Faddeev approach to atomic three-body problems*

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The Faddeev equations for the (e^-, H) system have been solved numerically using separable expansions for both screened and unscreened versions of the Coulomb t matrix. By considering the equations in uncoupled form, the convergence behavior of the binding energy and the singlet scattering length have been examined as the number of terms in the representation of the electron-electron potential has been increased. One to three states have been included in the e-p interaction and up to twenty states in the e-e interaction. Although the unscreened values are reasonable in low orders of truncation, the convergence is poor as more terms are included in the separable representations. To improve the rate of convergence, a screened form of the Coulomb t matrix based on the Sturmian expansion of the Hulthén potential has been introduced. In the lowest trucation of the e-p system, strong shielding of the e-e interaction is necessary and convergence of both the binding energy and the scattering length can be achieved. In higher truncations of the e-p system, where the representation of the e-p interaction is more realistic, shielding is not effective in improving the rate of convergence within the practical limits of the calculations. The implications of the present calculations for the Faddeev approach to atomic three-body problems are discussed.

I. INTRODUCTION

Chen and co-workers in a number of papers[1-5] have applied the Faddeev equations to the three-body problem with Coulomb interactions. In order to obtain a numerically tractable set of equations, the basic integral equations of the theory are reduced in dimension by utilizing the Sturmian expansion[6] of the two-body Coulomb t matrix. Although calculations of three-body observables, such as the binding energy of the H^- ion and resonances in low-energy electron-hydrogen scattering, appear quite promising in low orders of truncation, the numerical results fluctuate markedly as more terms are included in the separable expansions of the two-body interactions. Indeed, it is not clear that the approximation scheme is in principle convergent, since, unlike the situation with short-ranged potentials, the Faddeev equations with Coulomb potentials are singular. Thus the feasibility of using the Faddeev equations for accurate calculations of the properties of atomic, three-body systems is questionable.

The problem of slow convergence (or even perhaps lack of convergence) arises from the well-known divergence of the Coulomb t matrix for scattering in the forward direction, which is associated with long-range tail of the Coulomb potential. It might be expected that the resulting logarithmic singularity of the kernel of the Faddeev equations could be handled easily with suitable quadrature rules on numerical integration of the equations. But it must be emphasized that apart from the divergence at zero-momentum transfer, the Sturmian expansion provides a poor representation of the Coulomb potential over an appreciable range of small momentum transfers, converging extremely slowly with large oscillations, both in period and magnitude.[3,7]

To improve the rate of convergence in three-particle calculations, it appears necessary to modify the Sturmian expansion in a way which simulates the screening of the potential at large distances. In this paper the effect of screening on the convergence rate is investigated by considering the Sturmian expansion for the Hulthén potential[8] $V^a(r) = ze^2a^{-1}(e^{r/a} - 1)^{-1}$, which, for distances r which are small compared with the screening radius a behaves like the Coulomb potential $V(r) = ze^2/r$, and which for large r decreases exponentially.

In Sec. II a separable expansion of the t matrix for the Hulthén potential, which is suitable for three-body calculations, is introduced. This expansion has three desirable properties. First, the series of separable terms converges smoothly in the forward direction for moderate values of the screening radius. Second, in the limit that the screening radius becomes infinite, the expansion reduces to the usual Sturmian expansion of the unscreened Coulomb t matrix. Finally, as in the case of the Sturmian expansion of the unshielded Coulomb t matrix, the kernels of the Faddeev equations can be constructed in closed form without the need for numerical integration. The expansion for the Hulthén potential is only obtained explicitly for the angular-momentum zero projection of the potential in momentum space. In Sec. II a shielded form of the Coulomb t matrix based on the Hulthén expansion, which is easily

applied in all partial waves, is also proposed.

In Secs. III and IV calculations of the binding energy and singlet scattering length of the (e^-, H) system using both screened and unscreened forms of the Coulomb potential are described. These calculations are not intended to compete in accuracy with the standard variational calculations, but provide a test of the practicality of the Faddeev method using shielded interactions. Our aim is to study the rate of convergence as the number of terms in the representations of the two-body interactions is increased. If the same number of terms is included in all three pair interactions, the problem of numerical solution rapidly gets out of hand. However, if the exchange symmetry of the two electrons is taken into account, the Faddeev equations may be uncoupled. In uncoupled form it is possible to include a large number of terms in the repulsive electron-electron interactions without increasing the dimension of the numerical inversion problem. Hence a fixed number of terms is taken in the electron-proton system and the convergence of the three-body binding energy and scattering length is examined as the number of terms in the electron-electron interaction is increased. (It is perhaps worth noting that for values of the three-body energy close to the two-body bound-state poles, the first few terms make the major contribution to the Sturmian expansion for the attractive e-p t matrix, whereas there is no such pole dominance for the repulsive e-e interaction.)

In Sec. IV the results of the calculations are presented. One to three terms have been included in the e-p interactions and up to twenty terms in the e-e interaction. The only practical limitation on the number of terms included in the e-e interaction arises from the difficulty of computing the matrix elements of the kernel with sufficient numerical accuracy. The calculations show that the convergence rate may be significantly improved by introducing screening, but that a screening radius which is sufficiently small to produce rapid convergence generates large over-all shifts in the binding energy. Nevertheless, convergence to the true binding energy can be achieved by taking an appropriate value of the screening radius. In a scattering problem the screening radius might be regarded as an arbitrary parameter, which is fixed in each truncation of the e-p system by requiring that the correct binding energy be predicted. As a test of this approach, the singlet scattering length has also been calculated for a range of shielding radii. It is found that although the screened t matrix produces acceptable values for both the binding energy and the scattering length in the lowest truncation of the e-p system, the introduction of screening is not effective in obtaining satisfactory results within the practical limits of the calculation in higher truncations of the e-p system.

Our conclusions and the general implications of our results for the Faddeev approach to atomic problems are discussed in Sec. V.

II. SCREENED COULOMB t MATRIX

In terms of the eigenvectors ϕ_λ and eigenvalues γ_λ of the kernel of the Lippmann-Schwinger equation,

$$VG_0(E)\phi_\lambda(E) = \gamma_\lambda(E)\phi_\lambda(E), \tag{2.1}$$

the two-body t matrix at energy E,

$$t(E) = V + VG_0(E)t(E) \tag{2.2}$$

may be expressed in separable form[8] as

$$t(E) = \sum_\lambda \phi_\lambda^*(E)\phi_\lambda(E)[1-\gamma_\lambda(E)]^{-1}, \tag{2.3}$$

where V is the potential and $G_0(E) = (E - p^2/2\mu)^{-1}$ is the free propagator, with μ the reduced mass of the two-body system. The eigenvectors ϕ_λ satisfy the orthonormality condition

$$(\phi_\lambda, G_0^{-1}\phi_{\lambda'}) = \delta_{\lambda\lambda'}. \tag{2.4}$$

For the case of the Coulomb potential in momentum space,

$$V_l(p,p') = \frac{ze^2}{pp'}\, Q_l\!\left(\frac{p^2+p'^2}{2pp'}\right), \tag{2.5}$$

the partial-wave form of the integral equation (2.1) for orbital angular momentum l may be solved exactly. The eigenvectors $\phi_{\lambda l}$ are then the well-known Sturmian functions[3,6]

$$\phi_{\lambda l}(p,s) = \left(\frac{2^{4l+3}\lambda(\lambda-l-1)!}{\mu(\lambda+l)!}\right)^{1/2} l!\, s^{(2l+3)/2} \times \frac{p^l}{(p^2+s^2)^{l+1}}\, C_{\lambda-l-1}^{l+1}\!\left(\frac{p^2-s^2}{p^2+s^2}\right), \tag{2.6}$$

where $s^2 = -2\mu E$ and $C_{\lambda-l-1}^{l+1}$ are Gegenbauer polynomials.[9] (As far as possible the notation and normalization conventions of Ref. 3 are followed.)

The associated eigenvalues are

$$\gamma_{\lambda l} = -\lambda s/ze^2\mu, \tag{2.7}$$

and the partial-wave Coulomb t matrix in separable form becomes

$$t_l(p,p';s) = \sum_\lambda [1-\gamma_{\lambda l}(s)]^{-1}\phi_{\lambda l}(p,s)\phi_{\lambda l}(p',s). \tag{2.8}$$

In the limit $s \to \infty$, t_l approaches V_l, and we obtain a separable expansion for the potential,

$$V_l(p,p') = -\sum_\lambda \gamma_{\lambda l}^{-1}(s)\phi_{\lambda l}(p,s)\phi_{\lambda l}(p',s)\,. \quad (2.9)$$

This series at best converges conditionally, since the terms approach zero like λ^{-1} (λ is a positive integer) multiplied by functions of oscillating sign.[7] When $p=p'$, the associated Legendre function of the potential [Eq. (2.5)] has a logarithmic singularity and the series (2.9) diverges. Furthermore, numerical calculations show that when p is close to p', the series converges very slowly with large oscillations in both period and magnitude. An example of this behavior is shown in Fig. 1. Further examples may be found in the work of Chen and Ishihara.[3] Their extensive calculations also show that the remainder of the expansion for t, i.e.,

$$t_l(p,p',s) - V_l(p,p') = \sum_\lambda \{[1-\gamma_{\lambda l}(s)]\gamma_{\lambda l}(s)\}^{-1} \times \phi_{\lambda l}(p,s)\phi_{\lambda l}(p',s)\,, \quad (2.10)$$

is well behaved and converges reasonably smoothly. Thus the major problem with the expansion (2.8) for practical three-body calculations results from the poor behavior of the Born term (2.9) in the neighborhood of the logarithmic singularity of the potential at $p=p'$.

Consider now the expansion (2.3) for the Hulthén potential[8,10] $V^a(r) = ze^2a^{-1}(e^{r/a}-1)^{-1}$, which may be regarded as a screened form of the Coulomb potential $V(r)=ze^2/r$ with screening radius a. Our discussion is limited to s waves, so that we drop the angular-momentum suffix l. Defining

$$\Theta_\lambda(r,s) = rV^{-1}(r)\phi_\lambda(r,s)\,, \quad (2.11)$$

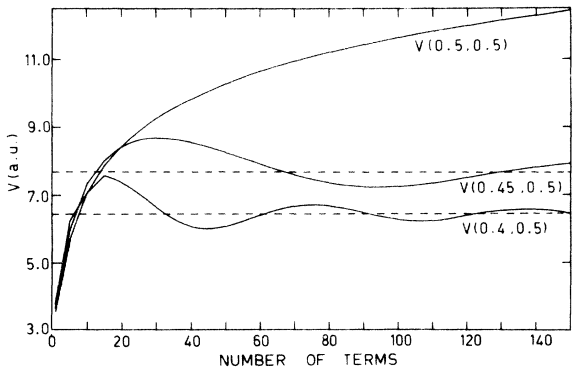

FIG. 1. Convergence behavior of the Sturmian expansion of the Coulomb potential $V(p,p')$. The broken lines indicate the exact values of V; for equal arguments the expansion diverges. Note that the value of the series for V has been plotted after every fifth term, and that the choice $s=1$ has been made in Eq. (2.9).

we see from Eq. (2.1) that Θ_λ satisfies a Schrödinger equation,

$$\left(\frac{d^2}{dr^2} - s^2 - \gamma_\lambda^{-1}(s)V(r)\right)\Theta_\lambda(r,s) = 0\,, \quad (2.12)$$

where the energy is fixed and the potential strength allowed to vary. With a suitable change of variables Eq. (2.12) can be transformed to the hypergeometric equation with normalized solutions which vanish at $r=0$ given by

$$\Theta_\lambda(r,s) = (1-e^{r/a})e^{-rs}P_{\lambda-1}^{(1,2sa)}(2e^{r/a}-1)\,, \quad (2.13)$$

where $P_{\lambda-1}^{(1,2sa)}$ are Jacobi polynomials.[9] The associated eigenvalues are

$$\gamma_\lambda^a = -(\lambda^2+2\lambda sa)/2\mu z e^2 a\,. \quad (2.14)$$

The functions $\phi_\lambda^a(p,s)$ normalized according to Eq. (2.4) are then found by Fourier transformation of Eq. (2.11),

$$\phi_\lambda^a(p,s) = N_\lambda p^{-1}\int_0^\infty \sin(pr)\,e^{r/a(1+sa)}P_\lambda^{(1,2sa)}(2e^{-r/a}-1)\,dr\,, \quad (2.15)$$

with

$$N_\lambda = \left\{\frac{2(\lambda+2as)^2(\lambda+as)}{\mu a^3}\right\}^{1/2}.$$

After using the explicit expression for the Jacobi polynomials,[9] the integral may be evaluated to obtain ϕ_λ^a in a form which is suitable for insertion in the Faddeev equations,

$$\phi_\lambda^a(p,s) = N_\lambda \sum_{j=1}^{\lambda} b_j^\lambda [p^2+(s+ja^{-1})^2]^{-1}\,, \quad (2.16)$$

with

$$b_j^\lambda = \binom{\lambda-1}{j-1}\frac{\Gamma(2as+\lambda+j)(-1)^{j+\lambda}}{\Gamma(2as+j)(\lambda-1)!(2as+\lambda)}\,. \quad (2.17)$$

In the Appendix it is shown that in the limit of infinite screening radius,

$$\phi_\lambda^a(p,s) \to \mu^{-1/2}\frac{(2s)^{3/2}}{p^2+s^2}C_{\lambda-1}^1\left(\frac{p^2-s^2}{p^2+s^2}\right), \quad (2.18)$$

which is equal to $\phi_{\lambda 0}(p,s)$ of Eq. (2.6). Also in this limit the eigenvalues (2.14) reduce to the eigenvalues (2.7) and the usual Sturmian expansion of the unscreened Coulomb t matrix is recovered.

Numerical calculations comparing the Sturmian expansions of V and t for the Hulthén and Coulomb potentials have been performed for a wide range of momenta energy and screening radii. As shown in Fig. 2, the screened form is finite for $p=p'$. As expected, the rate and smoothness of convergence are improved as the range of the potential is decreased. Of course, when the screening is made stronger, the potential is effectively weakened and the screened values are shifted further

from the unscreened values. Several examples are shown in Fig. 3.

Let us now return to the problem of introducing screening into the Coulomb t matrix. Since the poor convergence of the Sturmian expansion arises from the Born term (2.9), we split off the tail of the potential in the following way:

$$t = V^a + VG_0t + V - V^a \equiv t^a + V - V^a . \tag{2.19}$$

The separable expansions for V^a and VG_0t and hence t^a are well behaved. We also note that t^a has the same set of poles as the full t matrix; only the singularity at $p = p'$ has been smoothed. Consequently for the attractive potential, the bound-state poles and their residues, i.e., the two-body binding energies and bound states, are not altered. Hopefully, in three-particle calculations which are not sensitive to the tail of the Coulomb potential, the difference between the Coulomb potential V and the Hulthén potential V^a may be treated as a perturbation.

In the s wave the screened form of t used in the calculations of Sec. III is then

$$t_0^a(p,p',s) = \sum_\lambda \{[\gamma_{\lambda 0}(1-\gamma_{\lambda 0})]^{-1}\phi_{\lambda 0}(p,s)\phi_{\lambda 0}(p',s) - (\gamma_\lambda^a)^{-1}\phi_\lambda^a(p,s)\phi_\lambda^a(p',s)\}, \tag{2.20}$$

where $\gamma_{\lambda 0}$, $\phi_{\lambda 0}$, γ_λ^a, and ϕ_λ^a are defined by Eqs. (2.7), (2.6), (2.14), and (2.16), respectively.

The form of the expansion for the Hulthén potential also suggests a simple way of smoothing the logarithmic singularity in the Coulomb t matrix in all partial waves: The eigenvalues (2.7) in the Born term are replaced by the eigenvalues (2.14),

$$\gamma_{\lambda l} \to \gamma_{\lambda l}^a = -(\lambda^2 + 2\lambda sa)/2\mu z e^2 a , \tag{2.21}$$

yielding

$$t_l^a(p,p';s) = \sum_\lambda \{[\gamma_\lambda{}_l^{-1}(1-\gamma_{\lambda l})^{-1} - (\gamma_{\lambda l}^a)^{-1}] \times \phi_{\lambda l}(p,s)\phi_{\lambda l}(p',s)\} . \tag{2.22}$$

This method of screening has also been tested in the calculations of Sec. III.

III. THREE-BODY CALCULATIONS

In Sec. IV we wish to compare results of calculations of the binding energy and singlet scattering length for the (e^-, H) system, using unscreened [Eq. (2.8)] and screened versions [Eqs. (2.20) and (2.22)] of the Coulomb t matrix in the Faddeev equations.

The integral equations solved in the present work are essentially Eqs. (4.17) of Ref. 2; they are not repeated in detail here. In this section we outline a brief derivation which shows clearly that the indistinguishability of the electrons allows a large number of terms to be included in the separable expansion of the repulsive e-e interaction.

The Faddeev equations for the bound state ψ of energy E_0 of the (e^-, H) system may be written as

$$\psi_i = t_i(E_0)G_0(E_0)\sum_{j\neq i}\psi_j \quad (i,j=1,2,3) . \tag{3.1}$$

Here t_1 and t_2 are the t matrices for the attractive Coulomb interactions between electrons 1 and 2 and the proton, while t_3 is the Coulomb t matrix for the repulsive e-e interaction. The orbitals ψ_i are defined by $\psi_i = V_i\psi$, V_i being the Coulomb potentials, and $G_0 = (E - H_0)^{-1}$ is the resolvent

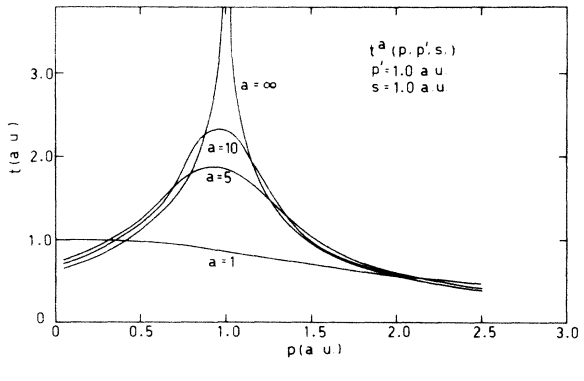

FIG. 2. Comparison of the half-off-shell t matrix $t^a(p,p',s)$ for the Hulthén potential as a function of the off-shell momentum p for shielding radii $a = 1$, 5, and 10, with the Coulomb t matrix ($a = \infty$). The variables p and s have fixed values $p = 1.0$ and $s = 1.0$.

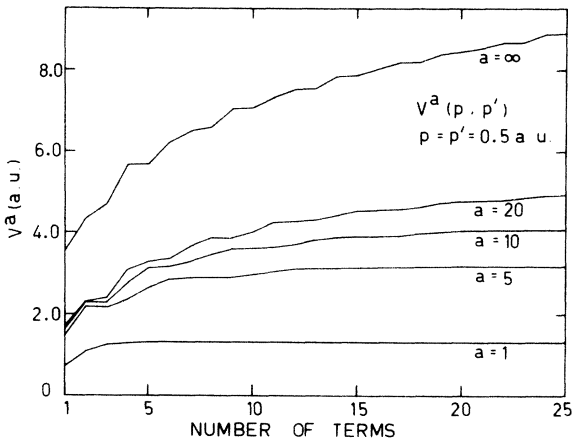

FIG. 3. Convergence of the Sturmian expansion for the Hulthén potential $V^a(p,p)$ with $p = 0.5$ for various screening radii.

operator for the kinetic energy of the three particles.

Let P be the operator that exchanges the spatial coordinates of the electrons, then in the singlet state $\psi_1 = P\psi_2$, since ψ is symmetric in the space observables. Thus Eq. (3.1) reduces to the following pair of equations:

$$\psi_1 = t_1 G_0 (P\psi_1 + \psi_3) , \qquad \psi_3 = t_3 G_0 (\psi_1 + P\psi_1) , \tag{3.2}$$

which may be uncoupled to obtain

$$(1 - t_1 G_0 P - t_1 G_0 t_3 G_0 - t_1 G_0 t_3 G_0 P)\psi_1 = 0 . \tag{3.3}$$

If a separable expansion of the form (2.3) is assumed for the e-p interaction, the operator t_1 acting in the three-particle space, becomes

$$t_1(E) = \sum_i \int \left| \phi_i\left(E - \frac{k_2^2}{2m}\right) \right\rangle |\vec{k}_2\rangle \tau_i \times \left(E - \frac{k_2^2}{2m}\right) \langle \vec{k}_2| \left\langle \phi_i\left(E - \frac{k_2^2}{2m}\right) \right| d^3k_2 . \tag{3.4}$$

When the integral is approximated by a numerical quadrature rule, the momentum variable $\vec{k}_2$ of electron 2 takes a discrete set of values and t_1 is replaced by a matrix operator, which we write symbolically as

$$t_1(E) = \sum_\alpha |\phi_\alpha(E)\rangle \tau_\alpha(E) \langle \phi_\alpha(E)| . \tag{3.5}$$

With the help of Eq. (3.5), Eq. (3.3) becomes a set of linear equations and the binding energy is determined by the determinantal equation

$$\det[\delta_{\alpha\beta} - A_{\alpha\beta}(E)\tau_\beta(E)] = 0 , \tag{3.6}$$

with

$$A_{\alpha\beta}(E) = \langle \phi_\alpha | G_0 P - G_0 t_3 (1 + P) G_0 | \phi_\beta \rangle .$$

Hence a tractable numerical problem is achieved without specific assumptions about the e-e interaction.

In order to study the effect of screening on the convergence of the Sturmian expansion, a separable expansion for t_3 is also assumed. The matrix A then has the form

$$A_{\alpha\beta} = K^{12}_{\alpha\beta} + 2 \sum_\gamma K^{13}_{\alpha\gamma} K^{31}_{\gamma\beta} . \tag{3.7}$$

After angular momentum analysis, it may be shown that the matrices K are the matrix representatives of the kernels of Eqs. (4.17) of Ref. 2 and that the basic equation (3.3) is just the uncoupled form of these equations.

If n and m are the number of terms included in the series for the e-p and e-e interactions, respectively, and n_0 is the number of quadrature points included in the integration over k in Eq. (3.4), A and K^{12} are $N \times N$ square matrices and K^{13} is an $N \times M$ rectangular matrix with $N = n \times n_0$ and $M = m \times n_0$.

Although not an essential restriction, for simplicity we have only considered angular momentum zero states in the various separable expansions. One to three terms have been included in the e-p system and up to twenty terms in the e-e interaction. Gaussian quadratures with $n_0 = 12$, 16, and 24 were used to obtain the matrix (3.7).

IV. RESULTS FOR THE (e^-,H) SYSTEM

We first consider the results for the Coulomb t matrix without shielding. In the simplest approximation, only the $1s$ state is retained in the e-p interaction, and the e-e interaction is ignored entirely. We refer to this as the $(1s, 0s)$ truncation. The calculated three-body energy of the H^- ion is -1.644 Ry, corresponding to a binding energy of 0.644 Ry. Of course, if the e-e interaction is omitted, the three-body system is exactly soluble (the static approximation in which the mass of the proton is infinite is assumed here), and the ground-state energy is -2.0 Ry, which is just the sum of the energies of the two electrons. All the remaining terms in the Sturmian expansion for the e-p system contribute only 0.356 Ry.

When the $1s$ state for the repulsive e-e interaction is included, the energy of the H^- ion becomes -1.0510 Ry, which is remarkably close to the accurate value of -1.0555 Ry obtained by Pekeris.[11] If further terms are added to the e-e potential, the (e^-, H) system no longer binds. This is not surprising, as the attractive e-p interaction has been weakened by truncation to the $1s$ state. More seriously, the determinant on the left-hand side of Eq. (3.6) does not appear to approach a limiting value, even after twenty terms have been included in the representation of the e-e interaction.

The very poor convergence of the standard Sturmian expansion is made more apparent when the singlet scattering length is calculated from the inhomogeneous form of Eq. (3.3). In the $(1s, 1s)$ truncation the singlet scattering length obtained in the present calculation is 6.304 a.u.. This result is in reasonable agreement with the value 6.337 a.u. obtained in a similar calculation by Chen, Chung, and Kramer,[2] and the accurate variational value of 5.965 a.u.[12] However, as shown in Fig. 4, the scattering length increases rapidly as more terms are added to the e-e inter-

action, and is still increasing in the $(1s, 20s)$ truncation.

The inclusion of further terms in the e-p interaction improves the result for the binding energy, but has little effect on the scattering length. In the $(3s, 0s)$ truncation, the three-body energy is -1.989 Ry, which is very close to the exact value of -2.0 Ry. In the $(3s, 3s)$ truncation, the binding energy is 0.0565 Ry. On the addition of further terms, the binding energy remains nearly constant, decreasing slightly to the value 0.0536 Ry in the $(3s, 20s)$ truncation. On the other hand the scattering length moves further from the correct value increasing from 6.47 a.u. in the $(3s, 3s)$ truncation to 15.1 a.u. in the $(3s, 20s)$ truncation.

We now consider the effect of replacing the Sturmian expansion (2.8) by the screened representation (2.20). Here convergence in the limit of large λ is expected since the potential has finite range. In Table I the binding energy is listed for various screening radii in the $(1s, ns)$ truncation. As expected, the convergence rate is improved by using small shielding radii. At the same time the binding energy is very sensitive to the choice of shielding radius. Whereas in the unscreened case the H^- ion was not bound in higher orders of truncation, by taking a screening radius of 3.77 a.u., convergence to the correct binding energy can be achieved. In Fig. 4 the scattering length is plotted for various orders of truncation of the e-e t matrix and various screening radii. Again, convergence is improved by taking sufficiently small shielding radii. With a screening radius of $a = 3.77$ a.u., the scattering length is 5.51 a.u., which is not unreasonable, in view of the severe truncation of the e-p system.

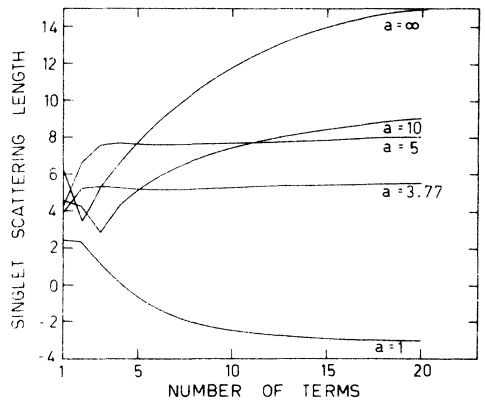

FIG. 4. Singlet scattering length of the (e^-, H) system in the $(1s, ns)$ truncation for various screening radii. The screened form Eq. (2.20) of the Coulomb t matrix was used in this calculation.

When the $2s$ and $3s$ terms are added to the e-p interaction, it is no longer possible to obtain satisfactory values for the scattering length and the binding energy, even with an arbitrary choice of screening radius. For example, to obtain the right magnitude for the scattering length, a screening radius of about 5.4 a.u. must be used. With this strong shielding, the binding energy is shifted by about 0.18 Ry from the correct value. On the other hand, a screening radius of the order of 300 a.u. produces the correct binding energy in the $(3s, 20s)$ truncation, but this weak screening makes little difference to the rate of convergence of the scattering length.

It appears that as the representation of the e-p interaction is made more realistic, the e-e t matrix requires less screening, and consequently the number of terms in the separable expansion required to produce convergence exceeds the practical limits of the calculation.[13]

V. SUMMARY AND CONCLUSIONS

The Faddeev equations for the (e^-, H) system have been solved using separable expansions for both screened and unscreened versions of the Coulomb t matrix. Although in low orders of truncation the unscreened values for the binding energy and singlet scattering length are in good agreement with the results of variational calculations, there is no indication that convergence has been obtained with the number of terms used in the present calculations.

To improve this rate of convergence, a screened form of the Coulomb t matrix, which smooths the logarithmic singularities in the kernel of the Faddeev equations, has been introduced. In the lowest truncation of the e-p system, strong shielding of the e-e interaction is necessary, and satisfactory convergence of both the binding energy and the scattering length can be achieved with a few terms of the e-e interaction. When further terms are included in the e-p interaction, the weak screening of the e-e interaction, which is

TABLE I. Energy of the H^- ion in the $(1s, ns)$ truncation (in Ry).

	Screening radius (a.u.)						
n	$a = \infty$	$a = 10$	$a = 7$	$a = 5$	$a = 3.77$	$a = 2$	$a = 1$
1	1.051	1.118	1.144	1.178	1.212	1.316	1.465
2	...	...	1.006	1.039	1.079	1.204	1.388
3	...	...	...	1.021	1.059	1.182	1.365
4	...	...	...	1.017	1.056	1.178	1.359
5	...	...	...	1.016	1.055	1.177	1.358
6	...	...	...	1.016	1.055	1.177	1.358

necessary to produce the correct value for the binding energy, is not effective in improving the rate of convergence.

The present calculations seem to indicate that the chief difficulty in applying the Faddeev equations to atomic problems lies not in the Coulomb potential *per se*, but in the poor convergence properties of the Sturmian expansions used to simplify the equations[7]; even when the logarithmic singularity is removed by modifying the $1/r$ dependence of the potential at large distances, the convergence of the separable expansion of the resulting *finite-range* potential is still too slow for calculations of satisfactory accuracy.

In view of the fundamental nature of the Faddeev equations for the (e^-, H) system, accurate solutions with which the standard close-coupling approximations[14] could be compared, would be of great interest. In the author's opinion, alternative methods of solution of the Faddeev equations which do not employ separable expansions of the t matrix[15] should be investigated for the Coulomb problem.

APPENDIX

In this Appendix we prove the relation (2.18), which implies that the separable expansion for the Hulthén potential reduces to the usual Sturmian expansion for the Coulomb potential in the limit of infinite screening. In the limit $a \to \infty$, Eq. (2.15) becomes

$$\phi_\lambda^\infty = \mu^{-1/2}(2s)^{3/2} \int_0^\infty \sin(pr) e^{-sr} L_\lambda^1(2sr)\, dr\,.$$

With the help of the generating function for the associated Laguerre polynomials[9]

$$(1-z)^{-2} \exp\left(\frac{xz}{z-1}\right) = \sum_{\lambda=0}^{\infty} L_\lambda^1(x) z^\lambda\,,$$

we have

$$\begin{aligned}
\mu^{1/2}(2s)^{3/2} \sum_{\lambda=0}^{\infty} z^\lambda \phi_\lambda^\infty &= (1-z)^{-2}\, \mathrm{Im} \int_0^\infty \exp[ipr - sr \\
&\qquad + 2rsz/(z-1)]\, dr \\
&= \frac{1}{s^2+p^2} \left((z^2+1) - 2z \frac{p^2 - s^2}{p^2+s^2} \right)^{-1} \\
&= \frac{1}{s^2+p^2} \sum_{\lambda=0}^{\infty} z^\lambda C_\lambda^1 \left(\frac{p^2-s^2}{p^2+s^2} \right),
\end{aligned}$$

since the expression in large parentheses is the generating function for the Gegenbauer polynomials.[9] The result (2.18) follows.

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[1]J. S. Ball, J. C. Y. Chen, and D. Y. Wong, Phys. Rev. 173, 202 (1968).
[2]J. C. Y. Chen, K. T. Chung, and P. J. Kramer, Phys. Rev. 184, 64 (1969).
[3]J. C. Y. Chen and T. Ishihara, Phys. Rev. 186, 25 (1969).
[4]J. C. Y. Chen and K. T. Chung, Phys. Rev. A 2, 1449 (1970).
[5]P. J. Kramer and J. C. Y. Chen, Phys. Rev. A 3, 568 (1971).
[6]M. Rotenberg, Ann. Phys. (N.Y.) 19, 262 (1962).
[7]I. M. Sloan, Phys. Rev. A 7, 1016 (1973).
[8]S. Weinberg, Phys. Rev. 131, 440 (1963).
[9]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965), Chap. 22.
[10]A. G. Sitenko, V. F. Kharchenko, and N. M. Petrov, Phys. Lett. B 28, 308 (1968).
[11]C. L. Pekeris, Phys. Rev. 112, 1649 (1958).
[12]C. Schwartz, Phys. Rev. 124, 1468 (1961).
[13]The matrix elements of the kernel, Eq. (3.7), are calculated as the sum of a series of large numbers of alternating sign. With single precision arithmetic on the CDC 6400 computer, the maximum value of n in the $(1s, ns)$ truncation is limited to about 20; with double precision the matrix elements can be computed for $n \lesssim 35$.
[14]K. Smith, R. P. McEachran, and P. A. Fraser, Phys. Rev. 125, 553 (1962); P. G. Burke and H. M. Schey, Phys. Rev. 126, 149 (1962); P. G. Burke, S. Ormonde, and W. Whittaker, Phys. Rev. Lett. 17, 800 (1966).
[15]For two such approaches for finite-range local potentials see Y. E. Kim, J. Math. Phys. 10, 1491 (1969); Phys. Lett. B 29, 411 (1969); W. M. Kloet and J. Tjon, Phys. Lett. B 37, 460 (1971).