Sturmian Expansion of the Coulomb t Matrix*

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The convergence of the Sturmian expansion (i.e., the Weinberg series) for the Coulomb t matrix at negative energies is discussed. It is pointed out that the series for the full three-dimensional t matrix diverges, and that the series for the partial-wave t matrix converges conditionally at best and sometimes diverges because of the long range of the Coulomb potential. The t matrix is rigorously expressed as the limit of a power series at a point on its circle of convergence, with the power series itself at that point being just the Sturmian expansion. The possibility of finding alternative separable expansions with better convergence behavior is discussed, the conclusion being reached that the poor convergence is an inevitable result of the long range of the Coulomb potential.

I. INTRODUCTION

In a number of recent papers,[1-6] the Coulomb t matrix at negative energies has been written as a Sturmian or Weinberg[7] series, i.e., as an infinite sum of Sturmian functions[8] for the Coulomb potential. Some of these papers have been concerned with the full three-dimensional t matrix,[1-3] others with the partial-wave t matrix.[1,4-6] In the partial-wave case the convergence of the expansion has received some attention, including some useful numerical calculations by Chen and Ishihara,[5] but for the three-dimensional case the convergence seems to have received little discussion.

Most strikingly, it does not appear to have been pointed out that the Sturmian expansion for the three-dimensional t matrix[1-3] (together with the similar expansion for the three-dimensional Coulomb Green's function[9,10]) does not converge at all.[11] We shall see that the lack of convergence in this case is not at all a subtle matter: The series does not converge because the terms in the series do not approach zero. In the partial-wave case the behavior is better, and here the convergence question is more delicate. It appears, however, that even here the convergence is conditional at best, and that in some cases (specifically, if the two momenta are equal, or if one of them is zero) even the partial-wave series diverges.

The aim of this paper is to study the convergence behavior of the Sturmian expansions for the negative-energy Coulomb problem, and to understand the reason why this behavior is so bad. Also, since the convergence difficulties cast doubt on many of the manipulations that have been carried out with the Sturmian expansions in the past, we obtain an alternative expression for the t matrix which avoids these convergence difficulties. In this expression, the t matrix is given rigorously as the limit of a power series at a point on its circle of convergence, and the Sturmian expansion is recognized as just the power series itself at that point.

The recent interest in the Sturmian expansions has been stimulated largely by interest in the three-body problem for three charged particles, for example, the problem of bound states and resonances of the H^- ion, or of $e^{\pm}$-H scattering below the ionization threshold.[4] The terms in the partial-wave Sturmian expansion are separable in the momenta, thus making the Faddeev equations[12] for the three-body problem tractable if the Sturmian expansion is suitably truncated. The kernels in the resulting equations involve an integration over the two-body variable, and this can be expected[4] to improve the convergence behavior over that of the partial-wave Coulomb t matrix itself. However, in practice it has been found[4,13] that the convergence is still disappointing, and it has been concluded[13] that the method is limited to describing the qualitative features of the problem of three charged particles.

The question naturally arises, then, as to whether it is possible to find another separable expansion for the Coulomb t matrix with better convergence properties. The reason for the poor convergence of the Sturmian expansion is, of course, the long range of the Coulomb potential. We shall look at the way the long range appears in the mathematics, and it then becomes apparent that the same essential problems must be expected to occur with *any* separable expansion. At the end of the paper we discuss an apparent counterexample; namely the Coulomb wave-function expansion of Chen and Ishihara.[5] The essential conclusion is that the good convergence in this case is achieved through an approximation that has the effect of leaving out the long-range tail of the Coulomb potential.

Though a good separable expansion of the t matrix itself may not be possible, the situation is much better for $T - V$, the difference of the t matrix from the Coulomb potential, since, as pointed out by Chen and Ishihara,[5] the main convergence

difficulties in the series for the t matrix come from the potential contribution. The present work confirms the rapidity of the convergence of the partial-wave Sturmian series for $T-V$, provided the momenta are not too small, and proves rigorously that for nonzero momenta the series converges to the correct value.

The Sturmian functions are defined and written out explicitly in Sec. II, and in Sec. III the Sturmian expansion for the three-dimensional t matrix is defined, its divergence is noted, and a rigorous relation (described above) between the Sturmian expansion and the t matrix is established. In Sec. IV the partial-wave expansions of the t matrix T and of the difference $T-V$ are studied. Finally, in Sec. V we consider the question of alternative separable expansions of the t matrix, and discuss in particular the Coulomb wave-function expansion of Chen and Ishihara.[5]

II. STURMIAN FUNCTIONS

The Sturmian functions[8] at a fixed negative energy E are the normalizable solutions of the eigenvalue equation

$$[H_0 - E + \gamma_\lambda(E)V]\,|\psi_\lambda(E)\rangle = 0\,, \tag{2.1}$$

or equivalently,

$$\frac{1}{E-H_0}\,V|\psi_\lambda\rangle = \frac{1}{\gamma_\lambda}\,|\psi_\lambda\rangle\,, \tag{2.2}$$

where H_0 is the kinetic energy and V is the potential. Both the eigenfunctions $|\psi_\lambda\rangle$ and the eigenvalues γ_λ^{-1} depend on the energy E.

It is sometimes convenient to work instead with functions $|\phi_\lambda(E)\rangle$ defined by

$$|\phi_\lambda\rangle = (E-H_0)\,|\psi_\lambda\rangle\,, \tag{2.3}$$

which are also called Sturmian functions and which satisfy the eigenvalue equation

$$V\,\frac{1}{E-H_0}\,|\phi_\lambda\rangle = \frac{1}{\gamma_\lambda}\,|\phi_\lambda\rangle\,. \tag{2.4}$$

It follows from this equation that $\langle\phi_{\lambda'}|(E-H_0)^{-1}|\phi_\lambda\rangle$ vanishes if $\gamma_{\lambda'}\neq\gamma_\lambda$, so that on adopting a convenient normalization we have

$$\langle\phi_{\lambda'}|\,\frac{1}{E-H_0}\,|\phi_\lambda\rangle = -\,\delta_{\lambda'\lambda}\,, \tag{2.5}$$

the minus sign coming from the negative definite character of $E-H_0$.

For the particular case of the Coulomb potential, the Sturmian functions are known analytically, because they are simply related to the bound-state wave functions of the hydrogen atom. We write the Coulomb potential as

$$V(r) = z_1 z_2 e^2/r\,, \tag{2.6}$$

or, in momentum space,

$$V(\vec{p}\,',\vec{p}) = z_1 z_2 e^2/2\pi^2\,|\vec{p}\,'-\vec{p}\,|^2\,, \tag{2.7}$$

and write the energy as

$$E = -p_0^2/2\mu\,, \tag{2.8}$$

where μ is the reduced mass. It is also convenient to replace λ by the standard hydrogen-atom quantum numbers n, l, and m.

The eigenvalues $\gamma_{nlm}\equiv\gamma_n$ are easily obtained by noting from Eq. (2.1) that $\gamma_n V$ is the potential that causes the nth hydrogenic bound state to occur at the energy E. In this way we obtain

$$\gamma_n = -n/\eta\,,\quad n=1,2,\ldots, \tag{2.9}$$

where

$$\eta = z_1 z_2 e^2\mu/p_0\,. \tag{2.10}$$

Then the Sturmian function $\psi_{nlm}(\vec{p};E)$ is simply the corresponding solution of the momentum-space Schrödinger equation with the potential $\gamma_n V$; i.e., it is the solution of the bound-state Coulomb problem[14,15] for charge $\gamma_n z_1 z_2 e^2 \equiv -np_0/\mu$.

In this way it is easily found that the Sturmian functions defined by (2.3) and by the normalization condition (2.5) are[4]

$$\begin{aligned}&\phi_{nlm}(\vec{p};E) = (\mu\pi)^{-1/2}\phi_{nl}(p;E)Y_{lm}(\hat{p})\,,\\ &l=0,1,\ldots,n-1,\qquad m=-l,\ldots,l\,,\end{aligned} \tag{2.11}$$

where Y_{lm} is the spherical harmonic,

$$\phi_{nl}(p;E) = \left(\frac{2^{4l+3}(l!)^2 n(n-l-1)!}{(n+l)!}\right)^{1/2} \times \frac{p_0^{l+3/2}p^l}{(p_0^2+p^2)^{l+1}}\,C_{n-l-1}^{l+1}\!\left(\frac{p_0^2-p^2}{p_0^2+p^2}\right)\,, \tag{2.12}$$

and C_i^ν is the Gegenbauer polynomial,[16] a polynomial of degree i defined by

$$(1-2hz+h^2)^{-\nu} = \sum_{i=0}^{\infty} C_i^\nu(z)h^i,\qquad |h|<|z\pm(z^2-1)^{1/2}|\,. \tag{2.13}$$

The original Sturmian functions that satisfy (2.1) are then given by [see Eq. (2.3)]

$$\psi_{nlm}(\vec{p};E) = -\,2\mu(p_0^2+p^2)^{-1}\phi_{nlm}(\vec{p};E)\,.$$

However, in the remainder of this paper the phrase "Sturmian function" refers to the ϕ functions of (2.11) rather than to these ψ functions.[17]

III. STURMIAN EXPANSION OF $T(\vec{p}\,',\vec{p};E)$

The t matrix $T(\vec{p}\,',\vec{p};E)$ is the solution of the Lippmann–Schwinger equation

$$T(\vec{p}\,',\vec{p};E) = V(\vec{p}\,',\vec{p}) + \int \frac{V(\vec{p}\,',\vec{p}\,'')T(\vec{p}\,'',\vec{p};E)}{E-p''^2/2\mu}\,d\vec{p}\,'' \tag{3.1}$$

or, more concisely, of

$$T(E) = V + V\frac{1}{E - H_0}T(E) . \tag{3.2}$$

Using Eqs. (2.4) and (2.5), and assuming that the Sturmian functions form an appropriately complete set for the purpose, it is a simple matter to write down a formal solution in terms of Sturmian functions,

$$T(E) = -\sum_{\lambda} |\phi_\lambda(E)\rangle \frac{1}{\gamma_\lambda(E) - 1} \langle\phi_\lambda(E)| , \tag{3.3}$$

and a corresponding expansion for V,

$$V = -\sum_{\lambda} |\phi_\lambda(E)\rangle \frac{1}{\gamma_\lambda(E)} \langle\phi_\lambda(E)| . \tag{3.4}$$

However, since the completeness and convergence properties are not obvious (indeed, our contention is that these series do not converge at all in the pointwise sense), we prefer not to follow this formal approach, but rather to begin again, starting from an explicit expression for the Coulomb t matrix.

A convenient starting point is the integral representation[18]

$$T(\vec{p}', \vec{p}; E) = \frac{z_1 z_2 e^2}{2\pi^2 |\vec{p}' - \vec{p}|^2} \times \left(1 + 4\eta \int_0^1 t^\eta \frac{1}{\epsilon(1-t)^2 - 4t}\, dt\right) , \qquad \eta > -1 , \tag{3.5}$$

where

$$\epsilon = -\frac{(p_0^2 + p'^2)(p_0^2 + p^2)}{p_0^2 |\vec{p}' - \vec{p}|^2} , \tag{3.6}$$

which is obtained from Schwinger's representation[9] of the Coulomb Green's function $G(\vec{p}', \vec{p}; E)$ through the identity

$$G(E) = \frac{1}{E - H_0} + \frac{1}{E - H_0} T(E) \frac{1}{E - H_0} . \tag{3.7}$$

Obviously the t matrix (like the potential) is singular at $\vec{p}' = \vec{p}$, so that we can exclude this case in the following discussion.

As it stands, Eq. (3.5) is valid only for $\eta > -1$, but this restriction could be removed[9] by replacing the integral by a contour integral,

$$\int_0^1 dt\, t^\eta (\cdots) \to \frac{1}{e^{2\pi i\eta} - 1} \int_C dt\, t^\eta (\cdots) , \tag{3.8}$$

where C begins at $t = 1 + i0$ with $\arg t = 0$, and terminates at $t = 1 - i0$ after encircling the origin within the unit circle. For the moment we retain the restriction on η, in order to keep the argument as transparent as possible.

It is easy to see from (3.6) that $\epsilon \le -1$, and from this it follows that the two zeros in the denominator of the integrand in Eq. (3.5) lie at complex conjugate points on the unit circle, but never at $t = 1$ for energies in $0 > E > -\infty$, if $\vec{p}' \neq \vec{p}$. With the aid of (2.13), we can express the denominator part of the integrand as a power series,

$$\frac{1}{\epsilon(1-t)^2 - 4t} = \frac{1}{\epsilon} \sum_{n=1}^{\infty} C_{n-1}^1 \left(1 + \frac{2}{\epsilon}\right) t^{n-1} , \quad |t| < 1 , \tag{3.9}$$

where

$$-1 \le 1 + (2/\epsilon) < 1 .$$

The power series does not converge at $t = 1$, since[16]

$$C_{n-1}^1(\cos\alpha) = \sin n\alpha / \sin\alpha , \tag{3.10}$$

which does not approach zero as $n \to \infty$, and therefore we should be cautious about integrating the series term by term up to $t = 1$.

Let us instead write the integral in Eq. (3.5) as

$$\int_0^1 t^\eta \frac{1}{\epsilon(1-t)^2 - 4t}\, dt = \lim_{\rho \to 1-} \int_0^\rho t^\eta \frac{1}{\epsilon(1-t)^2 - 4t}\, dt .$$

We know that this limit exists, because the integrand is regular at $t = 1$ if $\vec{p}' \neq \vec{p}$. Since the series (3.9) is uniformly convergent in $0 \le t \le \rho < 1$, we can integrate term by term up to $t = \rho$, thus obtaining

$$T(\vec{p}', \vec{p}; E) = \frac{z_1 z_2 e^2}{2\pi^2 |\vec{p}' - \vec{p}|^2} \left[1 - \frac{4}{\epsilon} \lim_{\rho \to 1-} \sum_{n=1}^{\infty} \frac{1}{\gamma_n(E) - 1} \times C_{n-1}^1 \left(1 + \frac{2}{\epsilon}\right) \rho^n \right] , \tag{3.11}$$

where $\gamma_n(E)$ is given by Eq. (2.9). It is easy to check that the same result can be obtained for all real values of η by using Eq. (3.8), and then using a similar limiting process, and therefore the restriction $\eta > -1$ is no longer necessary.

A similar expression can be obtained for the potential (2.7) by writing it as

$$V(\vec{p}', \vec{p}) = \frac{2 z_1 z_2 e^2 p_0^2}{\pi^2 (p_0^2 + p'^2)(p_0^2 + p^2)} \lim_{\rho \to 1-} \frac{\epsilon}{\epsilon(1-\rho)^2 - 4\rho} ,$$

and then using Eq. (3.9) to obtain

$$V(\vec{p}', \vec{p}) = \frac{2 z_1 z_2 e^2 p_0^2}{\pi^2 (p_0^2 + p'^2)(p_0^2 + p^2)} \lim_{\rho \to 1-} \sum_{n=1}^{\infty} C_{n-1}^1 \left(1 + \frac{2}{\epsilon}\right) \rho^n . \tag{3.12}$$

Finally, on recognizing that the first term of Eq. (3.11) is just $V(\vec{p}', \vec{p})$, we can write the t matrix as

$$T(\vec{p}', \vec{p}; E) = \frac{2 z_1 z_2 e^2 p_0^2}{\pi^2 (p_0^2 + p'^2)(p_0^2 + p^2)} \times \lim_{\rho \to 1-} \sum_{n=1}^{\infty} \frac{\gamma_n(E)}{\gamma_n(E) - 1} C_{n-1}^1 \left(1 + \frac{2}{\epsilon}\right) \rho^n . \tag{3.13}$$

On using Eqs. (3.10) and (2.9), it is very obvious that the power series in Eqs. (3.12) and (3.13) certainly do not converge at $\rho = 1$, since the terms in the series do not approach zero. But these divergent series with $\rho = 1$ are just the Sturmian expansions (3.3) and (3.4), as we shall now show.[19]

For this purpose we need the identity

$$C^{1}_{n-1}\left(1+\frac{2}{\epsilon}\right)=\sum_{l=0}^{n-1} 4^{2l}(2l+1)\,\frac{(n-l-1)!\,(l!)^2}{(n+l)!}$$
$$\times\left(\frac{p_0^2 p' p}{(p_0^2+p'^2)(p_0^2+p^2)}\right)^{l} C^{l+1}_{n-l-1}\left(\frac{p_0^2-p'^2}{p_0^2+p'^2}\right)$$
$$\times C^{l+1}_{n-l-1}\left(\frac{p_0^2-p^2}{p_0^2+p^2}\right) P_l(\hat{p}'\cdot\hat{p})\,, \quad (3.14)$$

which is easily obtained from (3.6) and the addition theorem for Gegenbauer polynomials.[16] Then, on using this and Eqs. (2.9)–(2.12) in (3.13), we obtain

$$T(\vec{p}',\vec{p};E)=-\lim_{\rho\to 1-}\sum_{n=1}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l}\phi_{nlm}(\vec{p}';E)$$
$$\times\frac{1}{\gamma_n(E)-1}\,\phi^{*}_{nlm}(\vec{p};E)\rho^n\,. \quad (3.15)$$

Similarly, from (3.12) we obtain

$$V(\vec{p}',\vec{p})=-\lim_{\rho\to 1-}\sum_{n=1}^{\infty}\sum_{l=0}^{n-1}\sum_{m=-l}^{l}\phi_{nlm}(\vec{p}';E)$$
$$\times\frac{1}{\gamma_n(E)}\,\phi^{*}_{nlm}(\vec{p};E)\rho^n\,. \quad (3.16)$$

These expressions would be just the Sturmian expansions (3.3) and (3.4), if only it were valid to take the limit $\rho\to 1$ in each term of the sums; but that of course would not be valid, because, as noted before, the resulting series diverge. We conclude that the Sturmian expansion of the three-dimensional t matrix does not converge, and that the formula (3.15) is as close as we can come to the Sturmian expansion with a rigorously correct expression for the t matrix.

Formally, the power series in (3.15) with $\rho = 1$ agrees with the expansions of $T(\vec{p}',\vec{p};E)$ written down by previous authors,[1–3] if we use Eqs. (3.7) and (3.14) and the relation

$$C^{l+1}_{n-l-1}(\cos\alpha)=\frac{1}{2^l l!\,n}\,\frac{d^{l+1}}{d(\cos\alpha)^{l+1}}(\cos n\alpha)\,,$$

which follows from Eq. 3.15(30) of Ref. 16 and from Eq. (3.10), to establish the connections. In the case of Rajagopal and Shastry,[2] however, it is perhaps worth observing that, although their Sturmian functions are essentially correct, the integral equation that defines them [their equation (3.1)] is not, since it is just the Sturmian equation (2.4), but with the eigenvalue missing. That is perhaps the reason for their incorrect assertion that for the case of a repulsive potential the Sturmian functions do not satisfy the corresponding eigenvalue problem. On the contrary, it is entirely clear that if a Sturmian function satisfies (2.4) for a Coulomb potential with a particular charge, then it also satisfies (2.4) for any value of the charge, positive or negative, but of course with an eigenvalue γ_λ^{-1} that is proportional to the charge.

Finally, we note that Eq. (3.13) suggests a way of numerically calculating the three-dimensional t matrix, in spite of the obvious unsuitability of (3.13) as it stands. The suggestion is to replace the truncated power series by diagonal Padé approximants[20] of increasing order, evaluated at $\rho = 1$. The Padé approximants provide an explicit analytic continuation in the variable ρ of the power series, and might be expected to be rather effective in this case, because the continuation has only to be carried as far as the circle of convergence. A slight variant of this scheme would actually be rather more sensible, namely, to apply the Padé technique to the difference $T - V$, since it is obvious from (3.12) and (3.13) that the power series for the difference converges much faster than the series for T and V separately.

IV. PARTIAL-WAVE STURMIAN EXPANSIONS

We can also write down a formula similar to (3.15) for the partial-wave t matrix, defined by

$$T(\vec{p}',\vec{p};E)=\frac{1}{4\pi^2\mu}\sum_{l=0}^{\infty}(2l+1)T_l(p',p;E)P_l(\hat{p}'\cdot\hat{p})\,. \quad (4.1)$$

In fact, it follows immediately from (3.15) and (2.11) that

$$T_l(p',p;E)=-\lim_{\rho\to 1-}\sum_{n=l+1}^{\infty}\phi_{nl}(p';E)$$
$$\times\frac{1}{\gamma_n(E)-1}\,\phi_{nl}(p;E)\rho^n\,. \quad (4.2)$$

Similarly, from (3.16) the partial-wave potential $V_l(p',p)$ is

$$V_l(p',p)=-\lim_{\rho\to 1-}\sum_{n=l+1}^{\infty}\phi_{nl}(p';E)\frac{1}{\gamma_n(E)}\,\phi_{nl}(p;E)\rho^n\,. \quad (4.3)$$

If we were to replace ρ by 1 in each term of the sum then (4.2) would become exactly the same as the partial-wave Sturmian expansion written down by Ball *et al.*[4]

We are of course interested in the convergence of the Sturmian expansions. The behavior for large values of n follows from the asymptotic formula for the Gegenbauer polynomials[21]:

$$C_j^{\nu}(\cos\theta)_{j\sim\infty} \frac{j^{\nu-1}}{2^{\nu-1}\Gamma(\nu)} \frac{\cos[(j+\nu)\theta - \frac{1}{2}\nu\pi]}{(\sin\theta)^{\nu}} \times[1+O(j^{-1})] , \quad (4.4)$$

uniformly for θ in $0<\delta\leq\theta\leq\pi-\delta<\pi$. From this and Eq. (2.12) it follows that for $p\neq 0$:

$$\phi_{nl}(p;E)_{n\sim\infty} \frac{(2p_0)^{1/2}}{p} \sin(n\theta - \tfrac{1}{2}l\pi)[1+O(n^{-1})] , \quad (4.5)$$

uniformly for p in any closed interval that excludes $p=0$, with θ being given by

$$\cos\theta = (p_0^2-p^2)/(p_0^2+p^2) , \quad 0<\theta<\pi . \quad (4.6)$$

Hence for large values of n the terms of (4.2) [or of (4.3), since both behave the same way for large n] with ρ replaced by 1 have the asymptotic formula

$$\frac{2z_1z_2e^2\mu}{p'p} \frac{\sin(n\theta' - \frac{1}{2}l\pi)\sin(n\theta - \frac{1}{2}l\pi)}{n}[1+O(n^{-1})] , \quad (4.7)$$

provided that $p'\neq 0$, $p\neq 0$. The quantity θ' is defined by (4.6) with p replaced by p'.

We see from Eq. (4.7) that the partial-wave Sturmian expansions are much better behaved than the three-dimensional expansions, since the terms of the partial-wave expansions do at least approach zero as $n\to\infty$. (For the present we exclude the case $p=0$ or $p'=0$.) However, since they approach zero only like n^{-1} multiplied by oscillating functions, it appears that the convergence cannot be absolute, and that if the series converge at all, they can do so only because of the sign fluctuations produced by the sine functions in the numerator of (4.7). (The conditional convergence of the series has not been proved, however; nor has it been proved, if the conditional convergence exists, that the series converge to the correct values.)

For the particular case $p'=p$ we observe that there are no sign fluctuations in the numerator of (4.7), and the partial-wave Sturmian expansions diverge logarithmically. This is no surprise, because the potential $V_l(p',p)$ itself is singular at $p'=p$. This is apparent from the explicit formula

$$V_l(p',p) = \frac{z_1z_2e^2\mu}{p'p} Q_l\left(\frac{p'^2+p^2}{2p'p}\right) , \quad (4.8)$$

which follows from (2.7). Here $Q_l(z)$ is the Legendre function of the second kind.[16] There is a logarithmic singularity in $V_l(p',p)$ at $p'=p$, because of the logarithmic singularity in $Q_l(z)$ at $z=1$.

The physical origin of the singularity in $V_l(p',p)$ at $p'=p$, and hence of the divergence of the Sturmian expansions at $p'=p$, is the long range of the Coulomb force. The logarithmic singularity in the partial-wave potential is a remnant of the much stronger singularity in the three-dimensional potential [Eq. (2.7)] at $\vec{p}'=\vec{p}$, which in turn is easily seen[15] to be caused by the long range. For example, it can be noted that the screened Coulomb (Yukawa) potential in momentum space[15] is regular for all finite screening lengths R, but becomes singular at $\vec{p}'=\vec{p}$ in the limit $R\to\infty$.

So far we have excluded the case $p=0$ or $p'=0$, because the asymptotic form (4.5) does not hold for $p=0$. However, it is easy to consider this as a special case. For $l>1$ all terms of the Sturmian expansions vanish, because in this case $\phi_{nl}(0;E)$ vanishes [see Eq. (2.12)]. But for $l=0$ the terms do not vanish, and in fact the behavior of the Sturmian expansions for the $p=0$ case is rather bad: In this case it follows from Eq. (3.10) that

$$C_{n-1}^1(1) = n ,$$

and therefore the value of the Sturmian function at $p=0$ is

$$\phi_{n0}(0;E) = 2\sqrt{2}\, p_0^{-1/2} n ;$$

thus the asymptotic formula for the nth term of the Sturmian expansions is not (4.7), but instead is

$$\frac{4\eta}{p'} \sin(n\theta')[1+O(n^{-1})] , \quad l=0,\ p=0,\ p'\neq 0 . \quad (4.9)$$

We observe therefore that the S-wave Sturmian expansions certainly do not converge for the $p=0$ case, because the terms of the expansions do not even approach zero. The strong divergence occurs in spite of the fact that the Coulomb potential itself certainly exists in this limit. This is perhaps seen most clearly by noting that if one of the momenta is zero then the S-wave part of the potential (apart from a constant factor) is just the full three-dimensional potential. Specifically, we have

$$V_0(p',0) = 2z_1z_2e^2\mu/p'^2 . \quad (4.10)$$

As before, the convergence difficulty is associated with the long range of the Coulomb potential. This time it shows up in the strong singularity in Eq. (4.10) at $p'=0$. The Sturmian expansion for the $p=0$ case is faced with the problem of reproducing this singularity by means of a linear combination of Sturmian functions, each of which is finite at $p'=0$.

Let us summarize the convergence behavior that we have found for the partial-wave Sturmian expansions of T and V: If $p'=p$ the expansions diverge logarithmically. If $p'=0$ or $p=0$ the terms in the expansions for $l>1$ all vanish, but the terms in the S-wave expansions do not even approach zero. For other values of p' and p the convergence is conditional at best, since the nth term in the

series behaves asymptotically as in Eq. (4.7), i.e., as n^{-1} multiplied by trigonometric functions that fluctuate in sign.

Chen and Ishihara[5] have carried out very useful numerical calculations with the partial-wave Sturmian expansions which emphasize how bad the behavior shown in Eq. (4.7) really is. They find large oscillations in the partial sums even at the largest values of n they considered ($n=40$ or 50). It is also worth noting from Eq. (4.7) that the size of these oscillations will only be halved, even if twice as many terms are retained.

An interesting aspect of their numerical calculations is that the oscillations in the calculated partial sums, as the maximum value of n is increased, show very clearly the two periods implied by the numerator of Eq. (4.7), namely, a short period $2\pi/(\theta'+\theta)$ and a long period $2\pi/|\theta'-\theta|$. The latter approaches infinity as $p'\to p$, and turns out in fact to be so large in one of the cases considered numerically[22] that the first node of the slow oscillation happens to occur at the point where the calculations stopped, thus creating a false impression of convergence in this case.

Chen and Ishihara[5] also observed in their numerical calculations that the partial-wave Sturmian expansion for $T-V$, quite unlike the separate expansions for T and V, converges quite rapidly. This is easily understood by writing down $T-V$ explicitly: With the aid of (4.2) and (4.3) we get

$$T_l(p',p;E)-V_l(p',p)=-\lim_{\rho\to 1-}\sum_{n=l+1}^{\infty}\phi_{nl}(p';E)\times\frac{1}{\gamma_n(E)[\gamma_n(E)-1]}\phi_{nl}(p;E)\rho^n\ . \quad (4.11)$$

Clearly, the Sturmian expansion for $T-V$ (i.e., the series obtained by putting $\rho=1$) has an extra power of n in the denominator [coming from the factor $\gamma_n(E)$, Eq. (2.9)], compared with the Sturmian expansion of T. Thus we see from Eq. (4.7) that the Sturmian expansion for $T-V$ can be dominated by a series of the form $\sum an^{-2}$, and is therefore absolutely convergent, provided that p' and p are not zero. It follows that in this case we can take the limit $\rho\to 1$ term by term in Eq. (4.11), thus obtaining

$$T_l(p',p;E)-V_l(p',p)=-\sum_{n=l+1}^{\infty}\phi_{nl}(p';E)\frac{1}{\gamma_n(E)[\gamma_n(E)-1]}\phi_{nl}(p;E)\quad \text{if } p'\neq 0,\ p\neq 0\ . \quad (4.12)$$

The present argument allows us to say not only that the Sturmian expansion (4.12) converges for all p', $p\neq 0$, but also to say with certainty that it does indeed converge to the desired value $T-V$. Furthermore, it is easy to see from the discussion given previously that the convergence is uniform for p' and p in $0<\delta\leq p,p'\leq P<\infty$, thus allowing us to deduce that $T_l(p',p;E)-V_l(p',p)$ is continuous at $p'=p$. In other words, the singularity in the exact t matrix $T_l(p',p;E)$ at $p'=p$ is just the singularity that comes from the potential term.

The worst behavior of the Sturmian expansion for $T_l(p',p;E)-V_l(p',p)$ occurs, naturally, when $p'=0$ or $p=0$, since we recall that in this case the terms of the Sturmian expansions for $T_l(p',p;E)$ and $V_l(p',p)$ separately [given by the asymptotic formula (4.9)] do not even approach zero. The corresponding asymptotic formula for the nth term of the difference $T_l(p',0;E)-V_l(p',0)$ is

$$\text{const}\times\frac{\sin(n\theta')}{n}[1+O(n^{-1})],\quad l=0,\ p=0,\ p'\neq 0$$

so that in this extreme case the Sturmian expansion for the difference does not converge absolutely. Even in this case, however, it should be easy to sum the expansion numerically, with the Padé-approximant technique mentioned at the end of Sec. III.

V. ALTERNATIVE EXPANSIONS

Is it possible to find alternative separable expansions for the Coulomb potential or t matrix, with better convergence properties than the Sturmian expansions? We believe that essentially the answer is no, because the poor convergence behavior is directly linked to the long range of the Coulomb potential.

Any such expansion of $V_l(p',p)$ could be written in the form

$$V_l(p',p)=\sum_{n',n}\chi'_{n'l}(p')\chi_{nl}(p)\ , \quad (5.1)$$

for some choice of functions χ and χ'. If such an expansion is to be valid for all p',p, then it *must* diverge when $p'=p$, because, as noted in Sec. IV, $V_l(p',p)$ itself has a logarithmic singularity at $p'=p$, the singularity being a direct result of the long range of the Coulomb potential. But if the series diverges when $p'=p$, then it seems that the only way it can converge for other values of p',p is if there is cancellation between different terms; in other words, the convergence could only be conditional at best. Similar remarks also apply to the difficulty faced by any separable expansion when one of the momenta is zero.

We conclude with a brief examination of an expansion that at first sight contradicts the above claim, namely, the Coulomb wave-function expansion proposed by Chen and Ishihara.[5] For convenience we now consider the specific case of the hydrogen atom; i.e., in atomic units we put $z_1=-z_2=e=\mu=1$.

This expansion is obtained by expanding the potential in the form

$$V_l(p',p)=\left(\sum_n+\int\right)A_{nl}(p')\psi_{nl}(p)\ , \qquad (5.2)$$

where the $\psi_{nl}(p)$ are hydrogen wave functions, normalized in the discrete case to

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

and with a similar δ-function normalization for the continuum states.

With the aid of the orthogonality relation, we get an explicit expression for the coefficients $A_{nl}(p')$ in Eq. (5.2),

$$A_{nl}(p')=\int_0^\infty V_l(p',p)\psi_{nl}(p)p^2dp\ ,$$

and then using the Schrödinger equation we obtain

$$A_{nl}(p')=\pi(\epsilon_n-\tfrac{1}{2}p'^2)\psi_{nl}(p')\ ,$$

where ϵ_n is the energy of the state ψ_{nl}. For the discrete part of the spectrum we have, of course, $\epsilon_n=-(2n^2)^{-1}$. Thus the Coulomb wave-function expansion of $V_l(p',p)$ is

$$V_l(p',p)=\pi\left(\sum_n+\int\right)\psi_{nl}(p')\,(\epsilon_n-\tfrac{1}{2}p'^2)\psi_{nl}(p)\ . \qquad (5.3)$$

[Alternatively, since the expansion is not explicitly symmetric, one can use an explicitly symmetrized expansion[5] instead of (5.3). The following arguments apply equally to the symmetrized expansion.]

In practical applications[23] of the Coulomb wave-function expansion, the expansion is approximated by omitting the continuum contribution to (5.3). Chen and Ishihara[5] studied the remaining discrete part of the expansion numerically and found that it converged rapidly for all values of p' and p considered.

It is easy to see theoretically that the convergence is indeed rapid, at least for values of p' and p not too near zero, by using the explicit expression for $\psi_{nl}(p)$ (Ref. 15),

$$\psi_{nl}(p)=\left(\frac{2^{4l+5}(n-l-1)!}{\pi(n+l)!}\right)^{1/2} l!\,\frac{n^{l+2}p^l}{(n^2p^2+1)^{l+2}} \times C_{n-l-1}^{l+1}\left(\frac{n^2p^2-1}{n^2p^2+1}\right)\ .$$

Since the argument of the Gegenbauer polynomial lies between -1 and 1, the value of the Gegenbauer polynomial is bounded[24] by its value at 1,

$$\left|C_{n-l-1}^{l+1}\left(\frac{n^2p^2-1}{n^2p^2+1}\right)\right|\le\left|C_{n-l-1}^{l+1}(1)\right|=\frac{(n+l)!}{(n-l-1)!\,(2l+1)!}\ .$$

It follows that if p' and p are nonzero, the terms in the discrete part of the Coulomb wave-function expansion ultimately decrease with increasing n like n^{-3}, and the sum over n converges absolutely and uniformly for all p' and p in $0<\delta\le p',p$. (However, the convergence is very nonuniform in the neighborhood of $p=0$ or $p'=0$, and if either p or p' is actually equal to zero, it is easy to see that the S-wave series does not converge at all.)

Given that the discrete part of (5.3) converges, the important question then is what is the value it converges to? Or equivalently, what is the error in leaving out the continuum contribution to (5.3)? Chen and Ishihara[5] found numerically that the error depended sensitively on p' and p but was generally small. This conclusion may be to some degree misleading, however, since the fact is that the error can be arbitrarily large, if p' and p are chosen sufficiently close. This follows from the fact noted in Sec. IV that $V_l(p',p)$ has a logarithmic singularity at $p'=p$, whereas we can see that the discrete part of the Coulomb wave-function expansion does not, since the uniform convergence implies that it is continuous at $p'=p$.

We conclude, therefore, that within the framework of the Coulomb wave-function expansion the logarithmic singularity in the potential comes entirely from the part of the expansion that is omitted in practice, namely, the continuum part of (5.3). But in Sec. IV it was pointed out that the logarithmic singularity is a direct consequence of the long range of the Coulomb potential. We conclude, therefore, that by omitting the continuum contribution to the Coulomb wave-function expansion we are in some sense omitting the effect of the long-range tail of the Coulomb potential. This might well be a good approximation in some applications, but in practice the errors introduced by this approximation would seem very difficult to assess.

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Elastic Electron-Neutral-Atom Interaction Measurements in Helium at Ultralow Energies

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The cross section σ_{MT} for the elastic momentum transfer of electrons with helium atoms at ultralow energies has been deduced from measurements of the microwave absorptivity of a transient cryogenic afterglow plasma. The electrons were selectively heated by an adjustable-microwave electromagnetic field. This cross section can be approximated as a function of the incident electron kinetic energy u_e between 2×10^{-4} and 10^{-1} eV by $\sigma_{MT}(\mathrm{cm}^2)=5.15\times10^{-16}[u_e(\mathrm{eV})/2\times10^{-4}]^{0.02}$.

I. INTRODUCTION

There has been considerable recent theoretical interest in the energy dependence of the cross section for elastic scattering between low-energy electrons and helium atoms.[1–5] However, owing to many technical difficulties, most measurements at very low energies are not completely satisfactory. Following the pioneering works of Ramsauer and Kollath, of Brode, and of Normand,[6] Golden and Bandel[7] have made, in 1965, a very detailed direct measurement of the total electron-helium scattering cross section with electron-beam techniques. But these methods are difficult to extend to energies lower than 0.3 eV. In this low-energy range, elastic scattering cross sections are usually deduced from electron transport-coefficient measurements by dc or ac swarm methods; the corresponding analysis techniques have been considerably refined throughout the years. Measurements have been made down to electron temperatures of about 77 °K, yielding useful experimental data down to about 10^{-3} eV.[8]

Direct-current swarm techniques have been used recently by a variety of workers, down to gas temperatures near 77 °K. Extensive discussions of these techniques have been given in papers by Phelps and co-workers[9,10] and by Crompton *et al.*[11,12] Recent measurements by various groups are in good agreement with each other, and represent a consistent set of data down to 10^{-2} eV.[8]

Microwave methods—which are essentially ac swarm techniques—have been also used by many authors, following the pioneering works of Gold-