General Method for Handling the Hard Core with Shell-Model Wave Functions

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The left-unitary operators that introduce the correlations of the hard core in an uncorrelated bound-state wave function of a finite number A of particles are explicitly determined up to a unitary transformation. Left unitarity is required in order to keep orthonormality. Using a shell-model basis, transformed according to the correlation operator, it is possible to diagonalize the Hamiltonian in a subspace of the full Hilbert space with the technique of Bloch and Horowitz. Ground as well as excited states are treated on the same footing. In practice, the diagonalization is accomplished using the original single-particle basis and transforming back the Hamiltonian. This results in an A-body operator for which a cluster expansion is possible. In this cluster expansion, there are three- and four-body terms easy to evaluate, because they factorize. A particularly interesting application can be made to few-body systems, evaluating the integrals numerically. The unique approximation is then connected with the cut of the basis. The method developed seems comparatively simple and is free of the mathematical problems of the hard core.

1. INTRODUCTION

We shall consider the time-independent Schrödinger equation for a finite system of particles mutually interacting by a two-body potential having an infinite core. It is a partial differential equation that holds for particle separation distances greater than the core radius, with the condition that the wave functions vanish on the surface of the cores. With standard symbols we can write for a system of A particles

$$\{\sum_{i}^{A}{}_{1} \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j}^{A}{}_{1} V_{ij} - E\}\Psi = 0, \tag{1.1}$$

for $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| > c$, where c is the core radius,

$$\Psi = 0 \quad \text{for} \quad r_{ij} = c. \tag{1.2}$$

Inside the cores the wave function is defined by

$$\Psi = 0 \quad \text{for} \quad r_{ij} < c. \tag{1.3}$$

For more than two particles, the problem cannot be solved exactly, and perturbation theory must be used. This cannot be done in the standard way, as matrix elements of single-particle wave functions with hard cores are meaningless.

Two approaches have been attempted so far in order to handle the problem: (i) the well-known Brueckner-Goldstone theory,[1] (ii) the method of the correlation operators.[2]

Correlation operators are left-unitary operators that introduce the correlations (1.2) and (1.3) in an uncorrelated basis. Left-unitarity is needed in order to keep orthonormality. To perform calculations, in absence of an explicit form for the correlation operators, the authors cited make assumptions and approximations leading to the method (i). One of such assumptions is that the correlation operators can be written as e^{iS}, and S can be approximated by a sum of two-body terms.

As far as point (i) is concerned, the situation is that there is no mathematical proof of convergence, and that the present results are ambiguous. On this subject we have already made some observations[3] that we hope to extend in a subsequent paper.

Method (ii), on the other hand, since no correlation operator is known, is at the stage of a variational approach, where the approximated correlation operators serve to introduce a trial wave function starting from an uncorrelated wave function.

Neither of the methods goes practically further than the study of two-body correlations. The importance of three- or more-body terms is very difficult to evaluate in (i) and impossible in (ii).

In this paper, we exactly determine the left-unitary correlation operators for bound systems of a finite number of particles. They differ from one another by an arbitrary unitary transformation. In Sec. 2 we shall consider the case of two particles in order to introduce the method, while in Secs. 3 and 4 we shall consider the most general case.

In order to perform calculations it is convenient to use an uncorrelated basis and transform back the Hamiltonian. This will be made in Secs. 5 and 6. Using the techniques of Bloch and Horowitz,[4] it is pos-

[1] For an extensive review on this subject see B. H. Brandow, Rev. Mod. Phys. **39**, 771 (1967).

[2] T. Tagami, Progr. Theoret. Phys. (Kyoto) **21**, 533 (1959); N. Austern and P. Iano, Nucl. Phys. **18**, 672 (1960); P. H. Wackman and N. Austern, *ibid.* **30**, 529 (1962); F. Villars, in *Proceedings of the International School of Physics "Enrico Fermi", Course XXIII*, edited by V. F. Weisskopf (Academic Press Inc., New York, 1963); J. S. Bell, in *Lectures on the Many-Body Problem, Bergen, 1961*, edited by C. Fronsdal (W. A. Benjamin, Inc., New York, 1962); J. Da Providencia and C. M. Shakin, Ann. Phys. (N.Y.) **30**, 95 (1964); C. M. Shakin, J. P. Svenne, and Y. R. Waghmare, Phys. Letters **21**, 209 (1966); D. M. Brink and M. E. Grypeos, Nucl. Phys. **A97**, 81 (1967); C. M. Shakin, Y. R. Waghmare, M. Tomaselli, and M. H. Hull, Jr., Phys. Rev. **161**, 1015 (1967).

[3] C. Natoli and F. Palumbo (to be published).

[4] C. Bloch and J. Horowitz, Nucl. Phys. **8**, 91 (1958). Better for our purpose is the version of M. Macfarlane in Proceedings of the International School of Physics "Enrico Fermi," Course XL.

sible to diagonalize the transformed Hamiltonian in a finite subspace of the full Hilbert space using shell-model wave functions as a basis.

The transformed Hamiltonian is an A-body operator, because of the appearance of a collective variable, and this is true separately for the transformed kinetic energy and the transformed two-doby potentials. This gives the possibility of a numerical investigation about the rate of convergence of a cluster expansion, as the many-body terms are explicitly determined. To zeroth order in the cluster expansion, the transformed potentials involve only two-body terms (and this holds to all orders for a potential of zero range outside the core), but the transformed kinetic energy involves two-, three-, and four-body terms.[5] These are easy to evaluate because they factorize. Now, for sufficiently dilute systems the cluster expansion will converge rapidly, but we are afraid that with the nuclear parameters the convergence is slow.[6] If so, the crucial point is: How good is the zeroth-order approximation? In fact, the method is of practical use in the measure in which the zeroth-order approximation is good. The answer requires a numerical investigation. In any case, the method is free of the mathematical problems peculiar to the hard core, is comparatively simple, allows a check of the rate of convergence of the cluster expansion, and ought to improve the approximation obtained in this field with the inclusion of the factorizable three- and four-body terms. Moreover, calculations on the few-body problem can be performed to any degree of accuracy by making numerical integrations.

We emphasize that because of the left unitarity the method allows us to treat on the same footing the ground state as well as the excited ones and is particularly suitable for calculating moments and transition amplitudes very sensitive to the hard-core region.

We shall be concerned only with the bound-state problem, and shall use bound-state single-particle wave functions for the many-particle basis. The separation of the c.m. motion from the internal motion can be obtained with a method previously developed.[7]

2. TWO-BODY CASE

Let us introduce the uncorrelated basis $\Phi_n(\mathbf{r}_1, \mathbf{r}_2)$. We shall sometimes use the c.m. position vector $\mathbf{R}$ and the polar coordinates ρ, ω for the relative position vector $\mathbf{r}_{12}$. The momentum canonically conjugate[8] to ρ is (putting $\hbar=1$) $p_\rho=-i(\partial/\partial\rho+1/\rho)$. When using the variables ρ, ω, $\mathbf{R}$ we shall write $\varphi_n(\rho, \omega, \mathbf{R})$ for $\Phi_n(\mathbf{r}_1, \mathbf{r}_2)$.

Let us define the operator

$$\mathfrak{N}=\exp(-icp_\rho)\theta(\rho), \qquad \theta(\rho)=1, \quad \rho>0 \qquad =0, \quad \rho<0 \tag{2.1}$$

and set

$$\lambda_n=\mathfrak{N}\varphi_n. \tag{2.2}$$

Theorem I: If the basis Φ_n is such that for $\rho\to 0$, $\Phi_n\sim\rho^\alpha$, $\alpha>-1$ (a condition generally satisfied), then the two-particle wave-functions λ_n satisfy (1.2) and (1.3), and are orthonormal if the Φ_n are; i.e., $\mathfrak{N}$ is a correlation operator. Proof: First of all we show that $\mathfrak{N}$ has the left inverse $\mathfrak{N}^\dagger$. For

$$\mathfrak{N}^\dagger\mathfrak{N}=\theta(\rho)\,\exp(icp_\rho)\,\exp(-icp_\rho)\theta(\rho)=[\theta(\rho)]^2=1. \tag{2.3}$$

This enables us to write

$$\lambda_n=\mathfrak{N}\varphi_n=\exp(-icp_\rho)\theta\varphi_n\exp(icp_\rho)\,\exp(-icp_\rho)1.$$

With a simple series expansion, we derive

$$\exp(\pm icp_\rho)\rho\,\exp(\mp icp_\rho)=\rho\pm c, \qquad \exp(\pm icp_\rho)1=(\rho\pm c)/\rho, \tag{2.4}$$

so that Eq. (2.2) becomes

$$\lambda_n=[(\rho-c)/\rho]\theta(\rho-c)\varphi_n(\rho-c, \omega, \mathbf{R}). \tag{2.5}$$

This satisfies (1.3) and (1.2) by virtue of the assumption $\varphi_n\sim(\rho-c)^\alpha$, $\alpha>-1$ for $(\rho-c)\to 0$. To complete the proof we must show that the λ_n are orthonormal if the φ_n are. For

$$\langle\lambda_n\,|\,\lambda_m\rangle=\int d\mathbf{R}\int d\omega\int_0^\infty d\rho\rho^2\left(\frac{\rho-c}{\rho}\right)^2\theta(\rho-c) \times\varphi_n^*(\rho-c, \omega, \mathbf{R})\varphi_m(\rho-c, \omega, \mathbf{R}),$$

from which, putting $\rho-c=x$, and taking into account the fact that $\varphi\to 0$ for $x\to\infty$, one gets

$$\int d\mathbf{R}\int d\omega\int_0^\infty dx\,x^2\varphi_n^*(x, \omega, \mathbf{R})\varphi_m(x, \omega, \mathbf{R}) =\langle\varphi_n\,|\,\varphi_m\rangle, \quad \text{QED.}$$

By passing, we note that $\mathfrak{N}^\dagger$ is not the right inverse of $\mathfrak{N}$. For

$$\mathfrak{N}\mathfrak{N}^\dagger=\exp(-icp_\rho)\theta(\rho)\theta(\rho)\,\exp(icp_\rho)=\theta(\rho-c)\neq 1. \tag{2.6}$$

Thus $\mathfrak{N}$ is not unitary. This is obvious, as $\mathfrak{N}$ changes the physical properties of the wave functions.

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[5] It may appear to be nonsense for the zeroth order to involve three- and four-body terms, but it is not so. For, clustering is not synonymous with the occurrence of many-body terms, but with close spatial correlation among many bodies; thus it must be represented by an operator *not factorizable* in single- or two-body operators.

[6] This is shown, for example, by T. Stovall and D. Vinciguerra [Lettere al Nuovo Cimento 1, 100 (1969)], who find that 5 correlated pairs are also important in ^{4}He for reproducing the experimental electromagnetic form factor.

[7] F. Palumbo, Nucl. Phys. **A99**, 100 (1967).

[8] *Principles of Quantum Mechanics*, edited by P. A. M. Dirac (Oxford University Press, Oxford, 1947).

If the Φ_n are a complete system in the Hilbert space of bound-state wave functions, the λ_n are a complete system for bound-state wave functions satisfying (1.2) and (1.3).

So holds *Theorem II*: Any correlation operator $\mathfrak{N}'$ differs from $\mathfrak{N}$ by a unitary transformation. Proof: We shall use the fact that $\mathfrak{N}\mathfrak{N}^\dagger$ is the unity for wave functions satisfying (1.2) and (1.3), and that any operator $\mathfrak{N}'$ must satisfy (2.6), if it has to give a complete set for wave functions satisfying (1.2) and (1.3). Then putting $\lambda_n'=\mathfrak{N}'\varphi_n$,
we have

$$\mathfrak{N}\mathfrak{N}^\dagger\lambda_n'=\mathfrak{N}\mathfrak{N}^\dagger\mathfrak{N}'\varphi_n=\mathfrak{N}'\varphi_n,$$

from which

$$\mathfrak{N}'=\mathfrak{N}(\mathfrak{N}^\dagger\mathfrak{N}')=\mathfrak{N}\mathfrak{U},$$

where $\mathfrak{U}=\mathfrak{N}^\dagger\mathfrak{N}$ is unitary, as is very easy to verify.

3. MANY-BODY CASE

We shall make some preliminary considerations that will enable us to generalize the procedure of Sec. 2. This will be made in two steps. In this section, we shall construct for the general case an operator $\mathfrak{N}$ analogous to (2.1), but violating translational invariance. That invariance will be restored in Sec. 4.

The configuration space for A particles, S_{3A}, has $3A$ dimensions. Now

$$r_{ij}=c, \quad \text{in} \quad S_{3A}$$

is the equation of a $3(A-1)$-times degenerate quadric that is a rectangular cylinder. Its intersection with the space $S_{3(A-1)}$, defined by

$$\mathbf{r}_k=0, \qquad k\neq i, j, \qquad \mathbf{r}_i+\mathbf{r}_j=0,$$

is a sphere of radius c, i.e., a closed surface. Then, any cylinder separates S_{3A} in internal and external connected regions that are complementary. For A particles we have $\frac{1}{2}A(A-1)$ of such cylinders, that intersect with each other. There are points external to one of them that are internal to another one. The boundary conditions (1.2), holding separately on the surface of any cylinder, must also hold on the surface separating the points internal to at least one of them from the points external to all of them. The interior and the exterior of this surface will be referred to as regions I and II, respectively. These two regions are connected and complementary.

We want now to write down the equation of the boundary of region I. We shall use the generalized polar coordinates[9] $r=(\mathbf{r}_1^2+\cdots\mathbf{r}_A^2)^{1/2}$, and ω which synthetically represents all the angular variables. We do not need the explicit relation of polar to Cartesian coordinates, as we shall only use the relations

$$\mathbf{r}_i=r\boldsymbol{\alpha}_i(\omega), \tag{3.1}$$

$$\mathbf{r}_{ij}=r\boldsymbol{\alpha}_{ij}(\omega), \qquad \boldsymbol{\alpha}_{ij}=\boldsymbol{\alpha}_i-\boldsymbol{\alpha}_j, \tag{3.2}$$

$$r_{ij}=r\alpha_{ij}(\omega), \qquad \alpha_{ij}=|\boldsymbol{\alpha}_i-\boldsymbol{\alpha}_j|. \tag{3.3}$$

As the points of region I belong to at least one cylinder, fixed ω, their polar radius must satisfy at least one of the relations

$$r_{ij}=r\alpha_{ij}(\omega)\leq c, \qquad i<j=1, \cdots, A. \tag{3.4}$$

Fixed ω, the maximum value of r satisfying (3.4), is the polar radius of a point belonging to the boundary of region I. This maximum value is obtained for the minimum of the $\alpha_{ij}(\omega)$ at fixed ω, so that the equation of the boundary is

$$r=c/\min\{\alpha_{ij}(\omega)\}=\sigma(\omega), \tag{3.5}$$

which defines $\sigma(\omega)$.

Equation (1.1) must be solved in region II with the boundary condition

$$\Psi=0 \quad \text{for} \quad r=\sigma(\omega). \tag{3.6}$$

In region I, the wave function is defined by

$$\Psi=0 \quad \text{for} \quad r<\sigma(\omega). \tag{3.7}$$

We can generalize the procedure of Sec. 2, region I now playing the role of the sphere $\rho\leq c$. To this end, let us define the momentum canonically conjugate to r

$$p_r=-i[(\partial/\partial r)+(3A-1)/2r^{-1}]. \tag{3.8}$$

As above, we shall define the operator

$$\mathfrak{N}=\exp[-i\sigma(\omega)p_r]\theta(r), \tag{3.9}$$

and the wave functions

$$\chi_n=\mathfrak{N}\varphi_n.$$

Theorem III: If the basis Φ_n is such that for $r_{ij}\to 0$, $\Phi_n\sim r_{ij}^{\alpha}$, $\alpha>-1$ (a condition generally satisfied), the many-particle wave functions χ_n satisfy (3.6) and (3.7), and are orthonormal if the Φ_n are, i.e., $\mathfrak{N}$ is a correlation operator. The proof is as in theorem I. First, we show that $\mathfrak{N}$ has the left inverse $\mathfrak{N}^\dagger$

$$\mathfrak{N}^\dagger\mathfrak{N}=\theta(r)\,\exp[i\sigma(\omega)p_r]\exp[-i\sigma(\omega)p_r]\theta(r)=1.$$

As for theorem I we derive, writing $\varphi_n(r,\omega)$ for $\Phi_n(\mathbf{r}_1, \cdots, \mathbf{r}_A)$

$$\chi_n=\mathfrak{N}\varphi_n=\exp[-i\sigma(\omega)p_r]\theta(r)\varphi_n\exp[i\sigma(\omega)p_r]\times\exp[-i\sigma(\omega)p_r]1. \tag{3.10}$$

A simple series expansion gives

$$\exp[\pm i\sigma(\omega)p_r]r_{ij}\exp[\mp i\sigma(\omega)p_r]=r_{ij}\pm\sigma(\omega)\alpha_{ij},$$

$$\exp[\pm i\sigma(\omega)p_r]1=\{[r\pm\sigma(\omega)]/r\}^{(3A-1)/2}, \tag{3.11}$$

[9] *Fonctions Hypergéométriques et Hypersphériques—Polynomes d'Hermite*, edited by P. Appell and J. Kampé de Fériet (Gauthier-Villars et Cie, Paris, 1926).

so that Eq. (3.10) leads to

$$\chi_n=\{[r-\sigma(\omega)]/r\}^{(3A-1)/2}\theta[r-\sigma(\omega)]\varphi_n[r-\sigma(\omega),\omega]. \tag{3.12}$$

This satisfies[10] (3.6) and (3.7). To complete the proof we must show that the χ_n are orthonormal if the Φ_n are. Using the expression of the volume element in generalized polar coordinates,[9] we derive

$$\langle\chi_n\mid\chi_m\rangle=\int d\omega\int_0^\infty dr\, r^{3A-1}\left[\frac{r-\sigma(\omega)}{r}\right]^{3A-1}\theta[r-\sigma(\omega)]$$
$$\times\varphi_n^*[r-\sigma(\omega),\omega]\varphi_m[r-\sigma(\omega),\omega]=\langle\Phi_n\mid\Phi_m\rangle,\quad\text{QED.}$$

As for the two particle case, $\mathfrak{N}^\dagger$ is not the right inverse of $\mathfrak{N}$. For

$$\mathfrak{N}\mathfrak{N}^\dagger=\exp[-i\sigma(\omega)p_r]\theta(r)\theta(r)\exp[i\sigma(\omega)p_r]$$
$$=\theta[r-\sigma(\omega)]\neq 1.$$

As in theorem I we conclude observing that if the Φ_n are a complete system in the Hilbert space of bound-state wave functions, the χ_n are a complete system for bound-state wave functions satisfying (3.6) and (3.7). So holds *Theorem IV*: Any correlation operator $\mathfrak{N}'$ differs from $\mathfrak{N}$ by a unitary transformation. The proof is identical with that of theorem II.

The problem arises whether there is a "best" $\mathfrak{N}'$, i.e., whether the unitary operator can be chosen *a priori* in such a way as to simplify the calculations. Now, the possible unitary operators can be put into two classes: Those that leave unvaried the single-particle character of the basis Φ_n, and those that do not. In the first case the unitary operator changes only the single-particle wave functions, that have remained up to now arbitrary. Their best choice can be obtained in practice with the Hartree-Fock method. In the second case $\mathfrak{N}'\Phi_n$ differs from $\mathfrak{N}\Phi_n$ by a configuration mixing. A configuration mixing in practice can only be obtained by making a diagonalization in some subspace of the full Hilbert space.

Thus, it is not possible to find *a priori* an operator $\mathfrak{N}'$ "better" than $\mathfrak{N}$, and all the correlation operators $\mathfrak{N}'$ are *a priori* equivalent as far as the hard-core effects are concerned.

We conclude this section with the following remarks:

(i) Eq. (3.12) can be rewritten as

$$\chi_n=\left\{\prod_{l<m}\left[\frac{r_{lm}-\sigma\alpha_{lm}}{r_{lm}}\right]^{(3A-1)/[A(A-1)]}\theta(r_{lm}-c)\right\}$$
$$\times\varphi_n[r-\sigma(\omega),\omega].$$

This seems to imply a different way of approaching the relative distance c for two particles, according to the total number of particles.

(ii) For $A=2$ we have

$$\chi_n=\{[r_{12}-\sigma(\omega)\alpha_{12}]/r_{12}\}^{5/2}\theta[r-\sigma(\omega)]\varphi_n[r-\sigma(\omega),\omega], \tag{3.13}$$

a result different from that of (2.5). This difference is due to the fact that in Sec. 2 $\mathfrak{N}=\exp(icp_\rho)$, $\rho=|\mathbf{r}_{12}|$, while now $\mathfrak{N}=\exp(icp_r)$, $r=(\mathbf{r}_1^2+\mathbf{r}_2^2)^{1/2}$.

(iii) The operator $\mathfrak{N}$ of Sec. 2 commutes with the c.m. position vector, while now $\mathfrak{N}$ does not. The operator $\mathfrak{N}$ of the present section is not translation invariant.

Point (i) will be discussed in Appendix A, where it will be shown that the way of approaching the relative distance c for two particles irrespective of the others is independent of A. This result will be used in Sec. 7.

Points (ii) and (iii), that are closely connected, will be discussed in Sec. 5.

4. TRANSLATION-INVARIANT TRANSFORMATION

We saw that the operator $\mathfrak{N}$ changes the length of the vectors in S_{3A}, without changing their direction. Thus we have, for example (see Appendix A),

$$\mathfrak{N}^\dagger\mathbf{r}_i\mathfrak{N}=\mathbf{r}_i(1+c/r_M),\qquad \mathfrak{N}_M=\min\{\mathfrak{N}_{ij}\}$$
$$\mathfrak{N}^\dagger\mathbf{R}\mathfrak{N}=\mathbf{R}(1+c/r_M).$$

As a matter of fact, what we want is a transformation that changes relative distances, as these are relevant for the intrinsic motion, but leaves unchanged the c.m. position vector $\mathbf{R}$. To this end we replace the coordinates $\{\mathbf{r}_1,\cdots,\mathbf{r}_A\}$ with a new set of coordinates $\{\mathbf{z}_1,\cdots,\mathbf{z}_{A-1},\mathbf{R}\}$. The $\{\mathbf{z}_1,\cdots,\mathbf{z}_{A-1}\}$ are intrinsic variables that belong to the intrinsic motion space $S_{3(A-1)}$. We can define in $S_{3(A-1)}$ an operator similar to $\mathfrak{N}$, which we shall still call $\mathfrak{N}$. The procedure is described hereafter.

We shall use in $S_{3(A-1)}$ generalized polar coordinates $(\rho,\omega)\equiv\{\mathbf{z}_1,\cdots,\mathbf{z}_{A-1}\}$. The polar radius

$$\rho=(\mathbf{z}_1^2+\cdots\mathbf{z}_{A-1})^{1/2}$$

and ω is a system of angular variables. The relation of ρ to the vectors $\mathbf{z}_i$ is

$$\mathbf{z}_i=\rho\boldsymbol{\beta}_i, \tag{4.1}$$

where $\boldsymbol{\beta}_i=\boldsymbol{\beta}_i(\omega)$. We shall also use the equations[11]

$$\mathbf{r}_{ij}=\sum_k^{A-1}a_{ij}{}^k\mathbf{z}_k=\rho\sum_k^{A-1}a_{ij}{}^k\boldsymbol{\beta}_k,$$
$$r_{ij}=\rho\left|\sum_k^{A-1}a_{ij}{}^k\boldsymbol{\beta}_k\right|=\rho\beta_{ij}, \tag{4.2}$$
$$\mathbf{r}_i-\mathbf{R}=\sum_k^{A-1}b_i{}^k\mathbf{z}_k=\rho\sum_k^{A-1}b_i{}^k\boldsymbol{\beta}_k.$$

[10] As a matter of fact, (3.6) only requires $\Phi_n\sim r_{ij}{}^\alpha$, for $r_{ij}\to 0$, $\alpha>-(3A-1)/2$. However, the condition $\alpha>-1$ is necessary in order to ensure that $\int|\chi_n|^2$ on all the variables but r_{ij} behaves as $[(r_{ij}-c)/r_{ij}]^2$. This will be shown in Appendix A.

[11] Obviously, ω is different from ω of Sec. 3. Also, $\beta_{ij}\neq|\boldsymbol{\beta}_i-\boldsymbol{\beta}_j|$.

The boundary conditions (1.2) define in $S_{3(A-1)}$ the surfaces $r_{ij}=c$, with equations

$$r=c/\beta_{ij}, \tag{4.3}$$

that have been written using (4.2).

The discussion following (3.3) can be repeated in all details, and we arrive to the following equation for the boundary of region I, which we still call σ:

$$\rho=c/\min\{r_{ij}\}=c\rho/r_M=\sigma(\omega).$$

We can now repeat the procedure of Sec. 3, defining the momentum canonically conjugate to ρ in $S_{3(A-1)}$,

$$p_\rho=-i[(\partial/\partial\rho)+(3A-4)/2\rho^{-1}],$$

and the operator

$$\mathfrak{N}=\exp[-i\sigma(\omega)\,p_\rho]\theta(\rho).$$

Applying $\mathfrak{N}$ to the uncorrelated basis $\Phi_n(\mathbf{r}_1,\cdots,\mathbf{r}_A)\equiv\varphi_n(\rho,\omega,\mathbf{R})$, we obtain the new basis

$$\lambda_n=[(\rho-\sigma(\omega))/\rho]^{(3A-4)/2}\theta[\rho-\sigma(\omega)]\varphi_n[\rho-\sigma(\omega),\omega,\mathbf{R}]. \tag{4.4}$$

These still satisfy (3.6) and (3.7), and are orthonormal if the Φ_n are. The λ_n have the same properties as the χ_n as far as the intrinsic motion is concerned, and the same properties as the Φ_n with regard to the c.m. motion. For $A=2$,

$$\lambda_n=[(r_{12}-c)/r_{12}]\theta[r_{12}-c]\varphi_n[r_{12}-c,\omega,\mathbf{R}], \tag{4.5}$$

that are idential to (2.5).

It is very easy to prove that the λ_n gives rise to the same two-particle relative behavior as the χ_n near the core. This will be done in Appendix B.

5. TRANSFORMATION OF THE TWO-PARTICLE HAMILTONIAN

In the previous sections, we have obtained a correlated basis useful for handling the hard core, and we have studied some of its properties. However, in order to perform actual calculations, it is more convenient to consider the problem

$$\left\{\mathfrak{N}^\dagger\left[\sum_i^A{}_1\frac{\mathbf{p}_i^2}{2m}+\sum_{i<j}^A{}_1 V_{ij}\right]\mathfrak{N}-E\right\}\Phi=0,\qquad \Phi=\mathfrak{N}^\dagger\Psi \tag{5.1}$$

that is equivalent to (1.1) in virtue of the left unitarity of $\mathfrak{N}$.

Again we shall first consider the case $A=2$ for simplicity. Throughout the paper only central potentials will be considered, as we are only interested in general properties connected with the core. The transformation of other potentials is straightforward, using the formulas that will be developed for the kinetic energy.

The transformation in the two-particle case is immediately obtained. From Eq. (5.1), one gets

$$\{\mathfrak{N}^\dagger[(\mathbf{p}^2/m)+(\mathbf{P}^2/4m)+V(\rho)]\mathfrak{N}-E\}\Phi=0, \tag{5.2}$$

where $\mathbf{p}=\frac{1}{2}(\mathbf{p}_1-\mathbf{p}_2)$ and $\mathbf{P}=\mathbf{p}_1+\mathbf{p}_2$. Using $\mathbf{p}^2=p_\rho^2+\mathbf{l}^2/\rho^2$, $\mathbf{l}$ orbital angular momentum,

$$[p_\rho,\mathfrak{N}]=[\mathbf{l}^2,\mathfrak{N}]=0,\qquad \mathfrak{N}^\dagger(\mathbf{l}^2/\rho^2)\mathfrak{N}=\mathbf{l}^2/(\rho+c)^2,$$

and (2.4) and (5.2), we obtain

$$\left\{\frac{\mathbf{p}^2}{m}+\frac{\mathbf{P}^2}{4m}+\mathbf{l}^2\left[\frac{1}{(\rho+c)^2}-\frac{1}{\rho^2}\right]+V(\rho+c)-E\right\}\Phi=0,$$

i.e.,

$$\left\{\frac{1}{2m}(\mathbf{p}_1^2+\mathbf{p}_2^2)+\mathbf{l}^2\left[\frac{1}{(\rho+c)^2}-\frac{1}{\rho^2}\right]+V(\rho+c)-E\right\}\Phi=0. \tag{5.3}$$

In Eq. (5.3), the potentials are always evaluated outside the core. The new potential $\mathbf{l}^2[1/(\rho+c)^2-1/\rho^2]$ is zero for s states, and attractive for other states. It accounts for the fact that the centrifugal barrier is less effective because of the core.

6. TRANSFORMATION OF THE MANY-PARTICLE HAMILTONIAN

In this section, we shall derive the transformation of the many-particle Hamiltonian. Possibilities for practicle calculations will be discussed in Sec. 7.

Let us first consider the transformation of a central potential

$$\mathfrak{N}^\dagger V(r_{ij})\mathfrak{N}=V[r_{ij}+c(r_{ij}/r_M)]. \tag{6.1}$$

Observe that as $r_{ij}/r_M\geq 1$, the transformed potential is always evaluated outside the core. Moreover, if in Eq. (5.1) $r_{st}=0$, $(s,t)\neq(i,j)$, then $r_M=r_{st}=0$,

$$\mathfrak{N}^\dagger V(r_{ij})\mathfrak{N}=V(\infty)=0\qquad \text{for } r_{ij}\neq 0.$$

In the discussion of the importance of the clusters, the difference between geometrical clustering due to the boundary conditions and dynamical clustering due to the close approach of three or more particles must be considered. An example of geometrical clustering has been seen above. It consists in the effect on the interaction of the pair (i,j) of the close approach of the particles s, t, irrespective of the distance between the pairs (s,t) and (i,j). It can be easily seen that the geometrical clustering is more probable than the dynamical one. The expression (6.1) can be written more explicitly [see (A3)].

$$\mathfrak{N}^\dagger V(r_{ij})\mathfrak{N}=\sum_{s<t}^A{}_1 V\left(r_{ij}+c\frac{r_{ij}}{r_{st}}\right)\mathcal{P}_{st}$$

with

$$\mathcal{P}_{st}=\prod_{m<n}^{(s,t)}[1-\theta(r_{st}-r_{mn})]=1-\sum\theta+\sum\theta\theta-\cdots. \tag{6.2}$$

Possible approximation to (6.2) will be discussed in Sec. 7.

We now consider the kinetic energy split into its intrinsic and c.m. parts:

$$T=T_I+\mathbf{P}^2/2A, \qquad m=1.$$

The c.m. part is left unchanged by $\mathfrak{N}$, so that we need transform only

$$T_I=\frac{2}{A}\sum_{i<j}^{A}{}_1\,\mathbf{p}_{ij}^2, \qquad \mathbf{p}_{ij}=\tfrac{1}{2}(\mathbf{p}_i-\mathbf{p}_j). \tag{6.3}$$

A sketch of the transformation follows. We write the argument of Φ in such a way that only vectors that transform simply under $\mathfrak{N}$ appear:

$$\Phi=\Phi[(\mathbf{r}_1-\mathbf{R})+\mathbf{R},\ (\mathbf{r}_2-\mathbf{R})+\mathbf{R},\ \cdots,\ (\mathbf{r}_A-\mathbf{R})+\mathbf{R}].$$

Now $\mathbf{R}$ is invariant under $\mathfrak{N}$, while

$$\mathfrak{N}(\mathbf{r}_i-\mathbf{R})\mathfrak{N}^\dagger=\tau(\mathbf{r}_i-\mathbf{R}), \qquad \tau=(r_M+c)/r_M. \tag{6.4}$$

This enables us to derive simply that

$$\mathbf{p}_{ij}\mathfrak{N}\Phi=-i(\nabla_{ij}\tau^{(3A-4)/2})\Phi' + \sum_{k}^{A}{}_1\,\tau^{(3A-4)/2}\{\nabla_{ij}[\tau(\mathbf{r}_k-\mathbf{R})+\mathbf{R}]\}\Phi_k', \tag{6.5}$$

where

$$\Phi'=\mathfrak{N}\theta\Phi\mathfrak{N}^\dagger, \qquad \Phi_k'=\mathfrak{N}(\mathbf{p}_k\theta\Phi)\mathfrak{N}^\dagger.$$

This gives

$$\mathbf{p}_{ij}\mathfrak{N}\Phi=\{-i\tfrac{1}{2}(3A-4)\tau^{-1}(\nabla_{ij}\tau)\mathfrak{N} + \sum_{k}^{A}{}_1\,(\nabla_{ij}[\tau(\mathbf{r}_k-\mathbf{R})+\mathbf{R}])\mathfrak{N}\mathbf{p}_k\}\Phi;$$

thus,

$$\mathfrak{N}^\dagger T_I\mathfrak{N}=\frac{2}{A}\sum_{i<j}^{A}{}_1\{\mathfrak{N}^\dagger i\tfrac{1}{2}(3A-4)\tau^{-1}(\nabla_{ij}\tau) + \sum_{k}^{A}{}_1\,\mathbf{p}_k\mathfrak{N}^\dagger(\nabla_{ij}[\tau(\mathbf{r}_k-\mathbf{R})+\mathbf{R}])\} \times\{-i\tfrac{1}{2}(3A-4)\tau^{-1}(\nabla_{ij}\tau)\mathfrak{N} + \sum_{k}^{A}{}_1\,(\nabla_{ij}[\tau(\mathbf{r}_k-\mathbf{R})+\mathbf{R}])\mathfrak{N}\mathbf{p}_k\},$$

which, after some very tedious calculations, leads to

$$T_I-\tfrac{3}{4}(3A-4)(A-2)\frac{c^2}{r_M^2(r_M+c)^2} -A^{-1}\sum_{i<j}^{A}{}_1\,\mathbf{p}_{ij}\frac{2r_Mc+c^2}{(r_M+c)^2}\mathbf{p}_{ij} + \sum_{i,j}^{A}{}_1\,\mathbf{p}_i\cdot(\mathbf{r}_i-\mathbf{R})\frac{c^2}{r_M^2(r_M+c)^2}(\mathbf{r}_j-\mathbf{R})\cdot\mathbf{p}_j + \sum_{i}^{A}{}_1\,\mathbf{p}_M\cdot\mathbf{r}_M\frac{c}{r_M(r_M+c)^2}(\mathbf{r}_i-\mathbf{R})\cdot\mathbf{p}_i + \sum_{i}^{A}{}_1\,\mathbf{p}_i\cdot(\mathbf{r}_i-\mathbf{R})\frac{c}{r_M(r_M+c)^2}\mathbf{r}_M\cdot\mathbf{p}_M. \tag{6.6}$$

We remind the reader that $\mathbf{r}_M$ is the minimum of the $\{\mathbf{r}_{ij}\}$, and $\mathbf{p}_M$ is the momentum canonically conjugate.

Expression (6.6) for $\mathfrak{N}T_I\mathfrak{N}^\dagger$ is obviously translation-invariant and Hermitian. It commutes with $\mathbf{R}$ and $\mathbf{P}$, as can be seen by observing that we can everywhere replace $\mathbf{p}_i$ with $\mathbf{p}_i-(1/A)\mathbf{P}$.

Also the expression for the kinetic energy, like that for the potential, is an A-body operator, because of the appearance of the collective variable $\mathbf{r}_M$. Using (A3) and (6.2) a cluster expansion can be immediately obtained.

It is perhaps worth while to add that the some procedure can be applied for calculating matrix elements of any operators. In particular, for the mean-square nuclear radius

$$R_m=A^{-1}\sum_{i}^{A}{}_1\,(\mathbf{r}_i-\mathbf{R})^2,$$

the transformed operator is

$$\mathfrak{N}^\dagger R_m\mathfrak{N}=A^{-1}\sum_{i}^{A}{}_1\sum_{s<t}^{A}{}_1\,(\mathbf{r}_i-\mathbf{R})^2\left(\frac{r_{st}+c}{r_{st}}\right)^2\mathcal{O}_{st}.$$

As $\mathfrak{N}^\dagger R_m\mathfrak{N}$ is much different from R_m, it is difficult to choose *a priori* a basis giving the experimental mean-square nuclear radius. However, as

$$\sum_{s<t}^{A}{}_1\left(\frac{r_{st}+c}{r_{st}}\right)^2\mathcal{O}_{st}>1,$$

the single-particle basis Φ_n must give an expectation value of $\mathfrak{N}^\dagger R_m\mathfrak{N}$ greater than that of R_m.

7. POSSIBILITY OF ACTUAL CALCULATIONS

The formal theory so far developed has given a transformed Hamiltonian that is an A-body operator. This was to be expected, because if the fully correlated wave function Ψ is transformed to the uncorrelated Φ, the full correlation must be shifted to the Hamiltonian. The correlation appears via the collective variable r_M, which seems very untractable.

In the following, we make some speculations about the relative importance of the zeroth and higher orders in the cluster expansion, and about the rate of convergence. These are separate problems: We could have a good zeroth-order approximation with a slow convergence of the rest.

We start by considering a case in which the transformed potential is as simple as possible. This arises when the potential external to the core is of δ type

$$V(r_{ij})=\delta(r_{ij}-c)/(r_{ij}-c)^2. \tag{7.1}$$

The denominator is needed in order that V give non-vanishing matrix elements. In fact, it is shown in Appendix B that after the integration over all the variables but $\mathbf{r}_{ij}$, $|\lambda_n|^2$ behaves as $(r_{ij}-c)^2$ near the core.

In this simple case, we can exactly evaluate the ma-

trix elements $\langle\lambda_n \mid V \mid \lambda_m\rangle$. In fact,

$$\mathfrak{N}^\dagger \frac{\delta(r_{ij}-c)}{(r_{ij}-c)^2}\mathfrak{N} = \sum_{s<t}^{A}{}_1 \frac{\delta[r_{ij}+c(r_{ij}/r_{st})-c]}{[r_{ij}+c(r_{ij}/r_{st})-c]^2}\mathcal{P}_{st},$$

that gives nonvanishing contributions[12] only for $r_{ij}=r_{st}=0$. But $\mathcal{P}_{st}|_{r_{st}=0}=1$, and then

$$\mathfrak{N}^\dagger[\delta(r_{ij}-c)/(r_{ij}-c)^2]\mathfrak{N}=\delta(r_{ij})/r_{ij}^2=2\pi\delta(\mathbf{r}_{ij}).$$

Realistic potentials are not of course of type (7.1). Nevertheless, the above makes it plausible that for a potential of a sufficiently short range the cluster expansion of $\mathcal{P}_{st}$ will converge rapidly. Unfortunately, it seems that this is not the case in nuclear physics.[6] For, the feasibility of a cluster expansion requires that the integral of $\Phi_n{}^*\mathcal{P}_{st}\Phi_m$ on all the variables but r_{st} vary slowly (as a function of r_{st}) within the range of the potential. Let us call this integral $f^{m,n}(r_{st})$. We believe that $f^{m,n}(r_{st})$ has a range of the same order as the potential or less. Thus we are in a situation in which, if we evaluate the matrix elements with the exact $f^{m,n}(r_{st})$, the many-body corrections are not probably exceedingly large, but if we attempt to evaluate $f^{m,n}(r_{st})$ with a cluster expansion, we obtain a slow convergence. All the above is of course only speculative, but it may be checked by numerical calculations.

We turn now to the problem of evaluating matrix elements of the kinetic energy. Here the situation is worse, because the kinetic energy never reduces to two-body operators. The most favorable case obviously happens when c is so small that, to a good approximation,

$$\mathfrak{N}^\dagger T_I \mathfrak{N} \simeq T_I + c\Delta T_I,$$

$$\begin{aligned}\Delta T_I = \lim_{c\to 0}\Big\{ &-\tfrac{3}{4}(3A-4)(A-2)\frac{c}{r_M{}^2(r_M+c)^2} \\ &-A^{-1}\sum_{i<j}^{A}{}_1 \mathbf{p}_{ij}\frac{2r_M+c}{(r_M+c)^2}\mathbf{p}_{ij} \\ &+\sum_{i<j}^{A}{}_1 \mathbf{p}_i\cdot(\mathbf{r}_i-\mathbf{R})\frac{c}{r_M{}^2(r_M+c)^2}(\mathbf{r}_j-\mathbf{R})\cdot\mathbf{p}_j \\ &+\sum_{i}^{A}{}_1 \mathbf{p}_M\cdot\mathbf{r}_M[r_M(r_M+c)^2]^{-1}(\mathbf{r}_i-\mathbf{R})\cdot\mathbf{p}_i \\ &+\sum_{i}^{A}{}_1 \mathbf{p}_i\cdot(\mathbf{r}_i-\mathbf{R})[r_M(r_M+c)^2]^{-1}\mathbf{r}_M\cdot\mathbf{p}_M\Big\}. \quad (7.2)\end{aligned}$$

Using the identity

$$1/(x+c)^2=1/(x^2+c^2)-(2xc)/(x^2+c^2)(x+c)^2,$$

and the equations[13]

$$\lim_{c\to 0}\pi^{-1}[c/(x^2+c^2)]=\delta(x),$$

$$\lim_{c\to 0}[x/(x^2+c^2)]=\mathcal{P}/x, \qquad \text{(principal value)}$$

$$\lim_{c\to 0}\pi^{-1}[2xc/(x^2+c^2)^2]=-(\partial/\partial x)\delta(x)=-\delta'(x),$$

we can carry out the limits

$$\lim_{c\to 0}[c/r_M{}^2(r_M+c)^2]=\pi[\delta(r_M)/r_M{}^2],$$

$$\lim_{c\to 0}[(2r_M+c)/(r_M+c)^2]=2(\mathcal{P}/r_M)+\pi r_M\delta'(r_M)=2/r_M,$$

$$\begin{aligned}\lim_{c\to 0}[r_M(r_M+c)^2]^{-1} &= (1/r_M{}^2)(\mathcal{P}/r_M)+\pi[\delta'(r_M)/r_M] \\ &= (1/r_M{}^2)(\mathcal{P}/r_M)-\pi[\delta(r_M)/r_M{}^2],\end{aligned}$$

where it has been taken into account that $r\delta(r)=r\delta'(r)=0$, and that $\mathcal{P}/r$ can be replaced with $1/r$, whereas $(1/r^2)\mathcal{P}/r$ cannot be replaced with $1/r^3$. Then we have

$$\begin{aligned}\Delta T_I = &-\tfrac{3}{4}\pi(3A-4)(A-2)\sum_{s<t}^{A}{}_1\frac{\delta(r_{st})}{r_{st}{}^2} \\ &-A^{-1}\sum_{i<j}^{A}{}_1\sum_{s<t}^{A}{}_1 \mathbf{p}_{ij}\frac{2}{r_{st}}\mathcal{P}_{st}\mathbf{p}_{ij} \\ &+\pi\sum_{i<j}^{A}{}_1\sum_{s<t}^{A}{}_1 \mathbf{p}_i\cdot(\mathbf{r}_i-\mathbf{R})\frac{\delta(r_{st})}{r_{st}{}^2}(\mathbf{r}_j-\mathbf{R})\cdot\mathbf{p}_j \\ &+\sum_{i}^{A}{}_1\sum_{s<t}^{A}{}_1\left\{\left[\frac{1}{r_{st}{}^2}\frac{\mathcal{P}}{r_{st}}\mathcal{P}_{st}-\pi\frac{\delta(r_{st})}{r_{st}{}^2}\right](\mathbf{r}_i-\mathbf{R})\cdot\mathbf{p}_i\right. \\ &\left.+\mathbf{p}_i\cdot(\mathbf{r}_i-\mathbf{R})\left[\frac{1}{r_{st}{}^2}\frac{\mathcal{P}}{r_{st}}\mathcal{P}_{st}-\pi\frac{\delta(r_{st})}{r_{st}{}^2}\right]\right\}. \quad (7.3)\end{aligned}$$

If it were not for the principal-value contributions, we would have in (7.3) at most four-body terms easy to evaluate as their matrix elements factorize. However, because of the principal-value term, we are still faced with the $\mathcal{P}_{st}$. The importance of these terms is reduced from the short-range character of $f^{m,n}(r_{st})$, but again to take advantage of this we ought to be able to evaluate $f^{m,n}(r_{st})$ without recourse to a cluster expansion.

It is perhaps worth noting that the above terms introduce long-range correlations.

8. CONCLUSIONS

In this paper, we have determined a left-unitary correlation operator for bound-state wave functions, and we have shown that the most general correlation operator differs from this one by an arbitrary unitary

[12] In fact, for $(i,j)\neq(s,t)$,

$$\delta[r_{ij}+c(r_{ij}/r_{st})-c]\theta(r_{ij}-r_{st})=(1+c/r_{st})^{-1}\delta[r_{ij}-c/(1+c/r_{st})]\times\theta[-r_{st}/(1+c/r_{st})]=0.$$

Then only the contribution from $(i,j)=(s,t)$ survives, giving $\delta(r_{ij})/r_{ij}{}^2$.

[13] *The Quantum Theory of Radiation*, edited by W. Heitler (Oxford-Clarendon Press, 1953).

transformation. The correlation operators can be chosen to be translation-invariant.

Using the techniques of Refs. 4 and 7, it is then possible to diagonalize the Hamiltonian in a subspace of the full Hilbert space using shell-model wave functions as a basis, obtaining intrinsic motion eigenfunctions. Ground as well as excited states are treated in the same way.

The diagonalization, in practice, can be better accomplished using the original basis and the transformed Hamiltonian, which results in an A-body operator. For dilute systems it can be approximated by two-, three-, and four-body operators. The three- and four-body operators are very easy to evaluate.

Unfortunately, nuclei are not dilute systems, so we are faced with the problem of evaluating many-body terms, where a cluster expansion will give presumably a poor convergence. We emphasize that this is not imputable to the method, as the arbitrary unitary transformation in the correlation operator cannot be determined *a priori* in order to simplify the calculations. In any case, the method, to the approximation obtained in this field, is comparatively simple and free of the mathematical problems of the hard core. Moreover, to zeroth order in the cluster expansion we are able to include the three- and four-body terms that factorize.

The method also lends itself to an easy evaluation of matrix elements where most of the contribution to the integration comes from short interparticle distances, as in such a case, we can make a cluster expansion. These matrix elements are important because they are very sentive to the region of the core.

A particularly interesting application can be made to few-body problems, where the approximation is only due to the cut of the basis if many-body integrals are performed numerically.

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APPENDIX A

We must show that the way of approaching the relative distance c for two particles, irrespective of the others, is independent of A. To this end, we shall define a two-particle function $|\psi|^2$ (let us refer for definiteness to the particles 1 and 2) by

$$|\psi_n|^2=\int d\mathbf{r}_3'\cdots\int d\mathbf{r}_A'\,|\chi_n|^2. \tag{A1}$$

This is the probability of finding particle 1 at $\mathbf{r}_1$, particle 2 at $\mathbf{r}_2$, irrespective of the position of the other particles. We shall show that

$$\lim_{r_{12}\to c}|\psi_n|^2$$

is independent of A.

In order to evaluate (A1), we shall write

$$|\psi_n|^2=\int d\mathbf{r}_1'\int d\mathbf{r}_2'\cdots\int d\mathbf{r}_A'\chi_n^*\delta(\mathbf{r}_1'-\mathbf{r}_1)\delta(\mathbf{r}_2'-\mathbf{r}_2)\chi_n=\int d\mathbf{r}_1'\int d\mathbf{r}_2'\cdots\int d\mathbf{r}_A'\Phi_n^*\mathfrak{V}^\dagger\delta(\mathbf{r}_{12}'-\mathbf{r}_{12})\delta(\mathbf{R}_{12}-\mathbf{R}_{12})\mathfrak{V}\Phi_n$$
$$=\int d\mathbf{r}_1'\int d\mathbf{r}_2'\cdots\int d\mathbf{r}_A'\Phi_n^*\delta[\mathbf{r}_{12}'(1+\sigma/r)-\mathbf{r}_{12}]\delta[\mathbf{R}_{12}'(1+\sigma/r)-\mathbf{R}_{12}]\Phi_n. \tag{A2}$$

We need some explicit form of σ/r to evaluate (A2). We observe that Eq. (3.5) can also be written $\sigma/r=c/r_M$ with $r_M=\min\{r_{ij}\}$. Now an obvious representation for a function $f(r_M)$ is

$$f(r_M)=\sum_{i<j}^{A}{}_1 f(r_{ij})\prod_{l<m}^{(i,j)}\theta(r_{lm}-r_{ij}), \tag{A3}$$

where $\prod_{l<m}^{(i,j)}$ means the product of all the terms $l<m$, except the term $(l,m)=(i,j)$.

Using (A3), we have

$$\delta\left[\mathbf{r}_{12}'\left(1+\frac{c}{r_M}\right)-\mathbf{r}_{12}\right]\delta\left[\mathbf{R}_{12}'\left(1+\frac{c}{r_M}\right)-\mathbf{r}_{12}\right]$$
$$=\sum_{i<j}^{A}{}_1\delta\left[\mathbf{r}_{12}'\left(1+\frac{c}{r_{ij}'}\right)-\mathbf{r}_{12}\right]\delta\left[\mathbf{R}_{12}'\left(1+\frac{c}{r_{ij}'}\right)-\mathbf{R}_{12}\right]\prod_{l<m}^{(i,j)}\theta(r_{lm}'-r_{ij}').$$

Let us consider separately the contribution from $i=1, j=2$.

This will be shown to be the leading term in Eq. (A2) in the limit $r_{12}\to c$. In fact,

$$\delta\left[\mathbf{r}_{12}'\left(1+\frac{c}{r_{12}'}\right)-\mathbf{r}_{12}\right]\delta\left[\mathbf{R}_{12}'\left(1+\frac{c}{r_{12}'}\right)-\mathbf{R}_{12}\right]\prod_{l<m}^{(1,2)}\theta(r_{lm}'-r_{12}')=\left(\frac{r_{12}-c}{r_{12}}\right)^5\delta\left[\mathbf{r}_{12}'-\frac{r_{12}-c}{r_{12}}\mathbf{r}_{12}\right]$$
$$\times\delta\left[\mathbf{R}_{12}'-\frac{r_{12}-c}{r_{12}}\mathbf{R}_{12}\right]\prod_{l<m}^{(1,2)}\theta[r_{lm}'-(r_{12}-c)]. \tag{A4}$$

This, put into (A2), gives

$$\left(\frac{r_{12}-c}{r_{12}}\right)^5\theta(r_{12}-c)\int d\mathbf{r}_3'\cdots\int d\mathbf{r}_A'\prod_{l<m}^{(1,2)}\theta[r_{lm}'-(r_{12}-c)]\left|\Phi_n\left(\frac{r_{12}-c}{r_{12}}\mathbf{r}_1,\frac{r_{12}-c}{r_{12}}\mathbf{r}_2,\mathbf{r}_3',\cdots\mathbf{r}_A'\right)\right|^2, \quad \text{(A5)}$$

whose behavior for $r_{12}\to c$ does not depend on A. It can be easily seen following the above procedure that the remaining terms of (A2) give contributions that tend to zero at least as $[(r_{12}-c)/r_{12}]^9$.

We conclude observing that a factor $[(r_{12}-c)/r_{12}]^3$ disappears in (A5) when the integration over $\mathbf{R}_{12}$ is performed, and we are left with the relative behavior of Eq. (2.5).

APPENDIX B

We rewrite the defining Eq. (A1) replacing χ_n by

$$|\psi_n|^2=\int d\mathbf{r}_1'\cdots\int d\mathbf{r}_A'\Phi_n^*\delta\{\mathbf{r}_{12}'[1+(c/r_M)]-\mathbf{r}_{12}\}\mathfrak{N}^\dagger\delta[\mathbf{R}_{12}'-\mathbf{R}_{12}]\mathfrak{N}\Phi_n.$$

We need now the transformation of $\delta[\mathbf{R}_{12}'-\mathbf{R}_{12}]$. We are reminded that, while $\mathbf{r}_{12}'$ belongs to $S_{3(A-1)}$, $\mathbf{R}_{12}'$ does not. In order to find the transformation of $\mathbf{R}_{12}$, we write it as a sum of vectors belonging and not belonging to $S_{3(A-1)}$

$$\mathbf{R}_{12}'=\tfrac{1}{2}(\mathbf{r}_1'+\mathbf{r}_2')=\tfrac{1}{2}[(\mathbf{r}_1'-\mathbf{R}')+(\mathbf{r}_2'-\mathbf{R}')]+\mathbf{R}'.$$

Then,

$$\mathfrak{N}^\dagger\mathbf{R}_{12}'\mathfrak{N}=\frac{1}{2}\left(1+\frac{c}{r_M'}\right)[(\mathbf{r}_1'-\mathbf{R}')+(\mathbf{r}_2'-\mathbf{R}')]+\mathbf{R}'=\left(1+\frac{c}{r_M'}\right)\mathbf{R}_{12}'-\frac{c}{r_M'}\mathbf{R}'=\left[\left(1+\frac{c}{r_M'}\right)-\frac{2}{A}\frac{c}{r_M'}\right]\mathbf{R}_{12}'$$

$$-\frac{c}{r_M'}A^{-1}\sum_i^A{}_3\,\mathbf{r}_i'=\frac{r_M'+c-(2c/A)}{r_M'}\mathbf{R}_{12}'-\frac{c}{r_M'}A^{-1}\sum_i^A{}_3\,\mathbf{r}_i',$$

$$\mathfrak{N}^\dagger\delta[\mathbf{R}_{12}'-\mathbf{R}_{12}]\mathfrak{N}=\delta\left[\frac{r_M'+c-(2c/A)}{r_M'}\mathbf{R}_{12}'-\frac{c}{r_M'}A^{-1}\sum_i^A{}_3\,\mathbf{r}_i'-\mathbf{R}_{12}\right]$$

$$=\left(\frac{r_M'}{r_M'+c-(2c/A)}\right)^3\delta\left[\mathbf{R}_{12}'-\frac{c}{r_M'+c-(2c/A)}A^{-1}\sum_i^A{}_3\,\mathbf{r}_i'-\frac{r_M'}{r_M'+c-(2c/A)}\mathbf{R}_{12}\right].$$

If we consider the contribution due to $r_M'=r_{12}'$,

$$\delta\left[\mathbf{r}_{12}'\left(1+\frac{c}{r_{12}'}\right)-\mathbf{r}_{12}\right]\mathfrak{N}^\dagger\delta[\mathbf{R}_{12}'-\mathbf{R}_{12}]\mathfrak{N}=\left(\frac{r_{12}-c}{r_{12}}\right)^2\delta\left[\mathbf{r}_{12}'-\frac{r_{12}-c}{r_{12}}\mathbf{r}_{12}\right]\left(\frac{r_{12}-c}{r_{12}-(2c/A)}\right)^3$$

$$\times\delta\left[\mathbf{R}_{12}'-\frac{c}{r_{12}-(2c/A)}\frac{1}{A}\sum_i^A{}_3\,\mathbf{r}_i'-\frac{r_{12}-c}{r_{12}-(2c/A)}\mathbf{R}_{12}\right].$$

We find the relative behavior $(r_{12}-c)^5$ as in (A4). For $A=2$ we have (2.5) exactly.