radiative component a_{ij} and a radiative component ω_{ij}. Since $\omega_{13}^{L} = I_{L_1L_3}/N_1$, Table VIII gives $\omega_{13}^{L} = 0.011 \pm 0.005$ at $Z = 93$ and $\omega_{13}^{L} = 0.009 \pm 0.005$ at $Z = 96$. The radiative component of the total CK yield f_{13}^{L} thus appears to be about 2% of the total.

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Ground-State Energies of the He Atom and the Li^+ Ion in the Faddeev Approach

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The ground-state energies of the He atom and the Li^+ ion have been calculated using the Faddeev formalism. For the off-shell two-body collision amplitude (t matrix), Sturmian-function (SF) as well as Coulomb-function representations have been employed. For the He atom, calculations have been performed retaining $1s$, $1s$ and $2s$, and $1s$, $2s$, and $3s$ states in the SF representation for the two-body t matrix, whereas only the $1s$ term has been retained in the mixed-mode (MM) representation. For the Li^+ ion, computations have been done after retaining terms up to $2s$ in the SF representation and only the $1s$ term in the MM representation. The results obtained by retaining only the $1s$ term are in marked disagreement with the experimental values in both representations. It is noticed that the results for the MM representation are almost as much below the experimental values as those for the SF representation are above. The results for the MM representation are slightly better than those for the SF representation. This is seen more clearly in the case of the Li^+ ion. The results in the SF representation are found to be in good agreement with the experimental findings after inclusion of the $2s$ term.

I. INTRODUCTION

A rigorous mathematical formulation of the nonrelativistic three-body problem with pair interactions has been given by Faddeev.[1,2] For local potentials, the theory involves the solution of a set of coupled integral equations in at least two continuous variables. In the case of Coulomb potentials, Ball *et al.*[3] and Chen *et al.*[4] have used separable expansions for the off-shell two-body collision amplitude

(t matrix) with Sturmian-function and also Coulomb-function expansion bases. The representation in which Sturmian functions are used in the expansion of the t matrix for every pair, both attractive and repulsive, has been termed the Sturmian-function (SF) representation. When Coulomb functions are used for the attractive pairs and Sturmian functions for the repulsive one, the representation is called a mixed-mode (MM) representation. Single-variable integral equations are obtained when these separable representations are used for the t matrix. Thus these authors have given a practical method for solving the Faddeev equations with Coulomb potentials and have computed the energies of the H^- bound state and its resonant states, as well as the s-wave phase shifts in the e^--H elastic collision. Rajagopal and co-workers[5,6] have carried out calculations for the ground-state energies of some three-particle Coulomb systems, retaining only the $1s$ term in the SF representation. Calculations for the binding energy of the ground state of He atom have been performed by Banerji *et al.*[7] using the one-state and two-state approximations in the SF representation.

In the present work, calculations for the ground-state energy of the He atom have been extended by including the $3s$ term in the SF representation of the two-body t matrix with a view to studying the convergence of the result with the inclusion of higher states. The method has been further applied to calculate the binding energy of the Li^+ ion in the two-state approximation. We have also applied the formalism due to Chen *et al.*[4] for the calculation of the binding energies of both the He atom and the Li^+ ion in the MM representation with a one-state approximation, and the results have been compared with those for the SF representation. For the He case we obtain six one-dimensional coupled integral equations when terms up to $3s$ are retained in the expansion for the t matrix. These equations when converted into a matrix equation give rise to a matrix of large dimension when quadratures with a suitable number of points are used in the evaluation of the integrals. Thus, although the Faddeev approach is exact when all the states are included, an upper limit for retaining terms in the expansion, i.e., for increasing the number of coupled integral equations, is set up. When the number of coupled integral equations becomes very large, it becomes formidable to tackle such equations even with present-day fast computers.

II. MATHEMATICAL FORMULATION

In the SF representation, following Ball *et al.*,[3] we may express the off-shell three-particle collision amplitude $\Psi_i^{(i)}(p,q,s)$ in which the ith pair of particles undergo final-state interactions as

$$\Psi_i^{(i)}(p,q,s)=\Phi_i^{(i)}(p,q,s)+\sum_{n=1}^{\infty}\{\lambda_{nl}^{(i)}(s-q^2)/[1-\lambda_{nl}^{(i)}(s-q^2)]\}\,\phi_{nl}^{(i)}(p,s-q^2)\,\chi_{nl}^{(i)}(q,s), \quad (2.1)$$

where $\Phi_i^{(i)}(p,q,s)$ represents the amplitude in which particle i acts as a spectator, $\phi_{nl}^{(i)}(p,E)$ is the eigenfunction of the Lippman-Schwinger equation for the Coulomb potential with the eigenvalue $\lambda_{nl}^{(i)}(E)$, and the functions $\chi_{nl}^{(i)}(q,s)$ can be determined from the set of coupled single-variable integral equations

$$\chi_{nl}^{(i)}(q,s)=\eta_{nl}^{(i)}(q,s)+\sum_{n',l',j\neq i}\int_0^{\infty}dq_j^2\,\kappa_{nl,n'l'}^{(i,j)}(q,q_j;s)\times\chi_{n'l'}^{(j)}(q_j,s)\quad(i=1,2,3), \quad (2.2)$$

with

$$\kappa_{nl,n'l'}^{(i,j)}(q,q_j;s)=\int_{L_{ij}}^{U_{ij}}dp_j^2\,B_{ll'}^{(i,j)}(q,p_j,q_j;s)\,\lambda_{n'l'}^{(j)}(s-q_j^2)\times\frac{\phi_{nl}^{(i)}(p_i,s-q^2)\,\phi_{n'l'}^{(j)}(p_j,s-q_j^2)}{[1-\lambda_{n'l'}^{(j)}(s-q_j^2)]}, \quad (2.3)$$

$$\eta_{nl}^{(i)}(q,s)=\sum_{l',j\neq i}\int_0^{\infty}dq_j^2\int_{L_{ij}}^{U_{ij}}dp_j^2\,B_{ll'}^{(i,j)}(q,p_j,q_j;s)\times\phi_{nl}^{(i)}(p_i,s-q^2)\,\Phi_{l'}^{(j)}(p_j,q_j,s), \quad (2.4)$$

$$B_{ll'}^{(i,j)}(q,p_j,q_j;s)\equiv\frac{(-)^{l+l'}[(2l+1)(2l'+1)]^{1/2}}{4\pi\,\alpha_{ij}\beta_{ij}q(p_j^2+q_j^2-s)}\times P_l(\omega_i)\,P_{l'}(\bar{\omega}_j), \quad (2.5)$$

and the limits of integration given by

$$U_{ij}=(\alpha_{ij}q_j+q)^2/\beta_{ij}^2,\qquad L_{ij}=(\alpha_{ij}q_j-q)^2/\beta_{ij}^2 \quad (2.6)$$

and all other symbols have their usual meanings.[3] In Eq. (2.1) the SF expansion of the t matrix

$$t_i^{(i)}(p,p';E)=\textstyle\sum_n\{\lambda_{nl}^{(i)}(E)/[1-\lambda_{nl}^{(i)}(E)]\}\times\phi_{nl}^{(i)}(p,E)\,\phi_{nl}^{(i)}(p',E) \quad (2.7)$$

has been employed for every pair of particles.

In the MM representation the two-body t matrix for an attractive pair is expressed in terms of the orthonormal set of Coulomb wave functions $\psi_{nl}(np)$ which satisfy the Schrödinger equation

$$(p^2-\epsilon_n)\,\psi_{nl}(np)=-\pi^{-1}\int_0^{\infty}dp'^2p'\,V_l(p,p')\,\psi_{nl}(np'), \quad (2.8)$$

with the orthonormality relation

$$\int_0^{\infty}\psi_{nl}(np)\,\psi_{n'l}(n'p)\,p^2dp=\delta_{nn'}\,. \quad (2.9)$$

Thus for an attractive pair we have

$$t_l^{(i)}(p,p';E) = V_l(p,p') + \tfrac{1}{2}\pi \sum_n' [(p^2-\epsilon_n)(p'^2-\epsilon_n)/(E-\epsilon_n)] \times \psi_{nl}(np)\,\psi_{nl}(np'), \quad (2.10)$$

where the Coulomb potential $V_l(p,p')$ can be expressed in any one of the following ways:

$$V_l(p,p') = -\tfrac{1}{2}\pi \sum_n' (p^2-\epsilon_n)\,\psi_{nl}(np)\,\psi_{nl}(np') \quad (2.11a)$$

$$= -\tfrac{1}{2}\pi \sum_n' (p'^2-\epsilon_n)\,\psi_{nl}(np)\,\psi_{nl}(np') \quad (2.11b)$$

$$= -\tfrac{1}{4}\pi \sum_n' [(p^2-\epsilon_n)+(p'^2-\epsilon_n)]\,\psi_{nl}(np)\,\psi_{nl}(np'). \quad (2.11c)$$

The prime on the summation sign indicates summation over the discrete states and integration over the continuum states. Using the expression (2.11a) for the Coulomb potential, we then obtain the three-particle amplitude as

$$\Psi_l^{(i)}(p,q,s) = \Phi_l^{(i)}(p,q,s) + \tfrac{1}{2}\pi \sum_n' \frac{p^2-\epsilon_n^{(i)}}{s-\epsilon_n^{(i)}-q^2} \times \psi_{nl}^{(i)}(np)\,\chi_{nl}^{(i)}(q,s). \quad (2.12)$$

For the repulsive pair we have employed, as before, the SF as the expansion basis for the two-body amplitude. Choosing, for definiteness, the third pair (i.e., particles 1 and 2) to be repulsive, and pairs 1 and 2 to be attractive, Chen *et al.*[4] have shown that in the MM representation the functions $\chi_{nl}^{(i)}(q,s)$ satisfy the set of coupled single-variable integral equations

$$\chi_{nl}^{(i)}(q,s) = \eta_{nl}^{(i)}(q,s) + \sum_{n'l'}' \sum_{j\neq i, j\neq 3} \int_0^\infty dq_j^2\, \kappa_{nl,n'l'}^{(i,j)}(q,q_j;s)\,\chi_{n'l'}^{(j)}(q_j,s) + \sum_{n'l'} \int_0^\infty dq_3^2\, \kappa_{nl,n'l'}^{(i,3)}(q,q_3;s)\,\chi_{n'l'}^{(3)}(q_3,s) \quad (i=1,2), \quad (2.13a)$$

$$\chi_{nl}^{(3)}(q,s) = \eta_{nl}^{(3)}(q,s) + \sum_{n'l'}' \sum_{j\neq 3} \int_0^\infty dq_j^2\, \kappa_{nl,n'l'}^{(3,j)}(q,q_j;s)\,\chi_{n'l'}^{(j)}(q_j,s), \quad (2.13b)$$

with

$$\kappa_{nl,n'l'}^{(i,j)}(q,q_j;s) = -\frac{\pi}{2}\int_{L_{ij}}^{U_{ij}} dp_j^2\, B_{ll'}^{(i,j)}(q,p_j,q_j;s)\,\frac{(p_j^2+q_j^2-s)(p_j^2-\epsilon_{n'}^{(j)})}{s-\epsilon_{n'}^{(j)}-q_j^2}\,\psi_{nl}^{(i)}(np_i)\,\psi_{n'l'}^{(j)}(n'p_j), \quad (2.14a)$$

$$\kappa_{nl,n'l'}^{(i,3)}(q,q_3;s) = -\int_{L_{i3}}^{U_{i3}} dp_3^2\, B_{ll'}^{(i,3)}(q,p_3,q_3;s)\,\frac{p_3^2+q_3^2-s}{1-\lambda_{n'l'}^{(3)}(s-q_3^2)}\,\lambda_{n'l'}^{(3)}(s-q_3^2)\,\psi_{nl}^{(i)}(np_i)\,\phi_{n'l'}^{(3)}(p_3,s-q_3^2), \quad (2.14b)$$

$$\kappa_{nl,n'l'}^{(3,j)}(q,q_j;s) = \frac{\pi}{2}\int_{L_{3j}}^{U_{3j}} dp_j^2\, B_{ll'}^{(3,j)}(q,p_j,q_j;s)\,\frac{p_j^2-\epsilon_{n'}^{(j)}}{s-\epsilon_{n'}^{(j)}-q_j^2}\,\phi_{nl}^{(3)}(p_3,s-q^2)\,\psi_{n'l'}^{(j)}(n'p_j), \quad (2.14c)$$

$$\eta_{nl}^{(i)}(q,s) = -\sum_{l',j\neq i} \int_0^\infty dq_j^2 \int_{L_{ij}}^{U_{ij}} dp_j^2\, B_{ll'}^{(i,j)}(q,p_j,q_j;s)(p_j^2+q_j^2-s)\,\psi_{nl}^{(i)}(np_i)\Phi_{l'}^{(j)}(p_j,q_j,s), \quad i=1,2 \quad (2.15a)$$

$$\eta_{nl}^{(3)}(q,s) = \sum_{l',j\neq 3} \int_0^\infty dq_j^2 \int_{L_{3j}}^{U_{3j}} dp_j^2\, B_{ll'}^{(3,j)}(q,p_j,q_j;s)\,\phi_{nl}^{(3)}(p_3,s-q^2)\,\Phi_{l'}^{(j)}(p_j,q_j,s). \quad (2.15b)$$

To consider the effect of spin we must multiply[8] the kernels K by a factor which, however, is unity for our systems. For two spin-$\frac{1}{2}$ identical particles, t is zero for even l if the spin of the pair is $S=1$, and t is zero for odd l if $S=0$. Further, since the ground states of both the systems He and Li^+ are zero-total-angular-momentum states, restricting ourselves only to the $l=0$ state expansion, we have

$$\chi_{n0}^{(1)}(q,s) = \chi_{n0}^{(2)}(q,s). \quad (2.16)$$

Thus the three coupled integral equations for $\chi_{nl}^{(i)}(q,s)$, $i=1,2,3$ are reduced to a pair of coupled equations.

III. RESULTS AND DISCUSSION

For bound states, the inhomogeneous parts in the integral equations for the χ's are dropped. The limits of integration in these equations are changed to -1 and $+1$ by the transformations

$$q_i^2 = \frac{1+x_i}{1-x_i}, \quad q^2 = \frac{1+x}{1-x} \quad (3.1)$$

and the usual Gauss-Legendre quadrature is used to recast the integral equations into a matrix equation of the form

$$A\tilde{\chi} = 0. \quad (3.2)$$

The ground-state energies are found by searching for the energy at which the determinant of the corresponding matrix A is zero.

To test the efficiency of our transformations for change of variables and also to test the convergence

TABLE I. Magnitudes of the ground-state energies of the He atom and Li^+ ion (in units of e^2/a_0) obtained by using the Faddeev formalism.

System	Present results SF representation $1s$	$1s+2s$	$1s+2s+3s$	MM representation $1s$	Variational results of Stewart (Ref. 9)	Experimental values
He	2.532 95	2.925 73	3.045 04	3.267 09	2.9037	2.9040[a]
Li^+	6.186 43	7.232 51	•••	8.187 68	7.2799	7.2811[a]

[a]Reference 10.

problem, we have carried out our computations by using 12- and 16-point Gaussian quadrature for the SF and MM representations, respectively, and have checked the results by increasing the number of points to 16 and 20, respectively. The results are found to remain unchanged up to five decimal places.

In Table I, we have tabulated our results for the ground-state energies of the He atom and Li^+ ion in the SF and MM representations with different degrees of approximation, and have compared them with the variational results of Stewart[9] and the experimental findings.[10] For the He atom, it has been noticed that the retention of the $1s$ term alone in the SF representation leads to a value of the ground-state energy far above the experimental result. For the H^- case, on the other hand, the same approximation yields the ground-state energy as -1.0516 Ry, which is 93% of the total contribution. Therefore, inclusion of the $1s$ term alone in the He problem is not at all sufficient. When the $2s$ term is included in the expansion, we obtain the result $-2.925\,73e^2/a_0$, which agrees very closely with the experimental value $-2.9040e^2/a_0$, although slightly overshooting it.[7] Retention of terms up to $3s$ gives the value $-3.045\,04e^2/a_0$, which is slightly lower than the previous value obtained with the inclusion of the $1s$ and $2s$ states. Thus we notice that as we go on including terms up to $3s$ in the expansion for the t matrix, the results get gradually farther displaced from the exact value, in the same direction. Hence, the oscillatory behavior observed in the case of H^- by Ball *et al.*[3] is not manifested here.

Unlike Rajagopal and co-workers,[5,6] we have found that the MM representation does yield convergent results as the size of the matrix is increased. In the MM representation with the $1s$ state alone in the expansion for the t matrix, our result for the He ground-state energy is almost as far below the experimental value as the corresponding result in the SF representation is above it. For the Li^+-ion case also, we notice that our result for the ground-state energy with the $1s$ state alone in the SF representation lies far above the exact one. On inclusion of the $2s$ state, the ground-state energy falls down to $-7.232\,51e^2/a_0$, in close agreement with the experimental value $-7.2811e^2/a_0$. In the MM representation, inclusion of the $1s$ state alone gives the Li^+ ground-state energy as $-8.187\,68e^2/a_0$, which is also below the experimental value, as observed in the corresponding He problem. The MM representation with the $1s$ state alone gives, however, a better result than the corresponding SF representation, for both He and Li^+ ground states. This is more pronounced in the Li^+ case. It will be interesting to test the convergence of the results in the MM representation as more and more states are included in the expansion for the t matrix. Further investigations on the resonant states of the He atom are in progress.

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