac{1}{r^4}+\frac{2}{r^3\alpha_R}+\frac{1}{r^2\alpha_R{}^2}\right)e^{-2r/\alpha_R}-\frac{B_R}{r\alpha_R{}^2}e^{-r/\alpha_R}\right],$$

which, for B_R large and α_R of the order of the core radius, has the required properties.

In the problems that concern us the gross nature of S_{ij} will clearly be characterized by

$$\begin{aligned}&S_{ij}\underset{r\to 0}{\longrightarrow}-\infty,\\ &S_{ij}\underset{r>C}{\longrightarrow}0,\end{aligned}\tag{18}$$

which forces the wave function Ψ_γ of (4) to vanish very rapidly as two particles in the system come close together, and approach Φ_γ as all particles in the system recede from each other. The approach to Φ_γ is also very rapid if S_{ij} has very short range, as will often be the case. This is just the sort of behavior expected on physical grounds. The short-range two-particle repulsions quite evidently assist in the realization of saturation.

In our treatment we do *not* deal with hard cores, of the form

$$\begin{aligned}v_{ij}{}^R&=+\infty,\quad r\leqslant C,\\ &=\ 0\ ,\quad r>C,\end{aligned}$$

but this does not seem, at present, a disadvantage, since we can choose $v_{ij}{}^R$ to be extremely strong, and extremely singular, for small r.

4. SIMPLIFIED EXPRESSIONS FOR SOME MATRIX ELEMENTS OF PHYSICAL INTEREST

First of all, if we set $\Phi_\beta=\Phi_\alpha=\Phi$ in (8), $\langle H\rangle_{\beta\alpha}$ becomes just the expectation value of the energy of the system (in state α)

$$\langle H\rangle_{\alpha\alpha}\equiv\langle H\rangle$$
$$=\int e^{2S}\left\{\frac{\hbar^2}{2M}\sum_k\nabla_k\Phi^*\cdot\nabla_k\Phi+\Phi^*V_A\Phi\right\}\Big/\int e^{2S}\Phi^*\Phi,\tag{19}$$

$V_{ij}{}^R$ is taken finite at $r_{ij}=0$.) The radius C of the core is defined as that value of r_{ij} at which v_{ij} vanishes. Obviously, this quantity is somewhat state-dependent in the nuclear problem.

a formula upon which the major part of our work will be based. Specifically, what has happened is this: because of our choice for S (and hence, to some extent, for V_R), the contribution to the expectation value of the V_R term in the interaction part has been completely cancelled out by correlation contributions (both negative and positive) to the kinetic energy part, leaving the above form for $\langle H\rangle$, in which the only residual influence of the short-range repulsions is embodied in the correlation factor e^{2S}. Now the factor e^{2S} greatly diminishes the contribution to $\langle H\rangle$ of that portion of configuration space in which any two particles are very close together. In other words, the important contributions to $\langle H\rangle$ come from the region of configuration space in which the over-all interaction V is well approximated by V_A and Ψ well approximated by Φ. This interpretation supplies a strong physical argument for the usefulness of the form (19). For if the effect of correlations other than those generated by V_R (these other correlations being predominantly of longer range) is small, we see why it should be quite satisfactory to construct Φ from appropriate single-particle wave functions.

Before going on to outline in detail the evaluation of $\langle H\rangle$ for actual physical systems, we are led to study some other matrix elements which, when expressed in terms of the Φ's, might allow a similar analysis.

Some of the operators that interest us do not commute with S. To study examples of this type, let each particle of our system carry a charge e. Then in the presence of an external electromagnetic field with vector potetial $\mathbf{A}_T$ we must include in H a term

$$H_c{}'=-\frac{e}{c}\sum_k\mathbf{A}(\mathbf{r}_k)\cdot\mathbf{v}_k,\tag{20}$$

where $\mathbf{A}(\mathbf{r}_k)$ is the vector potential of the perturbing radiation field, evaluated at the position of the kth particle, and the velocity operator $\mathbf{v}_k$ of the kth particle is given in terms of its momentum operator $\mathbf{p}_k$ by

$$\mathbf{v}_k=\frac{1}{M}\left[\mathbf{p}_k-\frac{e}{c}\mathbf{A}_0(\mathbf{r}_k)\right],\quad \mathbf{A}_0=\mathbf{A}_T-\mathbf{A}.\tag{21}$$

In spite of the fact that $H_c{}'$ does not commute with S, its matrix element

$$(\Psi_\beta,H_c{}'\Psi_\alpha)/[(\Psi_\beta,\Psi_\beta)^{\frac{1}{2}}(\Psi_\alpha,\Psi_\alpha)^{\frac{1}{2}}]\equiv\langle H_c{}'\rangle_{\beta\alpha},\tag{22}$$

(which for spinless particles is just the usual first order nonrelativistic electromagnetic transition matrix element if the Ψ's are the true many-particle wave functions for the field absent) can still be reduced to a simple form in terms of Φ_α, Φ_β. For we have

$$\int e^S\Phi_\beta{}^*\mathbf{A}(\mathbf{r}_k)\cdot\nabla_k(e^S\Phi_\alpha)=\int\Phi_\beta{}^*\mathbf{A}(\mathbf{r}_k)\cdot e^{2S}(\nabla_kS)\Phi_\alpha$$
$$+\int e^{2S}\Phi_\beta{}^*\mathbf{A}(\mathbf{r}_k)\cdot\nabla_k\Phi_\alpha,$$

the first term of which may be transformed as follows:

$$\frac{1}{2}\int \Phi_\beta^*\mathbf{A}(\mathbf{r}_k)\cdot(\nabla_k e^{2S})\Phi_\alpha = -\frac{1}{2}\int e^{2S}\nabla_k\cdot[\Phi_\beta^*\mathbf{A}(\mathbf{r}_k)\Phi_\alpha],$$

so if the gauge is chosen such that $\nabla_k\cdot\mathbf{A}(\mathbf{r}_k)=0$, $(k=1,\cdots,N)$, the two terms collapse to

$$\int e^S\Phi_\beta^*\mathbf{A}(\mathbf{r}_k)\cdot\nabla_k(e^S\Phi_\alpha) = \frac{1}{2}\int e^{2S}\mathbf{A}(\mathbf{r}_k)\cdot[\Phi_\beta^*\nabla_k\Phi_\alpha - (\nabla_k\Phi_\beta^*)\Phi_\alpha].$$

Thus we obtain

$$\langle H_c'\rangle_{\beta\alpha} = -\frac{e}{2c}\int e^{2S}\sum_k \mathbf{A}(\mathbf{r}_k)\cdot\{\Phi_\beta^*\mathbf{v}_k\Phi_\alpha + (\mathbf{v}_k\Phi_\beta)^*\Phi_\alpha\} \Big/ \left(\int e^{2S}\Phi_\beta^*\Phi_\beta\right)^{\frac{1}{2}}\left(\int e^{2S}\Phi_\alpha^*\Phi_\alpha\right)^{\frac{1}{2}}. \quad (23)$$

Note that this may be generated from the matrix element in terms of Ψ_α, Ψ_β, written in the form

$$\langle H_c'\rangle_{\beta\alpha} = -\frac{e}{2c}\int \sum_k \mathbf{A}(\mathbf{r}_k)\cdot\{\Psi_\beta^*\mathbf{v}_k\Psi_\alpha + (\mathbf{v}_k\Psi_\beta)^*\Psi_\alpha\} \Big/ \left[\left(\int \Psi_\beta^*\Psi_\beta\right)^{\frac{1}{2}}\left(\int \Psi_\alpha^*\Psi_\alpha\right)^{\frac{1}{2}}\right], \quad (24)$$

merely by replacing Ψ by Φ and multiplying each volume element $\prod_n d\mathbf{r}_n$ by e^{2S}. Further,

$$\mathbf{j}_{\beta\alpha}{}^S(\mathbf{r}) = \tfrac{1}{2}\sum_k\sum_{m_k t_k}\int e^{2S} \times\{\Phi_\beta^* e\mathbf{v}_k\Phi_\alpha + (e\mathbf{v}_k\Phi_\beta)^*\Phi_\alpha\}\prod_{n\neq k} dx_n\,|_{\mathbf{r}_k=\mathbf{r}}, \quad (25a)$$

plays the role of

$$\mathbf{j}_{\beta\alpha}(\mathbf{r}) = \tfrac{1}{2}\sum_k\sum_{m_k t_k}\int \times\{\Psi_\beta^* e\mathbf{v}_k\Psi_\alpha + (e\mathbf{v}_k\Psi_\beta)^*\Psi_\alpha\}\prod_{n\neq k} dx_n\,|_{\mathbf{r}_k=\mathbf{r}}, \quad (25b)$$

the usual $\beta\alpha$ matrix element of the electric current density of the unperturbed system.[13]

A quite similar situation to that for $\langle H_c'\rangle_{\beta\alpha}$ exists for the expectation value

$$\langle\boldsymbol{\mu}_L\rangle = \frac{e\hbar}{2Mc}(\Psi, \sum_k \mathbf{l}_k\Psi)/(\Psi,\Psi), \quad (26)$$

of the orbital magnetic moment operator of our system of charged particles. Here $\mathbf{l}_k=(1/\hbar)(\mathbf{r}_k\times\mathbf{p}_k)$ is the orbital angular momentum operator of the kth particle. Again, due to the presence of the **p**-operators $\boldsymbol{\mu}_L$ *does not* commute with S. But following exactly the same procedure as before we are able to cast $\langle\boldsymbol{\mu}_L\rangle$ into

$$\langle\boldsymbol{\mu}_L\rangle = \frac{e\hbar}{4Mc}\int e^{2S}\sum_k\{\Phi^*\mathbf{l}_k\Phi + (\mathbf{l}_k\Phi)^*\Phi\} \Big/ \int e^{2S}\Phi^*\Phi, \quad (27)$$

which is, of course, to be compared with

$$\langle\boldsymbol{\mu}_L\rangle = \frac{e\hbar}{4Mc}\int \sum_k\{\Psi^*\mathbf{l}_k\Psi + (\mathbf{l}_k\Psi)^*\Psi\} \Big/ \int \Psi^*\Psi. \quad (28)$$

Other operators of concern to us commute with S: the spin interaction and spin magnetic moment operators, the nuclear β-decay interaction, the Coulomb potential, and the quadrupole moment operator. Their matrix elements,

$$(\Psi_\beta, \mathcal{O}\Psi_\alpha)/(\Psi_\beta,\Psi_\beta)^{\frac{1}{2}}(\Psi_\alpha,\Psi_\alpha)^{\frac{1}{2}}, \quad (29)$$

all revert to the form

$$\int e^{2S}\Phi_\beta^*\,\mathcal{O}\Phi_\alpha \Big/ \left[\left(\int e^{2S}\Phi_\beta^*\Phi_\beta\right)^{\frac{1}{2}}\left(\int e^{2S}\Phi_\alpha^*\Phi_\alpha\right)^{\frac{1}{2}}\right]. \quad (30)$$

The type of qualitative discussion we gave for the energy expectation value (19) may be repeated for each of these quantities. It is noteworthy that in some of the matrix elements, not only are independent particle Φ functions a reasonable choice, but also the e^{2S} factor may perhaps be omitted altogether without serious error. In this connection the expectation value of the ordinary nuclear magnetic moment operator and possibly the nuclear electromagnetic and β-decay transition matrix elements are likely candidates. Thus our method may throw some light on the success of the shell model in predicting these (and other) detailed nuclear properties. However, actual quantitative investigation of these points is required.

We should remark, of course, that since e^S is invariant under reflections and rotations of the coordinate axes and under rotations in isospin space, the parity, angular momentum, and isospin quantum numbers of our total trial function Ψ_γ must be the same as those of the model function Φ_γ.

5. CHOICE OF MODEL FUNCTIONS

In the rest of this paper we shall concentrate on the energies of N-particle fermion and boson systems for which V_A is expressible as a sum of particle-particle interaction potentials,

$$V_A = \sum_{(i,j)} V_{ij}{}^A, \quad (31)$$

with $V_{ij}{}^A$ well-behaved and predominantly attractive. It is further supposed that $V_{ij}{}^A$ is the same for all N; hence we write it as $v_{ij}{}^A$—its value for i, j isolated—

[13] H. A. Kramers, *Quantum Mechanics* (North-Holland Publishing Company, Amsterdam, 1957), first edition, p. 397.

and set

$$V_A=\sum_{(i,j)} v_{ij}{}^A. \tag{32}$$

(This assumption that V_A contains *two-body forces only* is certainly not essential, but it is one which is convenient, and often made in regard to V, the *total* particle-particle interaction sum.)

Unless otherwise noted, the Φ functions we assume are the following:

(1) Fermion systems (total wave function antisymmetric with respect to interchange of any two particles):

$$\Phi=\left(\frac{1}{N!}\right)^{\frac{1}{2}}\sum_{\nu}\theta_\nu\prod_i\varphi_{\nu i}(x_i), \tag{33}$$

where there are N distinct single-particle states $\varphi_{\nu i}(\nu_i=1,\cdots,N;\ i=1,\cdots,N)$, with one particle in each state, and we sum over all permutations

$$\nu=\begin{pmatrix}1\cdots N\\ \nu_1\cdots\nu_N\end{pmatrix}.$$

The quantity θ_ν is $+1$ or -1 according as ν is an even or an odd permutation of $1,\cdots,N$, respectively. For the ground state the φ's are chosen as those corresponding to the N lowest single-particle energies.

(2) Boson systems (total wave function symmetric with respect to interchange of any two particles):

$$\Phi=\left(\frac{g_1!\cdots g_{N'}!}{N!}\right)^{\frac{1}{2}}\sum_{\nu'}\prod_i\varphi_{\nu i}(x_i), \tag{34}$$

where there are N', $1\leq N'\leq N$, distinct single-particle states $\varphi_{\nu i}(\nu_i=1,\cdots,N';\ i=1,\cdots,N)$, with g_i particles in the ith state, and we sum all distinct permutations of $\nu_1\nu_2\cdots\nu_N$. For the ground state, all particles are assigned to the same single-particle state, namely that corresponding to the lowest single-particle energy; we write

$$\Phi_0=\varphi_0(x_1)\cdots\varphi_0(x_N)=\prod_i\varphi_0(x_i). \tag{35}$$

How are the necessary φ's determined?

For N extremely large, the answer is simple: we take for the complete (orthogonal) set of φ's the set of all plane waves satisfying periodic boundary conditions in a large box of volume Ω, the relevant single-particle energies (for choosing the correct φ's to use in a given Φ) being just the free-particle energies. Thus we consider as models perfect (noninteracting) Fermi and Bose gases. One free parameter is left when the corresponding Φ is inserted into $\langle H\rangle$—the particle density $\rho=N/\Omega$, or equivalently, the particle spacing parameter r_0 (radius of the sphere containing one particle); this is to be determined by variation of $\langle H\rangle$.

For N finite, but not small, the problem is much more difficult. The most convenient solution is to adopt a suitable independent-particle model on more or less intuitive grounds (say some species of shell model in the case of nuclei) and then deduce the φ's and their corresponding energy order. The resultant Φ will always contain at least one natural variational parameter. A more systematic prescription—and one whose realization would involve considerable labor, more labor than we would care to expend—is the following: Given a system of fermions, take for the φ's the complete orthogonal set of solutions of the Hartree-Fock type wave equation

$$-\frac{\hbar^2}{2M}\Delta_i\varphi_j(x_i)+\int\Big[\sum_l\sum_{l'}\varphi_l{}^*(x)(l',V_1{}^Al)\varphi_{l'}(x_i)\Big]\times\varphi_j(x)dx=\epsilon_j\varphi_j(x_i), \tag{36}$$

where

$$(l',V_1{}^Al)=\sum_k{}'(l'k,v_{12}{}^Alk)_a,$$

$$\equiv\sum_k{}'\int\int[\varphi_{l'}{}^*(x_1)\varphi_k{}^*(x_2)-\varphi_k{}^*(x_1)\varphi_{l'}{}^*(x_2)]\times v_{12}{}^A\varphi_l(x_1)\varphi_k(x_2)dx_1dx_2, \tag{37}$$

the sum extending over all *occupied* states k, and ϵ_j is the single-particle energy corresponding to the state j. Here we visualize particle i moving in state j through the system under the influence of a nonlocal average potential due to all the other particles. This is just a step in the procedure that might be followed to find the total energy of the system—to be computed from

$$E=\sum_j{}'\epsilon_j-\tfrac{1}{2}\sum_j{}'(j,V_1{}^Aj) \tag{38}$$

—if it were valid to neglect the last term on the left in the transformed Schrödinger equation (derived in Appendix B):

$$-\frac{\hbar^2}{2M}\sum_k\Delta_k\Phi+\sum_{(k,l)}v_{kl}{}^A\Phi-\frac{\hbar^2}{M}\sum_k\nabla_kS\cdot\nabla_k\Phi=E\Phi. \tag{39}$$

But, as we go on to point out in Appendix B, this term should *not* be left out, so (38) is likely to provide a bad approximation to the total energy. This does not mean, though, that the Φ function constructed from (36), (37) is not perfectly adequate for use in $\langle H\rangle$: in fact, since the region of configuration space in which the solution of (39) differs from that of (39) with the ∇_kS terms missing is quite unimportant in our special form of the energy expectation value, we expect such a model function to serve rather well. An analogous scheme may be set up for a system of bosons; in this case symmetrized two-particle matrix elements are involved in the definition of $(l',V_1{}^Al)$, rather than antisymmetrized ones.

For N small it is desirable to use a Φ depending on internal coordinates only—a Φ independent of center-of-mass coordinates. This is especially important for $N=2, 3, 4$. As is well known, a simple exact factoriza-

tion of the center-of-mass motion is possible if harmonic oscillator single-particle wave functions are used.

Note that if the φ's we pick are orthogonal and normalized to unity, so are the Φ functions (33)–(35). We shall henceforth assume *all* model functions have been normalized to one.

For N very small, we are likely to know something more definite about the structure of the (internal) wave function in the absence of repulsive cores, say from previous calculations (this, for example, being true of the triton). If so, we may by-pass the above discussions and proceed instead as follows: Write down a suitable functional form for Φ containing one or more variational parameters and minimize $\langle H\rangle$ (by numerical calculation) with respect to these parameters. Then since we presumably know e^S, this determines a fairly good wave function for the system.

How good is our total wave function (4) if an independent-particle type model function is used? We may easily obtain a qualitative idea from the following considerations.

There are, roughly speaking, three important types of correlation in the systems of interest to us, all of two-particle nature:

(1) the short-range correlations due to the repulsive cores (very effective in nuclei for, say, $|\mathbf{r}_i-\mathbf{r}_j|=r<0.5$ f; i, j any two nucleons, f=fermi=10^{-13} cm),

(2) intermediate-range correlations due to the attractive forces (effective in nuclei for, say, $0.5\text{ f}<r<3$ f), and

(3) longer-range correlations, also due to the attractive forces (not effective in nuclei).

For fermion systems the correlations of class (3) are defined as those corresponding to momentum transfers considerably less than the Fermi momentum. Hence they are forbidden by the exclusion principle except for the most energetic particles. For boson systems there is no such distinction between the second and third categories.

Let us write the *exact* wave function for our system as

$$\Psi_\gamma{}^E=F\Phi_\gamma. \tag{40}$$

Consider first the case $N\to\infty$. Then since Φ_γ is completely uncorrelated, the "model operator" F must properly introduce each of the above types of correlation into the total wave function $\Psi_\gamma{}^E$. Ignoring state dependence of the short-range correlations (as always), our wave function (4), coupled with the connection (15),[14] approximately includes all of (1), plus part of (2). [As seen in (15),[14] in general $V_{ij}{}^R$ is taken to contain, besides the core, a relatively weak attractive component of slightly longer range.] However, the majority of the intermediate and all the longer range correlations are omitted. To visualize these relations, we may set

$$F\cong e^S F', \tag{41}$$

where F' properly introduces the remainder of (2), and (3) if necessary.

The supposition that the effect of correlations (2) and (3) in the true wave function is slight does not seem to be too bad for nuclei, as indicated by the correlation structure results of Brueckner and Gammel,[15] and discussed by Amado.[16] Furthermore, Iwamoto and Yamada[4] achieve saturation in their study of the nuclear matter problem using simply a state-independent core correlation function. So in the nuclear case (4)—with Φ_γ given by (33)—is expected to be a rather good wave function. On the other hand, these longer range correlations are of vital importance in the liquid He^4 problem, because of the Bose statistics and the higher particle density. So in this case (4)—with Φ_γ given by (34)—is expected to be rather crude.

For a finite system the qualitative situation should not change greatly, but some two-particle correlations arising from the $v_{ij}{}^A$ will then be approximately included in the trial Φ_γ (which can no longer be constructed from plane waves).

Finally, even if a simple model function is not completely adequate, calculations with such functions can serve as the first step in a systematic perturbation procedure (as outlined in Appendix C).

6. ENERGY EXPECTATION VALUE FOR FEW-PARTICLE SYSTEMS

We now indicate a technique for the evaluation of $\langle H\rangle$ as given by (19) and (32) which is practical for N small. First write

$$\langle H\rangle=(\mathcal{K}+\mathcal{U})/\mathfrak{N}, \tag{42}$$

$$\mathcal{K}=\frac{\hbar^2}{2M}\int e^{2S}\sum_k \nabla_k\Phi^*\cdot\nabla_k\Phi, \tag{43}$$

$$\mathcal{U}=\int e^{2S}\Phi^*\sum_{(k,l)} v_{kl}{}^A\Phi, \tag{44}$$

$$\mathfrak{N}=\int e^{2S}\Phi^*\Phi. \tag{45}$$

Then note that

$$e^{2S}=\exp(2\sum_{(i,j)}S_{ij})=\prod_{(i,j)}(1+\eta_{ij}), \tag{46}$$

where

$$\eta_{ij}=e^{2S_{ij}}-1, \tag{47}$$

and insert the expanded form of the product,

$$e^{2S}=1+\sum_{(i,j)}\eta_{ij}+\tfrac{1}{2}\sum_{(i,j)\neq(k,l)}\sum\eta_{ij}\eta_{kl}+\tfrac{1}{6}\sum_{(i,j)\neq(k,l)\neq(m,n)\neq(i,j)}\sum\sum\eta_{ij}\eta_{kl}\eta_{mn}+\cdots \tag{48}$$

[14] Or (16), if appropriate.

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

[16] R. D. Amado (to be published).

into $\mathcal{K}$, $\mathcal{U}$, and $\mathfrak{N}$. If the system contains a finite number N of particles, the expansion (48) breaks off after $2^{N(N-1)/2}$ distinct terms, some pairs of which generate identical contributions to one (or more) of the integrals (43)–(45). For a small number of particles, it appears feasible to evaluate all of these (different) contributions.

Observe, incidentally, that in any case, N large or small, η_{ij} may be fitted to a simple analytic form for convenience in integrations.

If we consider $N=3$, there are only eight distinct terms in (48) (see Fig. 1). For a system of three fermions in its ground state, take a model wave function

$$\Phi_0=\phi_0(r_{12},r_{13},r_{23}) \sum_{\nu=\binom{1\ 2\ 3}{\nu_1\ \nu_2\ \nu_3}} \theta_\nu \prod_{i=1}^{3} \chi_{\nu_i}(m_i,t_i), \quad (49)$$

with ϕ_0 symmetric, normalized, and real.[17] Then the results for $\mathcal{K}$, $\mathcal{U}$, and $\mathfrak{N}$ are rather simple:

$$\mathcal{K}=\frac{\hbar^2}{2M}3\int\int\int\{(\nabla_1\phi_0(r_{12},r_{13},r_{23}))^2$$
$$+\eta_{12}[2(\nabla_1\phi_0(r_{12},r_{13},r_{23}))^2+(\nabla_3\phi_0(r_{12},r_{13},r_{23}))^2]$$
$$+\eta_{12}\eta_{13}[(\nabla_1\phi_0(r_{12},r_{13},r_{23}))^2+2(\nabla_2\phi_0(r_{12},r_{13},r_{23}))^2]$$
$$+\eta_{12}\eta_{13}\eta_{23}(\nabla_1\phi_0(r_{12},r_{13},r_{23}))^2\}d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3, \quad (50)$$

$$\mathcal{U}=\int\int\int\{\bar{v}_{12}{}^A+\eta_{12}\bar{v}_{12}{}^A+2\eta_{12}\bar{v}_{13}{}^A+2\eta_{12}\eta_{13}\bar{v}_{12}{}^A$$
$$+\eta_{12}\eta_{13}\bar{v}_{23}{}^A+\eta_{12}\eta_{13}\eta_{23}\bar{v}_{12}{}^A\}$$
$$\times\phi_0{}^2(r_{12},r_{13},r_{23})d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3, \quad (51)$$

$$\mathfrak{N}=1+\int\int\int\{3\eta_{12}+3\eta_{12}\eta_{13}+\eta_{12}\eta_{13}\eta_{23}\}$$
$$\times\phi_0{}^2(r_{12},r_{13},r_{23})d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3. \quad (52)$$

In (51),

$$\bar{v}_{ij}{}^A=\sum_{(k,l)}\sum_{m_it_i}\sum_{m_jt_j}$$
$$\times[\chi_k{}^*(m_i,t_i)\chi_l{}^*(m_j,t_j)-\chi_l{}^*(m_i,t_i)\chi_k{}^*(m_j,t_j)]$$
$$\times v_{ij}{}^A\chi_k(m_i,t_i)\chi_l(m_j,t_j). \quad (53)$$

(Specializing to the triton, with central, charge-independent forces, $\bar{v}_{ij}{}^A=\frac{3}{2}[v_{ij}{}^A(\text{singlet})+v_{ij}{}^A(\text{triplet})]$.) The integrals involved in the relations (50)–(52) may be further reduced, of course, by a proper choice of coordinate system. If for a system of three bosons in its ground state we take $v_{ij}{}^A$ as independent of spin and isospin, and hence just $\Phi_0=\phi_0(r_{12},r_{13},r_{23})$, again with ϕ_0 symmetric, normalized, and real, then the above answers for $\mathcal{K}$, $\mathcal{U}$, and $\mathfrak{N}$ may be used to calculate $\langle H\rangle$ for the system, *provided* $\bar{v}_{ij}{}^A$ is replaced by $v_{ij}{}^A$ in (51).

[17] Such a wave function appears satisfactory for the trition in the absence of core and tensor force. For example, see H. Feshbach and S. I. Rubinow, Phys. Rev. **98**, 188 (1955).

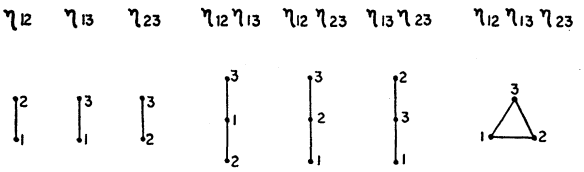

FIG. 1. Terms contributing to the cluster expansion of the correlation function e^{2S} for a system of three particles.

This complete cluster expansion approach should be most useful in studies of very light nuclei. Calculations which include the effect of the tensor force are now in progress for H^3, He^3, and He^4. Numerical results will be reported in a forthcoming paper. Extensions to the p shell may be possible if certain approximations are found to hold in these s-shell problems. In regard to few-boson systems, it is of interest to see whether or not a configuration of a small number of He^4 atoms form a bound system; this question is also under investigation.

7. ENERGY EXPECTATION VALUE FOR MANY-PARTICLE SYSTEMS

When N is large, we cannot hope to treat individually more than a few of the vast number of cluster contributions to $\mathcal{K}$, $\mathcal{U}$, and $\mathfrak{N}$; thus we are forced to seek a convergent cluster development of $\langle H\rangle$ the first few terms of which provide the major part of the answer. The natural expansion parameter is $\xi_S=N\omega_S/\Omega$, where ω_S is the volume associated with the cores, or, more precisely,

$$\omega_S=\int\eta_{ij}d\mathbf{r}_{ij}, \quad \eta_{ij}=e^{2S_{ij}}-1, \quad (54)$$

and Ω is the normalization volume of the system. For nuclear matter,

$$\xi_S\sim(C/r_0)^3\cong\tfrac{1}{10},$$

(using $r_0\cong1.07$ fermis, determined from the Stanford electron scattering experiments, and $C\cong0.5$ fermi), so if the coefficients of all powers of ξ_S were of about the same magnitude, a calculation to first order would suffice.

Such an expansion, in powers of $\xi=N\omega/\Omega$, with $\omega=\int[f^*(r_{ij})f(r_{ij})-1]d\mathbf{r}_{ij}$, has been derived for *general* short range two-particle correlations $f(r_{ij})$ in a thorough investigation of the cluster method for many-particle fermion and boson systems by Iwamoto and Yamada[3] (I-Y). It is worthwhile to see what form the results of I-Y take for our special choice $f(r_{ij})=e^{S_{ij}}$. Consider first the quantities H_i, H_{ij}, H_{ijk} involved in their generalized normalization integral ($i, j, \cdots, q=1, \cdots, N$)

$$I(\beta)=\sum_\nu\theta_\nu\int\prod_i\varphi_{\nu_i}{}^*(x_i)\prod_{(j,k)}f^*(r_{jk})f(r_{jk})e^{\beta H_{jk}(x_j,x_k)}$$
$$\times\prod_{(l,m,n)}e^{\beta H_{lmn}(x_l,x_m,x_n)}\prod_p\varphi_p(x_p)e^{\beta H_p(x_p)}\prod_q dx_q, \quad (55)$$

which are so defined that

$$\langle H\rangle\equiv\frac{(\Psi,H\Psi)}{(\Psi,\Psi)}=\frac{\partial}{\partial\beta}\ln I(\beta)\Big|_{\beta=0}, \tag{56}$$

with $\Psi=[\prod_{(i,j)}f(r_{ij})]\Phi$, Φ being given by (33). [See I-Y Eq. (4).] For these quantities *we* have

$$H_i(x_l)=-\frac{\hbar^2}{2M}\frac{\Delta_l\varphi_i(x_l)}{\varphi_i(x_l)},$$

$$H_{ij}(x_l,x_m;\cdots)=-\frac{\hbar^2}{M}\Big[\frac{[\nabla_l\varphi_i(x_l)\cdot\nabla_l S_{lm}]}{\varphi_i(x_l)}+\frac{[\nabla_m\varphi_j(x_m)\cdot\nabla_m S_{ml}]}{\varphi_j(x_m)}-\sum_k(\nabla_k S_{lk}\cdot\nabla_k S_{km})\Big]+v_{lm}{}^A(x_l,x_m), \tag{57}$$

$$H_{ijk}(x_l,x_m,x_n)=-\frac{\hbar^2}{M}[(\nabla_l S_{ml}\cdot\nabla_l S_{ln})+(\nabla_m S_{nm}\cdot\nabla_m S_{ml})+(\nabla_n S_{ln}\cdot\nabla_n S_{nm})].$$

Since there are terms in the above H_{ij} involving the coordinates of three particles, let us instead define

$$\tilde{H}_i(x_l)=H_i(x_l),$$

$$\tilde{H}_{ij}(x_l,x_m)=-\frac{\hbar^2}{M}\Big[\frac{[\nabla_l\varphi_i(x_l)\cdot\nabla_l S_{lm}]}{\varphi_i(x_l)}+\frac{[\nabla_m\varphi_j(x_m)\cdot\nabla_m S_{ml}]}{\varphi_j(x_m)}\Big]+v_{lm}{}^A(x_l,x_m), \tag{58}$$

$$\tilde{H}_{ijk}(x_l,x_m,x_n)=0.$$

Recalling Eq. (13) from Sec. 3, we see that (56) still holds with H_i replaced by $\tilde{H}_i$, H_{ij} by $\tilde{H}_{ij}$, and H_{ijk} by $\tilde{H}_{ijk}$. Now if we carry through the derivation of a cluster expansion by exactly the same procedure as developed in I-Y, the result is the same as their (30)–(33) except that no Δf and also no $\nabla f\cdot\nabla f$ terms appear. Writing explicitly only the zeroth-order terms in ξ_S (for brevity), our modified expansion reads

$$\langle H\rangle=\langle\sum_i H_i(x_i)\rangle+\langle\sum_{(i,j)}\tilde{H}_{ij}(x_i,x_j)\rangle, \tag{59}$$

$$\langle\sum_i H_i(x_i)\rangle=-\frac{\hbar^2}{2M}\sum_i(i,\Delta_1 i)+\cdots, \tag{60}$$

$$\langle\sum_{(i,j)}\tilde{H}_{ij}(x_i,x_j)\rangle=-\frac{\hbar^2}{2M}\sum_{i,j}(ij,e^{2S_{12}}[\nabla_1 S_{12}\cdot\nabla_1+\nabla_2 S_{12}\cdot\nabla_2]ij)_a+\tfrac{1}{2}\sum_{i,j}(ij,e^{2S_{12}}v_{12}{}^A ij)_a+\cdots, \tag{61}$$

in a notation obvious from (37). For the ground state the φ's corresponding to the N lowest single-particle energies are to be used (as pointed out earlier).

Similar results may be derived for the analogous boson problem. But let us consider only the ground state of the boson system and adopt, for the moment, the trial Φ-function $\Omega^{-N/2}$ of I-Y, for which

$$H_i(x_l)=0,\qquad \tilde{H}_{ij}(x_i,x_m)=v_{lm}{}^A(x_l,x_m). \tag{62}$$

Then, corresponding to their [A4], we find

$$\langle H\rangle=\frac{N^2}{2\Omega^2}\int\int e^{2S_{12}}v_{12}{}^A dx_1dx_2+\frac{N^3}{2\Omega^3}\int\int\int e^{2S_{12}}\eta_{13}\eta_{23}v_{12}{}^A dx_1dx_2dx_3+\cdots \tag{63}$$

with the η's defined as in (54).

Actually, we would like a cluster development of the simplified form (19) of the energy expectation value. Following a program quite similar to that of I-Y, who start instead from the form (9), this can be realized without much trouble—at least for the ground state boson system. Consider the generalized normalization integral

$$I_S(\beta)=\int e^{2S}\Phi^* e^{\beta H'}\Phi. \tag{64}$$

Then clearly

$$I_S(0)=\int e^{2S}\Phi^*\Phi=\mathfrak{N},$$

and

$$\frac{\partial I_S(\beta)}{\partial\beta}\Big|_{\beta=0}=\int e^{2S}\Phi^* H'\Phi,$$

so that

$$\frac{\partial}{\partial\beta}\ln I_S(\beta)\Big|_{\beta=0}=\langle H\rangle, \tag{65}$$

$\langle H\rangle$ being given by (19) and (32), if we choose

$$H'=\frac{\hbar^2}{2M}\frac{\sum_k\nabla_k\Phi^*\cdot\nabla_k\Phi}{\Phi^*\Phi}+\sum_{(i,j)}v_{ij}{}^A. \tag{66}$$

For a boson system in its ground state we take the trial Φ function (35), which is somewhat more general than that of I-Y. Then

$$H'=\sum_i H_i'(x_i)+\sum_{(i,j)}H_{ij}'(x_i,x_j), \tag{67}$$

with

$$H_i'(x_l)=\frac{\hbar^2}{2M}\frac{\nabla_l\varphi_0{}^*(x_l)\cdot\nabla_l\varphi_0(x_l)}{\varphi_0{}^*(x_l)\varphi_0(x_l)},\qquad H_{ij}'(x_l,x_m)=v_{lm}{}^A(x_l,x_m); \tag{68}$$

consequently the generalized normalization integral

takes the separated form

$$I_S(\beta)=\int \prod_i \varphi_0(x_i) \prod_{(j,k)} e^{2S_{jk}} e^{\beta H_{jk}(x_j,x_k)} \prod_l \varphi_0(x_l) e^{\beta H_l(x_l)} \prod_m dx_m. \tag{69}$$

If we now apply the cluster expansion techniques of I-Y, this $I_S(\beta)$ generates the following formula for the energy expectation value:

$$\begin{aligned}\langle H\rangle = N\frac{\hbar^2}{2M}\int |\nabla_1\varphi_0(x_1)|^2 dx_1 + \frac{N^2}{2}\int\int e^{2S_{12}}\varphi_0^*(x_1)\varphi_0^*(x_2)v_{12}{}^A\varphi_0(x_1)\varphi_0(x_2)dx_1dx_2 \\ + N^2\frac{\hbar^2}{2M}\int\int \eta_{12}|\nabla_1\varphi_0(x_1)|^2|\varphi_0(x_2)|^2 dx_1dx_2 - N^3\left(\int\int \eta_{12}|\varphi_0(x_1)|^2|\varphi_0(x_2)|^2 dx_1dx_2\right) \\ \times\left(\int\int e^{2S_{12}}\varphi_0^*(x_1)\varphi_0^*(x_2)v_{12}{}^A\varphi_0(x_1)\varphi_0(x_2)dx_1dx_2 + \frac{\hbar^2}{M}\int\int \eta_{12}|\nabla_1\varphi_0(x_1)|^2|\varphi_0(x_2)|^2 dx_1dx_2\right) \\ + N^3\int\int\int e^{2S_{12}}(1+\tfrac{1}{2}\eta_{13})\eta_{23}\varphi_0^*(x_1)\varphi_0^*(x_2)v_{12}{}^A\varphi_0(x_1)\varphi_0(x_2)|\varphi_0(x_3)|^2 dx_1dx_2dx_3+\cdots.\end{aligned} \tag{70}$$

This expression has the great advantage that S_{ij} only appears in the form $e^{2S_{ij}}$—there are no Laplacians or gradients of S_{ij} in the expansion.

The procedure just outlined does not go through in a straightforward way for fermion systems because of the antisymmetry of Φ. However, an expansion of the energy expectation value having the desired form—devoid of S_{ij} except in $e^{2S_{ij}}$ and η_{ij} factors—can be derived from the modified I-Y result [of which the zeroth-order terms are given in (60), (61)] by a series of integration by parts relations

$$\begin{aligned}
&(ij,e^{2S_{12}}\Delta_1 ij)_a = -2(ij,e^{2S_{12}}\nabla_1 S_{12}\cdot\nabla_1 ij)_a - (\nabla_1 ij,e^{2S_{12}}\cdot\nabla_1 ij)_a,\\
&(ijk,e^{2S_{12}}\eta_{23}\Delta_1 ijk)_a = -2(ijk,e^{2S_{12}}\eta_{23}\nabla_1 S_{12}\cdot\nabla_1 ijk)_a - (\nabla_1 ijk,e^{2S_{12}}\eta_{23}\cdot\nabla_1 ijk)_a,\\
&(ijk,e^{2S_{12}}\eta_{23}\Delta_2 ijk)_a = -2(ijk,e^{2S_{12}}\eta_{23}\nabla_2 S_{12}\cdot\nabla_2 ijk)_a - 2(ijk,e^{2S_{12}+2S_{23}}\nabla_2 S_{23}\cdot\nabla_2 ijk)_a - (\nabla_2 ijk,e^{2S_{12}}\eta_{23}\cdot\nabla_2 ijk)_a,\\
&(ijk,e^{2S_{12}+2S_{23}}\Delta_2 ijk)_a = -2(ijk,e^{2S_{12}+2S_{23}}(\nabla_2 S_{12}+\nabla_2 S_{23})\cdot\nabla_2 ijk)_a - (\nabla_2 ijk,e^{2S_{12}+2S_{23}}\cdot\nabla_2 ijk)_a,\\
&(ijk,e^{2S_{12}}\eta_{13}\eta_{23}\Delta_1 ijk)_a = -2(ijk,e^{2S_{12}}\eta_{13}\eta_{23}\nabla_1 S_{12}\cdot\nabla_1 ijk)_a - 2(ijk,e^{2S_{12}+2S_{13}}\eta_{23}\nabla_1 S_{13}\cdot\nabla_1 ijk)_a\\
&\qquad\qquad - (\nabla_1 ijk,e^{2S_{12}}\eta_{13}\eta_{23}\cdot\nabla_1 ijk)_a,\\
&(ijk,e^{2S_{12}+2S_{13}}\eta_{23}\Delta_1 ijk)_a = -2(ijk,e^{2S_{12}+2S_{13}}\eta_{23}(\nabla_1 S_{12}+\nabla_1 S_{13})\cdot\nabla_1 ijk)_a - (\nabla_1 ijk,e^{2S_{12}+2S_{13}}\eta_{23}\nabla_1 ijk)_a,\\
&(ijkl,e^{2S_{12}}\eta_{34}\Delta_1 ijkl)_{a'} = -2(ijkl,e^{2S_{12}}\eta_{34}\nabla_1 S_{12}\cdot\nabla_1 ijkl)_{a'} - (\nabla_1 ijkl,e^{2S_{12}}\eta_{34}\cdot\nabla_1 ijkl)_{a'},\\
&\qquad\cdots
\end{aligned} \tag{71}$$

which allow us to transform away all terms linear in $\nabla_i S_{ij}$. [Here we adopt the shorthand notation

$$\begin{aligned}
(\nabla_1 ij,e^{2S_{12}}\cdot\nabla_1 ij)_a &= \int\int \{\nabla_1[\varphi_i^*(x_1)\varphi_j^*(x_2)-\varphi_j^*(x_1)\varphi_i^*(x_2)]\}e^{2S_{12}}\cdot\nabla_1\varphi_i(x_1)\varphi_j(x_2)dx_1dx_2,\\
(ijk,e^{2S_{12}}\eta_{23}\Delta_1 ijk)_a &= \int\int\int \sum_{\nu=\binom{i\ j\ k}{\nu_1\ \nu_2\ \nu_3}} \prod_{n=1}^{3}\varphi_{\nu_n}^*(x_n)e^{2S_{12}}\eta_{23}\Delta_1\varphi_i(x_1)\varphi_j(x_2)\varphi_k(x_3)dx_1dx_2dx_3,
\end{aligned} \tag{72}$$

etc., a generalization of that of (37).] The prime of the last relation in (71) has the same meaning as in (32) of I-Y. The connections given above are sufficient, in particular, for the revision of all the zeroth- and first-order terms in our expansion (59). [This may be seen for the first-order terms by referring to I-Y, Eq. (32).] In each case the first term on the right side is the one we are setting out to eliminate; the leftover terms on the right side linear in $\nabla_i S_{ij}$, if any, are either dealt with by a trivial extension of some prior relation or treated explicitly in a following one. The free sums [see I-Y, (31), (32)] over the state indices are an essential ingredient in the removal of some of the terms—for example, note the fourth and sixth relations. The transformed expansion has much to offer from the calculational standpoint. It would be interesting to work out the nuclear matter problem again, on the basis of this expansion, for more realistic forces than those used by Iwamoto and Yamada.

APPENDIX A. ESTIMATE OF THE THREE-BODY INTERACTION TERM OF EQUATION (15)

Write

$$X_{12}\equiv\sum_k(\nabla_k S_{1k}\cdot\nabla_k S_{k2})=\sum_k(\nabla_1 S_{1k}\cdot\nabla_2 S_{2k}),\quad\text{(A1)}$$

and replace the summation over the instantaneous positions of the k particles by a weighted average over their positions:

$$X_{12}\to\frac{N}{\Omega}\int e^{2(S_{13}+S_{23})}(\nabla_1 S_{13}\cdot\nabla_2 S_{23})d\mathbf{r}_3\equiv\bar{X}_{12}.\quad\text{(A2)}$$

Then we have ($\eta_{ij}=e^{2S_{ij}}-1$, $i,j=1,\cdots,N$)

$$\begin{aligned}\bar{X}_{12}&=\frac{N}{4\Omega}\int(\nabla_1 e^{2S_{13}}\cdot\nabla_2 e^{2S_{23}})d\mathbf{r}_3\\&=\frac{N}{4\Omega}\int(\nabla_1\eta_{13}\cdot\nabla_2\eta_{23})d\mathbf{r}_3\\&=\nabla_1\cdot\left[\nabla_2\frac{N}{4\Omega}\int\eta_{13}\eta_{23}d\mathbf{r}_3\right]\\&=-\left[\Delta_1\frac{N}{4\Omega}\int\eta_{13}\eta_{23}d\mathbf{r}_3\right]\end{aligned}\quad\text{(A3)}$$

for the effective two-particle interaction generated by the three-body forces.

But go back a step and note

$$\begin{aligned}\bar{X}_{12}&=-\left[\nabla_1\cdot\frac{N}{4\Omega}\int(\nabla_1\eta_{13})\eta_{23}d\mathbf{r}_3\right]\\&=-\left[\nabla_1\cdot\frac{N}{2\Omega}\int(\nabla_1 S_{13})e^{2S_{13}}\eta_{23}d\mathbf{r}_3\right]\\&=-\frac{N\omega_S}{\Omega}\int e^{2S_{13}}[(\nabla_1 S_{13})^2+\tfrac{1}{2}(\Delta_1 S_{13})]\eta_{23}d\mathbf{r}_3\Big/\omega_S\end{aligned}\quad\text{(A4)}$$

where

$$\omega_S=\int\eta_{ij}d\mathbf{r}_{ij}.\quad\text{(A5)}$$

Now if we replace $\eta_{23}/\int\eta_{23}d\mathbf{r}_3$ in the second factor by a Dirac delta function, there results

$$\bar{X}_{12}\sim-\frac{N\omega_S}{\Omega}e^{2S_{12}}[(\nabla_1 S_{12})^2+\tfrac{1}{2}(\Delta_1 S_{12})].\quad\text{(A6)}$$

This replacement is rather crude if $r_{12}<C$, but fairly good for $r_{12}>C$ [see (18)]. At any rate we see that $|\bar{X}_{12}|$ is smaller than the two-particle interaction $(\nabla_1 S_{12})^2$ by a factor of order $(N\omega_S/\Omega)e^{2S_{12}}$. For the nuclear matter problem, $N\omega_S/\Omega\sim\frac{1}{10}$, so

$$|\bar{X}_{12}|/(\nabla_1 S_{12})^2\sim\tfrac{1}{10}e^{2S_{12}},$$

which is certainly negligible when the nucleons are close ($r_{12}<C$) and small when they are not ($r_{12}>C$).

It looks plausible that the correlations and energy shift generated by $\mathcal{H}_{12}-\bar{X}_{12}$ may be ignored.

APPENDIX B. USEFULNESS OF THE TRANSFORMED SCHRÖDINGER EQUATION

Suppose we write the Schrödinger equation for our N-particle system as

$$-\frac{\hbar^2}{2M}\sum_k\Delta_k\Psi+(V_A+V_R)\Psi=E\Psi,\quad\text{(B1)}$$

with

$$V_R=\frac{\hbar^2}{2M}\sum_k[(\nabla_k S)^2+(\Delta_k S)],\quad\text{(6)}$$

and set

$$\Psi=e^S\Phi,\quad\text{(B2)}$$

S a function only of the $\mathbf{r}_k(k=1,\cdots,N)$. Then since

$$\Delta_k\Psi=[(\nabla_k S)^2\Phi+(\Delta_k S)\Phi+2(\nabla_k S\cdot\nabla_k\Phi)+(\Delta_k\Phi)]e^S,$$

the differential equation to be satisfied by Φ is

$$-\frac{\hbar^2}{2M}\sum_k\Delta_k\Phi+V_A\Phi-\frac{\hbar^2}{M}\sum_k\nabla_k S\cdot\nabla_k\Phi=E\Phi.\quad\text{(B3)}$$

Specializing to the deuteron, we have $V_A=v_{12}^A$ and

$$-\frac{\hbar^2}{2M}(\Delta_1+\Delta_2)\Phi(x_1,x_2)+v_{12}^A\Phi(x_1,x_2)-\frac{\hbar^2}{M}(\nabla_1 S\cdot\nabla_1+\nabla_2 S\cdot\nabla_2)\Phi(x_1,x_2)=E\Phi(x_1,x_2).$$

Let $S(=S_{12})=S(r)$, $r=|\mathbf{r}_1-\mathbf{r}_2|$, and choose a central $v_{12}^A=v^A(r)$. Then, separating out the motion of the center of mass, and appealing to the fact that the central deuteron is in a ^3S state, we are left with the wave equation

$$-\frac{\hbar^2}{M}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\phi(r)+v_3^A(r)\phi(r)-2\frac{\hbar^2}{M}\frac{dS}{dr}\frac{d\phi(r)}{dr}=\epsilon\phi(r)$$

for the relative motion, where v_3^A is the ^3S component of v^A, and $-\epsilon$ is to be identified with the binding energy of the system. As usual, write $\phi(r)=u(r)/r$; the resulting differential equation for u is

$$-\frac{\hbar^2}{M}\frac{d^2u}{dr^2}+v_3^A u-\frac{2\hbar^2}{M}\frac{dS}{dr}\left(\frac{du}{dr}-\frac{u}{r}\right)=\epsilon u.\quad\text{(B4)}$$

Note, in particular, the net replacement

$$(\nabla_1 S\cdot\nabla_1+\nabla_2 S\cdot\nabla_2)\Phi(x_1,x_2)\to 2\frac{dS}{dr}\frac{1}{r}\left(\frac{du}{dr}-\frac{u}{r}\right).$$

Now it has been found for some simple forms of S

and $v_3{}^A$ that the criterion

$$\int_0^\infty u_0 \frac{2\hbar^2}{M}\frac{dS}{dr}\left(\frac{du_0}{dr}-\frac{u_0}{r}\right)dr \ll \int_0^\infty u_0{}^2 v_3{}^A dr, \quad \text{(B5)}$$

where u_0 (taken real) is the solution of (B4) with the last term on the left absent, is not met, the two integrals being in fact about the same size for the empirical core radius ($\sim$0.5 fermi), and "correct" range and strength of $v_3{}^A$ (adjusted to fit the low energy scattering data and the deuteron binding energy). This indicates that we cannot ignore the non-Hermitian terms in (B3), that they are instead quite appreciable. Thus—for nuclear problems, at least—it would appear there is little recourse but to follow a variational approach.

APPENDIX C. A PERTURBATION METHOD FOR SYSTEMS WITH STRONG SHORT-RANGE REPULSIONS

First we select an orthonormal set of functions $\Phi_1, \Phi_2, \cdots, \Phi_m, \cdots$ and define the Hermitian matrix elements

$$\mathcal{H}_{mn}=\int e^{2S}\left\{\frac{\hbar^2}{2M}\sum_k \nabla_k\Phi_m{}^*\cdot\nabla_k\Phi_n+\Phi_m{}^* V_A \Phi_n\right\}, \quad \text{(C1)}$$

$$\mathfrak{N}_{mn}=\int e^{2S}\Phi_m{}^*\Phi_n. \quad \text{(C2)}$$

Then the model function

$$\Phi=\sum_m c_m\Phi_m, \quad \text{(C3)}$$

introduced into (8) with $\Phi_\beta=\Phi_\alpha=\Phi$, yields ($\langle H\rangle \to E$)

$$E=\sum c_m{}^* c_n \mathcal{H}_{mn}/\sum c_p{}^* c_q \mathfrak{N}_{pq}, \quad \text{(C4)}$$

so that the extremum conditions $\partial E/\partial c_m=0$ ($m=1, 2, \cdots$) require

$$\sum_n c_n[\mathcal{H}_{mn}-E\mathfrak{N}_{mn}]=0. \quad \text{(C5)}$$

These equations provide the possibility of computing the energy eigenvalue E, and the expansion coefficients c_m, to an arbitrary degree of accuracy. For example, if

$$\begin{aligned} &\frac{\mathcal{H}_{11}}{\mathfrak{N}_{11}} < \frac{\mathcal{H}_{mm}}{\mathfrak{N}_{mm}}, \quad m\neq 1, \\ &\left|\mathcal{H}_{1m}-\mathcal{H}_{11}\frac{\mathfrak{N}_{1m}}{\mathfrak{N}_{11}}\right| \ll \left|\frac{\mathcal{H}_{11}}{\mathfrak{N}_{11}}-\frac{\mathcal{H}_{mm}}{\mathfrak{N}_{mm}}\right|, \quad m\neq 1, \end{aligned} \quad \text{(C6)}$$

we find easily

$$E=\frac{\mathcal{H}_{11}}{\mathfrak{N}_{11}}+\sum_{m=2}^{\infty}\left|\mathcal{H}_{1m}-\mathcal{H}_{11}\frac{\mathfrak{N}_{1m}}{\mathfrak{N}_{11}}\right|^2 \Bigg/ \left[\mathfrak{N}_{11}\mathfrak{N}_{mm}\left(\frac{\mathcal{H}_{11}}{\mathfrak{N}_{11}}-\frac{\mathcal{H}_{mm}}{\mathfrak{N}_{mm}}\right)\right]. \quad \text{(C7)}$$

The complete formal series for the energy and expansion coefficients will be presented in a later paper, together with a discussion and evaluation of the correction term of (C7). (For this evaluation a cluster development must again be employed. In the many-particle case some slight generalizations of the I-Y technique will be necessary.)

The extensive calculations of configuration interaction corrections to the shell-model energy spectrum and other shell-model properties involve matrix elements like $\mathcal{H}_{mn}$ and $\mathfrak{N}_{mn}$ except for the presence of the correlation factor e^S. It is not likely that this factor can *always* be replaced by unity without occasionally incurring serious error.