Reduced-Hamiltonian method in the theory of bound states of systems of identical particles

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The Schrödinger equation for a system of identical particles has a hidden symmetry due to the indistinguishability of the particles. This symmetry can be used to eliminate the antisymmetrization operator from the equation and to obtain functional differential equations for the components of the wave function. In these equations there remains only a reduced two-particle Hamiltonian which is the minimal essential part of the many-particle Hamiltonian. The review is devoted to an exposition of the consequences of the symmetry and to a method of solution of functional differential equations for bound states of a system based on expansion of the components with respect to a complete basis of eigenfunctions of the reduced Hamiltonian.

INTRODUCTION

The theory of nonrelativistic systems of interacting particles began more or less simultaneously with the creation of quantum mechanics and has achieved since then significant successes. However, the appearance of constructions of a complexity not hitherto encountered—realistic internucleon potentials—showed that the traditional methods of solving the Schrödinger equation were not well suited for such problems. By "traditional" we mean here all the methods of solving many-fermion problems in which antisymmetry of the model wave functions is guaranteed irrespective of the dynamics, i.e., irrespective of the nature of the interaction between the particles, before the actual Schrödinger equation is solved. Included here are expansions of the exact wave function with respect to a rigidly fixed basis, as well as the *a priori* construction of a trial function with free parameters or even fragments of a function, which is matched as well as is possible to the exact function by varying the parameters or fragments. A characteristic example of this kind is the Hartree–Fock approximation, in which the antisymmetry of the wave function, which depends on single-particle variables, can be ensured before the radial functions are particularized. In the oscillator shell model[1–3] it is in principle possible both to extend the fixed basis and to vary with respect to the parameters of the wave functions. In the method of hyperspherical functions[4] and its generalizations,[5] antisymmetry of the functions is ensured by a fixed part (hyperspherical harmonics), which depends on the angular and spin–isospin variables, while the fragments of functions, which depend on the collective variables, are determined from dynamical equations.

One can even carry out a certain classification of methods of this kind on the basis of the number of degrees of freedom whose functions are not fixed in order to simplify the antisymmetrization, but remain free and can be adapted to the dynamics of the particular problem. Of course, one must also include here free parameters whose variation can achieve a similar result. This list must begin with the oscillator shell model (one parameter) and the method of hyperspherical functions (one degree of freedom). Then comes the shell model in a deformed average field (two or three parameters) and, still later, the method of generalized hyperspherical functions, in which the number of degrees of freedom of this kind can be increased to six. For comparison it should be noted that in the Hartree–Fock method for an atom the number of radial functions that are free from this point of view is $\sim N^{2/3}$. It is this that guarantees the high quality of the corresponding wave function. In our case, of course, the success of the method is not always directly proportional to this number. For everything still depends on the physics of the phenomenon. For example, in the resonating-group method[6] only one degree of freedom usually "works," but this is quite sufficient to explain clustering effects.

Basically, such hybrid methods in nuclear theory are very effective, but the convergence of the expansions, particularly for potentials with a Coulomb core (such as the Reid potential[7]), leaves something to be desired.[8,9] The reasons for this can be analyzed before any calculations are made. The point is that for realistic internucleon potentials the exact wave function must correspond to a probability density distribution in the system that, crudely speaking, resembles the density distribution in a sponge, i.e., the wave function must be "expelled" from regions of the configuration space corresponding to small internucleon distances. But the infrastructure of the model bases mentioned above corresponds rather, if we may follow the parallel, to the density distribution in an onion. It is therefore not surprising that the solution of the problem in such a case requires very long (for a hard core, infinite) expansions.

More or less convincing methods of solution of these difficulties, i.e., of adequate allowance for the two-particle correlations, can be constructed only for nuclear matter and heavy nuclei,[10,11] i.e., for systems in which it is justified to use certain simplifications of a different kind and the model basis is exceptionally simple. For finite nuclei the greatest success in recent times has been achieved by the method of calculation based on the use of variational techniques for trial functions with correlation factors of Jastrow type.[12,13] This can hardly be regarded as a great success of theoretical physics. The method itself has long been known, and all that has changed has been the purely technical possibilities of realizing stochastic computational algorithms for real systems. The essence of the method is that a simple model wave function of the ground state of the system (of the shell model or the method of hyperspherical functions), the antisymmetry of which can be ensured relatively easily, is multiplied by a completely symmetric factor, equal, as a rule, to a product of identical functions for each pair of particles. These func-

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tions, the correlation factors, which depend in the first place on the relative coordinate of the pair, are chosen in such a way as to ensure the above-mentioned deformation of the model wave function. Although such a trial function has a rather simple appearance, in the actual use of it there arise not only technical but also apparently fundamental difficulties due to its very antisymmetry[12] (a many-fermion wave function changes sign repeatedly in the configuration space, and this makes it impossible to use the Monte Carlo algorithm directly). On the other hand, even if this method could be successfully used for light nuclei, the picture would hardly become clearer, since, first, the result depends to some extent on how felicitously the trial function is chosen and, second, the methods of direct integration process the input information in such a way that it is extremely difficult to note any clear connection between the quality of the obtained wave function and the type of potential. But the aim of the calculation is, besides everything else, to use nuclear data to improve the internucleon potential itself. One of the examples of this kind is the long noted almost linear correlation between the characteristics of three-, four-, and two-nucleon systems[14] (for example, between the triton binding energy and the D-wave admixture in the deuteron, between the triton and α-particle binding energies, etc.). These phenomena are clearly revealed in numerous calculations, but their origin does not become clearer and is not amenable to unambiguous and transparent interpretation.

Thus, we appear to be in a difficult situation with no way out. Antisymmetrization of the function after solution of the Schrödinger equation becomes quite inappropriate, since it is necessary to filter out a large number of spurious solutions, i.e., solutions for which the wave function becomes identically zero when an attempt is made to antisymmetrize them. Antisymmetrization before solution of the dynamical problem has already been discussed. Neither the one nor the other is acceptable. Fortunately, there is another possibility. It is well known that the antisymmetrization operator commutes with the Hamiltonian of a system of identical particles, and therefore this operation can be carried out at any stage of solution of the Schrödinger equation, including simultaneously with it. It was found, and this will be shown below, that this has in practice long been done when the Schrödinger equation is reduced to the Faddeev[15] or Faddeev–Yakubovskiĭ[16] equations. The point is (to be specific we shall speak of the differential form of these equations) that a component of the wave function that has a lower degree of antisymmetry is an unknown in these equations. The sum of a necessary number of such components is antisymmetric and, apart from the normalization, is equal to the wave function of the system. Unfortunately, the structure of the operators in these equations is such that the main method of their solution is direct numerical integration. With increasing number of particles this method becomes less and less convenient, and it is desirable to construct hybrid methods based not only on solution of simpler equations than the Schrödinger equation but also on expansion of the components with respect to bases adapted to the real dynamics and therefore better suited to taking into account pair correlations.

Precisely such a possibility is presented by functional differential equations that contain as an operator a two-particle reduced Hamiltonian, the construction, spectrum, and eigenfunctions of which can be readily determined. Expansions of the many-particle wave functions with respect to such a basis is the very foundation of the reduced-Hamiltonian method.

1. PERMUTATIONAL SYMMETRY OF THE SCHRÖDINGER EQUATION FOR A SYSTEM OF IDENTICAL FERMIONS

Faddeev's differential equations for a system of three bodies,[17,18]

$$(H_0+V_\alpha-E)\Phi_\alpha=-V_\alpha\sum_{\beta\neq\alpha}\Phi_\beta,$$

where the notation of Ref. 18 has been used, form a system of three equations corresponding to the three possible partitions $\alpha=(1)(23)$, $(2)(31)$, and $(3)(12)$. The formal derivation of these equations consists of representing the wave function Ψ as a sum of components that each has the form

$$\Phi_\alpha=-R_0(E+i0)V_\alpha\Psi,$$

and of applying to both sides of this equation the operator H_0-E. This leads to an equation convenient for subsequent calculations:

$$(E-H_0)\Phi_\alpha=V_\alpha\Psi.$$

For $\alpha=(1)(23)$, V_α in this equation is simply the potential energy V_{23} of the interaction between the second and third particles.

In the case of three particles, the components of the wave functions are uniquely determined after specificiation of the asymptotic boundary conditions.

For four or more particles one can also determine partitions of the same type (a_{N-1}), the corresponding components, and a system of equations for them:

$$(E-H_0)\Phi_{a_{N-1}}=V_{a_{N-1}}\Psi. \qquad (1)$$

In contrast to the case considered above, in order to obtain equations equivalent to compact integral equations for scattering problems a further reduction of the components, corresponding to different types of partitions, is necessary.

Because we are mainly interested in bound-state problems, we shall restrict ourselves to equations of the type given above.

Each of the equations in (1) can be characterized by a definite distinguished pair, and the sum of all $N(N-1)/2$ equations is identical to the Schrödinger equation. If the particles are identical, all the equations are identical. If an equation of such type were equivalent to the Schrödinger equation, this would be the simplification mentioned in the Introduction.

It is worth pointing out a further feature of these equations. The wave function of a many-fermion system must be antisymmetric. If the partition a_{N-1} is particularized in such a way that the pair $(N-1, N)$ is distinguished, then the antisymmetry of the right-hand side is spoilt (by the presence of $V_{N-1,N}$)—it is antisymmetric only with respect to permutations of the variables in the sets $(1, 2, \ldots, N-2)$ and $(N-1, N)$ separately. Because of the symmetry of $E-H_0$ it follows that the component must also have the symmetry characteristic of the right-hand side, i.e., the degree of its antisymmetry is lower than for the wave function. This is the key to the further simplifications.

Before we turn to their exposition, we introduce notation more convenient here. We shall denote the antisymmetric function of a system of N identical fermions by $\Phi(1, 2, \ldots, N)$, and the component with the antisymmetry just described by $\Phi(1, 2, \ldots, N-2; N-1, N)$, i.e., we shall use the semicolon to separate groups of single-particle indices with respect to the permutations of which the function is antisymmetric. With this notation, the last equation takes the form

$$(E - H_0)\,\Phi\,(1, \ldots, N-2; N-1, N) = V_{N-1,N}\Phi\,(1, \ldots, N). \qquad (2)$$

The origin of this and other equations for the components may be different from the formal derivation given above. To demonstrate this, we draw attention to a connection between the degrees of antisymmetry of a component and the wave function. The operator that antisymmetrizes the component in our case belongs to the left cosets with respect to the subgroup $S_{N-2} \times S_2$ of the group S_N,[99]

$$X_{1,\ldots,N-2;N-1,N} = \binom{N}{2}^{-1}\Big\{1 + \sum_{p=1}^{N-2}(P_{pN-1}P_{pN} + P_{pN}P_{pN-1}) + \sum_{p_1,p_2=1(p_1<p_2)}^{N-2} P_{p_1N-1}P_{p_2N}\Big\}. \qquad (3)$$

Here, P_{ij} are transposition operators that interchange all the single-particle variables of particles i and j.

Using it, we can not only write the wave function as a sum of components,

$$\Phi\,(1, \ldots, N) = X_{1,\ldots,N-2;N-1,N}\Phi\,(1, \ldots, N-2; N-1, N), \qquad (4)$$

but also represent the many-particle Hamiltonian as

$$H_{1,\ldots,N} = H_0 + \sum_{i,j=1\,(i<j)}^{N} v_{i,j} \equiv H_0 + X_{1,\ldots,N-2;N-1,N}V_{N-1,N},$$

where

$$V_{N-1,N} = \binom{N}{2} v_{N-1,N}.$$

After substitution of these last expressions in the Schrödinger equation, it can be represented in the form

$$X_{1,\ldots,N-2;N-1,N}\{QV_{N-1,N}\Phi\,(1, \ldots, N-2; N-1, N) - (E - H_0)\,\Phi\,(1, \ldots, N-2; N-1, N)\} = 0. \qquad (5)$$

The operator Q which appears in this expression is, like X, a certain sum of operators of permutations of the single-particle variables. It is determined from the condition

$$X^{(h)}_{1,\ldots,N-2;N-1,N}X^{(\phi)}_{1,\ldots,N-2;N-1,N} = X_{1,\ldots,N-2;N-1,N}Q. \qquad (6)$$

Here, the symbols (h) and (ϕ) appended to the operators mean that they act on the variables in the Hamiltonian and in the wave functions (or components), respectively. The absence of symbols means that an operator acts on the variables of all the functions to its right. Even for three particles, Eq. (6) has several independent solutions.[19] The only ones that are valuable are those that keep the same permutational symmetry of both terms in the curly brackets of the expression (5). For any N, they include the solution

$$Q = X^{(\phi)}_{1,\ldots,N-2;N-1,N}. \qquad (7)$$

It is readily seen that Eq. (2) can be obtained from (5) by substituting in the latter this expression for Q and eliminating the operator X. The validity of such an operation for functional differential equations will be proved below. In the considered case this operation can be immediately understood and justified as follows. Equation (5) can be represented schematically in the form

$$X_{1,\ldots,N-2;N-1,N}\eta\,(1, \ldots, N-2; N-1, N) = 0. \qquad (8)$$

Hence the attempt to antisymmetrize η gives zero, and this can occur only in two cases—either when η possesses some further symmetry, a possibility which contradicts the definition of a component, or when it is identically zero. This also makes it possible to simplify the Schrödinger equation for a system of identical particles. The remaining [different from (7)] solutions for Q (see Ref. 19) lead to solutions of different types, among which one can readily recognize different variants of the three-particle scattering equations.

For $N > 3$ Eq. (2) can be reduced, by a further reduction of the symmetry of the components, to the form of differential equations of the theory of many-particle scattering. For four particles such a reduction is carried out in Ref. 19. Thus, the equations can be obtained not only as a result of the well-known method (Schrödinger equation; integral equations of the theory of many-particle scattering; differential equations for the components), but also directly from the Schrödinger equation exclusively on the basis of an analysis of its symmetry and the possibility of a representation in the form (5), i.e., omitting the intermediate link. Of course, then there arise two old problems— the determination of the asymptotic boundary conditions for the components and the proof that the final equations are equivalent to the original equation. As is well known, the equivalence is usually proved precisely at the intermediate stage, so that for the equations formulated below this is a nontrivial problem. In what follows we shall not consider the first of these problems, since we restrict ourselves to the case of bound states, for which it can be solved trivially.

2. FUNCTIONAL DIFFERENTIAL EQUATIONS

It is readily seen that the expression (5) can also be simplified by a partition into two-particle fragments in H_0 as well, i.e., by using the representation

$$H_{1,\ldots,N} = \sum_{i,j=1\,(i<j)}^{N} h_{i,j} \equiv X_{1,\ldots,N-2;N-1,N}H_{N-1,N},$$

$$H_{N-1,N} = \binom{N}{2} h_{N-1,N}.$$

This makes it possible to cast the Schrödinger equation into the even simpler form

$$X_{1,\ldots,N-2;N-1,N}\,\{QH_{N-1,N}\Phi\,(1,\ \ldots,\ N-2;\ N-1,\ N)\\ -E\Phi\,(1,\ \ldots,\ N-2;\ N-1,\ N)\}=0.$$

All that was said above about equations of the type (5) applies also to this equation, and this means that if we equate to zero the expression in the curly brackets and thereby determine the component, then the wave function constructed from the sum of these components with permuted single-particle variables [the expression (4)] will satisfy the Schrödinger equation for the same eigenvalue E. In Ref. 19 a special case (ground state of a system of three one-dmensional particles with oscillator interaction) was considered, and solutions were obtained for these equations for all Q that satisfy Eq. (6). It is interesting that for different Q different expressions for the components are obtained; this is natural, since the representation (4) is a partition of the wave function into a finite number of terms. The mutually independent partitions of such type are determined by the type of the equations for the components, which in its turn depends on Q. The simplest possible solution of Eq. (6) is determined in the expression (7). In what follows, we shall use only this solution. In such a case the functional differential equations have the form

$$H_{N-1,N}X_{1,\ldots,N-2;N-1,N}\Phi\,(1,\ \ldots,\ N-2;\ N-1,\ N)\\ =E\Phi\,(1,\ \ldots,\ N-2;\ N-1,\ N). \qquad (9)$$

Compared with the many-particle Schrödinger equation, the many-particle Hamiltonian is here replaced by the reduced two-particle Hamiltonian, and the unknown is no longer the many-particle wave function but is a component with a lower degree of antisymmetry.

Before we turn to the proof that these equations are equivalent to the original Schrödinger equation and investigate the properties of their solutions, we shall determine the form of the reduced Hamiltonian for the simplest systems, and also the types of variables on which the component depends.

If the problem is such that there is no need to separate the center-of-mass motion of the system, and single-particle variables can be used, then every natural number i denotes the necessary discrete (spin, isospin, etc.) variables of particle i and also its spatial variables.

If the many-particle Hamiltonian is

$$H_{1,\ \ldots,\ N}=-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i+\sum_{i=1}^{N}U_i+\sum_{i,\ j=1(i<j)}^{N}V_{i,\ j},$$

then the reduced two-particle Hamiltonian is defined as

$$H_{N-1,\ N}\\ =\binom{N}{2}\left\{\frac{1}{N-1}\left[-\frac{\hbar^2}{2m}(\Delta_{N-1}+\Delta_N)+U_{N-1}+U_N\right]\right.\\ \left.+V_{N-1,\ N}\right\}. \qquad (10)$$

For an atom with a fixed core and in the approximation of a simple electrostatic interaction, a scaling transformation of the single-particle variables makes it possible to reduce this Hamiltonian to the form (apart from a factor)[20,21] of the Hamiltonian of a certain "two-electron atom" with "charge of the nucleus" equal to $Z^*=Z/(N-1)$, where N is the number of electrons, and Z is the charge of the nucleus.

But if it is necessary to ensure translational invariance of the wave function, we shall assume that $\Phi(1,\ldots,N)$ represents the internal function, i.e., does not depend on the center-of-mass coordinate. As internal variables we shall use the system of normalized Jacobi coordinates determined from the corresponding tree[19,22] with $2N-1$ vertices, of which N vertices are of the first degree. They must be placed on one line and labeled by the numbers $1, 2, \ldots, N$, which correspond to the single-particle coordinates $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N$. The remaining $N-1$ vertices (arranged below the first group) have the order two or three, are identified by the numbers $1, 2, \ldots, N-1$, and denote the Jacobi coordinates found for vertex i in accordance with the formula[19]

$$\xi_i=\sqrt{\frac{p_iq_i}{p_i+q_i}}\left[\frac{1}{p_i}\sum_{j\in\{p_i\}}\mathbf{r}_j-\frac{1}{q_i}\sum_{j\in\{q_i\}}\mathbf{r}_j\right],$$

where p_i is the number of vertices of the first degree that can be reached by moving from vertex i upward along the left-hand line, $\{p_i\}$ is the set of their numbers, and q_i is the same for the right-hand line.

Such a system of Jacobi coordinates is very convenient because if one determines

$$\xi_0=\frac{1}{\sqrt{N}}\sum_{j=1}^{N}\mathbf{r}_j,$$

then the transition from the single-particle coordinates $\mathbf{r}_1,\ldots,\mathbf{r}_N$ to the system $\xi_0,\ \xi_1,\ldots,\xi_N$ is determined by an orthogonal matrix. The transition is made in the same way from one set of Jacobi coordinates to another obtained after permutation of the single-particle coordinates.

After the construction of the Jacobi coordinates, it is necessary to associate with each of them certain spin and isospin coordinates (σ_i and τ_i), being guided by the following rule[19]: The number of single-particle spin–isospin variables to be associated with a vertex corresponding to a definite Jacobi coordinate is to be equal to the number of vertices of first degree that are directly connected to the given vertex.

We shall impose on all the Jacobi trees that are to be used below one further condition—the last two vertices, corresponding to the variables $\mathbf{r}_{N-1}$ and $\mathbf{r}_N$, must be connected directly to a vertex of third degree, i.e., the last Jacobi coordinate must have the form

$$\xi_{N-1}=\frac{1}{\sqrt{2}}(\mathbf{r}_{N-1}-\mathbf{r}_N).$$

In such a case the reduced two-particle Hamiltonian is particularly simple:

$$H_{N-1,\ N}=\binom{N}{2}\left[-\frac{\hbar^2}{mN}\Delta_{\xi_{N-1}}\right.\\ \left.+V\left(\sqrt{2}\,\xi_{N-1},\ \sigma_{N-1}\tau_{N-1}\sigma_N\tau_N\right)\right], \qquad (11)$$

i.e., it is a single-particle operator of Hamiltonian type. Following the recommendations that have been given, we shall group the variables in a component of such type as follows:

$$\Phi\,(\xi_1,\ \ldots,\ \xi_{N-2},\ \sigma_1\tau_1\ \ldots\ \sigma_{N-2}\tau_{N-2};\\ (\xi_{N-1},\sigma_{N-1}\tau_{N-1}\sigma_N\tau_N).$$

When the operators of permutations of the single-particle variables are applied to the Jacobi coordinates, they generate orthogonal transformations of them, and therefore the construction on the left-hand side of the expression (9) has a fairly complicated form.

For clarity, we shall write out all these equations in the case of a system of three one-dimensional particles with an interaction that does not depend on the spin–isospin variables. In addition, we shall consider the case when the spin–isospin part of the wave function is completely symmetric. In such a case, the Schrödinger equation has the form

$$\left\{-\frac{\partial^2}{\partial\xi_1^2}-\frac{\partial^2}{\partial\xi_2^2}+V(\xi_2)+V\left(-\frac{\sqrt{3}}{2}\xi_1-\frac{1}{2}\xi_2\right)+V\left(\frac{\sqrt{3}}{2}\xi_1-\frac{1}{2}\xi_2\right)\right\}\Psi(\xi_1,\xi_2)=E\Psi(\xi_1,\xi_2).$$

The wave function can be represented as a sum of three components:

$$\Psi(\xi_1,\xi_2)=\Phi(\xi_1;\xi_2)+\Phi\left(-\frac{1}{2}\xi_1+\frac{\sqrt{3}}{2}\xi_2;\ -\frac{\sqrt{3}}{2}\xi_1-\frac{1}{2}\xi_2\right)+\Phi\left(-\frac{1}{2}\xi_1-\frac{\sqrt{3}}{2}\xi_2;\ \frac{\sqrt{3}}{2}\xi_1-\frac{1}{2}\xi_2\right).$$

Here the Jacobi coordinates are

$$\xi_1=\frac{1}{\sqrt{6}}(x_1+x_2-2x_3),\quad \xi_2=\frac{1}{\sqrt{2}}(x_2-x_3).$$

The only condition for the components is that

$$\Phi(\xi_1;\ -\xi_2)=-\Phi(\xi_1;\ \xi_2).$$

In this case Faddeev's equation has the form

$$V(\xi_2)\Psi(\xi_1,\xi_2)=\left\{E+\frac{\partial^2}{\partial\xi_1^2}+\frac{\partial^2}{\partial\xi_2^2}\right\}\Phi(\xi_1;\xi_2),$$

and the functional differential equation is

$$\left\{-\frac{2}{3}\frac{\partial^2}{\partial\xi_2^2}+V(\xi_2))\right\}\Psi(\xi_1,\xi_2)=E\Phi(\xi_1;\xi_2).$$

It can be seen that the action of the permutation operator leads to transformations of the arguments of the components, and therefore the equations must be called functional differential equations.[23,24] However, it should be noted that their type is very special and has hitherto not been studied. It is precisely this circumstance that ensures that they have unique solutions in at least the space of square-integrable functions.

A characteristic feature of Eqs. (9) is the presence in them of only one simple operator of Hamiltonian type—the reduced two-particle Hamiltonian. If the interaction between the particles were a three-particle interaction, we would have a reduced three-particle Hamiltonian, and so forth. In any case it is the minimal essential part of the many-particle Hamiltonian, from which the latter can be uniquely recovered. One can also readily choose the operator X in an appropriate manner and arrive at analogous but more complicated equations.[19] In the case of a two-body interaction the reduced Hamiltonian is, as we have already noted, exceptionally simple, and its eigenvalues and eigenfunctions can be calculated with any accuracy. It is this circumstance that suggests the method of solution of the equations based on expansion of the components with respect to this basis,[25] i.e., a complete system of antisymmetric eigenfunctions of the problem

$$[H_{N-1,\,N}-\varepsilon]\,\zeta_{\varepsilon\lambda\mu}(N-1,\ N)=0. \qquad (12)$$

Here, λ labels the set of exact quantum numbers—the eigenvalues of the complete system of operators that commute with the two-particle reduced Hamiltonian. In the case of realistic internucleon interactions, for example, we have the quantum numbers $j\pi stm_t$ (total angular momentum, parity, spin angular momentum, isospin moment, and projection of the two-particle isospin). The projections of all quantum numbers having the character of moments and angular momenta on which the eigenvalues ε of the problem do not depend are denoted by μ. (In the given example the only such quantum number will be the projection m_j of the total angular momentum, since the form of the Hamiltonian does depend on m_t—in the case of a system of two protons it is necessary to take into account their Coulomb interaction.)

In general, this complete system will consist of functions of both the discrete and the continuous spectrum. However, one can facilitate the further treatment and make a restriction to square-integrable functions. For we merely need to point out that the entire proposed formalism is designed for the description of bound states of a system. Therefore, the functions of the continuous spectrum of the problem (12) serve only for expansions of the square-integrable components. In such a case it is entirely justified to introduce a different boundary condition that makes it possible to construct a complete orthonormalized basis in the interior region consisting of square-integrable functions. For this it is sufficient to require vanishing of all the functions ζ at some interparticle distance R_0. The value of this distance can be chosen in such a way as to satisfy the following conditions. First, R_0 must be appreciably greater than the characteristic ranges of the two-particle potential, and also greater than the dimension of the complete system. Second, it is expedient to choose R_0 in such a way that the values of the negative ε, calculated with reasonable accuracy, are not sensitive to a further increase of R_0. The practical fulfillment of these conditions in any case does not present difficulties.

Before we turn to the expansion of the components, it is necessary to put the notation for them in order. For simplicity, we have until now omitted identifiers of the investigated state of the system, i.e., the exact quantum numbers, from all wave functions and their components. We must now rectify this shortcoming, bearing in mind that each component must be characterized by the same quantum numbers as the corresponding wave function. The set of quantum numbers will be different for different particular systems, since it depends on the particle species and on the nature of the interaction. In the case of a nucleus, for example, the set will consist solely of the angular momentum, parity, and isospin projection. The simpler the potential, the richer the set. If we denote all this by the single letter Λ and all the necessary projections of the quantum numbers having the character of moments and angular momenta by the letter M, the complete set of identifiers of the state of the system will be $E\Lambda M$.

In such a case, the expression for the component takes the form

$$\Phi_{E\Lambda M}(1,\ \ldots,\ N-2;\ N-1,\ N)=\sum_{\varepsilon\lambda\mu}\chi_{E\Lambda M,\,\varepsilon\lambda\mu}(1,\ \ldots,\ N-2)\,\zeta_{\varepsilon\lambda\mu}(N-1,\ N).$$

The antisymmetric functions of the first $N-2$ Jacobi coordinates and discrete variables appearing in this expansion are defined as

$$\chi_{E\Lambda M,\,\varepsilon\lambda\mu}(1,\,\ldots,\,N-2)$$

$$=\sum_{\sigma_{N-1}\sigma_N\tau_{N-1}\tau_N}\int d\xi_{N-1}\zeta^*_{\varepsilon\lambda\mu}(N-1,\,N)$$

$$\times\Phi_{E\Lambda M}(1,\,\ldots,\,N-2;N-1,\,N).$$

The summation and integration here are over all the variables of the functions ζ. We expand them with respect to any complete orthonormal basis of square-integrable functions that depend on the same variables in accordance with the formula

$$\chi_{E\Lambda M,\,\varepsilon\lambda\mu}(1,\,\ldots,\,N-2)$$

$$=\sum_{\overline{\Gamma}\overline{\Lambda}\overline{M}}c^{E\Lambda M}_{\overline{\Gamma}\overline{\Lambda}\overline{M},\,\varepsilon\lambda\mu}\chi_{\overline{\Gamma}\overline{\Lambda}\overline{M}}(1,\,\ldots,\,N-2).$$

We have here introduced the notation $\overline{\Gamma}$ for all the remaining quantum numbers needed to ensure completeness of the basis. The coefficients of this expansion must satisfy the obvious condition

$$c^{E\Lambda M}_{\overline{\Gamma}\overline{\Lambda}\overline{M},\,\varepsilon\lambda\mu}=c^{E\Lambda}_{\overline{\Gamma}\overline{\Lambda},\,\varepsilon\lambda}\begin{bmatrix}\overline{\Lambda} & \lambda & \Lambda\\ \overline{M} & \mu & M\end{bmatrix},$$

where the factor on the right is the product of Clebsch–Gordan coefficients for quantities having the character of moments and angular momenta and Kronecker deltas for parities, isospin projections, etc.

With allowance for these expansions, the expression for the component can be represented in the form

$$\Phi_{E\Lambda M}(1,\,\ldots,\,N-2;\;N-1,\,N)$$

$$=\sum_{\overline{\Gamma}\overline{\Lambda},\,\varepsilon\lambda}c^{E\Lambda}_{\overline{\Gamma}\overline{\Lambda},\,\varepsilon\lambda}\Phi_{(\overline{\Gamma}\overline{\Lambda},\,\varepsilon\lambda)\Lambda M}(1,\,\ldots,\,N-2;\;N-1,\,N),\tag{13}$$

where

$$\Phi_{(\overline{\Gamma}\overline{\Lambda},\,\varepsilon\lambda)\Lambda M}(1,\,\ldots,\,N-2;\;N-1,\,N)$$

$$=\sum_{\overline{M},\,\mu}\chi_{\overline{\Gamma}\overline{\Lambda}\overline{M}}(1,\,\ldots,\,N-2)\,\zeta_{\varepsilon\lambda\mu}(N-1,\,N)\begin{bmatrix}\overline{\Lambda} & \lambda & \Lambda\\ \overline{M} & \mu & M\end{bmatrix}.\tag{14}$$

If we substitute this expression in Eq. (9), multiply both sides by

$$\Phi^*_{(\overline{\Gamma}\overline{\Lambda},\,\varepsilon\lambda)\Lambda M}(1,\,\ldots,\,N-2;\,N-1,\,N),$$

integrate over all the Jacobi coordinates, and sum over the discrete variables, the equation takes the form of a generalized algebraic eigenvalue problem[26]:

$$\boldsymbol{\varepsilon}\mathbf{X}\mathbf{c}=\mathbf{c}E.\tag{15}$$

The rows and columns of the matrices that occur in this expression are denoted by the set of quantum numbers $(\overline{\Gamma}\overline{\Lambda}\varepsilon\lambda)$.

If the dimensions of the employed basis is n, then $\boldsymbol{\varepsilon}_{n\times n}$ is a diagonal matrix constructed from the eigenvalues of the operator $H_{N-1,N}$. It is expedient to arrange them in a nondecreasing order. This makes it possible to select a convenient order for the basis functions that are taken into account.

The matrix $X_{n\times n}$ is symmetric and real, and its elements are determined in accordance with the formula

$$\int d\Omega_N\Phi^*_{(\overline{\Gamma}\overline{\Lambda},\varepsilon\lambda)\Lambda M}(1,\,\ldots,\,N-2;\,N-1,\,N)$$

$$\times X_{1,\,\ldots,\,N-2;\,N-1,\,N}\Phi_{(\overline{\Gamma}'\overline{\Lambda}'\varepsilon'\lambda')\Lambda M}(1,\,\ldots,\,N-2;\,N-1,\,N).\tag{16}$$

It is obvious that it is diagonal with respect to Λ and does not depend on M.

The column vector $\mathbf{c}_{n\times1}$ consists of unknown coefficients present in the expression (13).

The matrix $\mathbf{X}$ itself has numerous properties whose investigation is very important for what follows.

First, the operator X defined by the expression (3) is a projection operator, i.e., it satisfies the condition

$$X^2_{1,\ldots,N-2;\,N-1,\,N}=X_{1,\ldots,N-2;\,N-1,\,N}.\tag{17}$$

This can be seen by noting that every suitably normalized antisymmetrizer

$$A_{1,\,\ldots,\,N}=\frac{1}{N!}\sum_{P\in S_N}\delta_P\cdot P$$

(δ_P is the parity of the permutation P) is a projection operator and contains antisymmetrizers of all possible subsystems, i.e.,

$$A_{p_1,\ldots,p_k}A_{1,\ldots,N}=A_{1,\ldots,N},$$

if $k\leqslant N$, $1\leqslant p_i\leqslant N$, $p_i\neq p_j$.

To prove (17), it is now sufficient to recall that

$$A_{1,\ldots,N}=X_{1,\ldots,N-2;\,N-1,\,N}A_{1,\ldots,N-2}A_{N-1,\,N}.\tag{18}$$

Because of the reality and symmetry, the matrix of such an operator will be a projection in the employed basis.[26] This means that its eigenvalues will be only zeros or ones, and the eigenvectors $\mathbf{y}^{\alpha}$ corresponding to the unit eigenvalues will form an orthonormal system. Therefore, $\mathbf{X}$ itself can be represented in the form

$$\mathbf{X}=\sum_{\alpha=1}^{r}\mathbf{y}^{\alpha}\cdot\mathbf{y}^{\alpha+}=\mathbf{F}\cdot\mathbf{F}^{+}.\tag{19}$$

Here, r is the rank of the matrix, and is simply equal to its trace. The matrix $\mathbf{F}_{n\times r}$ is formed by the vectors $\mathbf{y}^{\alpha}$:

$$\mathbf{F}=\|\,\mathbf{y}^1\mathbf{y}^2\,\ldots\,\mathbf{y}^r\,\|.$$

The plus sign denotes the transpose. In addition,

$$\mathbf{F}^{+}\cdot\mathbf{F}=1.\tag{20}$$

For some of the calculations in what follows it will be convenient to construct the matrix $\boldsymbol{\varepsilon}$ in such a way that it is positive definite. To achieve this aim, it is sufficient to note the obvious property of the equations that if some constant d is added to the two-particle reduced Hamiltonian, its eigenfunctions are unchanged, while all the eigenvalues are shifted by the same amount. In particular, the value of d can be chosen in such a way that all the $\boldsymbol{\varepsilon}$ in (12) become positive. As a result of such an operation, the spectrum of the entire system is shifted by the amount $dN(N-1)/2$ and the expressions for the components are changed, though the total function preserves its form.

In what follows we shall assume that such an operation has already been carried out in Eq. (15).

For a diagonal and positive-definite matrix $\boldsymbol{\varepsilon}$ it is also easy to determine the matrices $\boldsymbol{\varepsilon}^{1/2}$ and $\boldsymbol{\varepsilon}^{-1/2}$ and reduce the equation to the form of a simple algebraic eigenvalue problem:

$$\boldsymbol{\varepsilon}^{1/2}\,[\boldsymbol{\varepsilon}^{1/2}\mathbf{F}\mathbf{F}^{+}\boldsymbol{\varepsilon}^{1/2} - E_{\alpha}]\,\boldsymbol{\varepsilon}^{-1/2}\mathbf{c}^{\alpha} = 0.$$

The $n\times n$ matrix $\boldsymbol{\varepsilon}^{1/2}\mathbf{F}\mathbf{F}^{+}\boldsymbol{\varepsilon}^{1/2}$ in this expression is real and symmetric, and therefore all its eigenvalues are real. They include at least $n-r$ zero eigenvalues, while the remainder will be equal to the eigenvalues of the $r\times r$ matrix $\mathbf{F}^{+}\boldsymbol{\varepsilon}\mathbf{F}$.[26] We denote the orthogonal matrix that diagonalizes it by $\mathbf{G}$, and the diagonal matrix of eigenvalues by $\mathbf{E}$, i.e., we define

$$\mathbf{G}^{+}\mathbf{F}^{+}\boldsymbol{\varepsilon}\mathbf{F}\mathbf{G} = \mathbf{E}. \tag{21}$$

It is now easy to show that $\mathbf{E}$ is a positive-definite matrix. We return to the original problem

$$[\boldsymbol{\varepsilon}\mathbf{F}\mathbf{F}^{+} - E_{\alpha}]\,\mathbf{c}^{\alpha} = 0.$$

In the brackets here we have an $n\times n$ matrix, but, as we have just explained, only its eigenvectors that correspond to nonzero values E_α are of value. It is easy to show that they are the columns of the $n\times r$ matrix $\boldsymbol{\varepsilon}\mathbf{F}\mathbf{G}$, i.e.,

$$\mathbf{c}^{\alpha} = (\boldsymbol{\varepsilon}\mathbf{F}\mathbf{G})_{*\alpha}, \tag{22}$$

and the corresponding eigenvalues are

$$E_{\alpha} = (\mathbf{G}^{+}\mathbf{F}^{+}\boldsymbol{\varepsilon}\mathbf{F}\mathbf{G})_{\alpha\alpha}.$$

The system of left eigenvectors is formed by the r rows of the matrix $\mathbf{G}^{+}\mathbf{F}^{+}$. After an appropriate normalization, one can make these systems quasibiorthogonal.

The expression for the system of orthonormalized wave functions is unexpectedly simple in such a formalism. Elementary application of Eq. (4) makes it possible to conclude that they correspond, as they must, to the same matrix of eigenvalues (21) and are columns of the matrix

$$\mathbf{F}\mathbf{G}. \tag{23}$$

Each of these functions is antisymmetric, since it corresponds to a unit eigenvalue of the antisymmetrizer of the complete system. This property of theirs can be proved by using the expression (18), the properties of the basis (14), and the fact that

$$\mathbf{X}\cdot\mathbf{F}\mathbf{G} = \mathbf{F}\mathbf{F}^{+}\mathbf{F}\mathbf{G} = \mathbf{F}\mathbf{G}.$$

In the antisymmetric basis the matrix of the Hamiltonian of the system is equivalent to the matrix of the operator

$$H_{N-1,\,N},$$

and therefore (21) indicates its diagonality.

This means that each of the basis functions—the columns of the matrix (23)—is an eigenfunction for the Hamiltonian of the system.

It only remains to show that the Schrödinger equation does not have other solutions apart from those determined by this expression.

If we omit the indices and arguments that are here unimportant, the equation for the components can be represented in the form

$$hY\Phi_0 - E\Phi_0 = 0. \tag{24}$$

Here, Y is the operator in the curly brackets in (3).

As was shown above, it is obtained if the complete Schrödinger equation is written as

$$Y\,(hY\Phi - E\Phi) = 0 \tag{25}$$

and vanishing of the expression in the brackets is required. This operation leads to a unique expression for the component Φ_0 [the solution of Eq. (23)] and the wave function, which by definition is

$$\Psi = Y\Phi_0.$$

It is obvious that Eq. (25) can in principle also have other solutions (components of the wave function) for which

$$hY\Phi_f - E\Phi_f = f; \tag{26}$$

$$Yf = 0. \tag{27}$$

Here, f is any function with the required symmetry corresponding to the symmetry of the left-hand side of (26) that satisfies the condition (27). Because of the positivity of all the possible E values and the condition just mentioned, Eq. (26) can be represented in the form

$$hY\left(\Phi_f + \frac{1}{E}f\right) - E\left(\Phi_f + \frac{1}{E}f\right) = 0.$$

Thus, it is equivalent to Eq. (24), the solutions of which are unique:

$$\Phi_0 = \Phi_f + \frac{1}{E}f.$$

This means that for each possible f we obtain a different expression for the components, but they all correspond to the same eigenvalues of the Schrödinger equation and the same wave function, since

$$\Psi = Y\Phi_0 = Y\Phi_f.$$

Concluding the study of the properties of the solutions of the functional differential equations, we must point out some important features of them.

The key aspects in the solution of the equations are, obviously, the construction of the projection matrix $\mathbf{X}$ and the determination of its spectral expansion (19). Taken together, these operations are equivalent to the traditional problem of calculating the coefficients of fractional parentage.[27] The connection with the original dynamical problem is ensured here by the fact that the basis in which $\mathbf{X}$ is defined is an eigenbasis for the reduced Hamiltonian. This makes it possible subsequently to avoid all operations with the Hamiltonian or its fragments. In what follows we shall present effective methods for determining both exact and approximate spectral expansions of $\mathbf{X}$. With regard to its actual calculation, there are here important simplifications, due in the first place to the fact that the basis $\chi\overline{\Gamma\Lambda M}(1,\ldots,N-2)$ has not yet been particularized and can even be chosen in such a way that the nondiagonal elements of the matrix of the Hamiltonian become minimal. If, as is usual, the original basis is not associated with the dynamics of the actual system, such a result cannot be achieved at this stage. The only inconvenience that then arises is associated with the need to ensure antisymmetry of the corresponding functions χ, which depend on the coordinates of the first $N-2$ particles. It is most convenient to solve this problem by using components with minimal antisymmetry and the equations for finding them determined in Refs. 19 and 27. The antisymmetry of these components is specified by the Jacobi tree. This means that the bases for their expansion require practically no further antisymmetrization, since the variables are divided into subsystems, each of which contains not more than two sets of single-particle spin–isospin variables. Of course, this is accompanied by a growth in the dimension of X, but the fundamental difficulties due to the need to antisymmetrize the basis are solved. The equations for such components are obtained by eliminating from the Schrödinger equation the following fragments of the antisymmetrizer in the same way that the operator X was eliminated at the first step. One can prove the existence of unique solutions of these equations and their one-to-one correspondence with the solutions of the Schrödinger equation.[27]

3. VARIOUS APPROXIMATIONS

The point of departure for the practical application of our method is the calculation of the spectrum and eigenfunctions of the reduced two-particle Hamiltonian. For the operator (11) this problem can be solved with any accuracy by direct numerical integration (see Refs. 28–30). For systems in an external field it is more complicated, and to achieve the desired accuracy it is necessary to use either variational functions or the well-known method based on expansions with respect to a fixed single-particle basis. However, the second method does not have such good convergence.

Below, we shall give arguments based on study of the physics of particular systems that offer hope that a reasonable result for the energy of a many-particle system can be obtained by taking into account a small number of excited states of the reduced Hamiltonian and that the convergence when the set of such states is extended must be good.

The second problem is to construct the matrix X. At the first glance it might appear that with increasing N the number of terms in the expression for the operator X becomes catastrophically large and that calculation of the integrals in accordance with (16) will be most laborious. Fortunately, this is not so. Because the basis has a high degree of antisymmetry, the integral of the operator X is equal to the integral of the operator (see, for example, Ref. 21)

$$\binom{N}{2}^{-1}\left\{1-2(N-2)P_{N-2,\,N}+\binom{N-2}{2}P_{N-3,\,N-1}P_{N-2,\,N}\right\}.$$

Thus, in any case one must calculate not more than two integrals of different permutation operators. In addition, the matrix X is a projection, i.e., it has characteristics known in advance. In modulus none of its elements can be greater than unity, its trace is equal to its rank, and the sum of the squares of all the elements of any row (column) is equal to the diagonal element.

On the other hand, its dimension must be high, and in the cases of greatest practical interest may even be infinite, and therefore there can be no talk of constructing the entire X and then finding its spectral expansion. It will be shown that for this purpose it is sufficient to calculate its fragments.

The problem of the spectral expansion of X (19) consists of finding an orthonormalized system [the condition (20)] of its eigenvectors corresponding to eigenvalue equal to unity or, in other words, in calculating a rectangular matrix F of dimension $n\times r$ that satisfies the condition

$$\mathbf{XF}=\mathbf{F}.$$

Because X itself is a projection,

$$\mathbf{X}\cdot\mathbf{X}=\mathbf{X},\quad \mathbf{X}^{+}=\mathbf{X},$$

and this means that each of its columns is an eigenvector corresponding to unit eigenvalue. Unfortunately, they are linearly dependent and not normalized, though these are problems of a different level of complexity, and their solution is fairly simple. The maximal number of linearly independent vectors of the matrix X is r, and this makes it possible to restrict the calculation to not more than r linearly independent rows of the matrix, i.e., a fragment of dimension $r\times n$, which can be denoted as $(\mathbf{X}_{11}\mathbf{X}_{12})$, where $\mathbf{X}_{11}$ is a square $r\times r$ matrix, and $\mathbf{X}_{12}$ is all the remainder. It is readily noted that because the matrix X is a projection its fragment $\mathbf{X}_{11}$ is the Gram determinant of these r vectors. As is well known, to construct an orthonormal basis it is sufficient to diagonalize this Gram determinant, and simple calculations lead to the result

$$\mathbf{F}=\begin{pmatrix}\mathbf{DZ}_{11}^{1/2}\\ \mathbf{X}_{12}^{+}\mathbf{DZ}_{11}^{-1/2}\end{pmatrix},$$

where D is the matrix that diagonalizes the Gramian $(\mathbf{X}_{11})$, and $\mathbf{Z}_{18}$ is the diagonal matrix of its positive eigenvalues, i.e.,

$$\mathbf{D}^{+}\mathbf{X}_{11}\mathbf{D}=\mathbf{Z}_{11}.$$

In such a case the matrix of the Hamiltonian

$$\mathbf{F}^{+}\varepsilon\mathbf{F},$$

whose eigenvalues give the spectrum of the many-particle Schrödinger equation, takes the form

$$\mathbf{E}=\mathbf{Z}_{11}^{-1/2}\mathbf{D}^{+}\{\mathbf{X}_{11}\varepsilon_{-}\mathbf{X}_{11}+\mathbf{X}_{12}\varepsilon_{+}\mathbf{X}_{12}^{+}\}\,\mathbf{DZ}_{11}^{-1/2}. \qquad (28)$$

In the previous expression ε is the diagonal matrix of eigenvalues of the reduced Hamiltonian, arranged in nondecreasing order in accordance with the order of the basis functions (14). This matrix can be split into two diagonal submatrices, namely, ε_{-}, which contains the r minimal eigenvalues, and ε_{+}, which contains the remaining $n-r$.

After diagonalization of (28) by means of some orthogonal matrix G [of dimension $r\times r$] we obtain a spectrum containing the r lowest eigenvalues of the Schrödinger equation. The corresponding eigenfunctions are the columns of the rectangular matrix

$$\mathbf{f}=\begin{pmatrix}\mathbf{DZ}_{11}^{1/2}\mathbf{G}\\ \mathbf{X}_{12}^{+}\mathbf{DZ}_{11}^{-1/2}\mathbf{G}\end{pmatrix}.$$

These results are obtained in the approximation of a finite rank of the matrix X. When this rank is increased, even calculation of the fragment $(\mathbf{X}_{11}\mathbf{X}_{12})$ may present great difficulties, and it is therefore necessary to consider approximations. The first of them is to consider the case when one can calculate only $m(1\leqslant m\leqslant r)$ rows of this fragment, i.e., when the dimension of $\mathbf{X}_{11}$ is $m\times m$. We complete the calculated part to a projection matrix; then

$$\mathbf{X}=\begin{pmatrix}\widetilde{\mathbf{X}}_{11} & \widetilde{\mathbf{X}}_{12}\\ \widetilde{\mathbf{X}}_{12}^{+} & \widetilde{\mathbf{X}}_{22}\end{pmatrix},$$

where $\widetilde{\mathbf{X}}_{22}$ is an unknown $(n-m)\times(n-m)$ submatrix. As before, we introduce an orthogonal $m\times m$ matrix $\widetilde{\mathbf{D}}$ which diagonalizes the Gramian of the first m rows, i.e., $\widetilde{\mathbf{X}}_{11}$. As a result of this operation we obtain a new projection matrix

$$\widetilde{Z}=\begin{pmatrix}\widetilde{\mathbf{D}}^{+} & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\widetilde{\mathbf{X}}_{11} & \widetilde{\mathbf{X}}_{12}\\ \widetilde{\mathbf{X}}_{12}^{+} & \widetilde{\mathbf{X}}_{22}\end{pmatrix}\begin{pmatrix}\widetilde{\mathbf{D}} & 0\\ 0 & 1\end{pmatrix}$$

$$=\begin{pmatrix}\widetilde{\mathbf{D}}^{+}\widetilde{\mathbf{X}}_{11}\widetilde{\mathbf{D}} & \widetilde{\mathbf{D}}^{+}\widetilde{\mathbf{X}}_{12}\\ \widetilde{\mathbf{X}}_{12}^{+}\widetilde{\mathbf{D}} & \widetilde{\mathbf{X}}_{22}\end{pmatrix}=\begin{pmatrix}\widetilde{\mathbf{Z}}_{11} & \widetilde{\mathbf{Z}}_{12}\\ \widetilde{\mathbf{Z}}_{12}^{+} & \widetilde{\mathbf{Z}}_{22}\end{pmatrix}. \tag{29}$$

Its spectral expansion can be represented in the form

$$\widetilde{\mathbf{Z}}=\begin{pmatrix}\mathbf{K}_{11} & \mathbf{K}_{12}\\ \mathbf{K}_{21} & \mathbf{K}_{22}\end{pmatrix}\begin{pmatrix}\mathbf{K}_{11}^{+} & \mathbf{K}_{21}^{+}\\ \mathbf{K}_{12}^{+} & \mathbf{K}_{22}^{+}\end{pmatrix}=\mathbf{K}\mathbf{K}^{+}.$$

The matrices here have the following dimensions: $m\times m$ for $\mathbf{K}_{11}$; $m\times(r-m)$ for $\mathbf{K}_{12}$; $(n-m)\times m$ for $\mathbf{K}_{21}$; $(n-m)\times(r-m)$ for $\mathbf{K}_{22}$. If $m=r$, then $\mathbf{K}_{12}=0$ and $\mathbf{K}_{22}=0$, and we obtain results as in the previous case.

It is readily noted that there is considerable freedom in the choice of $\mathbf{K}$, since

$$\mathbf{K}\mathbf{K}^{+}=(\mathbf{K}\mathbf{R})\,(\mathbf{K}\mathbf{R})^{+}\equiv\mathbf{M}\mathbf{M}^{+} \tag{30}$$

if the transformation is orthogonal, i.e.,

$$\mathbf{R}\mathbf{R}^{+}=\mathbf{R}^{+}\mathbf{R}=1.$$

This does not contradict the conditions of the spectral expansion, since by virtue of

$$\mathbf{K}^{+}\mathbf{K}=1$$

we also have

$$\mathbf{M}^{+}\mathbf{M}=(\mathbf{K}\mathbf{R})^{+}\,(\mathbf{K}\mathbf{R})=1. \tag{31}$$

As is well known, the orthogonal $r\times r$ matrix $\mathbf{R}$ has $r(r-1)/2$ free parameters. This fact makes it possible to fix arbitrarily the same number of elements in the matrix $\mathbf{M}$. The optimal requirement is to make the upper triangle of this matrix identically zero. Then $\mathbf{M}_{12}=0$, and the upper triangles $\mathbf{M}_{11}$ and $\mathbf{M}_{22}$ must be filled with zeros. In such a case the conditions (30) and (31) lead to the results

$$\mathbf{M}_{11}=\widetilde{\mathbf{Z}}_{11}^{1/2},\ \ \mathbf{M}_{21}=\widetilde{\mathbf{Z}}_{12}^{+}\widetilde{\mathbf{Z}}_{11}^{-1/2}. \tag{32}$$

$$\mathbf{M}_{21}^{+}\mathbf{M}_{22}=0. \tag{33}$$

This makes it possible to represent the matrix of the Hamiltonian in the form

$$\widetilde{\mathbf{E}}=\begin{pmatrix}\mathbf{M}_{11}^{+}\widetilde{\mathbf{D}}^{+}\tilde{\varepsilon}_{-}\widetilde{\mathbf{D}}\mathbf{M}_{11}+\mathbf{M}_{21}^{+}\tilde{\varepsilon}_{+}\mathbf{M}_{21} & \mathbf{M}_{21}^{+}\tilde{\varepsilon}_{+}\mathbf{M}_{22}\\ \mathbf{M}_{22}^{+}\tilde{\varepsilon}_{+}\mathbf{M}_{21} & \mathbf{M}_{22}^{+}\tilde{\varepsilon}_{+}\mathbf{M}_{22}\end{pmatrix}. \tag{34}$$

Here, as before, the matrix ε has been partitioned into submatrices: $\tilde{\varepsilon}_{-}$, which contains the m smallest eigenvalues of the reduced Hamiltonian, and $\tilde{\varepsilon}_{+}$, which contains the remaining $n-m$.

The transition that we have made to the matrix $\mathbf{M}$ has a deep physical significance. The point is that our basis states are in nondecreasing order of ε_i, the corresponding eigenvalues of the reduced Hamiltonian. The diagonality of $\mathbf{M}_{11}$ and the fact that $\mathbf{M}_{12}=0$ mean that only the first m columns of $\mathbf{M}$ (each of them describes a definite state of the system) are characterized by nonzero probabilities of the m lowest states of the reduced Hamiltonian, and this ensures the sinking of the corresponding eigenvalues. The diagonal submatrices $\widetilde{\mathbf{E}}$ (34) are clearly separated in accordance with the regions of distribution of their eigenvalues, while the nondiagonal submatrices are suppressed by virtue of the condition (33). It is therefore unnecessary to diagonalize the complete $\widetilde{\mathbf{E}}$; only its $m\times m$ submatrices need to be diagonalized. If $m=r$, this leads to the exact result (28); in other cases, as is shown by model calculations to be mentioned below, there is reasonable convergence. In other words, such an approximation corresponds to the assumption that the rank of the projection matrix $\widetilde{\mathbf{X}}$ is m, i.e., is equal to the number of rows that one can calculate. Thus, the considered variant is a special case of the first one. They both lead to upper bounds for the energies. As $m\to r$ the results converge to the exact values from above, since this operation corresponds to extension of the basis. In such a case the most accurate result corresponds to the approximation of finite rank r, and this, in its turn, gives only an upper bound on the true exact value if the problem in fact has infinite rank.

It could be that one of the most important aspects of the method is that it enables one to obtain, even more readily than upper bounds, lower bounds for the energies that converge to the exact values, and also the corresponding wave functions. The idea here is very simple. For a start we illustrate it by the explicit example of the expression (28). As we said above, the eigenvalues of the reduced Hamiltonian in the matrix ε are arranged in nondecreasing order. This means that any element in the matrix ε_{+} is not less than the $(r+1)$th eigenvalue, i.e., ε_{r+1}. Now the approximation

$$\varepsilon_{+}=\varepsilon_{r+1}\cdot 1$$

leads to lower bounds. Moreover, the second term in the curly brackets is in this case equal to

$$\varepsilon_{r+1}\mathbf{X}_{12}\mathbf{X}_{12}^{+}=\varepsilon_{r+1}\,(\mathbf{X}_{11}-\mathbf{X}_{11}^{2}).$$

This is true for fragments of any projection matrix. Ultimately we find that in the expression for the matrix of the Hamiltonian leading to the lower bounds only $\mathbf{X}_{11}$ occurs, i.e., the lower bounds can be determined for problems of infinite order, when $\mathbf{X}_{12}$ cannot be calculated even in principle, since it contains an infinite number of elements. Of course, in this case one cannot completely determine $\mathbf{X}_{11}$ either, since the matrix of $\mathbf{X}$ will certainly be infinite. However, it is readily noted that even in this case, when only part of the matrix $\widetilde{\mathbf{X}}_{11}$, whose dimension is $m\times m$ $(1\leqslant m\leqslant r)$, is determined, the approximation

$$\tilde{\varepsilon}_{+}=\varepsilon_{m+1}\cdot 1$$

leads to exact lower bounds, since because of the condition (33) the nondiagonal submatrices of the matrix $\widetilde{\mathbf{E}}$ determined by the expression (34) are zero, and its essential part with the minimal eigenvalues can be expressed in the form

$$\widetilde{\mathbf{E}}_{11}=\widetilde{\mathbf{Z}}_{11}^{1/2}\widetilde{\mathbf{D}}^{+}\widetilde{\varepsilon}_{-}\widetilde{\mathbf{D}}\widetilde{\mathbf{Z}}^{1/2}+\varepsilon_{m+1}(1-\widetilde{\mathbf{Z}}_{11}). \tag{35}$$

To obtain the expansion with respect to the employed basis states of the corresponding wave functions, it is necessary to look at this problem from a somewhat different point of view.

It is readily noted that all the previous treatment was based on the fact that the projection matrix **X** or at least some of its rows have already been constructed. The various approximations concerned only its spectral expansion if the available information was not sufficient to obtain an exact result. In this last case we have already assumed that we know only a square submatrix whose dimension is appreciably less than even the rank of **X**, which, incidentally, is also unknown. Now it is necessary to have recourse to approximations of the projection matrix itself (its recovery from a known fragment), since otherwise our formalism cannot be applied. Thus, the $m\times m$ fragment $\widetilde{\mathbf{X}}_{11}$ has been calculated. It belongs to a projection matrix, and therefore must have very specific properties. First, if any one of its diagonal elements is zero, then the entire row must also be identically zero, even though it is infinite, and so must the entire column at the intersection with which it stands. The same picture must be observed when the diagonal element is equal to unity. The first case (zero on the diagonal) means that this basis state must be excluded from consideration, since it cannot appear in the expansion of any antisymmetric function, while the second case means that this basis function itself is already antisymmetric and can be considered separately. If an orthogonal transformation is applied to the projection matrix, these properties are preserved, so that without loss of generality we can assume that all the eigenvalues of the submatrix $\widetilde{\mathbf{X}}_{11}$ are greater than zero but less than unity. The problem is to determine in the simplest possible way the submatrices $\widetilde{\mathbf{X}}_{12}$ and $\widetilde{\mathbf{X}}_{22}$, which complete $\widetilde{\mathbf{X}}_{11}$ to a projection matrix, and to find its spectral expansion, i.e., the simplest missing fragments $\widetilde{\mathbf{X}}$ and $\widetilde{\mathbf{F}}$ connected by the relations

$$\widetilde{\mathbf{X}}\equiv\begin{pmatrix}\widetilde{\mathbf{X}}_{11}\widetilde{\mathbf{X}}_{12}\\ \widetilde{\mathbf{X}}_{12}^{+}\widetilde{\mathbf{X}}_{22}\end{pmatrix}=\begin{pmatrix}\widetilde{\mathbf{F}}_{1}\\ \widetilde{\mathbf{F}}_{2}\end{pmatrix}(\widetilde{\mathbf{F}}_{1}^{+}\widetilde{\mathbf{F}}_{2}^{+})\equiv\widetilde{\mathbf{F}}\widetilde{\mathbf{F}}^{+};$$

$$\widetilde{\mathbf{F}}^{+}\widetilde{\mathbf{F}}=1.$$

These conditions already include the requirement of simplest continuation, since the rank of $\widetilde{\mathbf{X}}$ is taken equal to the rank of $\widetilde{\mathbf{X}}_{11}$, which in accordance with the adopted restrictions is equal to its order, i.e., m. It is convenient to apply a transformation of the type (29), which diagonalizes $\widetilde{\mathbf{X}}_{11}$, to $\widetilde{\mathbf{X}}$. After this we immediately find from the projection condition that

$$\widetilde{\mathbf{Z}}_{12}\widetilde{\mathbf{Z}}_{12}^{+}=\widetilde{\mathbf{Z}}_{11}-\widetilde{\mathbf{Z}}_{11}^{2}.$$

The simplest solution of this equation is

$$\widetilde{\mathbf{Z}}_{12}=\widetilde{\mathbf{Z}}_{12}^{+}=[\widetilde{\mathbf{Z}}_{11}(1-\widetilde{\mathbf{Z}}_{11})]^{1/2}.$$

Even more readily we find that

$$\widetilde{\mathbf{F}}=\begin{pmatrix}\widetilde{\mathbf{D}}\widetilde{\mathbf{Z}}_{11}^{1/2}\\ (1-\widetilde{\mathbf{Z}}_{11})^{1/2}\end{pmatrix}.$$

For the matrix of the Hamiltonian the already known result (35) is obtained. If it is reduced to diagonal form by means of a diagonal matrix $\widetilde{\mathbf{G}}$, then its eigenvectors are the columns of the matrix

$$\widetilde{\mathbf{f}}=\begin{pmatrix}\widetilde{\mathbf{D}}\widetilde{\mathbf{Z}}_{11}^{1/2}\widetilde{\mathbf{G}}\\ (1-\widetilde{\mathbf{Z}}_{11})^{1/2}\widetilde{\mathbf{G}}\end{pmatrix}. \tag{36}$$

The essence of the employed approximation is that only the first m basis functions are exactly known, while the remainder are not determined. Our result makes it possible to conclude that there exists a possibility of choosing them in such a way that the wave function becomes antisymmetric. The only thing known about these additional functions is that the eigenvalue of the reduced Hamiltonian for each of them is not lower than ε_{m+1} [the first m minimal ε_i ($\varepsilon_1\leqslant\varepsilon_2\leqslant\ldots\leqslant\varepsilon_m$) correspond to the basis functions taken into account]. It is this fact that was used to find the lower bounds on the eigenvalues of the many-particle Schrödinger equation.

It is well known that the Hall–Post method of obtaining lower bounds[31,32] is ultimately based on giving up the antisymmetry of the wave function. The imposition of subsidiary conditions on the density matrix[33] makes it possible to improve these results, but a possibility of constructing lower bounds that converge to the exact values appears only as a result of application of the above method, in which antisymmetry of the wave function is ensured but some of the basis functions remain undetermined. It is important that the expression (36) makes it possible to calculate the total weight of these functions, which gives a qualitative measure—the degree of its uncertainty. For the state i (column i of $\widetilde{\mathbf{f}}$) it is

$$g_i=\sum_{k=1}^{m}|\widetilde{\mathbf{G}}_{ki}|^2(1-\widetilde{\mathbf{Z}}_{11})_{kk}.$$

The weight of the known basis states is $1-g_i$, since each wave function is normalized to unity.

4. SOME RESULTS

In any approximation the method described here for solving the many-particle Schrödinger equation leads to a very simple expression for the energy of the system:

$$E_\Lambda=\sum_i\varepsilon_i w_{i,\Lambda}. \tag{37}$$

Here, ε_i are eigenvalues of the reduced Hamiltonian, and $w_{i,\Lambda}$ for bound states satisfy the condition

$$w_{i,\Lambda}\geqslant 0,\ \sum_i w_{i,\Lambda}=1$$

and therefore can be interpreted as the probabilities of occupation of the different i in the state of the system Λ.

The standard expression of such type has the form

$$E_\Lambda=\sum_{i,j}t_{i,j}q_{j,i;\Lambda},$$

where $t_{i,j}$ are quantities of the type of Talmi integrals, while $q_{j,i;\Lambda}$ are coefficients that are not amenable to a simple interpretation.

The simplicity of (37) is to some degree deceptive; for whereas the calculation of ε_i presents only certain technical difficulties, the determination of $w_{i,\Lambda}$, which, to be exact, are the diagonal matrix elements of the reduced two-particle density matrix of the system in the representation of the eigenfunctions of the reduced two-particle Hamiltonian, presents no small problem. At different times numerous attempts have been made to solve it,[21,34] but only the results presented above make it possible to give a more or less acceptable answer to this problem.

To demonstrate the value of this expression and the method as a whole, we consider two definite examples. The first is the model of a nucleus as a system of realistically interacting nucleons. The properties of the reduced Hamiltonian in such a case were studied in Refs. 29 and 30. This operator describes only the relative motion of the nucleons, and therefore the determination of its eigenfunctions is no more complicated than the corresponding problem for the deuteron; in addition, it has a very important property—the reduced effective mass in this formal structure, which does not describe any real subsystem, is directly proportional to N. For $N=2$, when it is identical to the ordinary Hamiltonian of the two-nucleon system, there is, as is well known, only one bound eigenvalue of such an operator in the state $^3S_1$–$^3D_1$, namely, the deuteron. For $N=3$, all realistic internucleon potentials ensure the appearance of a bound eigenvalue in the state $^1S_0$. With further increase of N, bound eigenvalues also begin to appear in other states, in which the phase shifts of nucleon–nucleon scattering change sign or are positive, though some of the channels in which the phase shifts are negative remain "closed" for any N. On the other hand, it is clear from the expression (37) that negative E_Λ are possible only for the Λ for which $\omega_{i,\Lambda}$ are large for negative ε_i (bound states of the reduced Hamiltonian) and small for positive ε_i, since the index of summation in general ranges over an infinite set of values. This set consists of all possible two-nucleon states ($^3S_1$–$^3D_1$, $^1S_0$, $^3P_2$–$^3F_2$, $^3D_2$, $^3P_0$, $^1D_2$, etc.), and also all possible eigenvalues of the reduced Hamiltonian in these states.

It can be shown that one can introduce the concept of the minimal rank of the two-particle reduced density matrix,[35] which determines the set of values of i that correspond to the maximal $w_{i,\Lambda}$ for each definite state Λ of the system. This set is determined by the need to ensure exact quantum numbers for the nuclear states. With increasing N it is strongly enlarged even for ground states, whereas the appearance of new negative ε is very limited. Ultimately this leads to the observed decrease in the stability of heavy nuclei with respect to decay into lighter fragments and termination of the stability valley. From this point of view the most favorable situation in all the lightest nuclei is for the ground states of the simplest systems: t, ^{3}He, and ^{4}He. As we have already mentioned, for $N \geqslant 3$ there are negative eigenvalues in the $^1S_0$ and $^3S_1$–$^3D_1$ channels for realistic potentials. Simultaneously, for $N \leqslant 4$ and the minimal possible J the minimal rank would permit a restriction to be made to only relative s states; however, such a function cannot be antisymmetrized because of the admixture of the D wave in the reduced Hamiltonian. This forces us to use a set of channels that is closed from the point of view of exact quantum numbers, namely, a set containing $^3D_1$, which, in its turn, must, because of the admixture of the F state in the $^3P_2$–$^3F_2$ channel, be extended further, and so forth. The set required to ensure antisymmetry of the wave function is infinite, but, as exact calculations showed,[36] an admixture of higher states is suppressed. In our language this can be readily understood, since each successive generation of channels enters with weight proportional to the admixture of the higher waves in states of the type $^3S_1$–$^3D_1$, $^3P_2$–$^3F_2$, etc. For this reason,the contribution of each following set is, roughly speaking, an order of magnitude smaller than the contribution of the previous one, and overall this leads to the reasonable convergence that was noted in Ref. 36.

As is clear from the formulation of the problem, it is sufficient to take into account the second approximation in order to elucidate the reason for the direct correlations mentioned earlier between the different characteristics of the few-nucleon systems. As was to be expected, an actual admixture of the D wave in the deuteron does not appear directly in our expression. Instead there is, generally speaking, a nonlinear dependence on a different parameter—the D-wave admixture in the $^3S_1$–$^3D_1$ channel of the corresponding reduced Hamiltonian. It is found[37] that both dependences are almost linear, and this, because of the exceptional importance of this channel in the description of few-nucleon systems, leads to the linear correlation that was mentioned. It should be noted here that study of the nature of these dependences is very important in nuclear theory, since only if we go beyond their framework can we hope for a more or less successful description of finite nuclei by means of a single nucleon–nucleon potential. For such potentials, like the Reid potential,[7] or the potentials with a supersoft core of the Orsay group,[38,39] one can reproduce already in the second approximation the fine details of the wave function obtained by solving Faddeev's differential equations for the triton.[36,40] This analysis was based on the use of natural bases for the expansion of nuclear wave functions[41] and the recursive scheme of calculation of the coefficients of fractional parentage,[42] and therefore its detailed exposition would occupy too much space, for which reason it is omitted.

As regards heavier nuclei, beginning with $N=5$ the Pauli principle requires an ever increasing probability of two-nucleon states of negative parity (whereas $w_{\pi=-1} \gtrsim 0.25$ for $N=5$, in the limit $N \to \infty$ we already have $w_{\pi=-1} \gtrsim 0.625$).[43] At the same time, for all the potentials that we have investigated new bound states arise only when $N > 8$. This makes it possible to explain why no single nucleus with $N \leqslant 9$ has more than one bound excited state. Moreover, the majority of them have no bound states at all, or just one such ground state. Of course, we are speaking here only of states that are bound from the point of view of the usually adopted nonrelativistic Hamiltonian of the nucleus, which takes into account only the nucleon–nucleon strong and Coulomb interactions. The significant jump in the number of bound states and in the distance to the nearest thresholds at $N=10$ indicate the relative stability of these and some heavier nuclei and are explained by the appearance of a negative eigenvalue in the $^3P_2$–$^3F_2$ channel. For different potentials this occurs at different $8 < N < 10$, since the phases in the higher states are determined with large errors, and this means that there can be appreciable differences even for potentials that are fairly good from the χ^2 point of view. For this reason the development of effective methods for calculating the probabilities $w_{i,\Lambda}$ is of very great interest. The point is that with increasing energy the phase shift becomes ever less sensitive to the detailed behavior of the potential in the region of its minimum, whereas in the reduced Hamiltonian (11) the levels that play a decisive part in the description of the nuclei sink deeper and deeper into the well with increasing N and depend more and more strongly on the details of its structure. For this reason, the use of nuclear data in such an approach may become an effective tool for more accurate determination of the internucleon potential itself.

With regard to other channels, bound states appear in them in the sequence given above when there is a further increase in the number of nucleons to $N = 20$. Moreover, in this range of N not more than one negative ε appears in any two-particle state. Of course, with increasing j the spread of the results for different potentials is still greater, but the general tendency is maintained—the provision of the necessary number of negative ε by realistic potentials lags well behind the demand for a steadily enlarged set of states essential to ensure the antisymmetry of the wave function, and therefore the total probability of states with $\varepsilon_i > 0$ in the expression (37) becomes greater than the total probability of the bound states in the channels. For the time being the presence of stable nuclei is ensured by the fact that with increasing N the lowest values of ε sink ever deeper into the corresponding wells, while the positive values are grouped near zero in the continuum. However, as is well known, it is not possible to fall below the bottom, and therefore heavy nuclei are either weakly stable or do not exist at all.

Ultimately, the expression (37) correctly reproduces the dependence of the binding energy on the number of nucleons at large N, since the reduced Hamiltonian (11) is essentially a single-particle operator, and the main contribution is made by its N lowest states, i.e., $w \quad \sim N$. On the other hand, $\varepsilon_i \sim N^2$ and therefore $E_\Lambda \sim N$.

Another example of those mentioned above concerns the ground state (^{2}S) of the three-electron lithium atom and the ions of its isoelectron sequence. It is very important from the methodological point of view, since if approximate eigenvalues of the reduced two-electron Hamiltonian (10) are constructed from a certain definite number of basis single-particle states, one can not only completely construct the projection matrix **X** in this approximation and calculate the "exact" spectrum but also verify in the same case the method of approximate solution and the system of lower bounds. In the considered case, when the two-particle functions are constructed from single-particle functions, it is necessary to solve only one dynamical problem, which consists of diagonalizing the matrix of the reduced Hamiltonian. The quality of the result depends here in the first place on the basis of the single-particle functions. Following the recommendations of Ref. 41, they were chosen as an extension, complementing the system of functions that are eigenfunctions for a certain integral operator whose kernel was constructed from two-parameter variational functions. If only single-particle s states are taken into account, such a basis of four functions ensures for the total energies of H$^-$ and He (the reduced two-electron Hamiltonian corresponds to $Z^* = 3/2$, i.e., is intermediate) the following results (all these are absolute values in atomic energy units): 0.5141 and 2.8787 (in the Hartree–Fock approximation the results are 0.4879 and 2.8617, respectively, while the radial limits, i.e., the best results when only the s states are taken into account, are 0.5145 and 2.8790, respectively). The basis set for expanding the components of the wave function of the three-electron atom in this case contains 64 functions. This is equal to the dimension of the matrix **X**, whose rank is 20. It is important that for the calculation of the matrix **X** itself, and also the matrix of the Hamiltonian **E** (28), it is not necessary to calculate even overlap integrals of the basis functions. We illustrate the characteristic final results for the example of the lithium atom. In the Hartree–Fock approximation the total energy is found to be 7.433, while the exact result is 7.478. Our results in the s-wave approximation are equal to the "exact" value 7.454, and the lowest approximation to it is 7.466. Because the rank of **X** is finite, it is not identical to the "exact" one. The uncertainty in the corresponding wave function is 1.4%.

It is well known that widely used methods of calculation of nuclei such as the translationally invariant shell model or the method of hyperspherical functions are of little use when an attempt is made to apply them directly to the calculation of atoms.[44,45] But an atom is a system of electrons between which the interaction is characterized by a repulsive "core" of the same type as in the Reid potential. This circumstance creates both problems, and the concrete results obtained indicate the importance of taking into account the specific nature of the problem already in the initial stages of its solution.

CONCLUSIONS

A large number of very interesting phenomena in many-fermion systems, beginning with the strange features of few-nucleon systems and ending with high-temperature superconductivity, are due to two-particle dynamical correlations generated by fine details of the interaction. Besides these there also exist kinematic (if one may use the expression) correlations due to the need to ensure antisymmetry of the wave functions and the exact quantum numbers of the states of the system. In contrast to the dynamical correlations, these cannot be ignored at all, since without exact quantum numbers it is impossible to identify states, and failure to make the wave function antisymmetric leads to the appearance of spurious, unphysical solutions of the Schrödinger equation. The most laborious operation is the one associated with this last difficulty, and therefore, as a rule, the technique of coefficients of fractional parentage[2,3,46] has always been developed independently of the dynamics of the system, the first consideration having been the simplification of the calculation, the completion of which is always a difficult problem. Most of the higher symmetries convenient for classifying the coefficients of fractional parentage are found, when tested, to be not viable under the conditions of the actual dynamics. Moreover, even if one of them is dominant, it is, as a rule, found that some important features of the system are determined precisely by a small admixture of other states. These contradictions appear particularly strikingly in nuclear theory, in which the dynamical correlations due to the presence of a core play a particularly important part. In other words, the difficulties avoided in the antisymmetrization stage return with new strength in the solution of the dynamical problem.

Ultimately, the method described here reduces in essence to the construction of a computational scheme in which the antisymmetrization (the calculation and spectral expansion of the matrix **X**) is made for a basis adapted to the specific dynamics, since one uses an expansion with respect to eigenfunctions of the reduced two-particle Hamiltonian. It was precisely this stage that was the most laborious in such a formulation of the problem, but the methods described above in Sec. 3 permit a significant simplification of it.

It is seen that the investment of work pays off, since instead of the antisymmetrization of each basis function in the traditional approach it is necessary to antisymmetrize once the entire wave function, in which the dynamical correlations are fully taken into account. This last assertion is based on the fact that if we use the eigenfunctions of the reduced two-particle Hamiltonian, it is no longer necessary to make such operations with the Hamiltonian of the system or its fragments.

An important feature of the method is the nature of the convergence of the eigenvalues. If, as is assumed, each basis function is antisymmetric and an expansion with respect to a complete set of them is used, then when the set is extended, if this is a particular concern, the eigenvalues of the Schrödinger equation converge to the exact values from above. We use a basis of functions that have a degree of antisymmetry of the component, i.e., less than for the wave function. If the rank of the wave function is infinite, then to ensure its antisymmetry it is necessary to use an infinite number of such basis functions. Since this cannot be done in practice, one must use a finite set, and the function belongs to a subspace that is somewhat larger than the subspace of antisymmetric functions. This makes it possible, through special efforts, to ensure uniform convergence from below to the exact values. Whereas in the usually adopted case the nature of the convergence can, as a rule, be gauged only from the proximity of the result to the exact result, for us there is a clear numerical measure for this purpose. Its origin is due to the fact that, whatever the rank of the wave function, it is in any case normalized. If a finite number of basis states is used, it is easy to determine the total weight that the remaining undetermined basis states make to the normalization. This is what is called the degree of uncertainty. Because the basis states are arranged in a definite sequence, knowledge of this quantity permits a conclusion to be drawn about the possible uncertainty of the other characteristics of the system in the studied state.

Ultimately, the reduced-Hamiltonian method leads to the simplest possible expressions for the eigenvalues of the Schrödinger equation (37). This is also of no little importance, since the transparency and clear physical meaning of this expression make it possible to recognize the connection, usually lost as a result of the calculation, between the nature of the two-particle potential and the properties of the many-particle system and to draw qualitative and sometimes even quantitative conclusions about its properties at any stage of the calculation. Here a direct analogy with the problem of a system of noninteracting fermions is suggested. It is well known that the eigenfunctions of the corresponding many-particle Schrödinger equation are determinants if they are constructed from single-particle functions that are eigenfunctions for the corresponding single-particle (reduced single-particle in the adopted terminology) Hamiltonian. In any other case it would be necessary to take a linear combination of determinants, and the solution of the problem, and also the expressions for the eigenvalues, would be significantly more complicated.

Concluding our account, we must also draw attention to one further circumstance. The attentive reader may have noted long ago that in the method of solution the concept of a component has completely disappeared, and the final results can, if one is sufficiently adept, be reproduced by starting directly from the Schrödinger equation. That is so, but this clarity appears only after all the expressions have been written out, and the equations for the components are important in that they indicate the most direct and natural way to obtain them. Undoubtedly, the importance of the equations is not restricted by this; for our derivation concerns only the reduced-Hamiltonian method, i.e., a very specific method of solving them in the special case of bound states, in which the expressions for the components (22) are even more complicated than the expressions for the wave functions (23) and the operation of their intermediate determination becomes meaningless. For any other method of solution the use of the symmetry of the Schrödinger equation for a system of identical particles leads to important simplifications of the problem, since the reduction of this equation to an equation for components, first carried out in the classical work of Faddeev, means, as we have shown above, nothing but the elimination of fragments of the antisymmetrizer from the many-particle Schrödinger equation.

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