Three-body Coulomb systems using generalized angular-momentum S states

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(Received 20 April 1972; revised manuscript received 23 April 1973)

An expansion of the three-body Coulomb potential in generalized angular-momentum eigenfunctions developed earlier by one of the authors is used to compute energy eigenvalues and eigenfunctions of bound S states of three-body Coulomb systems. The results for He, H^-, $e^-e^+e^-$, and $p\mu^-p$ are compared with the results of other computational approaches.

I. INTRODUCTION

The problem of three particles interacting via the Coulomb force has been the subject of rather intensive investigation in recent years.[1-12] The earliest mathematical treatments were based on the assumption that one or two of the particles have considerably larger masses than the others and can be considered infinitely heavy; the effect of finite masses is then introduced as a perturbation. Thus for the helium atom and its isoelectronic series, the most accurate results have been obtained by applying variational methods to wave functions of the type

$$\psi = \text{const} \times \exp(-\alpha r_1 - \alpha r_2) P(r_1, r_2, r_{12}), \qquad (1)$$

where P represents a polynomial in the interparticle distances or any equivalent polynomial expansion. This method was introduced by Hylleraas[1] and has been used by a large number of workers, culminating in the recent work of Pekeris[2] and coworkers.[3,4]

The approach mentioned does not serve as a satisfactory starting point when the masses of all three particles are of the same order of magnitude, as in the case of the μ-mesonic molecules $p\mu^-p$, $d\mu^-d$, and $p\mu^-d$ and the positronium ion $e^-e^+e^-$. To treat these systems without the assumption of infinite mass, Kolos *et al.*[5] and Carter[6] generalized the Hylleraas procedure and Frost *et al.*[7] used a Pekeris-series solution of equivalent length. While these variational procedures have been shown to lead to very accurate ground-state energies, they lead to long and complex analytical expressions, unlike other procedures which deal with symmetric representations of three bodies interacting Coulombically. Smith,[8] Whitten and Smith,[9] and other authors,[10-12] have explored the possibility of constructing a symmetrical representation of the quantum mechanics of three bodies. The coordinate system originally proposed by Smith[8] appears to be particularly well suited for some systems. In his approach, which we follow, the elements of the group SU(2) are exploited to simplify the mathematical manipulations. The purpose of the present paper is to report on applications of the coordinate system of Smith to specific problems and to show that it is capable of leading to simple analytical wave functions[13] of good accuracy in a variational treatment.

II. GENERALIZED ANGULAR MOMENTUM (GAM) METHOD

Because the GAM approach to the three-body problem has been thoroughly discussed elsewhere[8-12] we shall merely outline the general scheme, referring to an earlier paper[14] for details concerning the coordinate systems, the GAM operators, etc.

The Hamiltonian for the system is written in terms of the coordinates (ρ, Θ, Φ) as

$$H = -\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) - \frac{\Lambda^2}{\rho^2}\right] + V(\rho, \Theta, \Phi), \qquad (2)$$

where Λ^2 is the GAM scalar operator

$$\Lambda^2 = \frac{1}{\sin 4\Theta}\frac{\partial}{\partial\Theta}\left(\sin 4\Theta\frac{\partial}{\partial\Theta}\right) + \frac{1}{\cos^2 2\Theta} \times\left(\frac{\partial^2}{\partial\Phi^2} + \frac{\partial^2}{\partial\gamma^2} - \frac{\partial^2}{\partial\Phi\partial\gamma}\sin 2\Theta\right) - \frac{2}{\sin^2 2\Theta} \times\left(L^2 + \frac{\partial^2}{\partial\gamma^2}\right) + \frac{2\cos 2\Theta}{\sin^2 2\Theta}\left(L_{+1}^2 + L_{-1}^2\right). \qquad (3)$$

Here L^2 is the scalar-orbital angular-momentum operator and $L_{\pm 1}$ are the familiar ladder operators of orbital angular momentum. The eigenvalue equation satisfied by L^2 is $L^2 d^l_{mm'}(\alpha, \beta, \gamma) = l(l+1) \times d^l_{mm'}(\alpha, \beta, \lambda)$, where α, β, λ are the usual Euler angles of a body-fixed coordinate system with respect to a space-fixed system and the $d^l_{mm'}$ are the elements of the $(2l+1)$-dimensional representation of the rotation group $O(3)$. In the following analysis, we will consider only S states, where $L^2\psi_s = 0$ and Λ^2 simplifies to

$$\Lambda_s^2=\frac{1}{\sin4\Theta}\frac{\partial}{\partial\Theta}\left(\sin4\Theta\,\frac{\partial}{\partial\Theta}\right)+\frac{1}{\cos^2 2\Theta}\frac{\partial^2}{\partial\Phi^2}, \tag{4}$$

for which the solutions are the diagonal elements of the $(\frac{1}{2}\lambda+1)$-dimensional representation of the SU(2) group[15] $D^{\lambda/4}_{(\sigma/4)\sigma/4}(4\Phi, 4\Theta, 0)$, with $\lambda=0, 2, 4, 6, \ldots, -\lambda\leq\sigma\leq\lambda$, and

$$\Lambda^2\psi=\lambda(\lambda+4)\psi\,. \tag{5}$$

In Sec. III we shall look for solutions to the three-body Coulomb problem in which the eigenfunctions are expansions in the $D^{\lambda/4}_{(\sigma/4)\sigma/4}$,

$$\psi_s=\sum_{n,\lambda,\sigma} a^{\sigma}_{n,\lambda} f_{n,\lambda}(\rho) D^{\lambda/4}_{(\sigma/4)\sigma/4}\,. \tag{6}$$

We call the approach used in Sec. III "exact" with the understanding that a series truncation is involved just as the evaluation of $\sin x$ requires a series truncation. We shall show that

$$f_{n,\lambda}=e^{-x/2}x^{\lambda}L_n^{2\lambda+4}(x)$$

(where $L_n^{2\lambda+4}$ is a Laguerre polynomial) is a natural form to use from the standpoint of simplicity.

III. "EXACT" METHOD FOR THE THREE-BODY SYSTEM WITH COULOMB INTERACTION

In an earlier paper it was shown that the Coulomb interaction for three particles can be written[14]

$$\begin{aligned}V&=\sum_{i=1}^{3} V_i(\vec{r}_j-\vec{r}_k)\quad (i,j,k \text{ cyclical})\\&=\left(\frac{1}{\rho}\right)\frac{8\sqrt{2}}{\pi}\sum_{i=1}^{3} C_i e_j e_k \sum_{r=0}^{\infty}\frac{(r+1)(-1)^r}{(2r+1)(2r+3)}\\&\quad\times\sum_{\mu=-r}^{r} D^{r/2}_{(\mu/2)\mu/2}[4(\Phi+\delta_i), 4\Theta, 0],\end{aligned} \tag{7}$$

where e_j, e_k are the charges of the jth and kth particles, and

$$\begin{aligned}C_3&=\sqrt{2}/d\,,\\C_2&=\sqrt{2}d\,\sin\delta_2\,,\\C_1&=\sqrt{2}d\,\sin\delta_1\,,\end{aligned} \tag{8}$$

TABLE I. Values of parameters used in Eq. (11).

	Ω_1	Ω_2	δ
H_e [a]	$4\sqrt{2}$	1	$\frac{1}{4}\pi$
H^- [a]	$2\sqrt{2}$	1	$\frac{1}{4}\pi$
$e^-e^+e^-$	2	1	$\frac{1}{6}\pi$
$p\mu^-p$	0.842 68	0.480 51	$\sin2\delta=0.438\,42$

[a] Nucleus is assumed to be infinitely heavy.

with

$$\begin{aligned}d^2&=\frac{m_3}{\mu}\left(\frac{m_1+m_2}{m_1+m_2+m_3}\right),\\\mu^2&=m_1m_2m_3/(m_1+m_2+m_3);\end{aligned} \tag{9}$$

the phase angles δ_i are related to the particle masses by

$$\begin{aligned}\tan\delta_1&=\frac{1}{d^2}\left(\frac{m_1+m_2}{m_1}\right),\\\tan\delta_2&=-\frac{1}{d^2}\left(\frac{m_1+m_2}{m_2}\right),\\\tan\delta_3&=0\,.\end{aligned} \tag{10}$$

Note that the phases δ_i are not determined uniquely; for example, we can equally well take δ_3 to be 0 or π. We have resolved this problem by choosing $0\leq\delta_1\leq\frac{1}{2}\pi$, $0\geq\delta_2\geq-\frac{1}{2}\pi$, $\delta_3=\pi$. These choices for the δ's are similar to those employed by Zickendraht[11] and lead to the lowest-lying energy states.

Thus the potential for any three-body system with two identical particles is

$$\begin{aligned}V=\frac{e^2}{\rho}\frac{8\sqrt{2}}{\pi}&\sum_{r=0}^{\infty}\sum_{\mu=-r}^{r}\frac{(r+1)(-1)^r}{(2r+1)(2r+3)}\\&\times[\Omega_1\cos(2\delta\mu)-\Omega_2(-1)^{\mu}]\\&\times D^{r/2}_{(\mu/2)\mu/2}(4\Phi, 4\Theta, 0),\end{aligned} \tag{11}$$

with the values of the parameters $\Omega_1, \Omega_2, \delta$ given in Table I for the helium atom, the negative hydrogen ion, the positronium negative ion, and muonium $(p\mu^-p)$. Since the potential is of the form ρ^{-1}, we are led to look for hydrogenic radial functions

$$\psi\sim e^{-x/2}x^{\lambda}L_n^{2\lambda+4}(x)\,,$$

where $x=\alpha\rho$ with $\alpha=2k$ (k is related to the energy E by $E=-k^2\hbar^2/2\mu$), n is a positive integer or zero (required in order to satisfy boundary conditions at $\rho=\infty$), and the $L_n^{2\lambda+4}$ are Laguerre polynomials.

Before proceeding further we must ensure that the wave function is antisymmetric under interchange of the two identical particles in order to satisfy the Pauli exclusion principle. It is easy to show[11] that the angular part is of the form

$$D^{\lambda/4}_{(\sigma/4)\sigma/4}+(-1)^S D^{\lambda/4}_{(\sigma/4)\sigma/4},$$

where S is the spin of the system. Hence we have

$$\begin{aligned}\psi=\sum_{n,\lambda,\sigma} a^{\sigma}_{n,\lambda}\,e^{-x/2}x^{\lambda}L_n^{2\lambda+4}(x)\\\times[D^{\lambda/4}_{(\sigma/4)\sigma/4}+(-1)^S D^{\lambda/4}_{(\sigma/4)\sigma/4}]\,.\end{aligned} \tag{12}$$

The eigenvalue problem to be solved is thus (for $e^-e^+e^-$)

$$(H-E)\psi = 0 = -2\frac{\hbar^2 k^2}{\mu}\left\{\frac{d^2}{dx^2}+\frac{5}{x}\frac{d}{dx}-\frac{\Lambda^2}{x^2}-\frac{1}{4}+\frac{8(12)^{1/4}}{\epsilon x\pi}\sum_{r=0}^{\infty}(-1)^r\frac{(r+1)}{(2r+1)(2r+3)}\left[2\cos\left(\frac{\pi}{3}\mu\right)-(-1)^{\mu}\right]D^{r/2}_{(\mu/2)\mu/2}\right\}$$

$$\times\sum_{n,\lambda,\sigma}a^{\sigma}_{n,\lambda}e^{-x/2}x^{\lambda}L_n^{2\lambda+4}(x)[D^{\lambda/4}_{(\sigma/4)\sigma/4}+(-1)^S D^{\lambda/4}_{(\sigma/4)\sigma/4}], \tag{13}$$

where $\epsilon=\hbar^2k/(\mu e^2)$. Multiplying by

$$e^{-x/2}x^{\lambda}L_n^{2\lambda+4}(x)[D^{\lambda/4}_{(\sigma/4)\sigma/4}+(-1)^S D^{\lambda/4}_{(\sigma/4)\sigma/4}]$$

and integrating over space coordinates (with the weight function x^4) yields

$$\epsilon b^{\sigma}_{n,\lambda} = -\sum_{n',\lambda',\sigma'}\gamma^{\lambda\lambda'}_{\sigma\sigma'}b^{\sigma'}_{n',\lambda'}, \tag{14}$$

with

$$b^{\sigma}_{n,\lambda}=\left(\frac{(n+\lambda+\frac{5}{2})[\Gamma(n+2\lambda+5)]^3}{n!(\frac{1}{2}\lambda+1)}\theta_a(\sigma)\right)^{1/2}a^{\sigma}_{n,\lambda},$$

$$\gamma^{\lambda\lambda'}_{\sigma\sigma'}=\left[\left(\frac{\lambda}{2}+1\right)\left(\frac{\lambda'}{2}+1\right)\right]^{1/2}[(n+\lambda+\tfrac{5}{2})(n'+\lambda'+\tfrac{5}{2})\Gamma(n+2\lambda+5)\Gamma(n'+2\lambda'+5)]^{-1/2}\frac{\theta_b(\sigma,\sigma')}{[\theta_a(\sigma)\theta_a(\sigma')]^{1/2}}$$

$$\times\sum_{l}\frac{\Gamma(l+\lambda'+\lambda+5)}{l!(n-l)!(n'-l)![\Gamma(l+\lambda-\lambda'+1-n')/\Gamma(\lambda-\lambda'+1)]\Gamma(l+\lambda'-\lambda+1-n)/\Gamma(\lambda'-\lambda+1)}$$

$$\times\sum_{r}\left(\frac{8(12)^{1/4}(-1)^r}{(2r+1)(2r+3)\pi}\left\{\left[2\cos\left(\frac{\pi}{6}(\sigma-\sigma')\right)-(-1)\frac{\sigma-\sigma'}{2}\right](C^{(\lambda/4)(\lambda'/4)(r/2)}_{(\sigma/4)-(\sigma'/4)[(\sigma-\sigma')/4]})^2\right.\right.$$

$$\left.\left.+\left[2\cos\left(\frac{\pi}{6}(\sigma+\sigma')\right)-(-1)^{\sigma+\sigma'/2}\right](C^{(\lambda/4)(\lambda'/4)(r/2)}_{(\sigma/4)(\sigma'/4)[(\sigma+\sigma')/4]})^2\right\}\right), \tag{15}$$

where

$$\theta_a(\sigma)=\begin{cases}2 & \text{if } \sigma\neq 0,\\ 1 & \text{if } \sigma=0,\end{cases}$$

$$\theta_b(\sigma,\sigma')=\begin{cases}2 & \text{if } \sigma \text{ and } \sigma'\neq 0,\\ 1 & \text{if } \sigma \text{ or } \sigma'\neq 0,\\ \frac{1}{2} & \text{if } \sigma \text{ and } \sigma'=0,\end{cases} \tag{16}$$

and the $C^{ll'l''}_{mm'm''}$ are the Clebsch-Gordan coefficients of SU(2) in an obvious notation.

Since γ is a symmetric matrix, it can, after truncation, be diagonalized by standard techniques using a high-speed digital computer.[16] The result for $e^-e^+e^-$ of a truncation at $n=2$, $\lambda=6$ is $-E=0.20948$ a.u.,[17] which is to be compared with a much more precise value of 0.2620 obtained by variational methods.[7] The energy eigenvalues for various truncations and the eigenfunction expansion coefficients for truncation at $n=2$, $\lambda=6$ (the corresponding normalization constant is $(n!/8\pi^2)^{1/2}$ for all basis functions reported in this paper) are given in Table II for $e^-e^+e^-$ and $p\mu^-p$.

A similar approach was tried for the helium atom, muonium ($p\mu^-p$), and the hydrogen molecule ion (pe^-p). The computed energies for He and $p\mu^-p$ (−2.7922 and −62.928, respectively, with 39 and 37 terms in the expansion) are also much too small [the accurate values are −2.9033 a.u. (252-term wave function)[2] and −102.21 a.u. (55-term wave function)].[6] We attribute the error to very slow convergence of the series expansion which is reminiscent of the slow convergence obtained using a configuration-interaction treatment with hydrogenic wave functions.[18] Convergence did not occur for pe^-p. The truncation for finite n and λ is not, of course, unique since λ and n are independent parameters. In addition to the ground-state energy eigenvalues and eigenfunctions, those of excited states are also obtained during the diagonalization process; one eigenfunction is obtained for each term in the expansion. However, the excited-state energies obtained in this manner are even poorer than the ground-state values and so we do not present them here.

Obviously, these values for the energies of the various systems considered are not satisfactory. Because of the great success experienced with the use of variational methods, it is profitable to see

TABLE II. Energy values and coefficients for $e^-e^+e^-$ by the method of Sec. III.

Term No.	n	λ	σ	Energy $E(n)$ of n-term wave function (a.u.) $(E=-\frac{1}{2}\epsilon^2\mu)$	Coefficient b_σ^λ for 28-term wave function
1	0	0	0	−0.115 28	0.731 220 5
2	0	2	2	−0.168 85	−0.500 815
3	0	4	4	−0.169 02	$-0.972\,438\times10^{-1}$
4	0	4	0	−0.175 50	0.219 562
5	0	6	6	−0.177 40	0.125 515
6	0	6	2	−0.178 55	$-0.739\,908\times10^{-1}$
7	0	8	8	−0.178 95	$-0.354\,438\times10^{-1}$
8	0	8	4	−0.179 04	$-0.257\,319\times10^{-1}$
9	0	8	0	−0.179 57	$0.422\,006\times10^{-1}$
10	0	10	10	−0.179 59	$-0.115\,527\times10^{-1}$
11	0	10	6	−0.179 88	$0.309\,674\times10^{-1}$
12	0	10	2	−0.179 99	$-0.162\,713\times10^{-1}$
13	0	12	12	−0.180 10	$0.169\,977\times10^{-1}$
14	0	12	8	−0.180 16	$-0.100\,467\times10^{-1}$
15	0	12	4	−0.180 18	$-0.813\,436\times10^{-2}$
16	0	12	0	−0.180 25	$0.123\,049\times10^{-1}$
17	1	0	0	−0.197 04	−0.274 591
18	1	2	2	−0.198 99	−0.101 297
19	1	4	4	−0.198 99	$-0.438\,095\times10^{-1}$
20	1	4	0	−0.201 23	0.103 236
21	1	6	6	−0.203 10	$0.792\,090\times10^{-1}$
22	1	6	2	−0.204 27	$-0.514\,650\times10^{-1}$
23	2	0	0	−0.204 74	$0.428\,111\times10^{-1}$
24	2	2	2	−0.205 66	$-0.609\,569\times10^{-1}$
25	2	4	4	−0.205 69	$-0.289\,145\times10^{-1}$
26	2	4	0	−0.206 92	$0.774\,687\times10^{-1}$
27	2	6	6	−0.208 56	$0.854\,825\times10^{-1}$
28	2	6	2	−0.209 48	$-0.557\,822\times10^{-1}$

TABLE III. Variational energy values and coefficients for the ground state of helium; $\alpha=\frac{4}{5}\mu\xi_0^0, \mu=0.9997$.[a]

Term No.	n	λ	σ	ν	$E(n)$ (a.u.)	Coefficient b_σ^λ of 28-term wave function
1	0	0	0	0	−2.4996	0.965 406 7
2	0	2	2	1	−2.5294	$-0.709\,454\,3\times10^{-1}$
3	0	4	4	1	−2.7044	−0.190 329 4
4	0	4	0	1	−2.7823	0.115 739 4
5	0	6	6	1	−2.7823	$-0.290\,549\,6\times10^{-3}$
6	0	6	2	1	−2.7829	$-0.591\,431\,8\times10^{-2}$
7	0	8	8	2	−2.8034	$0.477\,521\,2\times10^{-1}$
8	0	8	4	2	−2.8312	$-0.516\,926\,6\times10^{-1}$
9	0	8	0	2	−2.8443	$0.331\,187\,8\times10^{-1}$

[a] See NAPS document No. 02309 for 8 pages of supplementary material. Order from ASIS/NAPS c/o Microfiche Publications, 305 E. 46th St., New York, N.Y. 10017. Remit in advance for each NAPS accession number $1.50 for microfiche or $5.00 for photocopies. Make checks payable to Microfiche Publications.

whether or not we can so improve on the results obtained in this section. Variational approaches using GAM are the subject of Sec. IV.

IV. VARIATIONAL MODIFICATION

For the cases (e.g., $e^-e^+e^-$, He, $p\mu^-p$) in which the expansion of the wave function in the GAM quantum numbers (λ, σ) is a convergent one, energy computed in Sec. III is still at least 15% greater than the true energy. As we shall see, a variational approach can be employed to substantially improve the results.

We begin our development by modifying our wave function as follows:

$$\psi = \sum_{n,\lambda,\sigma} a^{\sigma}_{n,\lambda} e^{\alpha\rho/2} (\alpha\rho)^{\nu} L_n^{2\nu+4}(\alpha\rho) \times [D^{\lambda/4}_{(\sigma/4)\,\sigma/4} + (-1)^S D^{\lambda/4}_{\sigma/4,\,-\sigma/4}] . \tag{17}$$

Here both ν, which is a function of λ, and α as well as the a^{λ}_{σ} are free parameters which can be used to minimize the energy; recall that in Sec. III we set $\alpha = 2k$. We first compute $(\psi, H\psi)$ and (ψ, ψ) and vary the $a^{\sigma}_{n,\lambda}$ such that the energy E,

$$-E = (2\mu/\hbar^2\alpha^2)(\psi, H\psi)/(\psi, \psi), \tag{18}$$

is a minimum ($\partial E/\partial a^{\sigma}_{n,\lambda} = 0$). After symmetrizing the resultant set of linear equations, we get

$$(\epsilon - \tfrac{1}{4}) b^{\sigma}_{n\lambda} + \sum_{n'} \beta^{\lambda\sigma}_{nn'} b^{\sigma}_{n'\lambda} - \left(\frac{2\mu e^2}{\hbar^2\alpha} \xi^0_0\right) \sum_{n'\lambda'\sigma'} \gamma^{\sigma\sigma'}_{nn',\lambda\lambda'} b^{\sigma'}_{n'\lambda'} = 0, \tag{19}$$

with

$$\beta^{\lambda\sigma}_{nn'} = \left([\lambda(\lambda+4) - \nu(\nu+4)] \sum_{l=0}^{\{n'\}} \frac{(l+2\nu+2)!\,(n-l+1)!\,(n'-l+1)!}{l!\,(n-l)!\,(n'-l)!} + (n+\nu+\tfrac{5}{2}) \sum_{l=0}^{\{n'\}} \frac{(l+2\nu+3)!}{l!} \right)$$

$$\times \left(\frac{n!\,n'!}{(2\nu+4+n)!\,(2\nu+4+n')!} \right)^{1/2} \frac{1}{(\frac{1}{2}\lambda+1)^{1/2}},$$

$$\gamma^{\sigma\sigma'}_{nn',\,\lambda\lambda'} = \left[\left(\frac{n!\,n'!\,(\frac{1}{2}\lambda+1)(\frac{1}{2}\lambda'+1)}{(n+2\nu+5)!\,(n+2\nu'+5)!} \right) \right]^{1/2} \sum_{l} \frac{(\nu+\nu'+5+l)!}{l!\,(n-l)!\,(n'-l)!} (-1)^{n+n'}$$

$$\times \frac{\theta_b(\sigma, \sigma')}{[\Gamma(l+\nu-\nu'-n'+1)/\Gamma(\nu-\nu'+1)]\,\Gamma(l+\nu'-\nu-n+1)/\Gamma(\nu'-\nu+1)} \tag{20}$$

$$\times \frac{1}{[\theta_a(\sigma)\sigma_a(\sigma')]^{1/2}} \sum_{r\geq 1} \frac{(-1)^r}{(r+1)} [\zeta^2_{\sigma-\sigma'/2} (C^{(\lambda/4)(\lambda'/4)(r/2)}_{(\sigma/4)(\sigma'/4)[(\sigma-\sigma)'/4]})^2 + \zeta^r_{\sigma+\sigma'/2} (C^{(\lambda/4)(\lambda'/4)(r/2)}_{(\sigma/4)(\sigma'/4)[(\sigma+\sigma)/4]})^2],$$

$$b^{\sigma}_{n,\lambda} = \left(\frac{[(n+2\nu+5)!]^3}{n!\,(\frac{1}{2}\lambda+1)} \theta_a(\sigma) \right)^{1/2} a^{\sigma}_{n,\lambda} .$$

Here

$$\zeta^r_{\mu} = \xi^r_{\mu}/\xi^0_0, \tag{21}$$

$$\xi^r_{\mu} = \frac{8\sqrt{2}}{\pi} \frac{(-1)^r(r+1)}{(2r+1)(2r+3)} [\Omega_1 \cos(2\delta\mu) - \Omega_2(-1)^{\mu}] .$$

We now seek the combination of $\nu(\lambda)$ and α which yield the best energy. Unfortunately, we could find no practical method of minimizing the energy analytically; instead we had to resort to trial and error to find a "best" combination of $\nu(\lambda)$ and α, taking care that the series still converged.

The results for He, H^-, $e^-e^+e^-$, and $p\mu^-p$ are shown in Table III. The computed energy for He (−2.90107 a.u.) is about 0.075% less than the value (−2.9033 a.u.) of Pekeris[2] while the energies for H^-, $p\mu^-p$, and $e^-e^+e^-$ (−0.52727, −102.16, and −0.2612 a.u., respectively) are about 0.03, 0.05, and 0.3% less than the values of Pekeris[2] (−0.52743 a.u. for H^-), Carter[6] (−102.21 a.u. for $p\mu^-p$), and Frost[7] (−0.2620 a.u. for $e^-e^+e^-$). The agreement with previous results is thus excellent, and we have the additional advantage that we do not use directly interelectronic coordinates. All integrals are evaluated analytically so that the only large computational task is diagonalization of the Hamiltonian matrix which is quite straight forward. It is quite possible that the energies reported here could be improved somewhat by trying other combinations of n and ν and different truncations of the triple series.

One may wonder why so much better energies result from the variational approach. It is apparent that by letting ν differ from λ, we are bringing

in higher-order Laguerre polynomials without the necessity of using expansions which are hundreds of terms long. This improvement occurs at the expense of the beauty of the method of Sec. III.

V. CONCLUSION

The foregoing presents a new approach to the computation of wave functions and energy eigenvalues of three-body bound S states. The computed energies of Sec. IV are in fact nearly as good as those found with the configuration-interaction Hylleraas methods. Our method is conceptually a very simple one which does contain correlation effects, and which yields results within, at most, a few tenths of a percent of the true energies; hopefully, it is susceptible to considerable improvement. For the case of two heavy particles and a light particle (e.g., pe^-p), the choice of basis functions employed in the present treatment is undoubtedly inappropriate; probably some generalization of the elliptic coordinates used in the usual treatments is required.

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