The three-body problem: generalized exponential expansion; arbitrary states in a correlated basis, and the binding energy of muonic molecules

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A simple scheme is given for solution of the three-body problem in a correlated basis for states with arbitrary L. An effective correlated basis is proposed, consisting of a generalized exponential expansion. It is shown that the corresponding system of functions is complete. For arbitrary L simple analytic formulas have been obtained for the matrix elements of the Hamiltonian and other typical operators in correlated bases. A reduction of the problem to a system of three-dimensional radial equations of simple form is carried out. The rate of convergence of the expansions in correlated basis functions is studied for muonic-molecule systems. General methods of increasing the accuracy of the variational calculation are pointed out. The usual formulas for the matrix elements of irreducible tensor operators are modified.

1. INTRODUCTION

In Refs. 1 and 2 the levels of three-particle muonic molecules were calculated, including the states responsible for the resonance mechanism of production of $dd\mu$ and $dt\mu$. The properties of the latter states include extremely weak binding, $L \neq 0$, and stringent requirements on accuracy of the calculation. As a result it was necessary to devote attention to the selection and development of a method for solving the problem. In the present work we present for solution of this problem a simple self-consistent scheme of solution of the three-particle problem (with a non-operator interaction) in a correlated basis for states with arbitrary orbital angular momenta L.

In Section 2 we propose an effective three-particle correlated basis—a generalized exponential expansion. It is shown that the corresponding system of functions is complete. We use suitable functions of the three-particle Euler angles Ω.[3] In Section 3 we obtain for arbitrary L general formulas for the matrix elements of the Hamiltonian, corresponding to expansion in such functions. In the Schrödinger equation we have separated the angles Ω, and in the general case it is reduced to a system of three-dimensional radial equations. These equations are much simpler than the analogous equations obtained previously[4] with use of the three-particle D functions $D^{L}_{MM'}(\Omega)$.

In Section 4 we calculate in general form the matrix elements over Ω of the Hamiltonian and other typical operators for arbitrary L. We note in this connection also Refs. 5 and 6. The remaining radial matrix elements are calculated analytically in Section 5 for the basis from Section 2 and for a generalized Hylleraas basis.

In Section 6 we discuss the rate of convergence of the expansions from Section 2, and in particular those for muonic molecules. We indicate general methods of increasing the accuracy of the variational calculation.

In Appendix 2 we indicate the necessary changes of the usual formulas for the matrix elements of irreducible tensor operators. In Appendix 3 we give simple explicit formulas for all matrix elements of the three-particle Coulomb Hamiltonian in states $L = 1^-$. (These states determine the efficiency of muon catalysis of dd and dt reactions.)

The rapid convergence and, of special importance, the possibility of simple analytical calculation of the matrix elements make the expansion given in Section 2 in many cases, apparently, the most effective way to solve the three-particle problem with adequate accuracy. Previously the S and P states of three-particle systems have primarily been considered in the literature, but recently there has been a tendency to study states with larger L values (see for example Ref. 7). Discussion of such states in a correlated basis with an appropriate formalism, however, is extremely difficult, and in this respect the results of the present article are very timely. The results presented are necessary also for solution of the problem of $dt\mu^*(L = 1)$, which is important for muon catalysis.

2. GENERALIZED EXPONENTIAL EXPANSION

Consistent inclusion of two-particle correlations for small $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ frequently is the basic condition for achieving high accuracy. For this purpose one requires a quasifactorized dependence of the basis functions on r_{ij}—a correlated basis. The widely used functions of the Hylleraas type satisfy this requirement. For a long time they were the only means of solution of the Coulomb problem with spectroscopic accuracy. In several studies, however, initially for muonic molecules,[8,9] a competitive exponential S-wave basis was used:

$$\varphi_i = \exp[-\alpha_1(i)r_{23} - \alpha_2(i)r_{13} - \alpha_3(i)r_{12}]. \qquad (1)$$

In Ref. 8 the great technical simplicity resulting from the use of Eq. (1) was demonstrated, and in Ref. 9 it was shown that the resulting expansion converges rapidly. It has no less flexibility than the Hylleraas functions for describing short-range correlations. The rate of convergence depends to a certain degree on the choice of the arguments $\alpha_p(i)$ from Eq. (1). It is possible[10] to make choices which are more efficient than was done in Ref. 9. We note some additional related

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calculations.[1,2,11-13] The basis (1), as is easy to understand, is better suited than the Hylleraas polynomials for describing weakly bound states. Therefore we have also applied this basis to the problem of the weakly bound molecules $dd\mu^*(L=1)$ and $dt\mu^*(L=1)$, generalizing it to $L>0$.[1]

For the purpose of generalizing Eq. (1) to states with any orbital angular momenta L, we propose the expansions

$$\Psi_{LM}=\sum_{l=0}^{L}\sum_{i=1}^{N} C_l(i)\mathcal{Y}_{LM}^{l,L-l}(\mathbf{r}_{13},\mathbf{r}_{23}) \times \exp[-\alpha_{1l}(i)r_{23}-\alpha_{2l}(i)r_{13}-\alpha_{3l}(i)r_{12}], \tag{2a}$$

$$\Psi_{LM}=\sum_{l=1}^{L}\sum_{i=1}^{N} C_l(i)\mathcal{Y}_{LM}^{l,L+1-l}(\mathbf{r}_{13},\mathbf{r}_{23}) \times \exp[-\alpha_{1l}(i)r_{23}-\alpha_{2l}(i)r_{13}-\alpha_{3l}(i)r_{12}]. \tag{2b}$$

Here $C_l(i)$ are the coefficients of the expansion, $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$, and

$$\mathcal{Y}_{LM}^{l_1l_2}(\mathbf{x},\mathbf{y})=x^{l_1}y^{l_2}Y_{LM}^{l_1l_2}(\mathbf{n}_x,\mathbf{n}_y),$$

where

$$Y_{LM}^{l_1l_2}(\mathbf{m},\mathbf{n})=\sum_{m_1+m_2=M} C_{l_1m_1l_2m_2}^{LM}Y_{l_1m_1}(\mathbf{m})Y_{l_2m_2}(\mathbf{n}). \tag{3}$$

The functions (2a) and (2b) correspond to states of parity $(-1)^L$ and $(-1)^{L+1}$. The convenient variables for the work below will be r_{ij} and the Euler angles Ω of the system. The dependence on Ω is contained in the functions $Y_{LM}^{l,L-l}$ and $Y_{LM}^{l,L+1-l}$ from Eq. (2). For a given L, M has $2L+1$ such functions. As was shown in Ref. 3, these functions form a complete system of functions of Ω and therefore can replace $2L+1$ D functions $D_{MM'}^{L}(\Omega)$. Functions of the type $Y_{LM}^{l,L-1}$, $Y_{LM}^{l,L+1-l}$ were used previously for the lowest L values in combination with Hylleraas polynomials in calculations of the atom $^\infty$He. Whereas with use of $D_{MM'}^{L}(\Omega)$ after integration over Ω a three-particle singularity arises in the remaining matrix elements over r_{ij},[4] so that these matrix elements cannot be calculated analytically, when $Y_{LM}^{l,L-1}$, $Y_{LM}^{l,L+1-l}$ is used the corresponding matrix elements are regular, and below we have calculated them analytically. We note also that in Ref. 14 in the problem of two particles in a force field in the case of P states of negative parity, basis functions corresponding to (2a) were constructed; however, we introduced the basis (2) in muonic-molecule calculations[15] before we learned about Ref. 14.

Elucidation of the general properties of the basis from Eq. (2) is not the subject of the present work. We shall prove only the simplest property of completeness. Let the arguments of the exponentials used in (2) satisfy one of the following conditions. We use the notation $\beta_{1l}(i)=\alpha_{2l}(i)+\alpha_{3l}(i)$, etc. Assume 1) that there is an infinite number of $\beta_{pl}(i)$, such that $\beta_{pl}(i)>C$, where C is some positive constant, and

$$\sum_{i=1}^{\infty}(\beta_{pl}(i))^{-1}=\infty.$$

Alternatively 2) let the values of the arguments depend also on N:

$$\alpha_{pl}(i)\to\alpha_{pl}(i,N),\quad \beta_{pl}(i)\to\beta_{pl}(i,N).$$

There exist positive constants C_1 and C_2 such that the number of $\beta_{pl}(i,N)$ lying between them rises without limit as $N\to\infty$. Then the system of basis functions of the form (2) [and (1)] is complete in $L^2(R^6)$: an arbitrary normalizable function $\psi_{LM}(\mathbf{r}_{13},\mathbf{r}_{23})$ can be approximated as accurately as desired by sums of the functions (2) in the sense of smallness of the integral

$$\iint d\mathbf{r}_{13}\,d\mathbf{r}_{23}[\psi_{LM}(\mathbf{r}_{13},\mathbf{r}_{23})-\Psi_{LM}(\mathbf{r}_{13},\mathbf{r}_{23})]^2. \tag{4}$$

The structure of the proof is as follows. Without loss of generality we can consider ψ_{LM} to be falling off exponentially at large r_{ij}. Using an expansion of the type (10) of such ψ_{LM} in $Y^{l\bar{l}}$ and taking into account (12), we integrate the expression (4) over $d\Omega$. We obtain an expression of the form

$$\int d\tau_r \sum_{l,l'} F_{l'l}^{L}\left[f_L{}^{l'}-\sum_i C_{l'}(i)\exp(\ldots')\right] \times\left[f_L{}^{l}-\sum_i C_l(i)\exp(\ldots)\right], \tag{5}$$

where $F_{l'l}^{L}$ is defined below in (14) and f_L^l is from Eq. (10). It is sufficient [cf. Eq. (33)] to establish that it is possible to make the integrals

$$\int\left[f_L{}^{l}-\sum_i C_l(i)\exp(\ldots)\right]^2 r_{13}^{2l+1}r_{23}^{2\bar{l}+1}r_{12}\,dr_{12}\,dr_{13}\,dr_{23} \tag{6}$$

arbitrarily small. We shall separate from f_L^l and the set of exponentials $\exp(\ldots)$ the factor $x=\exp(-\gamma\Sigma r_{ij})$; $f_L^l=\bar{f}_L^l x$, $\exp(\ldots)=\exp(\ldots'')x$, so that $\bar{f}_L^l$ and all $\exp(\ldots'')$ nevertheless fall off exponentially at large r_{ij}. This is possible in view of the statement above regarding f_L^l and $\beta_{pl}(i)$. We use the notation $\omega=r_{13}^{2l+1}r_{23}^{2\bar{l}+1}r_{12}x^2$. Below we shall use the bounded nature of ω. In order to make the integrations independent of each other,[16] we shall go over in addition to the well known parametric coordinates

$$u_1=\tfrac{1}{2}(r_{12}+r_{13}-r_{23}),\quad u_2=\tfrac{1}{2}(r_{12}+r_{23}-r_{13}),$$
$$u_3=\tfrac{1}{2}(r_{13}+r_{23}-r_{12}). \tag{7}$$

(The limits of integration in the variables r_{ij} consist of the three planes $r_{ij}+r_{jk}=r_{ik}$. In the transition to the variables u_i these limits according to Eq. (7) go over into three boundary planes $u_i=0$, which makes the integrations over u_i independent.) As a result we shall rewrite the expression (6) in the form

$$2\int_0^\infty du_1\int_0^\infty du_2\int_0^\infty du_3\left[\bar{f}_L{}^{l}-\sum_{i=1}^{N}C_l(i)\exp\left(-\sum_{p=1}^{3}\beta_{pl}'(i)u_p\right)\right]^2\omega, \tag{8}$$

where $\beta'_{pl}=\beta_{pl}-2\gamma$.

Let us consider first the integrals of the form (8) with $\omega=1$. (This is equivalent to narrowing the class of permissible $\bar{f}_L^l$.) In the case $\omega=1$ the completeness follows from the Müntz approximation theorem. Its three-dimensional formulation which we need is obtained as follows. Let us con-

sider the approximation integral

$$\int_0^1 dt_1 \int_0^1 dt_2 \int_0^1 dt_3 \,[t_1^{k} t_2^{m} t_3^{n} - \sum_{i=1}^{N} c(i)\, t_1^{\beta_{1l}''(i)} t_2^{\beta_{2l}''(i)} t_3^{\beta_{3l}''(i)}]^2, \qquad (9)$$

where $\beta_{pl}'' = \beta_{pl}' - 1/2$. The quantities β_{pl}' satisfy the same conditions as indicated above for β_{pl}. These conditions guarantee the possibility of arbitrarily accurate approximation in the one-dimensional case corresponding to (9) (see Appendix 1). We shall establish the same property in the case (9) by using successive one-dimensional approximations. Since $t_1^k t_2^m t_3^n$ is a closed system of functions in a unit cube, from this the completeness of the system of basis functions $\Pi t_p^{\beta'' pl(i)}$ follows from (9). The usual substitution of variables $t_i = e^{-u_i}$ establishes the completeness of the system of exponentials from (8) in the sense of the integral (8) with $\omega = 1$.

However, from this, as usual,[16] a similar property follows also for any bounded ω. The essential idea is that it is possible as a first step to approximate $\bar{f}_L^l$ by a function $\tilde{f}$ so that the integral of the form (8) with replacement of $\Sigma_{i=1}^N \cdots$ by $\tilde{f}$ is arbitrarily small, and on the other hand so that $(\tilde{f})^2$ is integrable with $\omega = \text{const}$. In view of the boundedness of ω the latter permits the question of approximation, which arises in the integral of the form (8) with $\bar{f}_L^l \to \tilde{f}$ to be reduced to the question for $\omega = 1$ discussed above.

James and Coolidge[16] established the completeness in the sense of (4) of the S-wave Hylleraas basis. Writing formulas of the type (5)–(8), we obtain an analogous completeness property in the case of the basis (10) and (38).

3. STRUCTURE OF THE MATRIX ELEMENTS; RADIAL EQUATIONS

The Schrödinger equation $(H-E)\psi = 0$ goes over into a system of algebraic equations for the coefficients of the expansion (2). Below we calculate the matrix elements which give these equations. The calculations will be carried out for a more general expansion which includes the case (2):

$$\Psi_{LM}(\mathbf{r}_{13}, \mathbf{r}_{23}) = \sum_{l=\varepsilon}^{L} \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{r}_{13}, \mathbf{r}_{23})\, f_L{}^l(r_{12}, r_{13}, r_{23}). \qquad (10)$$

Here and below for brevity we shall use the following notation: $\varepsilon = 0$ and $\varepsilon = 1$ respectively in the cases $\pi = (-1)^L$ and $\pi = (-1)^{L+1}$, $\bar{l} = L + \varepsilon - l$. The desired matrix elements are

$$\int d\tau (\mathcal{Y}_{LM}^{l'\bar{l}'}(\mathbf{r}_{13}, \mathbf{r}_{23}))^* f_L{}^{l'}(r_{12}, r_{13}, r_{23}) \times (H-E)\mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{r}_{13}, \mathbf{r}_{23}) f_L{}^l(r_{12}, r_{13}, r_{23}). \qquad (11)$$

The expression for $d\tau$, as is well known, can be written as

$$d\tau = d\mathbf{r}_{13} d\mathbf{r}_{23} = d\tau_r d\Omega, \qquad (12)$$

$$d\tau_r = r_{12} r_{13} r_{23} dr_{12} dr_{13} dr_{23}, \quad d\Omega = \sin\theta d\theta d\varphi d\psi, \qquad (13)$$

where θ, φ, ψ are angles giving the orientation of the coordinate system rigidly attached to the triangle formed by the three particles, relative to the laboratory system. (The expressions (13) can be obtained as follows. We carry out the integration over $d\mathbf{n}_{23}$ in (12), choosing $\mathbf{n}_{13}$ as the z axis. Then

$$d\mathbf{r}_{13} d\mathbf{r}_{23} = r_{13}^2 dr_{13} \sin\theta_{13} d\theta_{13} d\varphi_{13} r_{23}^2 dr_{23} d\varphi_{23} dx,$$

where x is defined below in (32). Writing $dx = (r_{13} r_{23})^{-1} r_{12} dr_{12}$ and choosing $\theta_{13}, \varphi_{13}, \varphi_{23}$ as the Euler angles, we obtain (13). Here the z' and x' axes corresponding to the movable coordinate system lie in the plane of the triangle formed by the three particles. Other corresponding choices of the Euler angles give the same result (cf. Ref. 17).)

In this section we shall reduce the integration in (11) over $d\Omega$ to standard integrals,

$$F_{l'l}^{L}(r_{12}, r_{13}, r_{23}) = \int d\Omega (\mathcal{Y}_{LM}^{l'\bar{l}'}(\mathbf{r}_{13}, \mathbf{r}_{23}))^* \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{r}_{13}, \mathbf{r}_{23}), \qquad (14)$$

and the matrix elements (11) to integrals over $d\tau_r$ from (13). The Hamiltonian in the center-of-mass system has the form

$$H = k_{13}\Delta_{r_{13}} + k_{23}\Delta_{r_{23}} + 2k_3 \nabla_{r_{13}} \nabla_{r_{23}} + V(r_{12}, r_{13}, r_{23}). \qquad (15)$$

Here and below we use the notation

$$k_i = -\hbar^2 (2m_i)^{-1}, \quad k_{ij} = k_i + k_j. \qquad (16)$$

We take into account that $\mathcal{Y}$ are homogeneous harmonic polynomials:

$$\begin{aligned} &\Delta_{\mathbf{x}} \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}) = \Delta_{\mathbf{y}} \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}) = 0, \\ &(\mathbf{x}\nabla_{\mathbf{x}}) \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}) = l \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}), \\ &(\mathbf{y}\nabla_{\mathbf{y}}) \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}) = \bar{l} \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}), \end{aligned} \qquad (17)$$

and we shall also use the following properties:

$$(\nabla_{\mathbf{x}} \nabla_{\mathbf{y}}) \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}) = 0, \qquad (18)$$

$$\begin{aligned} &(\nabla_{\mathbf{x}} y) \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}) = A(l, \bar{l}) \mathcal{Y}_{LM}^{l-1,\bar{l}+1}(\mathbf{x}, \mathbf{y}), \\ &(\mathbf{x}\nabla_{\mathbf{y}}) \mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{x}, \mathbf{y}) = A(\bar{l}, l) \mathcal{Y}_{LM}^{l+1,\bar{l}-1}(\mathbf{x}, \mathbf{y}), \end{aligned} \qquad (19)$$

$$A(l, \bar{l}) = [(l-\varepsilon)(\bar{l}+1-\varepsilon)(2l+1)(2\bar{l}+3)^{-1}]^{1/2}. \qquad (20)$$

Equation (18) follows from the fact that the action of the operator from (18) on $\mathcal{Y}_{LM}^{l_1 l_2}(\mathbf{x},\mathbf{y})$ obviously gives $\Delta L = 0$, $\Delta l_1 = \Delta l_2 = -1$. However, in the cases $l_1 + l_2 = L$ or $l_1 + l_2 = L + 1$, as in (18), this would give $l_1' + l_2' < L$, so that we obtain zero. The relations (19) are obtained from similar considerations, and the quantity (20) is calculated below.

We next introduce the notation

$$\partial_{ij} = \frac{1}{r_{ij}} \frac{\partial}{\partial r_{ij}}, \qquad \hat{L}_{ij} = \frac{\partial^2}{\partial r_{ij}^2} + \frac{2}{r_{ij}} \frac{\partial}{\partial r_{ij}}.$$

If we write (15) as $\hat{T} + V$, then straightforward calculations with inclusion of Eqs. (17)–(19) give

$$\begin{aligned} &\hat{T}[\mathcal{Y}_{LM}^{l\bar{l}}(\mathbf{r}_{13}, \mathbf{r}_{23}) f_L{}^l(r_{12}, r_{13}, r_{23})] \\ &= (\hat{O}_1{}^l f_L{}^l) \mathcal{Y}_{LM}^{l\bar{l}} + (\hat{O}_2{}^l f_L{}^l) \mathcal{Y}_{LM}^{l-1,\bar{l}+1} + (\hat{O}_3{}^l f_L{}^l) \mathcal{Y}_{LM}^{l+1,\bar{l}-1}, \end{aligned} \qquad (21)$$

where the operators are

$$\hat{O}_1{}^l = \hat{O}_0 + 2[k_{13} l \partial_{13} + k_{23} \bar{l} \partial_{23} + (k_1 l + k_2 \bar{l}) \partial_{12}], \qquad (22)$$

$$\hat{O}_2{}^l = 2A(l, \bar{l})(k_3 \partial_{23} - k_1 \partial_{12}), \quad \hat{O}_3{}^l = 2A(\bar{l}, l)(k_3 \partial_{13} - k_2 \partial_{12}). \qquad (23)$$

In Eq. (22), $\hat{O}_0$ is the well known operator for the S state:

$$\hat{O}_0 = k_{12}\hat{L}_{12} + k_{13}\hat{L}_{13} + k_{23}\hat{L}_{23} + k_1(r_{12}^2 + r_{13}^2 - r_{23}^2)\partial_{12}\partial_{13} + k_2(r_{12}^2 + r_{23}^2 - r_{13}^2)\partial_{12}\partial_{23} + k_3(r_{13}^2 + r_{23}^2 - r_{12}^2)\partial_{13}\partial_{23}. \quad (24)$$

Using (21) and the definition (14), we obtain for the desired matrix elements (11) the following expression:

$$\int d\tau_r f_L{}^{l'}(r_{12}, r_{13}, r_{23}) [F^L_{l'l}(r_{12}, r_{13}, r_{23})(\hat{O}_1{}^l + V - E) + F^L_{l',l-1}(r_{12}, r_{13}, r_{23})\hat{O}_2{}^l + F^L_{l',l+1}(r_{12}, r_{13}, r_{23})\hat{O}_3{}^l] f_L{}^l(r_{12}, r_{13}, r_{23}). \quad (25)$$

The quantities (14) entering into (25) are given in Section 4; the final calculation of the matrix elements (25) is carried out in Section 5. The expression (25) has been obtained in a form which does not reveal explicit symmetry in l and l', which is dictated by the requirement of simplicity of the answer. Symmetry in l and l' can be used as a test in the numerical calculations.

We note also that the calculations which have been made permit reduction of the Schrödinger equation to a system of simple $(L-\varepsilon)$ three-dimensional "radial" equations. For this purpose we equate to zero the coefficients of the expansion of the quantity $(H-E)\Psi_{LM}$ in $\mathcal{Y}^{\overline{II}}_{LM}$ using (21)–(23). We obtain the following equations:

$$(\hat{O}_1{}^l + V - E) f_L{}^l + \hat{O}_2{}^{l+1} f_L{}^{l+1} + \hat{O}_3{}^{l-1} f_L{}^{l-1} = 0, \quad l = \varepsilon, \ldots, L. \quad (26)$$

Here in (26) $f^\lambda_L = 0$ for $\lambda < \varepsilon$ and $\lambda > L$. Solving (26), it is convenient to go over in the operators (22) and (23) to the coordinates (7). (For $\hat{O}_0$ in (24) see Ref. 18.)

If particles (1) and (2) are identical: $(1\hat{2})\Psi_{LM} = \pm\Psi_{LM}$, where $(\hat{1}\,\hat{2})$ is the transposition of the particles, then when the relation

$$(1\hat{2})\ \mathcal{Y}^{l\bar{l}}_{LM} = \mathcal{Y}^{\bar{l}l}_{LM}(-1)^\varepsilon$$

is included in the treatment we should have

$$(1\hat{2})\ f_L{}^l(r_{12}, r_{13}, r_{23}) = (\pm)(-1)^\varepsilon f_L{}^{\bar{l}}(r_{12}, r_{13}, r_{23}). \quad (27)$$

This permits representation of (10), for example, in the form

$$\Psi_{LM} = [1 \pm (1\hat{2})] \sum_{l=\varepsilon}^{[1/2(L+\varepsilon)]} \mathcal{Y}^{l\bar{l}}_{LM}(\mathbf{r}_{13}, \mathbf{r}_{23}) f_L{}^l(r_{12}, r_{13}, r_{23}), \quad (28)$$

where $[\ldots]$ is the integral part of the number and f^l_L, in contrast to (10), already do not obey the requirement of symmetry. In (25) instead of $f_L{}^{l'}F^L_{l'l}$ and $f_L{}^{l'}F^L_{l',l\pm1}$ we have respectively

$$2[f_L{}^{l'}(r_{12}, r_{13}, r_{23})F^L_{l'l}(r_{12}, r_{13}, r_{23}) \pm (-1)^\varepsilon f_L{}^{l'}(r_{12}, r_{13}, r_{23})F^L_{\bar{l}'l}(r_{12}, r_{13}, r_{23})]$$

and the same expressions with $l \to l \pm 1$. Here $l \leqslant [\frac{1}{2}(L+\varepsilon)]$, $l' \leqslant [\frac{1}{2}(L+\varepsilon)]$.

4. ANGULAR MATRIX ELEMENTS

Together with the quantities (14) and (20) we shall consider also the matrix elements of other typical operators. A quantity of the form (14) was calculated in Ref. 5a and partly in Ref. 6. In Ref. 5b more general angular matrix elements containing the operator $Y^{k_1k_2}_{KQ}(\mathbf{n}_{13}, \mathbf{n}_{23})$ were also calculated. [Here the Y were defined as in (3).] We shall present expressions for these matrix elements in a somewhat different form. The method of derivation (of the type in Ref. 5a) is substantially simpler than that in Ref. 5b.

Let us consider the quantity

$$\int d\Omega\, Y^{l_1'l_2'}_{L'M'}(\mathbf{n}_{13}, \mathbf{n}_{23}) Y^{k_1k_2}_{KQ}(\mathbf{n}_{13}, \mathbf{n}_{23}) Y^{l_1l_2}_{LM}(\mathbf{n}_{13}, \mathbf{n}_{23}), \quad (29)$$

which contains all three of the Y symmetrically. The desired matrix element contains $(Y^{l_1'l_2'}_{L'M'})^*$ and is obtained from (29) by the substitution $M' \to -M'$ and multiplication by $(-1)^{l_1'+l_2'+L'-M'}$. Let us expand the product $Y^{l_1'l_2'}_{L'M'}$, $Y^{l_1l_2}_{LM}$ of bipolar harmonics from (29) in series in $Y^{\lambda_1\lambda_2}_{L'',M+M'}$ (see the formulas in Ref. 19). We expand the products arising as a result $Y^{\lambda_1\lambda_2}_{L'',M+M'}$, $Y^{k_1k_2}_{KQ}$ again in series in $Y^{\lambda\lambda''}_{JM_j}$. However, of the latter series only the terms with $J=0$ can give a nonzero contribution to the integral (29). These terms have the form $Y^{\lambda\lambda}_{00}$, i.e., $\lambda'' = \lambda$ in them. They arise only from the contributions with $L'' = K$. These terms themselves do not depend on Ω:

$$Y_{00}{}^{\lambda\lambda}(\mathbf{m}, \mathbf{n}) = (4\pi)^{-1}(-1)^\lambda(2\lambda+1)^{1/2}P_\lambda(\mathbf{mn}).$$

As a result, $9j$ symbol with a zero element simplifies and we obtain for the quantity (29) the expression

$$\delta_{M+M'+Q,0}\begin{pmatrix} L' & K & L \\ M' & Q & M \end{pmatrix}\sum_\lambda a_\lambda P_\lambda(x), \quad (30)$$

$$a_\lambda = (8\pi)^{-1}(-1)^{K+\lambda} \times\{[L'][L][K][l_1'][l_2'][l_1][l_2][k_1][k_2]\}^{1/2}[\lambda] \times\sum_{\lambda_1\lambda_2}[\lambda_1][\lambda_2]\begin{pmatrix} l_1' & l_1 & \lambda_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_2' & l_2 & \lambda_2 \\ 0 & 0 & 0 \end{pmatrix} \times\begin{pmatrix} \lambda & k_1 & \lambda_1 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \lambda & k_2 & \lambda_2 \\ 0 & 0 & 0 \end{pmatrix} \times\begin{Bmatrix} k_1 & k_2 & K \\ \lambda_2 & \lambda_1 & \lambda \end{Bmatrix}\begin{Bmatrix} l_1' & l_2' & L' \\ l_1 & l_2 & L \\ \lambda_1 & \lambda_2 & K \end{Bmatrix}, \quad (31)$$

where $[p] = 2p+1$. In (30) and below we use the notation

$$x = \mathbf{n}_{13}\mathbf{n}_{23} = (2r_{13}r_{23})^{-1}(r_{13}^2 + r_{23}^2 - r_{12}^2). \quad (32)$$

Drake[5b] used a diagram technique to obtain an expression which, if we take it in the form (29) and take into account the symmetry properties of the $3j$ and $9j$ symbols, is obtained from (30) and (31) by interchange of the set of four numbers l_1', l_2', L', M' and k_1, k_2, K, Q. In view of the symmetry of (20) this substitution is permissible. Expression (29) includes a matrix element of the operator $P_k(\mathbf{n}_{13}, \mathbf{n}_{23}) \propto Y^{kk}_{00}(\mathbf{n}_{13}, \mathbf{n}_{23})$. For this case (31) can be simplified, for which the form (31) is particularly convenient, and not the form given in Ref. 5b. Setting $K=0$ in (31), we have, as should be the case, $L' = L$, $\lambda_1 = \lambda_2$, and the $9j$ symbol reduces to a $6j$ symbol.[19] For the quantity (14), in particular, we have (here $k_1 = k_2 = K = 0$, $\lambda_1 = \lambda_2 = \lambda$)

$$F_{l'l}^{L}=r_{13}^{l+l'}\,r_{23}^{\bar{l}+\bar{l}'}\cdot{}^{1}/_{2}(-1)^{L}\{[l][l'][\bar{l}][\bar{l}']\}^{1/2}$$

$$\times\sum_{\lambda}(-1)^{\lambda}[\lambda]\begin{pmatrix} l & l' & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \bar{l} & \bar{l}' & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l' & \bar{l}' & L\\ \bar{l} & l & \lambda\end{Bmatrix}P_{\lambda}(x). \quad (33)$$

Here the $6j$ symbol is degenerate.[19] To simplify a formula of the type (31) in the case of the operator $Y_{kq}(\mathbf{n}_{13})\infty Y_{kq}^{k0}$ it is convenient to use the form given in Ref. 5b. In the expression of Ref. 5b for the matrix element of this operator it is necessary to omit the factor $(2k+1)^{1/2}$.

The matrix elements of a number of operators which depend on the momenta were discussed in Ref. 5b, but there functions of the form $Y_{LM}^{l_1l_2}(\mathbf{n}_x,\mathbf{n}_y)$ were used, where l_1 and l_2 are arbitrary, and not the functions $\mathscr{Y}_{LM}^{ll}(\mathbf{x},\mathbf{y})$. This greatly complicates the formulas, since the properties (17)–(19) no longer hold. To obtain (20) we shall use Appendix 2. We write, corresponding to (A.2),

$$(\nabla)_{\mu}\mathscr{Y}_{lm}(\mathbf{x})=-C_{lm1\mu}^{l-1,m'}(2l+1)\left(\frac{l}{2l-1}\right)^{1/2}\mathscr{Y}_{l-1,m'}(\mathbf{x}), \quad (34)$$

$$y_{\mu}\mathscr{Y}_{lm}(\mathbf{y})=C_{lm1\mu}^{l+1,m'}\left(\frac{l+1}{2l+3}\right)^{1/2}\mathscr{Y}_{l+1,m'}(\mathbf{y})$$

$$-C_{lm1\mu}^{l-1,m'}\left(\frac{l}{2l-1}\right)^{1/2}\mathscr{Y}_{l-1,m'}(\mathbf{y}).$$

Here

$$m'=m+\mu, \quad \mathscr{Y}_{lm}(\mathbf{r})=r^{l}Y_{lm}(\mathbf{n}).$$

By means of (A.7), taking into account that $\mathbf{x}\nabla_y=(x^{(1)}\cdot\nabla_y^{(1)})$, we directly calculate (20). We can proceed similarly in the other cases. For example, for the operator $[\mathbf{r}_{13}\nabla_{r23}]$, which enters into the Breit interaction, there is a formula of the same structure as (19), but the coefficient in this formula is calculated by means of (34) and (A.6). In addition to this operator and the operators from (17)–(19) in calculation of the matrix element from the Breit interaction it is necessary to consider the spin-orbit term $r_{12}^{-3}\mathbf{r}_{12}(\mathbf{r}_{12}\nabla_{r13})\nabla_{r23}$. The resulting contribution to the matrix element is easy to calculate if we rewrite this term in the form

$$r_{12}^{-3}[(\mathbf{r}_{13}\nabla_{r_{13}}-\mathbf{r}_{23}\nabla_{r_{23}}-1)(\mathbf{r}_{13}\nabla_{r_{23}}-\mathbf{r}_{23}\nabla_{r_{23}})], \quad (35)$$

acting successively with both factors enclosed in the brackets of (35) on $\mathscr{Y}_{LM}^{ll}f_L^l$, and using (17) and (19).

5. RADIAL MATRIX ELEMENTS

In the case in which (10) is the basis (2), the contribution to (25) of the kinetic energy and the contribution proportional to E, when (22), (23), and (33) are taken into account, reduce to integrals of the form

$$I_{\lambda}^{(N)}(n_1,n_2)=\int_0^{\infty}dr_{13}\int_0^{\infty}dr_{23}\int_{|r_{13}-r_{23}|}^{r_{13}+r_{23}}dr_{12}\,r_{13}^{n_1}r_{23}^{n_2}$$

$$\times\, r_{12}^{N-n_1-n_2}\exp(-ar_{12}-br_{13}-cr_{23})P_{\lambda}(x), \quad (36)$$

where the powers n_1 and n_2 take the values $l+l'$ and $\bar{l}+\bar{l}'$ or values greater by unity, and $N-n_1-n_2$ is equal to zero or unity. The contribution of V from (25) also reduces to integrals of the same form if V is the sum of the Coulomb interactions of the particles or, for example, the sum of short-range pairing interactions of the form[1)]

$$V(r_{ij})=\sum_p c_p\exp(-\gamma_p r_{ij}),$$
$$V(r_{ij})=\frac{1}{r_{ij}}\sum_p c_p\exp(-\gamma_p r_{ij}). \quad (37)$$

The matrix elements also reduce to integrals of the form (36) in the case in which in (10) the f_L^l are polynomials of the Hylleraas type:

$$f_L{}^{l}=\exp(-\alpha_{1l}r_{23}-\alpha_{2l}r_{13}-\alpha_{3l}r_{12})\sum_{m,n,p}c(m,n,p)\,r_{13}^{m}r_{23}^{n}r_{12}^{p}. \quad (38)$$

The expansion (10) and (38) generalizes the two-electron basis used in problems of the $^{\infty}$He type to the three-particle problem.

The values of λ in (36) are smaller than $L+\varepsilon$. In the case of the lowest L, calculation of (36) is easily carried out by expanding $P_{\lambda}(x)$ in powers of x and using (32). Since in (36) $\lambda\leqslant n_1$ and $\lambda<n_2$, as a result we have an integral of a polynomial in r_{ij} of low degree, multiplied by the exponential from (36). Such integrals are easily calculated analytically [see (40) and (41) below]. This also completes the calculation of the matrix elements (14). In Appendix 3 we have given explicit formulas for these matrix elements in the extremely important case $L=1$, $\pi=-1$.

In the case of higher L, the method described above for calculation of (36) is cumbersome. Furthermore, the general method from Ref. 5b when applied to (36) gives a recurrence relation with coefficients which depend on a, b, c, and with a number of terms which increases in each step. We shall give a simpler method. In (36) we write

$$P_{\lambda}(x)=\lambda^{-1}[(2\lambda-1)xP_{\lambda-1}(x)-(\lambda-1)P_{\lambda-2}(x)]$$

and then use (32). Using the notation

$$\delta I_l^{(N)}(n_1,n_2)=I_l^{(N)}(n_1+1,n_2-1)+I_l^{(N)}$$
$$\times(n_1-1,n_2+1)-I_l^{(N)}(n_1-1,n_2-1),$$

we obtain the recurrence relation

$$I_{\lambda}^{(N)}(n_1,n_2)=\lambda^{-1}[(\lambda-{}^{1}/_{2})\delta I_{\lambda-1}^{(N)}(n_1,n_2)-(\lambda-1)I_{\lambda-2}^{(N)}(n_1,n_2)], \quad (39)$$

where $\lambda>1$ and

$$I_1^{(N)}(n_1,n_2)={}^{1}/_{2}\delta I_0^{(N)}(n_1,n_2).$$

Equation (39) permits expression of the integrals (36) in terms of a set of $\frac{1}{2}(N+1)(N+2)$ integrals with $\lambda=0$:

$$I_0^{(N)}(n_1,n_2)=\int_0^{\infty}dr_{13}\int_0^{\infty}dr_{23}\int_{|r_{13}-r_{23}|}^{r_{13}+r_{23}}dr_{12}\,r_{13}^{n_1}r_{23}^{n_2}r_{12}^{N-n_1-n_2}$$

$$\times\exp(-ar_{12}-br_{13}-cr_{23}). \quad (40)$$

[In the case of the basis (2) we need $N=2(L+\varepsilon)+2$ and $N=2(L+\varepsilon)+3$.] Going over to integration over the parametric coordinates (7), the integrals (40) are easily represented in the form[6]

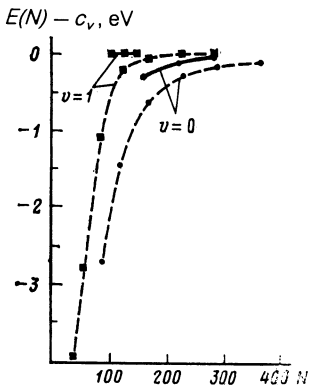

FIG. 1. Calculated binding energies $E(N)$ of the $dd\mu$ molecule in states with $L = 1$ as a function of the number of basis functions N. We have given the values $E(N) - c_v$, where $c_{v=0} = 226.7$ eV and $c_{v=1} = 1.97$ eV. The solid lines are the generalized exponential expansion (2a), and the dashed lines are the basis of the Hylleraas type from Ref. 21 of the form from Ref. 4.

$$I_0^{(N)}(n_1, n_2) = \frac{\partial^{N-n_1-n_2}}{\partial a^{N-n_1-n_2}} \frac{\partial^{n_1}}{\partial b^{n_1}} \frac{\partial^{n_2}}{\partial c^{n_2}} \left[\frac{2}{(a+b)(a+c)(b+c)} \right]. \tag{41}$$

A simple recurrence method of calculation of the set of quantities (41) is given in Ref. 20, which completes our calculation of the matrix elements (14).[2)]

6. APPLICATIONS, MUONIC MOLECULE SYSTEMS

The possibilities of the method discussed are partly demonstrated by the results of Refs. 1 and 2.[3)] We shall therefore confine ourselves to a few remarks. In Fig. 1 the rate of convergence of the expansion (2) for the $dd\mu$ system with $L = 1^-$ is compared with the same thing for a basis of the Hylleraas type[4] from Ref. 21. The results for the weakly bound state ($v = 1$) were calculated by Frolov in a supplement to the data in Ref. 2, and those for the ground state ($v = 0$) were taken from Ref. 1. The nonlinear parameters determining the argument of the exponentials from (2) (cf. below) were taken here to be the same for all N.

In Table I we have given the $tp\mu$ binding energies obtained by Frolov in the basis (2), which are considerably more accurate than the earlier ones.[1] The mass values are the same as in Ref. 1. The case of $tp\mu$ was chosen because it is one of the most unfavorable for this method. The "final" results were obtained by doing additional calculations for the same N (cf. Ref. 2), and the extrapolation to $N = \infty$ was as in Refs. 2 and 9. The results for $L = 0$ are considerably more accurate than the corresponding result from Ref. 21 of the Hylleraas type 213.829 eV with $N = 440$ (and all others in the literature). The results for $L = 1$ are less accurate than the result[21] 99.119 eV with $N = 440$, but their extrapolation shows that comparable accuracy will be achieved here. The results of Refs. 9 and 12, like the calculations of Frolov, show that the basis (1) provides high accuracy not only for the energy, but also for other typical observables, including the accuracy with which $\langle \delta(r_{ij}) \rangle$ is calculated.

The arguments $\alpha_{pl}(i)$ of the basis exponentials from (2) can be chosen as follows. A finite region $\{\alpha_{1l}, \alpha_{2l}, \alpha_{3l}\}$ is chosen in three-dimensional space, and the arguments are given quasirandomly inside this region, while its boundaries are optimized. A similar choice was used for the $^\infty$He atom[10–12] and was carried over to the basis (1) with $L = 0$ in Ref. 13. The number of optimized parameters was six. In Refs. 1 and 2 a similar selection was used with a number of parameters reduced basically to three. In the case of the He atom this is roughly equivalent to merely doubling the number of basis functions (cf. Ref. 2 with Ref. 12). Previously[9] a regular selection of the parameters in (1) was made: $\alpha_p(i) = c_p i$. For the ground states these selections give comparable results, but for the weakly bound states the quasirandom selection is preferable (the calculations of Frolov).

In our muon-molecule calculations,[15] which were carried out at the beginning of 1983, all $\alpha_{pl}(i)$, following the well known method, were optimized by means of random search. However, with reasonable calculation times this optimization is illusory and this method is not effective.

The arguments α_{pl} can also be negative, provided only that $\alpha_{pl} + \alpha_{ql} > 0$ for all p and q. This can be seen if one goes over to the variables (7).

The rate of convergence of expansions of the type (1) and (2) [or (10) and (38)] is well known to drop rapidly when we go over to adiabatic systems[4)] such as H_2^+. The reason is that the distribution in r_{12} in this case has a sharp peak near the point $r_{12} = (r_{12})_0$ corresponding to an equilibrium configuration of the nuclei. Since $(r_{12})_0 \neq 0$, to describe this peak it is necessary to have many basis exponentials. This applies also to muonic molecules.[22] The convergence can be accelerated in the following way. The following formal scheme of taking into account correlations was suggested in Ref. 23. The expansion $\Psi = \Sigma c_i \varphi$ is replaced by $\omega\Psi$, where ω is some function and $\omega = \Sigma_j a_j \overline{\varphi}_j$. This is equivalent

TABLE I

N	$L=0$	$L=1$
200	213.83914	99.02588
225	213.83945	99.05917
250	213.83978	99.07672
275	213.83986	99.08659
300	213.83992	99.09930
325	–	99.11017
350	–	99.11493
∞	213.8400	99.120

Note. The final results are: $L = 0$, 213.841 ± 0.001 eV; $L = 1$, 99.120 ± 0.005 eV.

to going over from a basis φ_i to the basis $(\Sigma_j a_j \overline{\varphi}_j)\varphi_i$. In our case we can take as $\omega = \omega(r_{12})$ a function which describes at least crudely the adiabatic motion of the nuclei, approximating it by exponentials:

$$\omega = \sum_j a_j \exp(-\gamma_j r_{12}).$$

As a result the basis exponentials in (2) are replaced by the functions

$$\sum_j a_j \exp[-\alpha_{1l}(i) r_{23} - \alpha_{2l}(i) r_{13} - (\alpha_{3l}(i) + \gamma_j) r_{12}].$$

A limitation on the increase of the number of basis functions N used in the calculation is imposed by loss of stability in solution of the system of algebraic equations which arise. Methods of the inverse-iteration type used in Refs. 1 and 2, as in Ref. 21, permit an advance to larger N but do not remove the difficulty completely. The following scheme may be useful here. If φ_i are the initial basis functions and one obtains

$$\Psi_1 = \sum_{i=1}^{N} c_i^{(1)} \varphi_i,$$

then instead of a further increase in the number of functions φ_i in the expansion we find

$$\Psi_2 = a\Psi_1 + \sum_{i=1}^{N} c_i^{(2)} \varphi_i^{(2)}, \ldots, \qquad \Psi_M = a\Psi_{M-1} + \sum_{i=1}^{N} c_i^{(M)} \varphi_i^{(M)},$$

where a and $c_i^{(M)}$ are the desired expansion coefficients and $\varphi_i^{(M)} \neq \varphi_i^{(M')}$ are the basis functions of the type entering into (2). In this way all new basis functions are connected and the result is improved without increasing the dimensions of the energy matrix.

The authors thank A. M. Frolov for carrying out the numerical calculations involved in Section 6. A question from L. D. Faddeev stimulated our discussion of the properties of the basis (2).

APPENDIX 1

A proof of the completeness of the system of functions $t^{\beta(i)-1/2}$ in the region [0,1], for the case in which the $\beta(i)$ satisfy a condition such as the condition (1) from Section 2, can be found for example in Ref. 24. We shall establish the completeness of this system for the case of the condition (2) from Section 2 (which occurred in the numerical calculations; see Section 6). Between the constants C_1 and C_2 determined in Section 2 let there be arguments with numbers 1, 2, . . . , $M(N)$. The completeness of the corresponding subsystem of functions is equivalent to fulfillment of the condition[24]

$$\lim_{N\to\infty} \prod_{i=1}^{M(N)} [n+1/2-\beta(i,N)]^2 [n+1/2+\beta(i,N)]^{-2} = 0, \qquad (A.1)$$

where $n \geqslant 0$ is any integer. Each factor from (A1) can be majorized by the quantity

$$[n+1/2-C]^2 [n+1/2+C]^{-2} < 1,$$

where C is one of the limiting values $C_1 > 0$ and $C_2 > 0$. From this equation (A1) also follows.

APPENDIX 2

The standard formulas for the matrix elements of tensor operators which are irreducible with respect to three-dimensional rotations can be represented in a form which is somewhat more general than in the usual handbooks and which is necessary for our calculations. For example, let $\varphi^{(1)}_{j_1 m_1}(\{x\})$ and $\varphi^{(2)}_{j_2 m_2}(\{y\})$ be functions with fixed j and m, and let $\hat{P}^{(1)}_{k_1 q_1}$ and $\hat{P}^{(2)}_{k_2 q_2}$ be irreducible tensor operators acting respectively on the variables $\{x\}$ and $\{y\}$. Let $\chi^{(1)}_{j_1' m_1'}(\{x\})$ and $\chi^{(2)}_{j_2' m_2'}(\{y\})$ be functions defined by means of the expansions

$$\hat{P}^{(i)}_{k_i q_i} \varphi^{(i)}_{j_i m_i} = \sum_{j_i'} C^{j_i', m_i+q_i}_{j_i m_i k_i q_i} \chi^{(i)}_{j_i', m_i+q_i}. \qquad (A.2)$$

We use the further notation

$$[\varphi^{(1)}_{j_1} \varphi^{(2)}_{j_2}]_{JM} = \sum_{m_1+m_2=M} C^{JM}_{j_1 m_1 j_2 m_2} \varphi^{(1)}_{j_1 m_1} \varphi^{(2)}_{j_2 m_2}, \qquad (A.3)$$

$$[\chi^{(1)}_{j_1'} \chi^{(2)}_{j_2'}]_{J'M'} = \sum_{m_1'+m_2'=M'} C^{J'M'}_{j_1' m_1' j_2' m_2'} \chi^{(1)}_{j_1' m_1'} \chi^{(2)}_{j_2' m_2'}, \qquad (A.4)$$

$$\{\hat{P}^{(1)}_{k_1} \hat{P}^{(2)}_{k_2}\}_{Kq} = \sum_{q_1+q_2=q} C^{Kq}_{k_1 q_1 k_2 q_2} \hat{P}^{(1)}_{k_1 q_1} \hat{P}^{(2)}_{k_2 q_2}. \qquad (A.5)$$

Then, for example, the following relation is valid:

$$\{\hat{P}^{(1)}_{k_1} \hat{P}^{(2)}_{k_2}\}_{Kq} [\varphi^{(1)}_{j_1} \varphi^{(2)}_{j_2}]_{JM} = [(2J+1)(2K+1)]^{1/2}$$

$$\times \sum_{j_1' j_2' J'} C^{J', M+q}_{JMKq} [(2j_1'+1)(2j_2'+1)]^{1/2} \times \begin{Bmatrix} k_1 & k_2 & K \\ j_1' & j_2' & J' \\ j_1 & j_2 & J \end{Bmatrix} [\chi^{(1)}_{j_1'} \chi^{(2)}_{j_2'}]_{J', M+q}. \qquad (A.6)$$

In particular, if we define

$$(\hat{P}^{(1)}_k \cdot \hat{P}^{(2)}_k) = (-1)^k (2k+1)^{1/2} \{\hat{P}^{(1)}_k \hat{P}^{(2)}_k\}_{00},$$

then we have

$$(\hat{P}^{(1)}_k \cdot \hat{P}^{(2)}_k)[\varphi^{(1)}_{j_1} \varphi^{(2)}_{j_2}]_{JM} = \sum_{j_1' j_2'} (-1)^{j_1+j_2'+J} [(2j_1'+1)(2j_2'+1)]^{1/2} \times \begin{Bmatrix} j_1' & j_1 & k \\ j_2' & j_2 & J \end{Bmatrix} [\chi^{(1)}_{j_1'} \chi^{(2)}_{j_2'}]_{JM}. \qquad (A.7)$$

Usually, assuming the basis of the type (A.3) to be orthonormalized, a relation for the matrix elements of the operator (A.5) is given in this basis. It is a particular case of (A.6). The metric properties of the functions (A.3) and (A.4) for validity of relations such as (A.6) are obviously unimportant in reality.

APPENDIX 3

For the case $L = 1$, $\pi = -1$ we shall give explicit formulas for the matrix elements of the nonrelativistic Coulomb Hamiltonian of three particles in the basis (2).[5] Here there are only two types of states: with $l = 1$ and with $l = 0$.

We shall denote them respectively as $\psi_i^{(13)}$ and $\psi_i^{(23)}$. The functions $\psi_i^{(p3)}$ used below differ from the corresponding basis functions from (2a) by numerical factors $12^{-1/2}(-1)^{1-l}$.

The matrix elements are expressed in terms of polynomials of quantities of the form

$$x_p=[\alpha_q(i)+\alpha_q(i')+\alpha_r(i)+\alpha_r(i')]^{-1}.$$

Here and below the numbers p, q, and r are any permutation of the numbers 1, 2, and 3. Notations of the form $\alpha_p(i),\alpha_p(i')$ replace notations of the form $\alpha_{pl}(i),\alpha_{pl'}(i')$ from (2); $\alpha_p(i)$ are arguments corresponding to the functions $\psi_i^{(13),(23)}$, and $\alpha_p(i')$, are arguments corresponding to the functions $\psi_{i'}^{(13),(23)}$. For brevity we shall use also the notation

$$X=x_1x_2x_3, \quad x_{ij}=x_i+x_j, \quad x_{ij}^{(n)}=x_i^n+x_j^n.$$

For the overlap integrals we obtain the expressions ($p=1,2$)

$$\langle\psi_{i'}^{(p3)}|\psi_i^{(p3)}\rangle=X\{x_q^2x_{p3}(x_{p3}^{(2)}+x_px_3)+2[x_p^4x_{q3}+x_3^4x_{pq}+X(x_{p3}^{(2)}+x_px_3)]+3x_p^2x_3^2x_{p3}\},$$

$$\langle\psi_{i'}^{(13)}|\psi_i^{(23)}\rangle=X[2x_3^4x_{12}+2x_3^3x_{12}^{(2)}+x_3^2x_{12}^{(3)}-x_1^2x_2^2x_{12}+Xx_3(x_{13}+x_{23})].$$

To write the further formulas we shall use the auxiliary polynomials

$$F(q)=1/6[2x_q^2x_{p3}^{(2)}+4x_p^2x_3^2+3x_p^3x_{q3}+3x_3^3x_{pq}+X(2x_q+3x_{p3})],$$

$$G(p,q,r)=1/2[x_p^3x_{qr}+x_r^3(3x_p+x_q)+4x_r^4+2x_p^2x_r^2+Xx_{pr}],$$

$$H(p,q,r)=1/6[3x_r^3x_{pq}+2x_r^2(x_p^2+2x_q^2)+3x_q^3(x_r-x_p)-2x_p^2x_q^2+X(x_q+3x_r)]. \qquad (A.8)$$

For the matrix elements of the Coulomb energy

$$V=\sum_{i<j}e_ie_jr_{ij}^{-1}$$

we obtain the expressions ($p=1,2$)

$$\langle\psi_{i'}^{(p3)}|V|\psi_i^{(p3)}\rangle=X[e_pe_3F(q)+e_1e_2G(p,q,3)+e_qe_3G(3,q,p)],$$

$$\langle\psi_{i'}^{(13)}|V|\psi_i^{(23)}\rangle=X[e_1e_3H(1,2,3)+e_2e_3H(2,1,3)+e_1e_2\times 1/6(12x_3^4+6x_3^3x_{12}+2x_3^2x_{12}^{(2)}-2x_1^2x_2^2+2Xx_3)].$$

To write the matrix elements of the kinetic energy $\hat{T}$ from (15) we use the additional notation

$$y_{pq}=x_p-x_q, \quad y_{pq}^{(n)}=x_p^n-x_q^n,$$
$$B_p=(2m_p)^{-1}(\alpha_q(i')\alpha_r(i)+\alpha_q(i)\alpha_r(i')),$$
$$C_p=\alpha_p(i')+\alpha_p(i),$$
$$A=1/2(m_1^{-1}A_{23}+m_2^{-1}A_{13}+m_3^{-1}A_{12}),$$
$$A_{pq}=\alpha_p(i')\alpha_p(i)+\alpha_q(i')\alpha_q(i).$$

In addition to (A.8) we use the polynomials

$$F_1(p,q,r)=6x_p^4x_{qr}+6x_r^4y_{pq}+3x_q^2y_{pr}^{(3)}+9x_p^2x_r^2x_{pr}+X(6x_p^2+4x_px_r+x_qy_{pr}),$$

$$G_1=x_1^2x_{23}+x_2^2x_{13}+x_3^2x_{12}+X,$$

$$H_1(p,q)=2x_3^4y_{pq}+2x_3^3y_{pq}^{(2)}+x_3^2y_{pq}^{(3)}-x_p^2x_q^2x_{pq}+X(x_3^2+x_q^2+x_3x_{pq}),$$

and also the notations k_p and k_{pq} from (16). For the "direct" matrix elements we obtain ($p=1,2$)

$$\langle\psi_{i'}^{(p3)}|\hat{T}|\psi_i^{(p3)}\rangle=t+X(t_1+t_2+t_3+t_4+t_5), \qquad (A.9)$$

$$t=A\langle\psi_{i'}^{(p3)}|\psi_i^{(p3)}\rangle, \quad t_3=-1/2k_{p3}G_1,$$
$$t_1=1/3(B_pF_1(p,q,3)+B_3F_1(3,q,p)),$$
$$t_2=B_q\{2x_p^4y_{q3}+2x_3^4y_{qp}+x_q^2x_{p3}^{(3)}-3x_p^2x_3^2x_{p3}+X[x_qx_{p3}+2(x_{p3}^{(2)}+x_px_3)]\},$$
$$t_4=k_{p3}C_qF(q), \quad t_5=k_3C_pH(q,p,3)+k_pC_3H(q,3,p).$$

The formulas for the crossing matrix elements are as follows:

$$\langle\psi_{i'}^{(13)}|\hat{T}|\psi_i^{(23)}\rangle=t'+X(t_1'+t_2'+t_3'+t_4'+t_5'), \qquad (A.10)$$

$$t'=A\langle\psi_{i'}^{(13)}|\psi_i^{(23)}\rangle \quad t_3'=-1/2k_3G_1,$$
$$t_1'=B_1H_1(1,2)+B_2H_1(2,1),$$
$$t_2'=1/3B_3[6x_3^4x_{12}+6x_3^3x_{12}^{(2)}+3x_3^2x_{12}^{(3)}+3x_1^2x_2^2x_{12}+X(6x_3^2-4x_1x_2-3x_{12}^{(2)}+x_3x_{12})],$$
$$t_4'=k_{13}\alpha_2(i)H(1,2,3)+k_{23}\alpha_1(i')H(2,1,3),$$
$$t_5'=k_3[\alpha_1(i)F(1)+\alpha_2(i')F(2)]-k_1\alpha_3(i)H(1,3,2)-k_2\alpha_3(i')H(2,3,1).$$

The formulas given were obtained with the matrix elements of the operator $\hat{T}$ in contrast to (25), written in the form of the product of the gradients of the basis functions. Here in (A.9) the quantities t, t_1, and t_2 correspond to terms with derivatives only of the exponentials, and t_3 corresponds to terms with derivatives only of $\mathcal{Y}_{1M}$, t_4, t_5—the crossing terms. The same terms correspond to the quantities from (A.10). Here the relation of the form (33) is reduced simply to

$$\int d\Omega x_M^*y_M=1/3\mathrm{xy}(8\pi^2).$$

[1)]A convenient method of approximation of an arbitrary pairing interaction by sums from (37) as is follows. First we carry out an approximation by one exponential, choosing the argument γ_1, for example, from the integral condition of the best mean-square approximation. Then we choose γ_2 from the condition of best approximation of the difference $V(r)-c_1\exp(-\gamma_1r)$, and so forth. Here the linear parameters c_p in each step are determined from solution of a system of linear equations corresponding to the condition mentioned above of the best approximation or its discrete analog.

[2)]We note, however, that, for example, in the case of the spin-orbit contribution to the Breit interaction the radial matrix elements which occur do not have the form of a product of an exponential and a polynomial in r_{ij}, and the analytic method of this section for calculating them is inapplicable.

[3)]See also Ref. 25. We note that only the results of specific calculations refer to the original results of the article.[25]

[4)]S. I. Vinitskiĭ kindly called our attention to this.

[5)]A. M. Frolov contributed to the derivation of these formulas.

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