Correlated wave functions for three-particle systems with Coulomb interaction: The muonic helium atom*

K.-N. Huang†
Department of Physics, University of Oregon, Eugene, Oregon 97403
(Received 1 October 1976)

A computational procedure for calculating correlated wave functions is proposed for ground and excited states of three-particle systems with Coulomb interaction. Calculations are performed for the muonic helium atom as an example. Hylleraas-type trial functions multiplied by appropriate angular factors are used as the basis of the correlated wave functions. The expansion coefficients and two nonlinear parameters are obtained variationally. Results for the states $(1s)_e(1s)_\mu$ $^{1,3}S$, $(1s)_e(2p)_\mu$ $^{1,3}P$, $(1s)_e(3d)_\mu$ $^{1,3}D$, $(1s)_e(4f)_\mu$ $^{1,3}F$, and $(1s)_e(5g)_\mu$ $^{1,3}G$ are listed.

I. INTRODUCTION

Interest in highly ionized atoms has increased in recent years, partly as a result of the observation of x-ray spectra from the solar corona and other astrophysical plasmas.[1-3] Furthermore, ion-atom collision and beam-foil techniques[4,5] make it possible to produce highly ionized atoms in the laboratory and study their spectra. In addition, the study of exotic atoms has opened up a fertile territory extending over atomic, nuclear, and elementary particle physics.[6-10] During the deexcitation cascade of an exotic atom, it becomes highly ionized through Auger transitions. The correlation between the remaining particles in highly ionized atoms is important, especially in the calculation of cascade processes.

In the present work a computational procedure for calculating correlated wave functions is proposed for three-particle systems interacting through Coulomb forces. The calculations, however, are carried out only for the muonic helium atom as an example. The results can be readily extended to electronic atoms, with proper allowance for exchange. Further works in this respect will be reported.

The recently observed muonic helium atom[11-13] is one of the simplest exotic atoms, in which one of the two electrons in a normal helium atom is replaced by a negative muon. It provides an interesting and potentially useful system for the study of a very different type of atomic structure, and also for the study of the μ^--e^- interaction and for the precise determination of the magnetic moment and mass of the negative muon as a test of CPT invariance.

Correlated wave functions for the muonic helium atom are required in the calculation of its hyperfine structure[12,14,15] and the muon capture and cascade processes.[13,16,17] In this work, variational wave functions which explicitly contain interparticle coordinates are presented for the ground and excited states; this has been proved to be the most effective way of handling the correlation in three-particle systems.[18-21]

II. REDUCTION OF THE TOTAL HAMILTONIAN

Consider a system of $(n+1)$ particles with coordinates $(\vec{R}_0, \vec{R}_1, \ldots, \vec{R}_n)$ whose total nonrelativistic Hamiltonian is, in atomic units,

$$\mathcal{H} = -\sum_{i=0}^{n} \frac{\vec{\nabla}_i^2}{2m_i} + V, \tag{1}$$

where i labels the ith particle, and V is the total potential energy depending only on relative coordinates. By introducing the coordinates of the center of mass and the relative coordinates,

$$\vec{R}_c = \sum_{i=0}^{n} m_i \vec{R}_i \Big/ \sum_{i=0}^{n} m_i ,$$
$$\vec{r}_i = \vec{R}_i - \vec{R}_0, \quad i = 1, 2, \ldots, n \tag{2}$$

we can separate the Hamiltonain of this system into two parts, $\mathcal{H} = H_{\mathrm{CM}} + H$.[22] The first part H_{CM} describes the motion of the center of mass, and the second part H pertains to the relative motion:

$$H = H_\infty + H_m , \tag{3}$$

where

$$H_\infty = -\sum_{i=1}^{n} \frac{\vec{\nabla}_i^2}{2m_i} + V , \tag{4}$$

$$H_m = -\frac{1}{2m_0}\left(\sum_{i=1}^{n} \vec{\nabla}_i\right)^2 , \tag{5}$$

where H_∞ is the Hamiltonian for the case of infinite nuclear mass, and H_m is the mass correction term, including reduced and correlated mass corrections. Now the $\vec{\nabla}_i$'s in (4) and (5) are gradients of the relative coordinates $\vec{r}_i$. The Schrödinger equation for a muonic atom with one electron and one muon hence reads

$$H\psi \equiv (H_\infty + H_m)\psi = E\psi ; \tag{6}$$

$$H_\infty = -\tfrac{1}{2}\vec{\nabla}_1^2 - \frac{1}{2m_2}\vec{\nabla}_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}},$$

$$H_m = -(1/2M_n)(\vec{\nabla}_1 + \vec{\nabla}_2)^2 .$$

Here, 1 and 2 stand for the electron and muon, respectively, r_{12} denotes the distance between them, and M_n is the mass of the nucleus.

III. VARIATIONAL WAVE FUNCTIONS AND MATRIX ELEMENTS

The ground-state wave function can be obtained by an expansion in the standard Hylleraas basis.[23] The calculation of excited-state wave functions is rendered more difficult, compared to that of the ground state, by the appearance of the subsidiary condition that the eigenfunction of every excited state must be orthogonal to the eigenfunctions of all lower states. The eigenfunctions belonging to two states of an atom are, however, automatically orthogonal to each other if either the total orbital angular momentum L or the total spin S (or both) have different values for the two states. The variational-method calculation of the lowest state belonging to a given L and S can therefore be treated without additional complications as long as those functions which have the appropriate symmetry and angular dependence are adopted as trial functions.[22]

The general Hylleraas-type trial functions used in this work are introduced by making use of the "solid harmonics." The normalized harmonic polynomial, or solid harmonic, is defined as[24]

$$\mathcal{Y}_{LM}(\vec{r}) = r^L Y_{LM}(\Omega) . \tag{7}$$

For the case in which the electron is in the 1s state, we use trial functions of the form[12]

$$U^{NL}_{lmn}(1,2) = \mathcal{Y}_{00}(1)\,\mathcal{Y}_{LL}(2) e^{-\alpha r_1 - \beta r_2/N} r_{12}^l r_1^m r_2^n , \tag{8}$$

where N and L are the principal and orbital-angular-momentum quantum numbers, respectively, of the muon, and $\mathcal{Y}_{00}(1) \equiv \mathcal{Y}_{00}(\vec{r}_1)$, etc. The variational wave function is taken to be the expansion

$$\psi_{NL}(\vec{r}_1, \vec{r}_2) = \sum_{l,m,n=0}^{l+m+n\le\omega} C_{lmn}\, U^{NL}_{lmn}(1,2) , \tag{9}$$

where the parameters α and β and the coefficients C_{lmn} are to be determined variationally. Here ω will be chosen later to have certain selected values. It is seen that the variational wave function (9) has the appropriate symmetry of the state with total angular momentum L, and reduces to the correct hydrogenic form when correlation is neglected.

The variational calculation can be carried out more easily by using a new set of coordinates r_1, r_2, r_{12}, t_1, t_2, and t_3 defined by[12]

$$\begin{aligned} &r_1 = |\vec{r}_1|, \quad r_2 = |\vec{r}_2|, \quad r_{12} = |\vec{r}_1 - \vec{r}_2|, \\ &t_1 = f_1(\hat{r}_1, \hat{r}_2), \quad t_2 = \mathcal{Y}_{LL}(\vec{r}_2), \quad t_3 = f_3(\hat{r}_1, \hat{r}_2) , \end{aligned} \tag{10}$$

where the unit vector $\hat{r}_i$ defines the orientation of the position vector $\vec{r}_i$. Here f_1 and f_3 are certain suitable functions which make up the last two independent variables. We do not have to know their exact forms because they depend only on the orientation of the whole system and do not appear in the trial functions.[25] The Hamiltonian for the case of infinite nuclear mass is[12]

$$\begin{aligned} H_\infty = &-\frac{1}{2r_1}\frac{\partial^2}{\partial r_1^2} r_1 - \frac{1}{2m_2 r_2}\frac{\partial^2}{\partial r_2^2} r_2 - \left(\frac{1}{2} + \frac{1}{2m_2}\right)\frac{1}{r_{12}}\frac{\partial^2}{\partial r_{12}^2} r_{12} + \left(\frac{r_2^2 - r_1^2 - r_{12}^2}{2r_1 r_{12}}\right)\frac{\partial^2}{\partial r_1 \partial r_{12}} \\ &+ \left(\frac{r_1^2 - r_2^2 - r_{12}^2}{2m_2 r_2 r_{12}}\right)\frac{\partial^2}{\partial r_2 \partial r_{12}} - \frac{Lt_2}{m_2 r_2}\frac{\partial^2}{\partial r_2 \partial t_2} - \frac{Lt_2}{m_2 r_{12}}\left(1 - \frac{\mathcal{Y}_{11}(1)}{\mathcal{Y}_{11}(2)}\right)\frac{\partial^2}{\partial r_{12}\partial t_2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} , \end{aligned} \tag{11}$$

and the matrix element can be written[12]

$$\begin{aligned} \langle U^{NL}_{l'm'n'} \,|\, H_\infty \,|\, U^{NL}_{lmn} \rangle = &-\tfrac{1}{8}(a^2 + b^2/m_2) A(i+2,j+2,k+2) + [\tfrac{1}{2}a(m+1+\tfrac{1}{2}l) - Z] A(i+2,j+1,k+2) \\ &+ [(b/2m_2)(n+1+L+\tfrac{1}{2}l) - Z] A(i+2,j+2,k+1) - \tfrac{1}{2}m(m+l+1) A(i+2,j,k+2) \\ &- (1/2m_2) n(n+l+1+2L) A(i+2,j+2,k) + A(i+1,j+2,k+2) \\ &- \tfrac{1}{2}l[(l+m+1) + (l+n+1+2L)(1/m_2)] A(i,j+2,k+2) \\ &+ \tfrac{1}{4}al[A(i,j+3,k+2) - A(i,j+1,k+4)] + (b/4m_2) l[A(i,j+2,k+3) - A(i,j+4,k+1)] \\ &+ \tfrac{1}{2}lm\, A(i,j,k+4) + (ln/2m_2) A(i,j+4,k) + (lL/m_2) A_y(i,j+2,k+2) , \end{aligned} \tag{12}$$

where $a = 2\alpha$, $b = 2\beta/N$, and $i = l' + l$, $j = m' + m$, $k = n' + n + 2L$. Here, $A(i+2,j+2,k+2)$ and $A_y(i+2,j+2,k+2)$

are defined by the integrals

$$A(i+2,j+2,k+2)=\int \frac{d^3r_1}{4\pi}\,\frac{d^3r_2}{4\pi}\,e^{-ar_1-br_2}r_{12}^i r_1^j r_2^k\,, \tag{13}$$

$$A_y(i+2,j+2,k+2)=\int \frac{d^3r_1}{4\pi}\,\frac{d^3r_2}{4\pi}\,e^{-ar_1-br_2}r_{12}^i r_1^j r_2^{k-2L}\,4\pi\,\frac{\mathcal{Y}_{11}(1)}{\mathcal{Y}_{11}(2)}\,\mathcal{Y}^*_{LL}(2)\mathcal{Y}_{LL}(2)\,. \tag{14}$$

The calculation of these integrals is described in Appendix A.

The mass correction term H_m, expressed in the new coordinates, is[12]

$$H_m=-\frac{1}{2M_n}\left[\frac{1}{r_1}\frac{\partial^2}{\partial r_1^2}\,r_1+\frac{1}{r_2}\frac{\partial^2}{\partial r_2^2}\,r_2+\left(\frac{r_1^2+r_2^2-r_{12}^2}{r_1 r_{12}}\right)\frac{\partial^2}{\partial r_1 r_2}+\frac{2Lt_2}{r_2}\frac{\partial^2}{\partial r_2\partial t_2}+\frac{2Lt_2}{r_1}\left(\frac{\mathcal{Y}_{11}(1)}{\mathcal{Y}_{11}(2)}\right)\frac{\partial^2}{\partial r_1\partial t_1}\right]\,; \tag{15}$$

its matrix element is[12]

$$\begin{aligned}\langle U^{NL}_{l'm'n'}\,|\,H_m\,|\,U^{NL}_{lmn}\rangle&=-\frac{1}{2M_n}\{\tfrac{1}{4}(a^2+b^2)A(i+2,j+2,k+2)-\tfrac{1}{2}a(2m+n+2)A(i+2,j+1,k+2)\\&-\tfrac{1}{2}b(2n+m+2+2L)A(i+2,j+2,k+1)+m(m+n+1)A(i+2,j,k+2)+n(m+n+1+2L)A(i+2,j+2,k)\\&-\tfrac{1}{4}ab[A(i+4,j+1,k+1)-A(i+2,j+1,k+3)-A(i+2,j+3,k+1)]\\&-\tfrac{1}{2}an[A(i+2,j+3,k)-A(i+4,j+1,k)]-\tfrac{1}{2}bm[A(i+2,j,k+3)-A(i+4,j,k+1)]\\&-mnA(i+4,j,k)+2L[mA_y(i+2,j,k+2)-\tfrac{1}{2}aA_y(i+2,j+1,k+2)]\}\,.\end{aligned} \tag{16}$$

The normalization matrix element is

$$\langle U^{NL}_{l'm'n'}\,|\,U^{NL}_{mn}\rangle=A(i+2,j+2,k+2)\,. \tag{17}$$

IV. VARIATIONAL CALCULATION

The variational wave function (9) has the general form

$$\psi=\sum_{i=1} C_i U_i\,. \tag{18}$$

The variational-principle equivalent to the Schrödinger equation (6) is

$$\delta\langle\psi\,|\,(H-E)\,|\,\psi\rangle=0\,. \tag{19}$$

Approximating the wave function ψ in (19) by an expansion of the form (18), we find

$$\delta\left\{\sum_{i=1}\sum_{j=1} C_i C_j[H_{ij}-EU_{ij}]\right\}=0\,, \tag{20}$$

where $H_{ij}=\langle U_i\,|H\,|\,U_j\rangle$ and $U_{ij}=\langle U_i\,|\,U_j\rangle$. Variation with respect to the coefficients C_i leads to the matrix eigenvalue problem[20]

$$\sum_{j=1}\{H_{ij}-EU_{ij}\}C_j=0\,. \tag{21}$$

The nonlinear parameters α and β in the variational wave function are also varied to obtain the lowest eigenvalue and corresponding eigenvector.

V. RESULTS AND DISCUSSION

For the ground state $(1s)_e(1s)_\mu\ ^{1,3}S$, the variational wave function (9) is computed for $\omega=0$, 1, 2, 3, and 4; the number of terms in the expansion is 1, 4, 10, 20, and 35, respectively. There is excellent convergence of the energy as the number of terms in the wave function is increased. The energies and wave function are listed in Tables I and II, respectively. For excited states, we only quote the energies obtained for 1- and 35-term wave functions in Table III. We find that

TABLE I. Ground-state energy (in atomic units) of the muonic helium atom computed from 1-, 4-, 10-, 20-, and 35-term wave functions.[a]

Wave function	Z_e[b]	Z_μ[c]	E
1-term	1.000 036 8	1.999 999 94	−402.641 012 67
4-term	0.994	2.000 0	−402.641 013 95
10-term	1.054	1.999 8	−402.641 014 05
20-term	1.138	1.999 8	−402.641 014 18
35-term	1.270	1.999 2	−402.641 014 36

[a] The fundamental physical constants used here are the electron mass $m_e=0.511\,003\,4$ MeV, the muon mass $m_\mu=105.659\,48$ MeV, the mass of the α particle $m_\alpha=4.002\,603$ amu, and the atomic mass unit 1 amu $=931.501\,6$ MeV.

[b] $Z_e=\alpha/M_e$, where M_e is the reduced mass of the electron with respect to the nucleus, and α is the variational parameter in Eq. (8).

[c] $Z_\mu=\beta/M_\mu$, where M_μ is the reduced mass of the muon with respect to the nucleus, and β is the variational parameter in Eq. (8).

TABLE II. Ground-state wave functions of the muonic helium atom. The format A (n) means $A \times 10^n$.

l m n	4-term	10-term	20-term	35-term
0 0 0	3.225 164 571 598 934 (4)	3.225 550 156 522 934 (4)	3.225 125 867 937 781 (4)	3.225 900 254 889 307 (4)
0 0 1	2.134 502 452 206 636	−1.289 217 948 947 425 (3)	−1.298 404 204 984 705 (3)	−5.167 245 794 062 952 (3)
0 1 0	5.271 784 185 417 956 (2)	2.162 534 247 490 955 (3)	4.405 222 528 879 461 (3)	7.776 026 629 013 713 (3)
1 0 0	−7.201 670 953 392 672 (2)	−4.310 730 587 184 210 (2)	5.225 494 845 594 197 (1)	8.949 298 538 365 987 (2)
0 0 2		4.271 747 146 912 845 (2)	7.454 109 271 511 015 (2)	1.255 055 621 112 182 (3)
0 1 1		−1.844 234 609 423 314 (4)	−6.369 487 120 073 833 (4)	−1.549 151 236 937 622 (5)
0 2 0		−1.017 837 423 728 196 (2)	4.991 938 099 955 998 (2)	3.111 022 291 831 306 (3)
1 0 1		1.836 324 494 078 106 (4)	6.352 109 947 753 359 (4)	1.534 495 787 557 413 (5)
1 1 0		6.152 571 782 104 603 (2)	8.097 211 117 492 863 (2)	−1.345 357 049 523 521 (2)
2 0 0		−4.609 799 684 710 024 (2)	−1.013 736 828 419 658 (3)	−1.749 110 249 921 565 (3)
0 0 3			−6.293 371 923 185 622 (3)	−3.169 879 510 759 632 (4)
0 1 2			3.675 090 508 043 885 (4)	2.846 449 846 018 038 (5)
0 2 1			2.615 385 046 630 319 (4)	1.342 564 901 871 183 (5)
0 3 0			2.121 292 565 892 837 (1)	−2.945 587 356 780 464 (2)
1 0 2			−3.691 589 067 790 872 (4)	−2.846 826 826 248 252 (5)
1 1 1			−2.104 594 029 611 347 (4)	−1.023 200 688 260 874 (5)
1 2 0			−1.851 134 145 358 710 (2)	−1.230 131 480 052 125 (3)
2 0 1			−5.123 938 050 679 311 (3)	−3.206 874 288 180 736 (4)
2 1 0			1.078 805 917 967 000 (2)	1.797 962 711 294 499 (3)
3 0 0			7.488 549 337 573 903 (1)	−1.978 686 066 875 219 (2)
0 0 4				7.245 695 514 300 020 (4)
0 1 3				−3.660 726 026 649 146 (5)
0 2 2				−2.041 229 668 970 605 (5)
0 3 1				2.665 674 999 640 809 (5)
0 4 0				−3.846 575 378 158 233 (1)
1 0 3				3.829 437 680 301 983 (5)
1 1 2				2.349 938 256 150 153 (5)
1 2 1				−8.639 753 539 916 517 (5)
1 3 0				8.856 047 059 290 417 (1)
2 0 2				−3.088 691 495 864 763 (4)
2 1 1				8.894 357 794 671 428 (5)
2 2 0				6.511 635 956 400 499 (2)
3 0 1				−2.920 615 508 406 978 (5)
3 1 0				−1.084 572 554 737 665 (3)
4 0 0				3.972 313 142 604 773 (2)

TABLE III. Excited-state energies of the muonic helium atom computed from 1- and 35-term wave functions.

		Z_e [a]	Z_μ [a]	E
$(1s)_e(2p)_\mu$ $^{1,3}P$	1-term	1.000 362 7	1.999 997 60	−101.035 320 27
	35-term	1.412	1.998 8	−101.035 345 15
$(1s)_e(3d)_\mu$ $^{1,3}D$	1-term	1.001 494 4	1.999 977 80	−45.182 775 76
	35-term	1.422	1.997 6	−45.182 982 68
$(1s)_e(4f)_\mu$ $^{1,3}F$	1-term	1.004 174 2	1.999 889 85	−25.635 162 14
	35-term	1.386	1.981 7	−25.635 968 26
$(1s)_e(5g)_\mu$ $^{1,3}G$	1-term	1.009 335 7	1.999 614 78	−16.588 756 27
	35-term	1.417	1.993 6	−16.590 963 87

[a] For definitions of Z_e and Z_μ, see footnotes b and c to Table I.

for 1-term wave functions, i.e., simple product wave functions, the variational calculation can be carried out explicitly by differentiation with respect to α and β. This is demonstrated in Appendix B, and the results for 1-term wave functions in Tables I–III were obtained by this method. All the energies are minimized to the last quoted digit. We have not attempted to find extrapolated energies,[20] as this procedure appears to be rather heuristic.

The flexibility in the choice of the exponential parameters α and β significantly reduces the number of terms required to achieve a given accuracy. All the nonlinear parameters are also optimized in this work to the last quoted digit. As can be seen from the variation of α and β, the effective charges cannot be defined unambiguously by the variational procedure because their optimum values with respect to the energy depend on the number of terms and the choice of basis functions in the variational expansion.

The merit of the present approach lies in its simplicity and its well-defined expansion sequence. With high-speed computers, it is possible to focus on the asymptotic behavior of wave functions with a large number of terms, rather than on the question of optimizing results with a given number of terms. Furthermore, the exact nonrelativistic Hamiltonian, including the mass correction, is used in the variational calculation. Accurate nonrelativistic wave functions obtained in this way can serve as a starting point in the calculation of relativistic, radiative, and nuclear-size corrections.

ACKNOWLEDGMENT

The author would like to thank Professor Bernd Crasemann for help in revising the manuscript and for many fruitful discussions.

APPENDIX A: EVALUATION OF INTEGRALS $A(l+2,m+2,n+2)$ and $A_y(l+2,m+2,n+2)$

We describe briefly the evaluation[12] of the integrals needed for the calculation of the matrix elements (12), (16), and (17). All the matrix elements of the operators are expressed in terms of the integrals

$$A(l+2,m+2,n+2) = \int \frac{d^3r_1}{4\pi} \int \frac{d^3r_2}{4\pi}\, e^{-ar_1-br_2}\, r_{12}^l r_1^m r_2^n \tag{A1}$$

and

$$A_y(l+2,m+2,n+2) = \int \frac{d^3r_1}{4\pi} \int \frac{d^3r_2}{4\pi}\, e^{-ar_1-br_2}\, r_{12}^l r_1^m r_2^{n-2L}\, 4\pi\, \frac{y_{11}(1)}{y_{11}(2)}\, y_{LL}^*(2) y_{LL}(2)\,, \tag{A2}$$

By the generalized Laplace's expansion to arbitrary powers of the interelectronic distance,[26] we have

$$r_{12}^l = \sum_{k=0}^{\infty} R_{lk}(r_1,r_2) P_k(\cos\theta_{12})\,, \tag{A3}$$

where the $P_k(\cos\theta_{12})$ are Legendre ploynomials. The radial functions $R_{lk}(r_1,r_2)$ are defined in terms of a hypergeometric function,

$$R_{lk}(r_1,r_2) = \frac{\Gamma(-\frac{1}{2}l+k)\Gamma(\frac{1}{2})}{\Gamma(-\frac{1}{2}l)\Gamma(k+\frac{1}{2})}\, r_>^l \left(\frac{r_<}{r_>}\right)^k \times {}_2F_1(k-\tfrac{1}{2}l\,,\, -\tfrac{1}{2}-\tfrac{1}{2}l\,;k+\tfrac{3}{2}\,,\, r_<^2/r_>^2)\,. \tag{A4}$$

The angular integrations in (A1) and (A2) can then be carried out easily with the results

$$A(l+2,m+2,n+2) = \int_0^\infty dr_1 \int_0^\infty dr_2\, e^{-ar_1-br_2} r_1^{m+2}\, r_2^{n+2} R_{l0}(r_1,r_2)\,, \tag{A5}$$

and

$$A_y(l+2,m+2,n+2) = \frac{1}{3}\int_0^\infty dr_1 \int_0^\infty dr_2\, e^{-ar_1-br_2} r_1^{m+3}\, r_2^{n+1} R_{l1}(r_1,r_2)\,. \tag{A6}$$

The integrals (A5) and (A6) are evaluated by means of the auxiliary functions

$$A_a(i) = \int_0^\infty e^{-ax} x^i\, dx\,, \tag{A7}$$

$$V_{ab}(m,n) = \int_0^\infty dx \int_x^\infty dy\, e^{-ax-by} x^m y^n\,,$$

$$m \geq 0\,, \quad (m+n) \geq -1\,. \tag{A8}$$

The recurrence relations are[27]

$$A_a(i) = (i/a)A_a(i-1)\,, \quad i \geq 1\,; \tag{A9}$$

$$V_{ab}(m,n) = (1/b)[nV_{ab}(m,n-1) + A_{(a+b)}(m+n)]\,,$$

$$m \geq 0\,, \quad (m+n) \geq 0\,. \tag{A10}$$

APPENDIX B: VARIATIONAL CALCULATION OF THE TOTAL ENERGY OF THREE-PARTICLE SYSTEMS WITH SIMPLE PRODUCT WAVE FUNCTIONS

We consider only states with the muon angular momentum quantum number $l = n-1$. The simple

product wave function is

$$\psi(\vec{r}_1,\vec{r}_2)=\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)\,;$$
$$\psi_1(\vec{r}_1)=(\alpha^3/\pi)^{1/2}e^{-\alpha r_1}\,, \tag{B1}$$
$$\psi_2(\vec{r}_2)=R_{n,(n-1)}(r_2)Y_{(n-1)m}(\Omega_2)\,,$$

where

$$R_{n,(n-1)}(r_2)=\left[\left(\frac{2\beta}{n}\right)^{2n+1}\frac{1}{(2n)!}\right]^{1/2}e^{-(\beta/n)r_2}r_2^{n-1}\,, \tag{B2}$$

The exact nonrelativistic Hamiltonian for uncorrelated wave functions is

$$H=-\frac{1}{2M_1}\vec{\nabla}_1^2-\frac{1}{2M_2}\vec{\nabla}_2^2-\frac{Z}{r_1}-\frac{Z}{r_2}+\frac{1}{r_{12}}\,, \tag{B3}$$

where M_1 and M_2 are the reduced masses with respect to the nucleus. By using wave function (B1) we can show that the energy expectation value is

$$E=\frac{a^2}{8M_1}+\frac{b^2}{8M_2}-\frac{Z}{2}\left(a+\frac{b}{n}\right)+\frac{1}{2}\frac{b}{n}\left(1-\frac{b^{2n}[(n+1)a+b]}{(a+b)^{2n+1}}\right), \tag{B4}$$

where $a=2\alpha$ and $b=2\beta/n$. Variation of the parameters a and b leads to the minimizing conditions

$$\frac{\partial E}{\partial a}=\frac{a}{4M_1}-\frac{Z}{2}+\frac{b^{2n+1}[2(n+1)a+b]}{(a+b)^{2n+2}}=0\,, \tag{B5}$$

$$\frac{\partial E}{\partial b}=\frac{b}{4M_2}-\frac{1}{2n}(Z-1)-\frac{b^{2n}[b^2+(2n+2)ab+(2n+1)(n+1)a^2]}{2n(a+b)^{2n+2}}=0\,. \tag{B6}$$

By introducing a new variable $x=b/a$, we can reduce (B5) and (B6) to

$$a=2M_1\left[Z-\frac{x^{2n+1}(x+2n+2)}{(x+1)^{2n+2}}\right], \tag{B7}$$

$$b=2\frac{M_2}{n}\left[Z-1+\frac{x^{2n}[x^2+(2n+2)x+(2n+1)(n+1)]}{(x+1)^{2n+2}}\right] \tag{B8}$$

and effect a further reduction to an equation of degree $(2n+3)$:

$$F(x)=[xZ-k(Z-1)](x+1)^{2n+2}-x^{2n}[x^3+(2n+2+k)x^2+(2n+2)kx+(2n+1)(n+1)k]=0\,, \tag{B9}$$

where $k=M_2/(nM_1)$. To find the desired root of (B9), we can employ the Newton process. Let x_0 be close to the desired root R, and

$$x_n=x_{n-1}-F(x_{n-1})/F'(x_{n-1})\,, \tag{B10}$$

then $x_n\to R$, as $n\to\infty$. For the muonic helium atom, the desired root $R\sim M_2/M_1\gg 1$; so we choose x_0 to be the root of the approximated equation

$$F(x)\approx x^{2n+1}(x+2n+2)(Zx-x-Zk)=0\,,$$

and get

$$x_0=kZ/(Z-1)\,. \tag{B11}$$

Alternatively, we can obtain the desired root from (B7) and (B8) by an iterative process, which automatically eliminates any local maximum of E. The root R obtained from either of the above methods may be checked by verifying that $(\partial^2E/\partial a^2)_{x=R}>0$ and $(\partial^2E/\partial b^2)_{x=R}>0$.

*Supported in part by the National Aeronautics and Space Administration (NGR 38-003-036) and by the U. S. Army Research Office (DAHC 04-75-G-0021).

† Present address: Dept. of Physics and Astronomy, Univ. of Nebraska, Lincoln, Neb. 68588.

[1]K. Evans and K. A. Pounds, Astrophys. J. 152, 319 (1968).

[2]K. G. Widing and G. D. Sandlin, Astrophys. J. 152, 545 (1968).

[3]A. H. Gabriel and C. Jordan, *Case Studies in Atomic Collision Physics II* (North-Holland, Amsterdam, 1972).

[4]I. Martinson and A. Gaupp, Phys. Rep. 15C, 115 (1974).

[5]D. J. Pegg and I. A. Sellin, *Beam Foil Spectroscopy* (Plenum, New York, 1976).

[6]C. S. Wu and L. Wilets, Ann. Rev. Nucl. Sci. 19, 527 (1969).

[7]G. Backenstoss, Ann. Rev. Nucl. Sci. 20, 467 (1970).

[8]E. H. S. Burhop, Contemp. Phys. 11, 335 (1970).

[9]L. Tauscher, in Proceedings of the Sixth International Conference on High-Energy Physics and Nuclear Structure, Santa Fe, New Mexico, 1975 (unpublished).

[10]F. Scheck and J. Hüfner, in *Muon Physics*, edited by V. W. Hughes and C. S. Wu (Academic, New York, 1976).

[11]P. A. Souder, D. E. Casperson, T. W. Crane, V. W. Hughes, D. C. Lu, H. Orth, H. W. Reist, M. H. Yam, and G. zu Putlitz, Phys. Rev. Lett. 34, 1417 (1975).

[12]K.-N. Huang, Ph.D. thesis (Yale University, 1974) (unpublished).

[13]K.-N. Huang, V. W. Hughes, M. L. Lewis, R. O. Mueller, H. Rosenthal, C. S. Wu, and M. Camani, in *Proceedings of the Fifth International Conference on High-Energy Physics and Nuclear Structure*, edited

by G. Tibell (North-Holland, Amsterdam, 1973), p. 312.
[14]V. W. Hughes and S. Penman, Bull. Am. Phys. Soc. 4, 80 (1959).
[15]K.-N. Huang, V. W. Hughes, and M. L. Lewis, Bull. Am. Phys. Soc. 18, 1503 (1973).
[16]M. Camani, Helv. Phys. Acta 46, 47 (1973).
[17]P. K. Haff and T. A. Tombrello, Ann. Phys. (N.Y.) 86, 178 (1974).
[18]C. L. Pekeris, Phys. Rev. 126, 1470 (1962).
[19]Y. Accad, C. L. Pekeris, and B. Schiff, Phys. Rev. A 4, 516 (1971).
[20]C. Schwartz, Phys. Rev. A 134, 1181 (1964).
[21]J. N. Silverman and G. H. Brigman, Rev. Mod. Phys. 39, 228 (1967).
[22]H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin, 1957).
[23]E. A. Hylleraas, Z. Phys. 54, 347 (1929).
[24]A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U.P., Princeton, N.J., 1957).
[25]An expression of the total Hamiltonian in terms of r_1, r_2, θ_{12}, and the Euler angles was given by A. K. Bhatia and A. Temkin [Phys. Rev. A 137, 1335 (1965)].
[26]R. A. Sack, J. Math. Phys. 5, 245 (1964).
[27]H. M. James and A. S. Coolidge, Phys. Rev. 49, 688 (1936).