

Analytic perturbation theory for screened Coulomb potentials: Nonrelativistic case*

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We have developed an analytic perturbation theory for screened Coulomb radial wave functions, based on an expansion of the potential of the form $V(r) = -(a/r)[1 + V_1\lambda r + V_2(\lambda r)^2 + V_3(\lambda r)^3 + \dots]$, where $\lambda \simeq \alpha Z^{1/3}$ is a small parameter characterizing the screening. The coefficients V_k may be chosen such that the above form converges rapidly and gives a good approximation to realistic numerical potentials, such as those of Herman and Skillman, in the interior of the atom. The screened radial wave functions are obtained as a series in λ with simple analytic coefficients, owing to the special symmetries of the unperturbed Coulomb problem. Both bound and continuum shapes are correctly treated in the region $\lambda r < 1$. For inner bound states, this includes all of the region where the wave function is large. Similarly, high-energy continuum wave functions will have completed several oscillations in this interval so that by $r \simeq \lambda^{-1}$ one has reached the asymptotic region. Consequently, expressions for bound-state normalizations can be given as series in λ , which are accurate, in general, for the K shell and for other low-lying levels of high- Z elements. The continuum normalizations which we obtain are valid for energies on the order of the K -shell binding energy above threshold. Bound-state energies and continuum phase shifts are also obtained in these circumstances.

I. INTRODUCTION

The purpose of this paper is to present an analytic perturbation theory for the calculation of nonrelativistic screened Coulomb wave functions, based on the behavior of the potential in the interior of the atom. In addition to bound and continuum radial wave-function shapes, we derive analytic expressions for their normalizations, for bound-state energy eigenvalues, and for continuum phase shifts. We find that the wave-function shapes which we obtain agree with exact solutions to the Schrödinger equation in the region $\lambda r < 1$, where λ is a small parameter characterizing the screening ($\lambda \simeq \alpha Z^{1/3}$). Thus for low-lying bound states (the K shell for most Z and the L shell for high Z), we obtain all of the region where the wave function is large. Similarly, for high-energy continuum states in this interval, the wave function will have completed several oscillations so that by $r \simeq \lambda^{-1}$ we have reached, essentially, the asymptotic region. Hence we also find that our expressions for normalizations and phase shifts give a good approximation to the exact values for reasonably high energies. Thus we obtain analytically a complete description of the solutions of the Schrödinger equation in the interior of an atom characterized by a screened Coulomb potential.

It is known¹ that at distances which are small on the atomic scale (Compton-wavelength distances), but still outside the nucleus, the primary effect of atomic screening, insofar as it can be described by a central potential, is to modify the normalization of the electron wave function. The *shape* of the wave function is essentially Coulombic. It is only at somewhat larger distances that

modifications of the shape of the wave function due to screening become appreciable. These conclusions of Ref. 1 have been extended in the present work, and the results have been explicitly incorporated into a perturbation theory which is especially convenient for the calculation of interior screened Coulomb wave functions.

There are essentially two features of our approach which differ from the usual Rayleigh-Schrödinger perturbation theory. First, since it makes use of certain special properties of the Coulomb wave function, our method is limited to problems involving screened atomic potentials which are Coulombic at the origin. Second, since it is based on an approximation to the potential which is valid only in the interior of the atom, it will yield wave functions which are likewise correct only in this region. Because of this specialization, however, we are able to derive easily, simple analytic expressions for screened electron wave functions which are accurate in the interior of the atom.

It has long been recognized that there are many atomic and nuclear processes which are characterized by the behavior of an electron wave function at the origin. (However, nuclear size effects usually must also be included.) One such process is orbital electron capture, since only the region of overlap between electron and nuclear wave functions contributes. Another is ordinary β decay. In electron capture, screening effects can be quite important, while in β decay the energy of the emitted electron is usually large enough so that screening effects are relatively unimportant. Wave-function normalizations are also needed for the interpretation of fine-structure and hyperfine-

structure splittings, isotope shifts, etc.

Somewhat more recently it has been realized that there are other processes which, although occurring outside the nucleus, are dominated by distances which are small on the atomic scale. In atomic photoeffect, for example, Pratt and Tseng¹ have argued that for a wide range of photon energies electron Compton-wavelength distances are of primary importance. Here, not only normalizations, but the actual screened wave function, at least for small r , would be desirable in order to fully include the effects of screening. Internal conversion,² threshold pair production,³ and single-quantum annihilation⁴ are also processes characterized by small distances on the atomic scale. In all these situations, it is often possible to simply relate the screened matrix elements to the corresponding point Coulomb matrix element. Since the shape of the screened wave function is Coulombic near the origin, to a good approximation, atomic electron screening may be ignored except as an external multiplicative factor determined by the ratio of screened to point Coulomb normalizations. This normalization screening theory has enjoyed considerable success. In this way, for example, the anomalously large photoeffect cross section in molecular hydrogen has recently been explained.⁵ Thus there is a growing appreciation of the importance of the small-distance properties of screened electron wave functions in the analysis of many processes of physical interest. One of the results of the present work will be to allow a systematic improvement in these predictions of normalization screening theory.

Even for processes in which the dominant region is not near the origin, but is still within the interior of the atom, a simple calculational scheme which yields tractable analytic wave functions for screened Coulomb potentials will be useful since, in any case, the Schrödinger equation cannot be solved exactly and either numerical methods or some form of perturbation theory is required. In the nonrelativistic case, the usual Rayleigh-Schrödinger perturbation theory, with the use of the closed-form expressions for the Coulomb Green's function, can be used to obtain expressions for the energy shifts and wave functions. The results, however, are generally rather complicated, require numerical work, and cannot easily be generalized to the relativistic case. Direct numerical calculations are often too time consuming for systematic studies and very often fail to give insight into the mechanisms of a process. Thus it is desirable to consider possible alternatives.

One of the simplest (and oldest) procedures for

constructing wave functions for general potentials is the WKBJ method.⁶ Because it is based on an analysis of the behavior of the wave function at large distances, the WKBJ method is complementary to the approach to be presented here. It is, then, somewhat ironic that one of the more useful sources of information concerning the wave function at small distances, the Fermi-Segrè formula⁷ for the square of the wave function of an S electron at the origin, is based on an application of the WKBJ method. It is, of course, true that the normalization involves the value of the wave function over all space. One hence understands that the Fermi-Segrè formula is more accurate for outer electrons, since it relates the normalization to the behavior at large distances. On the other hand, our approach to the normalization is based on an analysis of the smaller-distance behavior of the wave function and is valid for inner electrons. Thus the two methods should supplement each other.

There are, in fact, a number of approaches to the construction of screened Coulomb wave functions which are based on large-distance properties of the potential. The quantum-defect method,⁸ for example, is useful for the construction of screened wave functions for outer electrons at energies near threshold. This method takes advantage of the fact that for large r , the potential seen by an electron is essentially Coulombic. The effect of inner-electron screening, then, is only to change the normalization and phase of the exterior Coulomb wave function. For bound states, the energy shift is obtained by analytically continuing the phase shift to negative energies. The parameter which results is then identified as the quantum defect, μ , and the energy is simply $E_n = -\frac{1}{2}a^2/(n - \mu)^2$, where $\pi\mu = \delta(E_n)$. Of course, the normalization and phase shift must be obtained by matching to the appropriate solution of the Schrödinger equation in the interior region, or by semiempirical methods. If, for example, the experimental energies are known, then $\mu(E)$ may be analytically continued to positive energies—giving directly the low-energy phase shift. Again, this approach and our own should supplement each other.

Our method for the construction of screened Coulomb wave functions is motivated by the discussion of Pratt and Tseng,¹ which should be viewed as an introduction to this paper. Following their example, we consider central potentials for which it is possible to write an expansion of the form

$$V(r) = - (a/r) [1 + V_1\lambda r + V_2(\lambda r)^2 + V_3(\lambda r)^3 + \dots], \quad (1)$$

where λ is a small parameter characterizing the

screening (usually, $\lambda \approx \alpha Z^{1/3}$). The coefficients V_k are then of order unity and, in general, alternate in sign and decrease with increasing k . As noted in Ref. 1, this assumption, (1), is not particularly restrictive, since the coefficients V_k can be chosen to fit realistic numerical potentials such as the Herman-Skillman Hartree-Fock-Slater potentials. However, some care must be exercised in the choice of fitting procedure for nonanalytic potentials; a discussion of the procedure we have adopted and its philosophy will be found in Sec. IV. With Eq. (1) as a basis we will construct wave functions, energies, normalizations, and phase shifts⁹ which are characterized by an expansion in powers of λ . We note that the analysis of Pratt and Tseng indicates that if only low orders of the series in λ are retained, the resulting wave functions should then be accurate for small r . In fact, we find that our wave functions are valid wherever the expansion (1) gives a good approximation to the potential, and it is in this sense that our analysis gives screened Coulomb wave functions in the interior of the atom. This differs considerably from the usual perturbation theory in which the expansion is in powers of the perturbation. Because our approach is limited to potentials of the form (1), our results can be expressed in an especially compact form. Whereas Rayleigh-Schrödinger wave functions are expanded in an infinite sum of Coulomb wave functions, our results are given as a finite sum of functions which are essentially the configuration-space realization of the "tilted" wave functions used in calculations involving the SO(4,2) dynamical group.¹⁰

There are certain aspects of our perturbation theory which can be compared with other recent investigations of screened Coulomb potentials. Sherstyuk,¹¹ for example, has developed a perturbation theory for bound states which contains elements of the theory presented here and of the usual Rayleigh-Schrödinger perturbation theory. This approach has been applied to the Dirac equation with a central potential, and, for certain potentials, the wave function (at least to first order) can be obtained in closed form, the result being used to give the energy correct to third order. In general, however, in this approach, the wave function can be expressed only as an infinite (discrete) sum of the eigenfunctions of a certain Sturm-Liouville operator, while in our approach, owing to the restriction to small r , the wave function is expressed as a finite sum. Moreover, the Sherstyuk approach is not directly applicable to continuum states.

Bednář^{12(a)} has considered an algebraic approach to the construction of screened Coulomb wave functions which is based on the SO(4,2) dynamical

group. This treatment is similar to our procedure in that the results are expressed as a finite sum of Coulomb-like states, but the generalization to the relativistic case is not straightforward and continuum states are not treated. Moreover, it would be difficult to determine the region of validity of the wave functions in this theory. His approach can, however, be applied to certain noncentral potentials, whereas our approach cannot. Other recent considerations of analytic screened potentials are due to Green^{12(b)} and to McGuire,^{12(c)} while Fano, Theodosiou, and Dehmer^{12(d)} have used phase-amplitude and numerical results to discuss small-distance properties of continuum wave functions in the zero-energy limit. Finally, in addition to those more general methods, there have also appeared analytic treatments for special cases of modified Coulomb potentials, which exploit various symmetries or generating functions to sum the results of perturbation theory.¹³⁻¹⁶ These results for the bound-state wave functions are of somewhat limited usefulness, however, except as a check on the more general procedures, since the potentials are rather specialized.

In Sec. II we will outline our procedure for constructing nonrelativistic screened bound-state wave functions, including energy shifts and normalizations. In Sec. III we will consider continuum radial wave functions. We will also derive expressions for normalizations and phase shifts. In order to assess the range of validity of our approach, we present in Sec. IV a rather extensive comparison of our results with exact analytic and numerical solutions for screened Coulomb potentials. In separate papers we will apply our results to an analytic screened calculation of nonrelativistic photoeffect in dipole approximation¹⁷ and we will describe the extension of our theory to the relativistic case.¹⁸

II. BOUND STATES

Consider the radial Schrödinger equation

$$\frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} - \frac{l(l+1)}{r^2} R + 2(T - V)R = 0. \quad (2)$$

We use natural units, $\hbar = c = m_e = 1$, so that distances are measured in electron Compton wavelengths and energies in units of the electron rest-mass energy. $V(r)$ is the screened central potential and T is the energy of the (bound) electron. We now define a function $s(r)$ through the relation

$$R(r) = Nr^l \exp[-(-2T_c)^{1/2} r] s(r) \quad (3)$$

and make a change of variable, $x = 2(-2T_c)^{1/2} r$, where $T_c = -a^2/2n^2$ is the unperturbed Coulomb energy (n is the principal quantum number). N is

a normalization constant and will be discussed later. Here $a = \alpha Z$, where α is the fine-structure constant and Z the nuclear charge. We find that $s(x)$ satisfies

$$x s''(x) + [2l + 2 - x] s'(x) + (n - l - 1) s(x) = (x/4T_c)(\delta T - \delta V) s(x), \quad (4)$$

where

$$\delta T = T - T_c = \lambda T_1 + \lambda^2 T_2 + \lambda^3 T_3 + \dots \quad (5)$$

and

$$\delta V = V - V_c = -aV_1 \lambda - aV_2 \lambda^2 r - aV_3 \lambda^3 r^2 - \dots \quad (6)$$

(The notation is essentially that of Ref. 1.) For convenience, we standardize $s(x)$ such that $s(0) = 1$.

Equation (4) is the basic equation which we have to solve. We will show that it is possible to arrange the solution so that, to any finite order in λ , it can be expressed as a finite sum of eigenfunctions of the differential operator which appears on the left-hand side of (4). To proceed, we assume a solution of the form

$$s(x) = s_c(x) + \lambda A_1(x) + \lambda^2 A_2(x) + \lambda^3 A_3(x) + \dots, \quad (7)$$

where $s_c(x)$ is the unperturbed Coulomb solution standardized such that $s_c(0) = 1$. In order to illustrate our approach and also simplify the subsequent discussion, we will consider first the lowest-order correction to the energy and wave function. If we substitute (7) into (4) and equate like powers of λ , then for the first two terms we have

$$\left(x \frac{d^2}{dx^2} + (2l + 2 - x) \frac{d}{dx} + (n - l - 1) \right) s_c(x) = \mathfrak{D}_{n,l} s_c(x) = 0, \quad (8a)$$

$$P(x) = -\frac{n^2}{2a^2} (T_1 + V_1 a) \left(\beta_{-1}^1 M(l + 1 - n + 1, 2l + 2; x) \right.$$

$$\left. - \beta_{+1}^1 M(l + 1 - n - 1, 2l + 2; x) + \beta_0^1 \int_0^\infty dx' G(x, x') M(l + 1 - n, 2l + 2; x') \right), \quad (13)$$

where $G(x, x')$ is the Green's function for the operator $\mathfrak{D}_{n,l}$. The boundary condition on the wave function, that $R(r)$ be square integrable, implies $C_2 = 0$. The CHF's $M(l + 1 - n \pm 1, 2l + 2; x)$ behave asymptotically as $x s_c(x)$, so that they are consistent with this boundary condition. However, it can be shown that the last term on the right-hand side of (13) is of order e^x for large x . Thus the coefficient of this term must vanish.²⁰ Since $\beta_0^1 \neq 0$, we must have $T_1 = -V_1 a$. This determines the

$$\mathfrak{D}_{n,l} A_1(x) = - (x n^2 / 2a^2) (T_1 + V_1 a) s_c(x). \quad (8b)$$

The right-hand side of (8b) is rather simple, as it is proportional to $s_c(x)$, the unperturbed Coulomb solution, which is the regular solution of (8a) and is given by

$$s_c(x) = M(l + 1 - n, 2l + 2; x). \quad (9)$$

In Eq. (9), $M(a, b, x)$ is a regular confluent hypergeometric function (CHF). (The notation is that of *Handbook of Mathematical Functions*.¹⁹) Using the relation between contiguous CHF's

$$x M(a, b, x) = a M(a + 1, b, x) + (b - 2a) M(a, b, x) + (a - b) M(a - 1, b, x), \quad (10)$$

Eq. (8b) for $A_1(x)$ can be rewritten in the form

$$\mathfrak{D}_{n,l} A_1(x) = -\frac{n^2}{2a^2} (T_1 + V_1 a) \times \sum_{s=-1}^1 \beta_s^1(n, l) M(l + 1 - n + s, 2l + 2; x), \quad (11)$$

where, in general, none of the β_s^1 is zero.

The general solution of (11), following the usual procedure for linear differential equations, can be written

$$A_1(x) = C_1 s_c(x) + C_2 U_c(x) + P(x), \quad (12)$$

where U_c is the irregular Coulomb solution and $P(x)$ is a particular solution of the inhomogeneous equation. We see that $P(x)$ can be written

first-order energy shift. Since $s(0) = s_c(0) = 1$, we must also impose the condition that $A_k(0) = 0$. This implies $C_1 = 0$, and hence the entire first-order correction to the wave function vanishes. This result is also found in the work of Pratt and Tseng, and will considerably simplify the following discussion.

We note for future reference the following features of the considerations presented above: (i) The inhomogeneous part of the equation for $A_1(x)$

can be expanded in terms of associated CHF's;
(ii) These CHF's are eigenfunctions of $\mathfrak{D}_{n,l}$, i.e.,

$$\mathfrak{D}_{n,l}M(l+1-n-s, 2l+2; x) = -sM(l+1-n-s, 2l+2; x); \quad (14)$$

(iii) The coefficient of the CHF with eigenvalue zero in this expansion, i.e., the unperturbed Coulomb solution, must vanish if we are to satisfy the boundary condition that the wave function be square integrable. This requirement determines the correction to the energy eigenvalue in this order. These are general features, and we will find that provided T_k is properly chosen each $A_k(x)$ can be expressed as a finite sum of eigenfunctions of the operator $\mathfrak{D}_{n,l}$.

Let us now consider the higher-order terms. Taking cognizance of the fact that the first-order correction to the wave function vanishes, we write

$$s(x) = s_c(x) + \lambda^2 A_2(x) + \lambda^3 A_3(x) + \dots \quad (15)$$

The boundary conditions on the coefficients $A_k(x)$ are that they be polynomially bounded and that $A_k(0) = 0$. [The work of Pratt and Tseng also shows that in the nonrelativistic case $s(x) - s_c(x) = 0(x^2)$ for small x . Thus we should also find $A'_k(0) = 0$, which gives a convenient check on our results.] Substituting (15) into (4) and equating like powers of λ , we find, through fourth order,

$$\left(x \frac{d^2}{dx^2} + (2l+2-x) \frac{d}{dx} + (n-l-1)\right) s_c(x) = \mathfrak{D}_{n,l} s_c(x) = 0, \quad (16a)$$

$$\mathfrak{D}_{n,l} A_2(x) = -(xn^2/2a^2)(T_2 + \frac{1}{2}V_2 nx) s_c(x), \quad (16b)$$

$$\mathfrak{D}_{n,l} A_3(x) = -(xn^2/2a^2)[T_3 + (V_3/4a)n^2 x^2] s_c(x), \quad (16c)$$

$$\begin{aligned} \mathfrak{D}_{n,l} A_4(x) = & -(xn^2/2a^2)\{[T_4 + (V_4/8a^2)n^3 x^3] s_c(x) \\ & + (T_2 + \frac{1}{2}V_2 nx) A_2(x)\}, \end{aligned} \quad (16d)$$

with similar results for the higher-order terms. The set of equations which we have obtained yields a hierarchy for the coefficients $A_k(x)$. The equation for each $A_k(x)$ depends only on the solutions to the preceding equations. In particular, the equations for $A_2(x)$ and $A_3(x)$ are especially simple since the inhomogeneous parts involve only $s_c(x)$.

To solve the set of equations (16), we proceed by induction as follows: We assume that for $j < k$ we can write

$$A_j(x) = \sum_{s=-j}^j \alpha_s^j(n, l) M(l+1-n-s, 2l+2; x), \quad (17)$$

where the CHF's $M(l+1-n-s, 2l+2; x)$ are eigenfunctions of the operator $\mathfrak{D}_{n,l}$ with integer eigenvalues [cf. Eq. (14)]. Inspection of the set of equations (16) shows that if (17) is true for $j < k$, then by repeated use of the relation (10), the equation for $A_k(x)$ can be written in the form

$$\mathfrak{D}_{n,l} A_k(x) = \sum_{s=-k}^k \beta_s^k(n, l) M(l+1-n-s, 2l+2; x). \quad (18)$$

Employing Eq. (14), we can immediately write the solution to (18) in the form

$$A_k(x) = \sum_{s=-k}^k \alpha_s^k(n, l) M(l+1-n-s, 2l+2; x), \quad (19)$$

where

$$\alpha_s^k(n, l) = -\beta_s^k(n, l)/s, \quad (20)$$

provided the coefficient of the CHF with eigenvalue zero on the right-hand side of (18) vanishes, that is, if

$$\beta_0^k(n, l) = 0. \quad (21)$$

(We note that this is equivalent to the usual perturbation theory requirement that the perturbation have no component in the subspace spanned by the unperturbed solution.) As we established previously, this condition is necessary if our bound-state wave function is to be square integrable. Since the k th order correction to the energy has not been determined, T_k can be fixed such that the condition (21) is satisfied. To complete our argument, we note that the form (17) holds for $k=2$ [cf. Eq. (9)], so that by induction the result (19) is valid for all k .

Because of the particular form of the recursion relation (10), we find that only terms with $l+1-n-s \leq 0$ will contribute to (19) if n is an integer. Thus in the bound-state case, each of the coefficients $A_k(x)$ will be a polynomial of degree $k+n-l-1$. In order to satisfy the remaining boundary condition, $A_k(0) = 0$, we note that since Eqs. (16) are linear, we are free to add a solution of the homogeneous equation, $s_c(x)$, with arbitrary coefficient to (19). [Another way to say this is to point out that because of (21), $\alpha_0(n, l)$ is indeterminate. Thus we are free to choose it such that $A_k(0) = 0$.]

The explicit forms of the solutions to (16), through third order, are given below:

$$T_1(n, l) = -V_1 a, \quad (22a)$$

$$T_2(n, l) = \frac{1}{2} V_2 [-3n^2 + l(l+1)], \quad (22b)$$

$$A_2(n, l; x) = (n^2 V_2 / 4a^2) \left\{ -\frac{1}{2}n(n-l-2)(n-l-1)M(-2, x) + (n-l-1)[n(n-2) + l(l+1)]M(-1, x) \right. \\ \left. + [3n^2 + 2l(l+1)^2]M(0, x) - (n+l+1)[n(n+2) + l(l+1)]M(1, x) + \frac{1}{2}n(n+l+2)(n+l+1)M(2, x) \right\}, \quad (22c)$$

$$T_3(n, l) = -(n^2 V_3 / 2a) [5a^2 + 1 - 3l(l+1)], \quad (22d)$$

$$A_3(n, l; x) = (n^4 V_3 / 4a^3) \left\{ \frac{1}{6}(n-l-3)(n-l-2)(n-l-1)M(-3, x) - \frac{3}{2}(n-1)(n-l-2)(n-l-1)M(-2, x) \right. \\ \left. + \frac{1}{2}(n-l-1)[5n(n-3) + 3l(l+1) + 4]M(-1, x) + [10n^2 + \frac{5}{3}l(l+1)(2l+1)]M(0, x) \right. \\ \left. - \frac{1}{2}(n+l+1)[5n(n+3) + 3l(l+1) + 4]M(1, x) + \frac{3}{2}(n+1)(n+l+2)(n+l+1)M(2, x) \right. \\ \left. - \frac{1}{6}(n+l+3)(n+l+2)(n+l+1)M(3, x) \right\}, \quad (22e)$$

where $M(s, x) = M(l+1-n-s, 2l+2; x)$.

For future reference, we note that the coefficients α_s^k satisfy the relation

$$\alpha_s^k(n, l) = \alpha_{-s}^k(-n, l), \quad (23)$$

while the coefficients T_k satisfy

$$T_k(n, l) = T_k(-n, l). \quad (24)$$

We also find that $A_2(x)$ and $A_3(x)$ defined by (20) are of order x^2 for small x , so that our results are consistent with those of Pratt and Tseng. Explicitly, neglecting higher-order terms in x ,

$$A_2(x) \xrightarrow{x \rightarrow 0} (n^2 V_2 / 8a^2) [3n^2 - l(l+1)]x^2 / (2l+3), \\ A_3(x) \xrightarrow{x \rightarrow 0} (n^4 V_3 / 8a^3) [5n^2 - 3l(l+1) + 1]x^2 / (2l+3). \quad (25)$$

$$n=1, \quad l=0: \quad s(x) = 1 + \frac{\lambda^2 V_2}{8a^2} x^2 + \frac{\lambda^3 V_3}{4a^3} x^2 \left(1 + \frac{1}{6}x\right),$$

$$n=2, \quad l=0: \quad s(x) = 1 - \frac{1}{2}x + \frac{2\lambda^2 V_2}{a^2} x^2 \left(1 - \frac{1}{4}x\right) + \frac{2\lambda^3 V_3}{a^3} x^2 \left(7 - \frac{7}{6}x - \frac{1}{6}x^2\right), \quad (26)$$

$$n=2, \quad l=1: \quad s(x) = 1 + \frac{\lambda^2 V_2}{a^2} x^2 + \frac{2\lambda^3 V_3}{a^3} x^2 \left(3 + \frac{1}{3}x\right).$$

We recall that $x = 2ar/n$. For completeness, we also give the K - and L -shell binding energies. Through third order,

$$n=1, \quad l=0: \quad T = -\frac{1}{2}a^2 - \lambda V_1 a - \frac{3}{2}\lambda^2 V_2 - 3\lambda^3 V_3 a^{-1}, \\ n=2, \quad l=0: \quad T = -\frac{1}{8}a^2 - \lambda V_1 a - 6\lambda^2 V_2 - 42\lambda^3 V_3 a^{-1}, \\ n=2, \quad l=1: \quad T = -\frac{1}{8}a^2 - \lambda V_1 a - 5\lambda^2 V_2 - 30\lambda^3 V_3 a^{-1}. \quad (27)$$

To summarize, in general the correction to the Coulomb wave function of order k will have the form $\lambda^k r^l e^{-x/2} A_k(x)$, where $A_k(x)$ is a linear combination of $2k+1$ CHF's. For a bound state, the

From (25), we see that for given x the effective expansion parameter for our bound-state wave functions is essentially $\lambda n^2/a$. From Eq. (20), we note that the energy shift is also, effectively, an expansion in $\lambda n^2/a$. Since λ is a number of the order of $\alpha Z^{1/3}$, we find that our bound-state wave functions and energy shifts are given, essentially, as expansions in $n^2 Z^{-2/3}$. Thus we expect them to be valid for the K shell of all but the lowest- Z elements and for other low-lying levels of high- Z elements. At small distances the wave-function shapes for all n, Z will have the validity indicated in Eq. (25).

Although the corrections to the wave function (22) are given in terms of linear combinations of CHF's, for small values of n and l these expressions can be more simply expressed as polynomials in x . In particular, for K - and L -shell electrons we have, through third order in λ ,

CHF's which appear are generalized Laguerre polynomials, so that the solution to each order will be proportional to a finite polynomial. It should be noted, however, that these correction terms are not linear combinations of Coulomb wave functions. Instead, they are related to Coulomb wave functions by a scale transformation, so that if $f_c(n+s, l; r)$ is a Coulomb solution with principal quantum number $n+s$, then

$$f_c(n+s, l; r) \\ = N r^l e^{-nx/2(n+s)} M(l+1-n-s, 2l+2; [n/(n+s)]x). \quad (28)$$

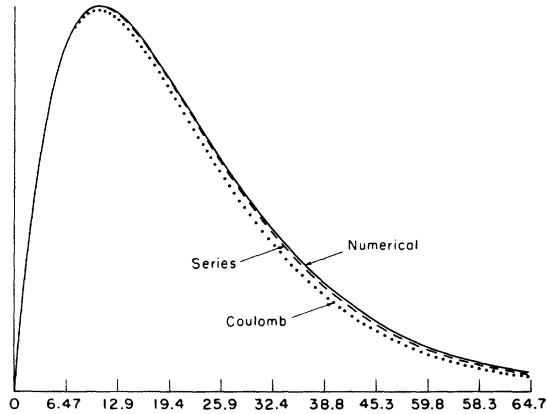


FIG. 1. Unnormalized radial function $u(r) = N^{-1}rR(r)$ for the 1S state of aluminum ($Z = 13$). The unbroken line is the numerical shape, obtained using our analytic fit to the HS-HFS potential, while the dashed line gives the analytic result. The dotted line is the point Coulomb shape for the same Z . Distances are in electron Compton wavelengths.

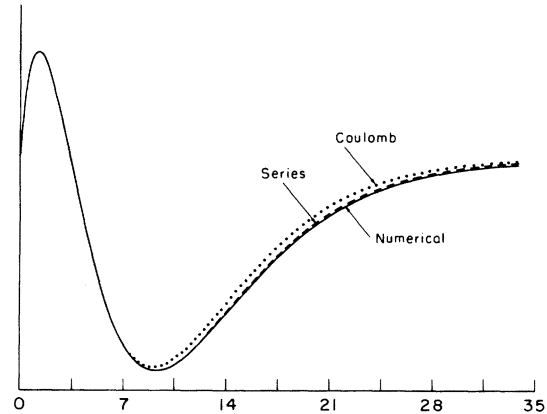


FIG. 2. Unnormalized radial function $u(r) = N^{-1}rR(r)$ for the 2S state of gold ($Z = 79$), assuming a Yukawa potential $V(r) = -(a/r)e^{-\lambda r}$. λ is the Thomas-Fermi radius. The unbroken line gives the exact numerical shape, while the dashed line gives the analytic result. The dotted line is the point Coulomb shape for the same Z . Distances are in electron Compton wavelengths.

It is easily seen, then, that our nonrelativistic wave functions are, in fact, expanded in terms of the (unnormalized) tilted wave functions which form a basis for the $SO(4, 2)$ dynamical group.¹⁰

The wave functions given above are standardized so that $s(0) = 1$. For completeness, we must also consider their normalization. Since our solutions are square integrable, the determination of the normalization is straightforward. Of course, one might question the validity of the normalization constant obtained from an analytic wave function which is presumed most accurate at small distances. However, in fact, our wave-function shapes, like our representation of the potential, are accurate over nearly the entire interior of the atom (cf. Figs. 1 and 2). In particular, for the K shell of all but very-low- Z elements and for other

low values of n and high Z , they are valid in the region which gives the principal contribution to the normalization integral. Hence at least for tightly bound inner electrons the normalization should be nearly exact. A comparison of our analytic normalization with exact numerical results is given in Sec. IV.

In order to determine the normalization, we consider the following:

$$R(r) = Nr^l e^{-ar/n} s_c(2ar/n) = Nr^l e^{-ar/n} [s_c(2ar/n) + \lambda^2 A_2(2ar/n) + \dots] \quad (29)$$

or

$$R(x) = N(n/2a)^l x^l e^{-x/2} [s_c(x) + \lambda^2 A_2(x) + \dots]. \quad (30)$$

Let

$$I = \int_0^\infty r^2 R^2(r) dr = \left(\frac{n}{2a}\right)^3 \int_0^\infty x^2 R^2(x) dx = N^2 \left(\frac{n}{2a}\right)^{2l+3} \int_0^\infty x^{2l+2} e^{-x} [s_c^2(x) + 2\lambda^2 A_2(x) s_c(x) + \dots] dx. \quad (31)$$

We note that the CHF's (Laguerre polynomials) which appear in (31) are orthogonal with respect to the weight function $x^{2l+1} e^{-x}$ in the interval $[0, \infty]$; that is,

$$\int_0^\infty x^{2l+1} e^{-x} M(l+1-n, 2l+2; x) M(l+1-m, 2l+2; x) dx = \delta_{m,n} \frac{(n-l-1)! [(2l+1)!]^2}{(n+l)!}. \quad (32)$$

The weight function which appears in (31), however, is $x^{2l+2} e^{-x}$. Since we wish to use the orthogonality of the CHF's to evaluate the normalization, we associate a factor of x with one of the factors in each term of the expression in square brackets in (31) so that we have

$$I = N^2 \left(\frac{n}{2a}\right)^{2l+3} \int_0^\infty x^{2l+1} e^{-x} [s_c(x) x s_c(x) + 2\lambda^2 A_2(x) x s_c(x) + \dots] dx. \quad (33)$$

It is easily seen that a general term of the expression in square brackets will be given by $A_{s-k}(x)xA_k(x)$, with $k \leq s-k$. Using Eq. (10), the factor $xA_k(x)$ can be expanded in terms of associated CHF's, after which the integral (32) can be employed. In this way, we find that $I(n, l)$ can be written in the form

$$I = N^2 \left(\frac{n}{2a} \right)^{2l+3} \frac{2n(n-l-1)! [(2l+1)!]^2}{(n+l)!} \left(1 + 2\lambda^2 \frac{n^2 V_2}{4a^2} [6n^2 + l(l+1)(2l+1)] \right. \\ \left. + 2\lambda^3 \frac{n^4 V_3}{4a^3} [20n^2 + \frac{1}{3}l(l+1)(10l-13) + 2] + \dots \right) \\ = N^2 N_c^{-2} [1 + 2\lambda^2 \gamma_2 + 2\lambda^3 \gamma_3 + \dots] = N^2 N_c^{-2}(n, l) \chi^{-2}(T_c, l), \quad (34)$$

where

$$N_c = \left(\frac{2a}{n} \right)^{l+3/2} \frac{1}{(2l+1)!} \left(\frac{(n+l)!}{2n(n-l-1)!} \right)^{1/2} \quad (35)$$

is the unperturbed Coulomb bound-state normalization and $T_c = -a^2/2n^2$. The γ_k are defined implicitly by (34). We find thus that the normalization factor is given by

$$N(n, l) = N_c(n, l) \chi(T_c, l) \equiv N_c [1 - \lambda^2 \gamma_2 - \lambda^3 \gamma_3 - \dots]. \quad (36)$$

From the explicit result for the normalization integral (34), we see that the effective expansion parameter is essentially $n^2 \lambda / a$. This is the same as for the energy, so that, again, for the K shell (other than for very low Z) and for other low-lying levels of sufficiently-high- Z elements, the series (36) should be valid.

For K - and L -shell electrons, in particular, we have the following simple forms for the normalization constants. Through third order we find

$$n=1, \quad l=0: \quad N = \frac{1}{\sqrt{2}} (2a)^{3/2} \left(1 - \frac{3}{2} \frac{\lambda^2 V_2}{a^2} - \frac{11}{2} \frac{\lambda^3 V_3}{a^3} \right), \\ n=2, \quad l=0: \quad N = \frac{1}{\sqrt{2}} a^{3/2} \left(1 - 24 \frac{\lambda^2 V_2}{a^2} - 328 \frac{\lambda^3 V_3}{a^3} \right), \\ n=2, \quad l=1: \quad N = \frac{1}{2} \frac{1}{\sqrt{6}} a^{5/2} \left(1 - 30 \frac{\lambda^2 V_2}{a^2} - 320 \frac{\lambda^3 V_3}{a^3} \right). \quad (37)$$

III. CONTINUUM STATES

We want to find solutions to the radial Schrödinger equation (2) with $T > 0$, which, for distances well inside the atom, give analytic screening corrections to the unperturbed Coulomb shape. We have shown that for bound states such wave functions can be constructed relatively easily in terms of the eigenfunctions of a certain differential operator, owing to the special symmetries of the Coulomb problem and the expansion (1) we have assumed for the potential. We will now extend these results to the continuum case. However, instead of simply repeating the derivation of Sec.

II, we will show that in this instance the positive-energy solutions to the Schrödinger equation can be obtained explicitly, by means of an analytic continuation, from the corresponding bound-state expressions (22). This considerably simplifies the discussion of the continuum case since the relevant formulas already have essentially been written down.

We note that because of our expansion of the potential, our analytic wave function, to any finite order in λ , will not have the correct asymptotic behavior, $(Nkr)^{-1} \sin[kr - \frac{1}{2}\pi l + \delta_l]$. Thus it is not possible to obtain directly an analytic expression for the normalization or phase shifts from our regular solution. However, comparison with numerical results indicates that our wave function is a good approximation to the exact screened solution in the interior of the atom. In particular, since the effective expansion parameter becomes $a\lambda/T$ in the continuum case, our expressions improve with increasing energy. At sufficiently high energy, the wave function will have achieved its asymptotic form in the region in which our expansion is valid. In such circumstances, it would appear that our knowledge of the wave function in the interior region should be sufficient to determine the normalization and phase shifts. One way to extract this information on normalization and phases is through the Jost function. Since the Jost function is determined by the behavior of the irregular (Jost) wave function at the origin, it should be possible, in this way, to determine the normalization and phase from the behavior of the wave function in the interior of the atom.

Thus in addition to the regular (scattering) solution, we will also consider the irregular (Jost) solutions. By decomposing our regular wave function into parts which are, asymptotically, purely incoming or outgoing waves, we obtain, up to a phase, explicit expressions for the screened Jost solutions which are valid in the interior of the atom. The residual phase, which is nonanalytic in λ , is a well-known feature of screened Coulomb wave functions and arises from the difference in asymptotic behavior of the screened and point

Coulomb solutions. By considering the asymptotic behavior of our Jost solution, we obtain some (but not complete) information on this exterior phase. From the Jost solutions determined in this way, we obtain analytic expressions for the Jost functions and hence the normalization and phase shifts. Our final results for the screened Coulomb normalization and phase shifts are in good agreement with numerical values.

For both the regular and irregular solutions, our approach differs from the usual perturbation theory in that we introduce a parameter $T_c > 0$ which, for convenience, we call the unperturbed Coulomb energy, since it plays a role analogous to that played by the Coulomb bound-state energy in the construction of screened bound-state wave functions. (For example, in the limit $\lambda \rightarrow 0$, $T_c \rightarrow T$.) Although the difference $\delta T = T - T_c$ is a specified function of T_c in our approach, no quantization is implied, since T_c is arbitrary, and T can assume any positive value.²¹ On the other hand, in the usual Rayleigh-Schrödinger perturbation theory, one sets $\delta T = 0$ in the continuum case. We note, however, that the work of Pratt and Tseng indicates that $\delta T = 0$ is not necessarily the best physical choice. For many processes, the matrix element may be substantially improved if one employs energy-shifted Coulomb wave functions. Moreover, we will see that considerable mathematical simplification results from the introduction of a continuum unperturbed Coulomb wave function whose energy is not equal to the energy eigenvalue which appears in the Schrödinger equation. Of course, in general, the selection of a specific form for δT is arbitrary. Our particular choice results in an especially simple and convenient form for the screened continuum wave function. The final justification of this choice, however, must come from the agreement of our analytic wave functions with the exact numerical results in the region of interest.

A. Regular solution

To proceed, we define the function $s(r)$ as in Sec. II by means of the relation

$$R(r) = Nr^l e^{-ik_c r} s(r) \quad (38)$$

and substitute $x = 2ik_c r$, where $T_c = \frac{1}{2}k_c^2$ and $R(r)$ is the radial continuum wave function. We find that $s(x)$ satisfies the equation

$$\left(x \frac{d^2}{dx^2} + (2l + 2 - x) \frac{d}{dx} + (-i\nu - l - 1) \right) s(x) = \mathfrak{D}_{-i\nu, l} s(x) = (x/4T_c)(\delta T - \delta V)s(x), \quad (39)$$

where $\nu = a/k_c$ and $\delta T = T - T_c = \lambda T_1 + \lambda^2 T_2 + \lambda^3 T_3$

$+ \dots$. (We assume throughout that the potential is attractive. For a repulsive potential it is necessary to replace a by $-a$ wherever it appears.²²) The boundary condition on $s(x)$ is that it be regular at the origin. Again for convenience, we standardize $s(x)$ such that $s(0) = 1$. In order to completely characterize Eq. (39), the form of δT must be specified. We choose δT such that it is given by the expression for the bound-state energy shift with the substitution $n \rightarrow -i\nu$. That is, we define²³

$$\begin{aligned} \delta T &= T - T_c \\ &= -\lambda V_1 a + \frac{1}{2} \lambda^2 V_2 \left(\frac{3a^2}{2T_c} + l(l+1) \right) \\ &\quad + \frac{a\lambda^3 V_3}{4T_c} \left(\frac{-5a^2}{2T_c} - 3l(l+1) + 1 \right) + \dots \end{aligned} \quad (40)$$

It is evident from (24) that δT will be real for real T_c . We note that the right-hand side of (40) depends explicitly on l . Thus for any given energy T , the corresponding unperturbed Coulomb energy T_c will necessarily be different for each radial wave function and must be chosen appropriately. With this choice (40) for the energy shift Eq. (39) for the continuum solution is identical to the Eq. (4) for the bound state, with the substitution $n \rightarrow -i\nu$. Moreover, the boundary condition that $s(x)$ be regular at the origin is the same in each case.²⁴ It then follows from a theorem of Poincaré²⁵ that the solution of (39) can be obtained from the solution of (4) with the substitution $n \rightarrow -i\nu$. Thus we can immediately write

$$s(x) = s_c(x) + \lambda^2 A_2(x) + \lambda^3 A_3(x) + \dots, \quad (41)$$

where $s_c(x)$ is the unperturbed Coulomb continuum solution with energy T_c . That is,

$$s_c(x) = M(l+1+i\nu, 2l+2; x). \quad (42)$$

The correction terms $A_k(x)$ can be written

$$A_k(x) = \sum_{s=-k}^k \alpha_s^k(-i\nu, l) M(l+1+i\nu-s, 2l+2; x), \quad (43)$$

where the coefficients $\alpha_s^k(-i\nu, l)$ are obtained from the corresponding bound-state expressions (22) by means of the substitution $n \rightarrow -i\nu$. We note that the CHF's which appear in (43) are not polynomials in the continuum case. Their properties, however, are similar to those of continuum Coulomb wave functions. In particular, for any process in which the point Coulomb results can be obtained explicitly, one can also evaluate the corrections owing to screening analytically, using our wave functions, since the integrals involved are formal-

ly the same.

The fact that our continuum solution can be written in the form (43) if we choose the expression (40) for the energy shift is the motivation for our selection of this form for δT . With a different expression for the energy shift, our continuum solution would contain terms involving integrals which depend on the radial Coulomb Green's function, as in Eq. (13). Thus we would probably not be able to obtain an explicit form for the continuum wave function, since the integrals are rather complicated. Moreover, since this choice for the energy shift allows us to use a simple analytic continuation to obtain the continuum solution from the corresponding bound-state solution, it guarantees that for each order in λ our continuum radial wave function reduces to the correct bound-state wave function when T is analytically continued to a physical bound-state energy eigenvalue. This is a necessary condition on any valid scattering solution of the Schrödinger equation, and it is trivially satisfied by our solution (41). Of course, it is not entirely novel that the continuum wave function can be obtained from the bound-state solution by analytic continuation. It has long been known explicitly for the Coulomb wave function,

$$rR(r) - rR_c(r) \xrightarrow{r \rightarrow \infty} \sum_{m=2}^k \lambda^m \sum_{s=0}^m B_s^m r^s \sin[k_c r + \nu \ln 2k_c r - \frac{1}{2}\pi(l+s) + \delta_{l+s}], \quad (46)$$

where the B_s^m are constants which depend on k_c , l , and the potential, and $\delta_{l+s} = \arg \Gamma(l+s+1-i\nu)$. $\Gamma(z)$ is the Euler gamma function. It is evident from (46) that our continuum wave function does not have the correct asymptotic behavior to any finite order in λ . Thus it is not possible to evaluate the normalization and phase shifts directly from the asymptotic form (46). This sort of behavior is to be expected, since the expansion (1) we have assumed for the potential is correct only in the interior of the atom. In this region, however, our screened wave functions give a very good approximation to the exact numerical results. (see Figs. 3 and 4). Evidently, our solutions are valid interior solutions to the Schrödinger equation with a screened Coulomb potential. Moreover, we will see subsequently, when we consider the irregular solutions, that the most divergent parts, at least, of the expression (46) in each order of λ do sum up to cancel the Coulomb logarithmic phase $\nu \ln 2k_c r$. Thus we will find that our final expressions for the normalization and phase shifts, which we will obtain from the Jost function, are in good agreement with the exact numerical values.

and it is true, in general, that the regular solution of the Schrödinger equation, as an analytic function of energy, gives both bound and continuum states as special cases.²⁶ However, it should be noted that with the choice (40) for δT , one could also obtain the same result, Eq. (41), directly by means of the analysis of Sec. II. In this case, the use of analytic continuation to obtain the continuum radial wave function serves merely to avoid unnecessary duplication of effort.

Certain properties of the radial wave functions defined by (38) and (41)–(43) follow immediately from those of the CHF's and of the coefficients $\alpha_s^k(-i\nu, l)$. In particular, we note that $R(r)$ is real since, from Krummer's identity,

$$[e^{-ik_c r} M(l+1+i\nu-s, 2l+2, 2ik_c r)]^* = e^{-ik_c r} M(l+1+i\nu+s, 2l+2, 2ik_c r), \quad (44)$$

and from (23),

$$[\alpha_s^k(-i\nu, l)]^* = \alpha_s^k(-i\nu, l), \quad (45)$$

(the asterisk denotes complex conjugation) and the sum (43) is symmetric about $s=0$. The asymptotic behavior of our screened continuum radial wave functions, including terms of order λ^k , is given by

B. Irregular solutions

We now consider the irregular solutions of the radial Schrödinger equation. Our motivation is to obtain an expression for the screened Coulomb Jost functions and hence the normalization and phase shifts. To obtain the Jost functions, it is convenient to work directly with the Jost solutions, which are related to the irregular Schrödinger wave functions as follows: Let $v(\pm k, l; r)$ be two linearly independent irregular solutions of Eq. (2) which behave asymptotically as pure incoming (outgoing) spherical waves. The Jost solution $f(\pm k, l; r)$ are then defined by the relation

$$f(\pm k, l; r) = r v(\pm k, l; r). \quad (47)$$

The phase of $v(\pm k, l; r)$ is fixed, conventionally, by requiring that $f(\pm k, l; r)$ satisfy the boundary condition

$$\lim_{r \rightarrow \infty} e^{\pm ikr} f(\pm k, l; r) = 1. \quad (48)$$

Given the Jost solutions, the Jost functions $f(\pm k, l)$ are defined by the relation

$$f(\pm k, l) = \lim_{r \rightarrow 0} (2l+1)r^l f(\pm k, l; r). \quad (49)$$

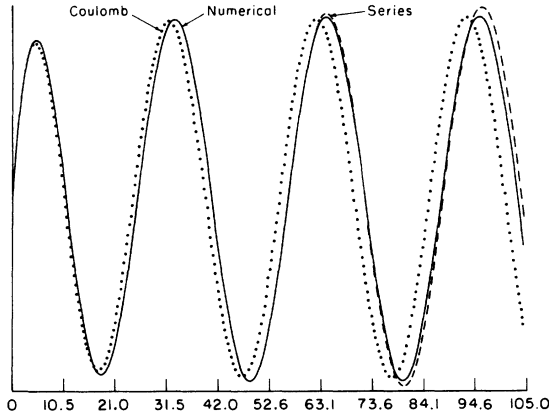


FIG. 3. 10-keV continuum S-wave radial function $u(r)/k = N^{-1}rR(r)$ for aluminum ($Z = 13$), using our analytic fit to the HS-HFS potential. The solid curve is the numerical shape, the dashed curve gives our analytic result, and the dotted curve is the point Coulomb shape for the same Z . Distances are in electron Compton wavelengths.

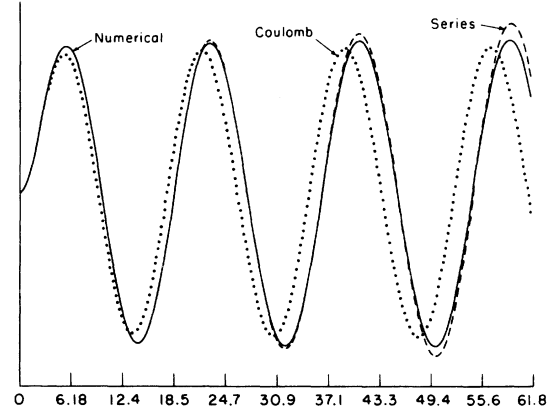


FIG. 4. 30-keV continuum P -wave radial function $u(r)/k = N^{-1}rR(r)$ for krypton ($Z = 36$) assuming a Yukawa potential $V(r) = -(a/r)e^{-\lambda r}$. λ is the Thomas-Fermi radius. The unbroken curve is the exact numerical shape, the dashed curve is our analytic result, and the dotted curve is the point Coulomb shape for this Z . Distances are in electron Compton wavelengths.

From the definitions (47)–(49) it follows that the regular solution of (2) can be written in the form

$$N^{-1}rR(r) = - (1/2ik) [f(-k)f(k, r) - f(k)f(-k, r)], \quad (50)$$

where we omit the angular momentum quantum number l for simplicity. We also note that for real k $f(-k, r) = f^*(k, r)$.²⁶ For convenience, we will refer to $f(k, r)$ as the Jost solution, since the properties of $f(-k, r)$ can be inferred from those of $f(k, r)$. Similarly, $f(-k, l) = f^*(k, l)$ for real k .

From (50) and (48) we can determine the normalization and phase shifts in terms of the Jost function. For example, assuming an asymptotic behavior of the form²⁷

$$rR(r) \rightarrow k^{-1} \sin(kr - \frac{1}{2}\pi l + \delta_l) \quad \text{as } r \rightarrow \infty, \quad (51)$$

the continuum normalization can be written

$$N(k, l) = | f(k, l) |^{-1}, \quad (52)$$

while the phase shift is essentially the phase of $f(k, l)$, that is,

$$f(k, l) = | f(k, l) | \exp[i\delta(k, l) - \frac{1}{2}i\pi l]. \quad (53)$$

In order to illustrate our procedure for determining the irregular screened solutions and also to introduce some results which will be needed later, we will consider first the unperturbed Coulomb Jost solutions. Of course, owing to the long range of the Coulomb potential, the definition of the Jost solution must be modified somewhat, since it is not possible to obtain solutions of the radial Schrödinger equation which behave asymptotically as pure spherical waves. In particular,

for the Coulomb case, the boundary condition (48) becomes

$$\lim_{r \rightarrow \infty} [\exp \pm (ik_c r + i\nu \ln 2k_c r)] f_c(\pm k_c, r) = 1, \quad (54)$$

where $\nu \ln 2k_c r$ is the usual logarithmic Coulomb phase.

To proceed, we write the regular Coulomb solution in the form

$$N_c^{-1}rR_c(r) = r^{i+1} e^{-x/2} M(l+1+i\nu, 2l+2; x), \quad (55)$$

where $x = 2ik_c r$. This solution can be separated into incoming and outgoing parts by means of the identity²⁸

$$M(a, b; x) = [\Gamma(b)/\Gamma(b-a)] e^{i\pi a} \psi(a, b; x) + [\Gamma(b)/\Gamma(a)] e^{i\pi(a-b)} e^x \psi(b-a, b; -x), \quad (56)$$

where $\psi(a, b; x)$ and $e^x \psi(b-a, b; -x)$ are linearly independent irregular solutions of the confluent hypergeometric equation. The properties of $\psi(a, b; x)$ which are relevant for our purposes are the following: At large x , we have the asymptotic behavior

$$\psi(a, b; x) \rightarrow x^{-a} \quad \text{as } x \rightarrow \infty, \quad (57)$$

while, at the origin,

$$\lim_{x \rightarrow 0} (b-1)x^{b-1} \psi(a, b; x) = \Gamma(b)/\Gamma(a). \quad (58)$$

Using (56), we can write the regular solution (55) in the form

$$N_c^{-1}rR_c(r) = \frac{-1}{2ik_c} \left((-2ik_c)^{-l} e^{-\nu} \frac{\Gamma(2l+2)}{\Gamma(l+1-i\nu)} x^{l+1} e^{-x/2} \psi(l+1+i\nu, 2l+2; x) \right. \\ \left. - (2ik_c)^l e^{-\nu} \frac{\Gamma(2l+2)}{\Gamma(l+1+i\nu)} (-x)^{l+1} e^{x/2} \psi(l+1-i\nu, 2l+2; -x) \right), \quad (59)$$

where from (57) we see that the first term of (59) is the incoming part, while the second term is outgoing. We can now identify the incoming part of (59) with the incoming part of (50) to obtain

$$f_c(-k_c) f_c(k_c, r) = (-2ik_c)^{-l} e^{-\nu} \left[\frac{\Gamma(2l+2)}{\Gamma(l+1-i\nu)} \right] \\ \times x^{l+1} e^{-x/2} \psi(l+1+i\nu, 2l+2; x) \quad (60)$$

for the Coulomb Jost solution. We note that this equation determines the Jost solution only up to a phase factor, since it involves the product $f_c(-k_c) f_c(k_c, r)$. Using the property of the irregular CHF (58) and the definition (49) we can determine the magnitude of $f_c(k_c)$ from (60). Using that result, we can write the Jost solution in the form

$$f_c(k_c, r) = e^{i\phi} e^{-\nu} x^{l+1} e^{-x/2} \psi(l+1+i\nu, 2l+2; x), \quad (61)$$

where, at this point, the phase ϕ is arbitrary. The corresponding Jost function is given by

$$f_c(k_c) = e^{i\phi} (2ik_c)^{-l} \frac{\Gamma(2l+2)}{\Gamma(l+1+i\nu)} e^{-\nu/2}. \quad (62)$$

The phase of $f_c(k_c, r)$ can now be determined from the boundary condition (54). Using (57), we find that this condition, Eq. (54), is satisfied if $\phi = 0$. As a final check, we note that $r^{-1} f_c(k_c, r)$ defined by (61) is, indeed, a solution of the Schrödinger equation (2) since $\psi(a, b; x)$ satisfies the same equation as $M(a, b; x)$. Thus by separating the regular solution into parts which are asymptotically incoming or outgoing, we can determine the Jost solution up to a phase. By imposing the asymptotic boundary condition, one determines this phase factor and hence the complete Jost solution.

Finally, we remark that the result (62) for the Coulomb Jost function gives the correct Coulomb normalization

$$N_c = |f_c(k_c)|^{-1} = (2k_c)^l \frac{|\Gamma(l+1+i\nu)|}{\Gamma(2l+2)} e^{\nu/2} \quad (63)$$

and the usual Coulomb phase shifts

$$\delta_c(k_c, l) = \arg f_c(k_c) + \frac{1}{2} \pi l = \arg \Gamma(l+1-i\nu). \quad (64)$$

We will now derive an expression for the screened Jost solution from our regular solution (41) using the same procedure as that outlined above for the Coulomb case. To proceed, we as-

sume that the screened Jost solution can be written in the form

$$f(k, r) = e^{i\phi(k_c)} (k/k_c)^{l/2} \left[f_c(k_c, r) + \lambda^2 f_2(k_c, r) \right. \\ \left. + \lambda^3 f_3(k_c, r) + \dots \right], \quad (65)$$

with the corresponding Jost function given by

$$f(k, l) = \lim_{r \rightarrow 0} (2l+1) r^l f(k, r) \\ = e^{i\phi(k_c)} (k/k_c)^{l/2} \left[f_c(k_c, l) + \lambda^2 f_2(k_c, l) \right. \\ \left. + \lambda^3 f_3(k_c, l) + \dots \right], \quad (66)$$

where the factor $(k/k_c)^{l/2}$ is chosen for consistency with Eq. (41) [cf. Eq. (71)]. In (65), $f_c(k_c, r)$ is the unperturbed Coulomb Jost solution of shifted energy. We have not included terms of first order in λ in this expansion, since our Jost solution is derived from the regular solution (41) in which, as we have shown, the first-order term vanishes. In order to satisfy the condition $f(-k, r) = f^*(k, r)$, we assume that $\phi(-k_c) = -\phi(k_c)$ and $f_n(-k_c, r) = f_n^*(k_c, r)$. We must verify later that this leads to an acceptable solution.²⁹ The additional (arbitrary) phase $\phi(k_c)$ allows for the fact that the screened and point Coulomb Jost solutions do not coincide in the limit $\lambda \rightarrow 0$. In this limit, as is well known, the screened Jost solution is equal to the point Coulomb Jost solution multiplied by a divergent phase. Thus $\phi(k_c)$ must contain terms which are nonanalytic in λ . We also find that our procedure for constructing $f(k, r)$, as in the Coulomb case, determines the screened Jost solution only up to an overall phase, which we incorporate in $\phi(k_c)$. To see this, we note that if $r^{-1} f(k, r)$ and $r^{-1} f'(k, r)$ are two solutions of the radial Schrödinger equation and, moreover, each satisfies incoming boundary conditions, then since the incoming and outgoing solutions are linearly independent, we must have

$$f'(k, r) = A f(k, r), \quad (67)$$

where A is an arbitrary constant. This result is well known. However, if the quantity $N^{-1} r R(r)$ is given, and if we also require that these solutions satisfy the relation

$$N^{-1} r R(r) = (-1/2ik) [f(-k)f(k, r) - f(k)f(-k, r)], \quad (68)$$

with $f(-k, r) = f^*(k, r)$, then it follows that for real k

$$\begin{aligned} & [f(-k)f(k, r) - f(k)f(-k, r)] \\ &= |A|^2 [f(-k)f(k, r) - f(k)f(-k, r)]. \end{aligned} \quad (69)$$

Hence $|A|^2 = 1$ and

$$f'(k, r) = e^{i\alpha(k)} f(k, r). \quad (70)$$

Thus with $N^{-1}rR(r)$ specified, the expression (68) determines the Jost solution up to an overall phase. Since we incorporate this arbitrary phase into the phase $\phi(k_c)$ which appears in (65), it is sufficient to find a particular incoming solution which satisfies (68). We will thus ignore possible

additional phase contributions in the subsequent discussion. Finally, of course, the resulting phase factor $e^{i\phi(k_c)}$ must be determined by requiring that our screened Jost solution satisfy the asymptotic boundary condition (48). It is, however, important to note that the *magnitude* of the Jost function is determined unambiguously by the particular method we use to evaluate $f(k, r)$. Hence for the solution which we will construct it is only the value of $\phi(k_c)$ which must be determined from the large-distance behavior of the wave function.

If we substitute (65) and (66) into the relation (68), we obtain

$$\begin{aligned} N^{-1}rR(r) &= (-1/2ik)[f(-k)f(k, r) - f(k)f(-k, r)] \\ &= (-1/2ik_c) \{ [f_c(-k_c)f_c(k_c, r) - f_c(k_c)f_c(-k_c, r)] \\ &\quad + \lambda^2 \{ [f_c(-k_c)f_2(k_c, r) + f_2(-k_c)f_c(k_c, r)] - [f_c(k_c)f_2(-k_c, r) + f_2(k_c)f_c(-k_c, r)] \} \\ &\quad + \lambda^3 \{ [f_c(-k_c)f_3(k_c, r) + f_3(-k_c)f_c(k_c, r)] - [f_c(k_c)f_3(-k_c, r) + f_3(k_c)f_c(-k_c, r)] \} + \dots \}, \end{aligned} \quad (71)$$

where the first term on the right-hand side of the second equation of (71) is just the unperturbed Coulomb wave function of shifted energy. It was to obtain this result that the factor $(k/k_c)^{1/2}$ was introduced in (65). The remaining terms give the corrections to the regular Coulomb solution owing to screening. Note that the phase $\phi(k_c)$ does not appear in (71). If we write the regular solution $N^{-1}rR(r)$ in the form

$$N^{-1}rR(r) = N^{-1}r[R_c(r) + \lambda^2 R_2(r) + \lambda^3 R_3(r) + \dots], \quad (72)$$

where $R_c(r)$ is the unperturbed Coulomb wave function, then from (38), (41), and (43) we obtain explicit expressions for the correction terms $R_n(r)$. For $n=2, 3$, we have

$$N^{-1}rR_n(r) = \sum_{s=-n}^n \alpha_s^n(-i\nu, l) r^{l+1} e^{-x/2} M(l+1+i\nu-s, 2l+2; x). \quad (73)$$

As in the Coulomb case, we can separate the incoming and outgoing parts of (73) by means of the identity (56). Thus for $n=2, 3$,

$$\begin{aligned} N^{-1}rR_n(r) &= \sum_{s=-n}^n \alpha_s^n(-i\nu, l) r^{l+1} e^{-x/2} \left(\frac{\Gamma(2l+2)}{\Gamma(l+1-i\nu+s)} e^{i\pi(l+1+i\nu-s)\psi} \psi(l+1+i\nu-s, 2l+2; x) \right. \\ &\quad \left. + \frac{\Gamma(2l+2)}{\Gamma(l+1+i\nu-s)} e^{-i\pi(l+1-i\nu+s)\psi} e^{x\psi} \psi(l+1-i\nu+s, 2l+2; -x) \right) \\ &= \frac{-1}{2ik_c} \left(f_c(-k_c) \sum_{s=-n}^n \frac{\Gamma(l+1-i\nu)}{\Gamma(l+1-i\nu+s)} \alpha_s^n(-i\nu, l) (-1)^s e^{-\pi\nu/2} x^{l+1} e^{-x/2} \psi(l+1+i\nu-s, 2l+2; x) \right. \\ &\quad \left. - f_c(k_c) \sum_{s=-n}^n \frac{\Gamma(l+1+i\nu)}{\Gamma(l+1+i\nu-s)} \alpha_s^n(-i\nu, l) (-1)^s e^{-\pi\nu/2} (-x)^{l+1} e^{x/2} \psi(l+1-i\nu+s, 2l+2; -x) \right), \end{aligned} \quad (74)$$

where in the second equation of (74) we have used the definition (62) of the Coulomb Jost function to extract the factors $f_c(\pm k_c)$. This decomposition, Eq. (74), into incoming and outgoing portions is unique, since the ψ functions which appear are linearly independent. If we equate the right-hand

sides of (71) and (72), the result must then hold for each order in λ . Moreover, to any given order in λ , the incoming and outgoing parts must separately be equal, owing to the uniqueness of this decomposition. In this way, using the result (74) we find, for $n=2, 3$, the relation

$$\begin{aligned}
& f_c(-k_c)f_n(k_c, r) + f_n(-k_c)f_c(k_c, r) \\
&= f_c(-k_c) \sum_{s=-n}^n \frac{\Gamma(l+1-i\nu)}{\Gamma(l+1-i\nu+s)} \alpha_s^n(-i\nu, l) (-1)^s e^{-r\nu/2} \\
&\quad \times x^{l+1} e^{-x/2} \psi(l+1+i\nu-s, 2l+2; x),
\end{aligned} \tag{75}$$

or

$$\begin{aligned}
f_n(k_c, r) &= -\frac{f_n(-k_c)}{f_c(-k_c)} f_c(k_c, r) \\
&+ \sum_{s=-n}^n \frac{\Gamma(l+1-i\nu)}{\Gamma(l+1-i\nu+s)} \alpha_s^n(-i\nu, l) (-1)^s e^{-r\nu/2} \\
&\quad \times x^{l+1} e^{-x/2} \psi(l+1+i\nu-s, 2l+2; x).
\end{aligned} \tag{76}$$

Equation (76), which defines implicitly the second- and third-order corrections to the Coulomb Jost solution, represents the first two equations in a hierarchy of equations for the correction terms

$f_n(k_c, r)$. For $n > 3$, similar, albeit more complicated, expressions would be obtained. In general, the expression for $f_n(k_c, r)$ would involve contributions from all lower-order corrections to $f_c(k_c, r)$. For $n = 2, 3$, however, the situation is once again rather simple, since the only lower-order term which appears is the unperturbed Coulomb solution $f_c(k_c, r)$. For our purposes, Eq. (76) is the basic equation we have to consider.

In order to solve this equation, we define $\chi_n(k_c)$ such that

$$f_n(k_c) = f_c(k_c) \chi_n(k_c). \tag{77}$$

Expression (76) then becomes

$$\begin{aligned}
f_n(k, r) &= -\chi_n(-k_c) f_c(k, r) \\
&+ \sum_{s=-n}^n \frac{\Gamma(l+1-i\nu)}{\Gamma(l+1-i\nu+s)} \alpha_s^n(-i\nu, l) (-1)^s e^{-r\nu/2} \\
&\quad \times x^{l+1} e^{-x/2} \psi(l+1+i\nu-s, 2l+2; x).
\end{aligned} \tag{78}$$

Multiplying (78) by $(2l+1)r^l$ and taking the limit $r \rightarrow 0$, we find

$$\begin{aligned}
f_n(k_c) = f_c(k_c) \chi_n(k_c) &= -\chi_n(-k_c) f_c(k_c) + f_c(k_c) \left(\sum_{s=-n}^0 (-1)^s \frac{\Gamma(l+1-i\nu)}{\Gamma(l+1-i\nu+s)} \frac{\Gamma(l+1+i\nu)}{\Gamma(l+1+i\nu-s)} \bar{\alpha}_s^n(-i\nu, l) \right. \\
&\quad \left. + \sum_{s=-n}^0 (-1)^s \frac{\Gamma(l+1+i\nu)}{\Gamma(l+1+i\nu+s)} \frac{\Gamma(l+1-i\nu)}{\Gamma(l+1-i\nu-s)} \bar{\alpha}_s^n(i\nu, l) \right),
\end{aligned} \tag{79}$$

where we define

$$\bar{\alpha}_s^n(-i\nu, l) = \begin{cases} \alpha_s^n(-i\nu, l), & s \neq 0, \\ \frac{1}{2} \alpha_s^n(-i\nu, l), & s = 0. \end{cases} \tag{80}$$

In the last term of (79), we have used the relation (45) to rearrange the sum. From (79) we find the particular solution

$$\begin{aligned}
\chi_n(k) &= \sum_{s=-n}^0 (-1)^s \frac{\Gamma(l+1-i\nu)}{\Gamma(l+1-i\nu+s)} \frac{\Gamma(l+1+i\nu)}{\Gamma(l+1+i\nu-s)} \\
&\quad \times \bar{\alpha}_s^n(-i\nu, l).
\end{aligned} \tag{81}$$

With this result, Eq. (81), the correction $f_n(k_c, r)$ to the Coulomb Jost solution is given by (78).

Having derived an expression for the corrections to the Coulomb Jost solution, it is essentially trivial to verify that the functions $r^{-1/2} f(\pm k, r)$ defined by (65) and (78) are in fact the irregular solutions to the Schrödinger equation to the order considered. We note that the functions $\psi(a, b; x)/\Gamma(b-a)$ satisfy the relation

$$\begin{aligned}
x \frac{\psi(a, b; x)}{\Gamma(b-a)} &= -a \frac{\psi(a+1, b; x)}{\Gamma(b-a-1)} + (b-2a) \frac{\psi(a, b; x)}{\Gamma(b-a)} \\
&\quad - (a-b) \frac{\psi(a-1, b; x)}{\Gamma(b-a+1)},
\end{aligned} \tag{82}$$

which is the analog of the relation (10), and that

$$\begin{aligned}
\mathfrak{D}_{-i\nu, l} \psi(l+1+i\nu-s, 2l+2; x) \\
= -s \psi(l+1+i\nu-s, 2l+2; x),
\end{aligned} \tag{83}$$

where $\mathfrak{D}_{-i\nu, l}$ is the differential operator defined by Eq. (39). One may then verify by direct substitution after eliminating the factor $r^l e^{-ik_c r}$ that Eq. (39) is satisfied to the order considered. We have thus found two linearly independent solutions to the screened Schrödinger equation which for $\lambda = 0$ give, except for a phase factor, the correct point Coulomb Jost solutions.³⁰

Although the expression we have given for $f(k, r)$ is in terms of a purely incoming (irregular) solution of the Schrödinger equation, our specification of the screened Coulomb Jost solution is not yet complete. We must also impose the asymptotic boundary condition (48) and hence determine the

phase $\phi(k_c)$. At this point, however, we can only give a heuristic derivation of this quantity. This is because of the fact that to any finite order in λ our solution explicitly violates the asymptotic boundary condition (48). It is only by generalizing the behavior of the lowest-order terms which we have obtained to all orders in λ that we are able to gain some information on the phase of $f(k, r)$. Thus we do not obtain an exact analytic expression for the phase shifts. By means of this heuristic argument, however, we can write down an explicit expression for the major part of the screened Coulomb phase shifts, including the correct non-analytic part, which had previously been determined by Taylor.³¹ Our final result for the phase shifts is in good agreement with exact numerical values. At the same time, it should again be noted that our result for the magnitude of the Jost function is independent of $\phi(k_c)$. As we have shown, using our procedure the quantity $|f(k)|$ is determined unambiguously from our regular solution. Hence our expression for the normalization, to the order considered, should be exact.

If we consider the asymptotic behavior of our expression (65) using the result (78), then to order λ^n we have

$$\lim_{r \rightarrow \infty} e^{ikr} f(k, r) = \lim_{r \rightarrow \infty} e^{i\phi(k_c)} e^{-i\nu \ln 2k_c r} \left(1 + \sum_{m=1}^n \lambda^m \sum_{s=0}^m C_s r^s \right), \quad (84)$$

where the C_s are constants which depend on k_c , l , and the potential. In addition to the Coulomb logarithmic phase $\nu \ln 2k_c r$, there are additional powers of r which diverge at large distances. Thus to any finite order in λ the form (84) will violate the asymptotic boundary condition (48). However, if we consider only the most divergent terms for each order in λ , and insert the explicit values of the C_m which we obtain from the result (78), using (57), then to the same order in λ we have

$$e^{-i\nu \ln 2k_c r} \left(1 + \sum_{m=1}^n C_m (\lambda r)^m \right) = \exp \left[\frac{i}{k_c} \int_{r_0}^r \frac{-a}{r'} \left(1 + \sum_{m=1}^n V_m (\lambda r')^m \right) dr' \right], \quad (85)$$

where $r_0 = \frac{1}{2} |k_c|^{-1} + O(\lambda)$. We recognize that the argument of the exponential on the right-hand side of Eq. (85) is just the integral of our expansion (1) for the potential. Returning now to (84), using the result (85) we conjecture that if the right-hand side of this equation could be calculated to all orders in λ and summed, then neglecting terms of relative order $1/r$ we would have for the asymptotic behavior of our solution

$$\lim_{r \rightarrow \infty} e^{ikr} f(k, r) = \lim_{r \rightarrow \infty} \exp \left(i\phi(k_c) + \frac{i}{k_c} \int_{r_0}^r V(r') dr' \right), \quad (86)$$

where

$$r_0 = \frac{1}{2} |k_c|^{-1} + O(\lambda). \quad (87)$$

Unfortunately, at this time we do not have a procedure for calculating the higher-order corrections to r_0 , since we are not able to write an unambiguous expression for the sum of the nonleading terms in (84). We note, however, that these higher-order terms will be analytic in λ . Hence we do obtain all of the nonanalytic part of $\phi(k_c)$. In any case, the expression (86) will yield a convenient representation for $\phi(k_c)$.

Assuming (86) is correct, there are two possibilities which must be considered: that of a neutral atom, and the ionic case. If $V(r)$ goes to zero faster than $1/r$ at large r , corresponding to a neutral atom, then from (86) we can immediately write

$$\phi(k_c) = -\frac{1}{k_c} \int_{r_0}^{\infty} V(r') dr'. \quad (88)$$

In this case, the right-hand side of (86) is equal to unity and the boundary condition (48) will be satisfied. We see explicitly that the integral (88) is not defined in the limit $\lambda \rightarrow 0$, so that $\phi(k_c)$ determined in this way is nonanalytic in λ . In fact, with r_0 defined by (87), the expression (86) gives precisely the result of Taylor³¹ for the nonanalytic part of the screened Coulomb phase shift. In the other case, we consider an electron which is removed from a neutral atom so that $V(r) \sim -1/r$ at large distances. For this ionic case, the screened Jost solution must satisfy the boundary condition (54), with the logarithmic Coulomb phase $\nu' \ln 2k_c r$ corresponding to a unit point charge. In this situation, we subtract from $V(r)$ the asymptotic Coulomb tail, and write

$$\phi(k_c) = -\frac{1}{k_c} \int_{r_0}^{\infty} \left(V(r') + \frac{1}{r'} \right) dr'. \quad (89)$$

Then, neglecting higher-order terms, (86) becomes

$$e^{ikr} f(k, r) \sim e^{-i\nu' \ln 2k_c r}, \quad (90)$$

where $\nu' = 1/k_c$. Hence (86) will give an asymptotic behavior which is appropriate for this case.

For certain potentials, the integral (88) can be evaluated explicitly. An example is the Yukawa potential, $V(r) = -ae^{-\lambda r}/r$. In this case, we obtain

$$\phi(k_c) = \nu E_1(\lambda r_0) = -\gamma\nu + \nu \ln |2k_c/\lambda| + O(\lambda), \quad (91)$$

where $E_1(x)$ is the exponential integral¹⁹ and $\gamma = 0.57722$ is the Euler constant. The logarithmic

dependence on λ in (91) seems to be characteristic of screened Coulomb problems although potentials can be written which have more singular terms.

C. Normalizations and phase shifts

Having, finally, obtained an expression for the screened Coulomb Jost function, we can write immediately the continuum normalization and phase shifts. Collecting our results, we have the following contributions to the screened Jost function through third order in λ :

$$f(k, l) = e^{i\phi(k_c)} (k/k_c)^{1/2} f_c(k_c, l) \times [1 + \lambda^2 \chi_2(k_c, l) + \lambda^3 \chi_3(k_c, l)], \quad (92)$$

where, from (81),

$$\chi_2(k_c, l) = \frac{-V_2}{8T_c} \{l(l+1)(2l+1) + \frac{1}{2}i\nu[\nu^2 - l(l-1)]\}, \quad (93)$$

$$\chi_3(k_c, l) = \frac{aV_3}{16T_c^2} \left\{ \frac{5}{3}l(l+1)(2l+1) - \frac{1}{2}i\nu[(l-1)(l-4) - \frac{7}{3}(\nu^2+1)] \right\},$$

and $\phi(k_c)$ is given by (88) or (89). The unperturbed Coulomb Jost function is given by (62). Employing (52), the continuum normalization is given through third order in λ by

$$N(k, l) = N_c(k_c, l) (k_c/k)^{1/2} [1 - \lambda^2 \text{Re} \chi_2(k_c, l) - \lambda^3 \text{Re} \chi_3(k_c, l)] \\ = N_c(k_c, l) (k_c/k)^{1/2} [1 + \lambda^2 (V_2/8T_c) l(l+1)(2l+1) - \lambda^3 (5aV_3/48T_c^2) l(l+1)(2l+1)], \quad (94)$$

where $N_c(k_c, l)$ is the point Coulomb normalization of shifted energy, Eq. (63). The factor $(k_c/k)^{1/2}$ can also be expanded in powers of λ . Using (40), we find, through third order,

$$k = k_c - \frac{\lambda V_1 a}{k_c} - \frac{\lambda^2}{2k_c} \left((V_1^2 - 3V_2) \frac{a^2}{k_c^2} - V_2 l(l+1) \right) - \frac{a\lambda^3}{2k_c^3} \left((V_1^3 - 3V_1 V_2 + 5V_3) \frac{a^2}{k_c^2} - (V_1 V_2 - 3V_3) l(l+1) - V_3 \right). \quad (95)$$

With this result, (94) can be rewritten in the form

$$N(k, l) = N_c(k, l) \left[1 + \frac{\lambda V_1 a}{4T_c} + \frac{\lambda^2}{8T_c} \left((5V_1^2 - 6V_2) \frac{a^2}{4T_c} + 2V_2 l^2(l+1) \right) \right. \\ \left. + \frac{a\lambda^3}{16T_c^2} \left(\frac{15}{4}(V_1^3 - 2V_1 V_2 + 4V_3) \frac{a^2}{2T_c} + V_1 V_2 l(l+1)(l-4) - \frac{1}{3} V_3 l(l+1)(10l-4) - V_3 \right) \right]. \quad (96)$$

Although the expression (96) is rather complicated, we note from (94) that the ratio

$$\frac{k^{1/2} N(k, l)}{k_c^{1/2} N_c(k_c, l)} = 1 + \lambda^2 \frac{V_2}{8T_c} l(l+1)(2l+1) - \lambda^3 \frac{5aV_3}{48T_c^2} l(l+1)(2l+1) \quad (97)$$

is considerably simpler and differs from unity only at second order in λ . In fact, for $l=0$ the correction terms vanish. Thus the entity $k^{1/2} N(k, l)$, compared to the corresponding point Coulomb quantity of shifted energy, is essentially independent of screening except at very low energy. This result, Eq. (97), verifies a conjecture made by Pratt and Tseng¹ based on empirical observations, and is of considerable importance to the normalization screening theory of processes such as photoeffect. This is because of the fact that for our particular normalization the matrix element is multiplied by the phase space factor $k^{1/2}$ for each final continuum electron. Since the

shape of the continuum wave function is largely independent of screening, it is the multiplicative factor $k^{1/2} N$ which gives the major correction for the effects of continuum electron screening. Our result (97) gives a simple means of obtaining this quantity from the corresponding point Coulomb expression. In fact, this simple result for the continuum normalization suggests that a more appropriate normalization for screened Coulomb wave functions is $k^{1/2} N(k, l)$, which corresponds to the asymptotic behavior

$$rR(r) \sim k^{-1/2} \sin[kr - \frac{1}{2}\pi l + \delta_l], \quad \text{as } r \rightarrow \infty. \quad (98)$$

This normalization is equivalent to the energy δ -function normalization of radial continuum states; that is, the asymptotic form (98) implies

$$\int_0^\infty r^2 dr R_E^*(r) R_{E'}(r) = \frac{1}{2}\pi \delta(E - E'). \quad (99)$$

Since this normalization gives the simplest result for the ratio of screened to point Coulomb normal-

izations, it is especially attractive from the point of view of normalization screening theory and may also clarify the discussion of other properties of screened Coulomb wave functions.

As a final note, we remark that it is also possible to obtain the bound-state normalization from the Jost function $f(k, l)$ by analytic continuation to negative energies. If the bound-state energy is written in the form $T = -\frac{1}{2}\kappa^2$, then the normalization is given by²⁶

$$N^2(\kappa, l) = \frac{(2\kappa)^2}{f(i\kappa, l)f'(-i\kappa, l)}, \quad (100)$$

where

$$f'(-i\kappa, l) = \frac{df(-i\kappa, l)}{d\kappa}.$$

If we use our result (92) in (100), then we find, using the fact that $f_c(-i\kappa_c, l) = 0$, where $\kappa_c = a/n$, that to third order³²

$$\begin{aligned} N^2(\kappa, l) &= \frac{(2\kappa_c)^2}{f_c(i\kappa_c, l)f'_c(-i\kappa_c, l)} \frac{\kappa}{\kappa_c} \frac{d\kappa}{d\kappa_c} \\ &\times [1 - \lambda^2 \operatorname{Re}\chi_2(-i\kappa_c, l) - \lambda^3 \operatorname{Re}\chi_3(-i\kappa_c, l)]^2 \\ &= N_c^2 [1 - \lambda^2 \gamma_2(n, l) - \lambda^3 \gamma_3(n, l)]^2, \end{aligned} \quad (101)$$

where this expression (101) is identical to the expression (36) which we obtained directly from the bound-state wave function. Hence our expression for the Jost function, Eq. (92), also gives the correct bound-state normalization when analytically continued to negative energies. This result is necessary if our expression for the screened Jost function is to be consistent with our previous results.

An expression for the screened Coulomb phase shifts can be derived from (92), using the relation (53). Through third order in λ , we have

$$\begin{aligned} \delta(k, l) &= \phi(k_c) + \delta_c(k_c, l) \\ &+ \tan^{-1} \frac{\lambda^2 \operatorname{Im}\chi_2(k_c, l) + \lambda^3 \operatorname{Im}\chi_3(k_c, l)}{1 + \lambda^2 \operatorname{Re}\chi_2(k_c, l) + \lambda^3 \operatorname{Re}\chi_3(k_c, l)} \\ &= \phi(k_c) + \delta_c(k_c, l) - \lambda^2 \frac{V_2}{16T_c} \nu[\nu^2 - l(l-1)] \\ &\quad - \lambda^3 \frac{aV_3}{32T_c^2} \nu[(l-1)(l-4) - \frac{7}{3}(\nu^2 + 1)], \end{aligned} \quad (102)$$

where $\delta_c(k_c, l)$ is the unperturbed Coulomb phase shift of shifted energy. As we have pointed out, our knowledge of the value of $\phi(k_c)$ is incomplete. In particular, we can give only a heuristic derivation of the nonanalytic part of $\phi(k_c)$; at this point we have not been able to evaluate the contributions to this term which vanish in the limit $\lambda \rightarrow 0$. This is because $\phi(k_c)$ is determined essentially by the

large-distance behavior of the wave function. Because of our expansion of the potential, we are not able to obtain sufficient information in this asymptotic region to determine the exterior phase $\phi(k_c)$ exactly. For many applications, however, this uncertainty in the value of $\phi(k_c)$ is unimportant. Since this part of the phase shift stems from the large-distance behavior of the wave function, and since the angular momentum term in the Hamiltonian is negligible in this region, $\phi(k_c)$ is essentially independent of l . It is well known, in fact, that the difference between screened and point Coulomb wave functions, in the limit $\lambda \rightarrow 0$, is only an infinite unobservable (l -independent) overall phase. And it is certainly true that the nonanalytic part of $\phi(k_c)$ which we have obtained does not depend on the angular momentum. On this basis, we conjecture that the exterior part of the phase shift is essentially independent of l . The l dependence of the phase shift is then given by the interior phase

$$\begin{aligned} \delta_{\text{int}}(k, l) &= \delta_c(k_c, l) + \lambda^2 (V_2/16T_c) \nu[\nu^2 - l(l-1)] \\ &\quad - \lambda^3 (aV_3/32T_c^2) \nu[(l-1)(l-4) - \frac{7}{3}(\nu^2 + 1)], \end{aligned} \quad (103)$$

which is determined by the behavior of the wave function in the interior of the atom. In fact, it has been noted by Tseng and Ron,³³ referring to numerical evaluations of screened Coulomb phase shifts, that the difference $\delta(k, l) - \delta_c(k_c, l)$ is virtually independent of l at high energy. We also find, from comparison with numerical results, that the relative phase $\delta(k, l) - \delta(k, 0)$ is given to a good approximation by the expression (103) alone. Since for many processes it is only the relative phase which is needed, our simple result (103) should be useful in these circumstances. At the same time, it should be noted that if we simply use $\phi(k_c)$ defined by (88) or (89), with $r_0 = \frac{1}{2}|k_c|^{-1}$, we also obtain results for the absolute phase shift which are in good agreement with numerical results, including energy dependence. For energies on the order of the K -shell binding energy above threshold or greater, our analytic expression for the screened Coulomb phase shifts agrees with exact numerical results to better than 1%. A comparison of our analytic results for the normalization and phase shifts is given in Sec. IV.

IV. EVALUATION AND COMPARISON WITH EXACT RESULTS

In the preceding sections we have given analytic expressions for screened Coulomb wave functions, including bound-state energy eigenvalues and normalizations and continuum normalizations and phase shifts. In this section we will discuss the

range of validity of our results. Because it would be difficult to give theoretically a precise assessment of the accuracy of our expansions, we have made rather extensive comparisons with numerical evaluations of the corresponding quantities and with exact analytic expressions wherever possible. There are, however, some preliminary remarks which can be made concerning the relative accuracy of our results as we vary the energy, angular momentum, and atomic number. In the case of bound-state shapes at fixed x , as well as bound-state energy shifts and normalizations, for example, we have already noted that the effective expansion parameter is essentially $n^2\lambda/a \approx n^2Z^{-2/3}$. Thus for a given shell we expect our results to improve with increasing Z . For a given element, our expressions will become less reliable as we go to higher shells. In particular, we expect that our results will be valid for the K -shell of all but the lowest- Z elements and for other low-lying levels of high- Z elements.

In general, our expressions for shapes, at least at small distances, will be better than the expressions for energy shifts or normalizations. This is because the corrections to the point Coulomb shape are of second order in λ and behave as r^2 for small r . At Compton-wavelength distances, these corrections are negligible and our wave functions reduce to the exact Coulomb form. For the bound state, the explicit form of the correction terms at small distances is given by

$$\begin{aligned} A_2(x) &- (n^2 V_2 / 8a^2) [3n^2 - l(l+1)] x^2 / (2l+3), \\ A_3(x) &- (n^4 V_3 / 8a^3) [5n^2 - 3l(l+1) + 1] x^2 / (2l+3), \end{aligned} \quad (104)$$

where $x = 2ar/n$. Since x also depends on Z , at small distances these shape corrections, as a function of r , are in fact essentially independent of the atomic number. This result was also noted by Pratt and Tseng.¹ From (104), we see that for fixed r within a given shell our expression for shapes, at least at small distances, should improve somewhat as l is increased. This stems not only from the factor $(2l+3)^{-1}$, but also from cancellation between the terms involving n and l in the square brackets. This corresponds to the fact that the number of nodes, $n - l - 1$, of the wave function decreases as l increases for fixed n , so that the radial wave-function shape becomes simpler as l increases within a given shell. From our expression for the energy shift, Eq. (22), we note the same cancellation between n and l in (104). Thus we also expect our expression for the bound-state energy to improve slightly as l is increased for fixed n . On the other hand, from (34) we see that there is no cancellation between n and l in our

expression for bound-state normalizations. Since the significant part of the wave function moves away from the origin for higher angular momenta, we expect that our expansion of the normalization should become less accurate as l is increased within a given shell.

In the continuum case, the effective expansion parameter becomes $\lambda a/T$. Thus our expressions for continuum shapes, normalizations, and phase shifts should improve as the energy is increased. Physically, this is reasonable since the effects of atomic electron screening become smaller at higher energies. For fixed energy, we expect that our results will be better for low- Z elements than for high Z in the continuum case. Again, this is a reflection of the fact that screening effects on continuum states are larger for higher Z .

As in the bound-state case, we expect that our expression for continuum shapes, at least at small distances, will be better in general than our expressions for normalizations and phase shifts. The continuum-shape corrections are of second order in λ and behave as r^2 for small r . Explicitly,

$$\begin{aligned} A_2(x) &- \frac{1}{16} (V_2/T_c) [\frac{3}{2}a^2/T_c + l(l+1)] x^2 / (2l+3), \\ A_3(x) &- \frac{1}{32} (-aV_3/T_c^2) [\frac{5}{2}a^2/T_c + 3l(l+1) - 1] x^2 / (2l+3), \end{aligned} \quad (105)$$

where $x = 2ik_c r$. Thus at Compton-wavelength distances these screening corrections will be negligible and our wave function reduces to the correct Coulomb form. For fixed r at a given energy, using (105), we expect that our expressions for screened continuum shapes will become less accurate as l increases. There is no cancellation between energy and angular momentum terms in the continuum case. Physically, this is reasonable, since the centrifugal barrier effect tends to keep continuum electrons away from the origin when l is large. From the explicit results (96) and (102) we also expect that our expressions for the continuum normalization and phase shifts will become less accurate as l increases for a given element at fixed energy.

For convenience, we summarize the estimates given above in Table I. In general, the trends observed in comparing our results with exact numerical values agree with these estimates. In some cases there may be minor variations, but the overall tendencies are as noted.

Before giving the comparisons of our results with exact analytic and numerical calculations, we should discuss the determination of the coefficients V_k for screened atomic potentials. We have assumed that in the interior of the atom, the potential can be written in the form

TABLE I. Variation in the relative accuracy of our expressions as a function of energy, angular momentum, and atomic number. In each case, all parameters are assumed to be fixed except the one considered.

Case	Quantity	Parameter	Relative accuracy
Bound states	Wave function at fixed $x = 2ar/n$	n increases	decreases
		l increases	increases
		Z increases	increases
	Energy shift	n increases	decreases
		l increases	increases
		Z increases	increases
	Normalization	n increases	decreases
		l increases	decreases
		Z increases	increases
Continuum states	Wave function at fixed $ x = 2k_c r$	T increases	increases
		l increases	decreases
		Z increases	decreases
	Normalization	T increases	increases
		l increases	decreases
		Z increases	decreases
	Phase shifts	T increases	increases
		l increases	decreases
		Z increases	decreases

$$V(r) = -(a/r)[1 + V_1 \lambda r + V_2 (\lambda r)^2 + V_3 (\lambda r)^3 \dots], \quad (106)$$

where, of course, it should be recognized that the determination of λ and of the V_k cannot be made independently. It is only the product $\lambda^k V_k$ which has significance. For concreteness, we have chosen λ such that it is equal to the reciprocal of the Thomas-Fermi radius of the atom. Thus,

$$\lambda = 2(4/3\pi)^{2/3} \alpha Z^{1/3} \approx 1.13 \alpha Z^{1/3}, \quad (107)$$

and distances such that $r < \lambda^{-1}$ comprise the interior of the atom, while $r > \lambda^{-1}$ refers to the exterior. Having fixed λ , the coefficients V_k must be chosen appropriately. For analytic potentials, such as the Hulthén, Yukawa, or modified Thomas-Fermi (TFC) potentials, the assumption (106) needs little justification. The parameters V_k can be determined explicitly by expanding $V(r)$ about the point $r=0$, and for $r < \lambda^{-1}$ the expansion will give a good approximation to the actual potential. These analytic potentials, however, are of limited utility in general. For applications of our theory we will wish to use more realistic approximations to the actual potential seen by an electron; for example, the Hartree-Fock (HF) or Hartree-Fock-Slater (HFS) approximations or their various modifications. Since these potentials are not given as analytic forms (and, in fact, may not even be analytic functions of r) but rather in tabulated form, the determination of the coefficients V_k becomes nontrivial. Moreover, even if we were to obtain an analytic expansion of the

HF or HFS potentials, based on an analysis of the self-consistent-field equations at the origin, the result would not be useful. This is because the very-short-distance behavior of these potentials does not characterize the behavior throughout the interior of the atom. In fact, extrapolating from the behavior at the origin obtained from the self-consistent-field equations, one finds rather sharp disagreement with the actual potential by distances on the order of one electron Compton wavelength.

For concreteness, the numerical potentials which we will discuss here are the self-consistent HFS potentials tabulated by Herman and Skillman (HS).³⁴ These potentials are readily available and give reasonable values for energies and wave functions. The use of other realistic potentials may modify the subsequent development, but the essential features should remain the same. We want to find an expansion of the form (106) which gives a good approximation to these potentials throughout the interior of the atom. There are, however, several features of the HS-HFS potentials which must be noted:

(i) These potentials are based on the Slater approximation to the exchange term. Since this approximation is not valid at small distances,³⁵ the HS potentials do not have the correct behavior at the origin.

(ii) There is considerable "scatter" in the data points given in the HS tables. Thus these data must be smoothed if we are to consider an analytic fit to the potential and its derivatives.

(iii) There is a discernible fine structure in the

TABLE II. Potential parameters from least-squares fits to HS-HFS potentials using the form $V(r) = -(a/r)[Z^{-1} + \xi e^{-\mu_1 r} + (1 - \xi - Z^{-1})e^{-\mu_2 r}]$, with $\lambda = 1.13\alpha Z^{1/3}$. For comparison, we also give the values of V_k for the Yukawa and Hulthén potentials.

Z	ξ	μ_1	μ_2	V_1	V_2	V_3	V_4
6	0.1153	0.035 20	0.010 76	-0.7866	0.5034	-0.2935	0.1543
8	0.0554	0.052 15	0.013 68	-0.8689	0.6041	-0.4439	0.3280
10	0.0264	0.079 67	0.016 74	-0.9417	0.6533	-0.5186	0.4735
12	0.3985	0.031 86	0.018 67	-0.9709	0.6535	-0.3359	0.1371
13	0.5038	0.030 28	0.008 63	-0.9734	0.6559	-0.3260	0.1256
16	0.4102	0.039 15	0.009 59	-1.016	0.7842	-0.4659	0.2164
18	0.3335	0.047 42	0.011 15	-1.047	0.8842	-0.6012	0.3239
20	0.4116	0.044 19	0.009 21	-1.034	0.8476	-0.5341	0.2612
26	0.3117	0.056 92	0.013 01	-1.072	0.9381	-0.6733	0.3848
36	0.4462	0.050 65	0.012 60	-1.074	0.8285	-0.4875	0.2237
50	0.4317	0.061 59	0.012 92	-1.108	0.9368	-0.6065	0.3046
54	0.4396	0.063 10	0.012 60	-1.109	0.9453	-0.6141	0.3084
74	0.4557	0.066 58	0.015 11	-1.108	0.8934	-0.5477	0.2606
79	0.4290	0.071 64	0.016 17	-1.124	0.9377	-0.6024	0.3014
86	0.5083	0.066 13	0.013 76	-1.105	0.8731	-0.5123	0.2311
92	0.5336	0.065 83	0.012 78	-1.100	0.8612	-0.4949	0.2177
Yukawa				-1.000	0.5000	-0.1667	0.0417
Hulthén				-0.5000	0.0833	0.000	-0.0014

HS potentials. That is, the general monotonic decrease of $V(r)$ is modified near the origin by small-amplitude but short-wavelength (on the order of one Compton wavelength) oscillations. This causes the higher derivatives of the potential to vary rapidly over relatively short distances when r is small. Because of these characteristics of the HS potentials, it is clear that the V_k cannot be obtained directly by evaluating the derivatives of $V(r)$ at the origin.

The procedure we have adopted for determining the coefficients V_k is to assume an analytic form for the atomic potential which has the correct Coulomb behavior at the origin, the appropriate asymptotic behavior,³⁶ and which has several free parameters which may be adjusted to give a least-squares fit to the HS data in the interior. From the resulting analytic approximation to the HS potential, the coefficients V_k are obtained by means of a Taylor expansion about $r=0$. We have found that the three-parameter form

$$U(r) = V(r)/V_c(r) = Z^{-1} + \xi e^{-\mu_1 r} + (1 - \xi - Z^{-1})e^{-\mu_2 r} \quad (108)$$

can reproduce the HS potential to better than 1% accuracy in the interior of the atom,³⁷ and gives values for energies and wave functions evaluated numerically which are likewise accurate at 1%. Other analytic forms have been investigated to determine whether the coefficients V_k are sensitive to the particular parametrization employed, but we have found the expression (108) the simplest to work with in general.

It is important to note that with the coefficients

V_k determined in the manner described above, it is really the average behavior of the potential in the interior of the atom which is being described by (106), and not, strictly, the behavior close to the origin.³⁸ From a physical point of view, this makes our results more reasonable since we do not expect that the extremely-short-distance behavior of $V(r)$ should have much effect on the determination of atomic energy levels, etc. The HS potentials themselves are a good indication of this. Thus we do not attempt to rigorously determine the coefficients V_k from an analysis of the HFS equations at the origin, since the result would certainly not adequately characterize the potential throughout the interior of the atom. Instead, we concentrate on the more general behavior of $V(r)$ in the region $\lambda r < 1$, since it is this which is significant in the determination of atomic properties.

In Table II, we give the results of our analytic fits to the HS potentials for Z in the range 6–92. In addition to the coefficients V_k we also give the values of the potential parameters for the form (108). Since the variation with Z is rather smooth, reasonable values for the coefficients V_k for other atomic numbers may be obtained by interpolation. For comparison, we also give values of the V_k for the Yukawa and Hulthén potentials. We note that the coefficients V_k do not decrease as rapidly with k for realistic potentials as for the Yukawa or Hulthén potentials. Hence our expressions for shapes, energies, normalizations, and phase shifts will, in general, be better for these analytic potentials than for more realistic atomic potentials. This can be seen explicitly when we compare our analytic results with the exact numerical

values.

For the comparison of our analytic expressions for screened electron wave functions with exact results, it is generally necessary to use numerical methods. However, in the case of the Hulthén potential

$$V(r) = -a\lambda e^{-\lambda r}/(1 - e^{-\lambda r}), \quad (109)$$

$$rR(r) = N \exp \left[- \left(\frac{a}{n} - \frac{n\lambda}{2} \right) r \right] \frac{-\Gamma(1 - 2a/n\lambda + n)}{2(a/n - \frac{1}{2}n\lambda)\Gamma(1 - 2a/n\lambda)\Gamma(1 + n)} F(-n, 2a/n\lambda; 1 + 2a/n\lambda - n; e^{-\lambda r}), \quad (110)$$

where $F(a, b; c; x)$ is the Gauss hypergeometric function. Although this wave function (110) could probably be expanded in terms of CHF's to obtain a result which has the form of our expansion (15), in fact we have not yet been able to prove this conjecture. Hence we will consider here only the results for bound-state energy eigenvalues and normalizations. Corresponding to the wave function (110), the exact $l=0$ bound state energies are given by

$$T_n = -\frac{a^2}{2n^2} + \frac{a\lambda}{2} - \frac{n^2\lambda^2}{8}, \quad (111)$$

where $n = 1, 2, 3, \dots, n_0$, with n_0 the largest integer smaller than $(2a/\lambda)^{1/2}$ (the number of bound states is finite). We see that this agrees with our perturbation results (22), with $V_1 = -\frac{1}{2}$, $V_2 = \frac{1}{12}$, $V_3 = 0$, to the order calculated. The normalization of the wave function (110) is given by

$$\begin{aligned} N(n) &= \frac{1}{\sqrt{2}} \left(\frac{2a}{n} \right)^{3/2} \left(1 - \frac{n^4\lambda^2}{4a^2} \right)^{1/2} \\ &= N_c(n) \left(1 - \frac{n^4\lambda^2}{8a^2} + O(\lambda^4) \right). \end{aligned} \quad (112)$$

Again we see that this agrees with our perturbation result (36) to the order considered.

For the S-wave continuum state of the Hulthén potential, one can also obtain the exact solution.

the Schrödinger equation can be solved exactly for $l=0$.³⁹ Since this screened potential is Coulombic at the origin, it can be treated using our perturbation theory. Thus in this case we can make some comparisons analytically. To proceed, we write the exact bound-state radial function in the form

If we consider just the Jost solution, we find

$$\begin{aligned} f(k, r) &= e^{-ikr} \\ &\times F \left(\frac{ik}{\lambda} - \frac{i}{\lambda} (k^2 - 2a\lambda)^{1/2}, \right. \\ &\quad \left. \frac{ik}{\lambda} + \frac{i}{\lambda} (k^2 - 2a\lambda)^{1/2}; 1 + 2i \frac{k}{\lambda}; e^{-\lambda r} \right). \end{aligned} \quad (113)$$

The corresponding Jost function is given by

$$f(k) = \frac{\Gamma(1 + 2ik/\lambda)}{\Gamma(1 + i\nu)\Gamma(1 + 2ik/\lambda - i\nu)}, \quad (114)$$

where $\nu = a/k_c$. In writing (114), we have used the fact the unperturbed Coulomb energy k_c , which according to our prescription is determined from (111) by the replacement $n - i\nu$, satisfies the relation

$$k = k_c + a\lambda/2k_c, \quad (115)$$

or solving for k_c ,

$$k_c = \frac{1}{2}k + \frac{1}{2}(k^2 - 2a\lambda)^{1/2}. \quad (116)$$

Using the asymptotic expansion given in Ref. 28 for the ratio of two Γ functions, we can expand the Hulthén-Jost functions (114) to obtain

$$f(k) = \frac{\Gamma(1 + 2ik/\lambda)}{\Gamma(1 + i\nu)\Gamma(1 + 2ik/\lambda - i\nu)} = f_c(k_c) e^{i\nu \ln(2k/\lambda)} \left[1 + \frac{a\lambda}{4k_c^2} - \frac{a^2\lambda^2}{32k_c^4} - \frac{a^4\lambda^2}{32k_c^6} + i \left(-\frac{a^2\lambda}{4k_c^3} + \frac{a\lambda^2}{48k_c^3} + \frac{a^3\lambda^2}{48k_c^5} \right) + O(\lambda^3) \right]. \quad (117)$$

From this expression we can write the exact S-wave continuum normalization for the Hulthén case in the form

$$\begin{aligned} N(k) &= |f(k)|^{-1} \\ &= N_c(k_c) \left[1 - \frac{1}{4}a\lambda/k_c^2 + \frac{3}{32}a^2\lambda^2/k_c^4 + O(\lambda^3) \right]. \end{aligned} \quad (118)$$

This expression is identical to our perturbation result (96) to the order considered. Finally, (117) gives the following result for the Hulthén phase shifts:

$$\delta(k) = \nu \ln \left(\frac{2k_c}{\lambda} \right) + \delta_c(k_c) + \frac{a^2\lambda}{4k_c^3} + \frac{a\lambda^2}{48k_c^3} - \frac{a^3\lambda^2}{24k_c^5} + O(\lambda^3). \quad (119)$$

TABLE III. Bound-state wave-function shapes for the Yukawa and HS potentials as a function of n , l , and Z . $R_{\max}(\epsilon)$, as defined in the text, is the radial distance at which the relative error ϵ achieves the specified value. All distances are given in terms of electron Compton wavelengths.

Z	n	l	$R_{\max}(\epsilon)$ for Yukawa		$R_{\max}(\epsilon)$ for HS		First Bohr orbit (a^{-1})	Thomas-Fermi radius (λ^{-1})
			$\epsilon = 0.1\%$	$\epsilon = 1.0\%$	$\epsilon = 0.1\%$	$\epsilon = 1.0\%$		
13	1	0	15	34	11	27	10.5	51.6
		2	0	4	10	3		
36	1	0	13	27	9	19	3.8	36.7
		2	0	4	22	3		
	2	1	6	16	4	10		
	3	0	2	5	1	3		
	3	1			1	4		
	3	2			2	6		
79	1	0	11	21	7	14	1.7	28.3
		2	0	10	16	2		
	2	1	6	14	4	9		
	3	0	2	9	1	3		
	3	1	3	6	2	4		
	3	2	4	9	2	5		

Although this expression is similar to our result (102), exact comparison is not possible since at present we are unable to determine the exterior phase $\phi(k_c)$ precisely.

Since the Hulthén potential is the only known example of a screened potential which is Coulombic at the origin for which analytic solutions of the Schrödinger equation can be obtained, we have made rather extensive comparisons of our analytic expressions for screened Coulomb wave functions with exact numerical results. We present below a summary of these comparisons for three elements, Al ($Z=13$), Kr ($Z=36$), and Au ($Z=79$), which show typical results for low, medium, and high Z . For these elements, we present data for both the Yukawa [$V(r) = -(a/r)e^{-\lambda r}$] and HS potentials. In the latter case, it should be noted that the numerical values given were obtained by solving the Schrödinger equation using our analytic fits to the HS potentials rather than the actual numerical potentials. The values so obtained will differ from the HS data by less than 1% and are somewhat easier to reproduce numerically.

If we consider first the bound-state case, then Table III gives a comparison of our analytic results for bound state shapes with exact numerical values, for both the Yukawa and HS potentials. In order to characterize the results simply, we have given the values of the radial distances $R_{\max}(\epsilon)$ (in Compton wavelengths), at which the relative error ϵ of our theoretical shapes compared to the exact numerical results reaches 0.1% and 1.0%. Because our expressions for shapes are valid even when the wave function has nodes, we have esti-

mated the relative error as follows: When there are no nodes, we define

$$\epsilon(r) = \frac{|\psi_{\text{num}}(r) - \psi_{\text{an}}(r)|}{|\psi_{\text{num}}(r)|} \quad (120)$$

where $\psi(r)$ is the appropriate radial wave function. If $\psi(r)$ has zeroes, then we define

$$\epsilon(r) = \frac{|\psi_{\text{num}}(r) - \psi_{\text{an}}(r)|}{(|\psi_{\text{num}}(r)|)_{\text{envelope}}}, \quad (121)$$

where the envelope is just the curve obtained by linear interpolation between peaks of $|\psi_{\text{num}}(r)|$. Since a detailed comparison of $\psi_{\text{an}}(r)$ and $\psi_{\text{num}}(r)$ indicates that our analytic wave functions give the positions of the nodes accurately for not-too-high values of n , and are usually accurate beyond the first node, this formula, Eq. (121), for the relative error gives a better estimate of the validity of our results than the expression (120). In Table III we also give values in Compton wavelengths for the first Bohr orbit ($=a^{-1}$) and the Fermi-Thomas radius of the atom ($=\lambda^{-1}$). We see that our analytic shapes reproduce the numerical results to an accuracy of better than 1% over nearly the entire region where the wave function is large in the case of the inner shells of high- Z elements and for the K shell of all but the lowest- Z elements. It is for this reason that we are able to obtain expressions for bound-state normalizations which are accurate in these circumstances. We note that these results go somewhat beyond the conclusions made by Pratt and Tseng,¹ so that by using our analytic expression for screened radial wave-function shapes, we can considerably extend

TABLE IV. Bound-state energies (in keV) for the Yukawa and HS potentials as a function of n , l , and Z . For comparison we also give the point Coulomb results.

Potential	Z	n	l	Bound-state energy (keV)			Fractional error			
				Numerical	Analytic	Coulomb	Analytic	Coulomb		
Yukawa	13	1	0	-1.488(0)	-1.484(0)	-2.999(0)	0.0027	0.55		
			36	1	0	-1.424(1)	-1.424(1)	-1.763(1)	0.000 16	0.24
			2	0	-1.692(0)	-1.615(0)	-4.408(0)	0.046	1.6	
			2	1	-1.566(0)	-1.504(0)	-4.408(0)	0.039	1.8	
	79	1	0	-7.495(1)	-7.495(1)	-8.491(1)	0.000 020	0.13		
				2	0	-1.250(1)	-1.245(1)	-2.123(1)	0.0043	0.70
				2	1	-1.225(1)	-1.221(1)	-2.123(1)	0.0035	0.73
	HS	13	1	0	-1.544(0)	-1.535(0)	-2.299(0)	0.0057	0.49	
				36	1	0	-1.413(1)	-1.412(1)	-1.763(1)	0.000 61
2				0	-1.833(0)	-1.563(0)	-4.408(0)	0.15	1.41	
			2	1	-1.676(0)	-1.479(0)	-4.408(0)	0.12	1.6	
79		1	0	-7.404(1)	-7.403(1)	-8.491(1)	0.000 10	0.15		
				2	0	-1.237(1)	-1.212(1)	-2.123(1)	0.020	0.72
				2	1	-1.199(1)	-1.180(1)	-2.123(1)	0.015	0.77

the range of validity of the normalization screening theory.

In Table IV we evaluate our expression for bound-state energies. We see that the difference between analytic and numerical results for the K shell is somewhat less than 1% even for low Z and improves as Z increases. For the L shell at low Z it is not sufficient to retain only the terms through third order in our expansion of the energy shift; the result does not give an accurate value for the bound-state energy. However, for medium and high Z , our results are generally good to

better than 5% and improve with increasing Z . There is also some improvement as l increases for fixed n, Z . For the M shell, our third-order results are not adequate except for very high Z . It is possible that inclusion of higher-order terms in λ may improve our results for the higher shells.

A comparison of our expression for bound-state normalizations with exact numerical results is given in Table V. The states considered are the same as for Table IV. We see that our results for the K shell are good to better than 1% for $Z \geq 13$ and improve with increasing Z . For the

TABLE V. Bound-state normalizations for the Yukawa and HS potentials as a function of n , l , and Z . For comparison we also give the point Coulomb results.

Potential	Z	n	l	Bound-state normalization			Fractional error			
				Numerical	Analytic	Coulomb	Analytic	Coulomb		
Yukawa	13	1	0	5.692(-2)	5.711(-2)	5.844(-2)	0.0033	0.027		
			36	1	0	2.674(-1)	2.674(-1)	2.693(-1)	0.000 26	0.0073
			2	0	8.618(-2)	8.933(-2)	9.521(-2)	0.036	0.10	
			2	1	6.306(-3)	6.582(-3)	7.220(-3)	0.044	0.15	
	79	1	0	8.731(-1)	8.731(-1)	8.754(-1)	0.000 035	0.0026		
				2	0	2.982(-1)	2.999(-1)	3.095(-1)	0.0057	0.038
				2	1	4.905(-2)	4.937(-2)	5.151(-2)	0.0067	0.050
	HS	13	1	0	5.664(-2)	5.699(-2)	5.844(-2)	0.0061	0.032	
				36	1	0	2.663(-1)	2.665(-1)	2.693(-1)	0.000 83
2				0	8.394(-2)	9.200(-2)	9.521(-2)	0.096	0.13	
			2	1	6.008(-3)	6.628(-3)	7.220(-3)	0.10	0.20	
79		1	0	8.714(-1)	8.715(-1)	8.754(-1)	0.000 15	0.0047		
				2	0	2.923(-1)	2.981(-1)	3.095(-1)	0.020	0.059
				2	1	4.758(-2)	4.861(-2)	5.151(-2)	0.022	0.083

TABLE VI. Continuum wave-function shapes for the Yukawa and HS potentials as a function of T , l , and Z . $R_{\max}(\epsilon)$, as defined in the text, is the radial distance at which the relative error ϵ achieves the specified value. All distances are given in terms of electron Compton wavelengths.

Z	T (keV)	l	$R_{\max}(\epsilon)$ for Yukawa		$R_{\max}(\epsilon)$ for HS		First Bohr orbit (a^{-1})	Thomas-Fermi radius (λ^{-1})	de Broglie wavelength	
			$\epsilon = 0.1\%$	$\epsilon = 1.0\%$	$\epsilon = 0.1\%$	$\epsilon = 1.0\%$				
13	3	0	16	30	14	28	10.5	51.6	58.0	
		1	16	25	14	22				
		2	15	24						
	10	0	30	57	25	47			31.8	
		1	21	47	19	39				
		2	18	29	17	25				
		4	15	24	13	22				
		6	13	21	11	19				
	30	0	39	72	31	57			18.3	
		1	33	66	28	54				
		2	20	51	16	42				
		4	15	22	13	20				
		6	13	20	11	18				
		8	11	19	10	17				
	36	30	0	17	31	12	24	3.8	36.7	18.3
1			13	27	10	19				
2			11	20	9	14				
4			10	16	8	13				
6			9	14	7	11				
8			8	13	6	10				
100		0	24	44	17	31			10.0	
		1	21	41	16	30				
		2	15	34	11	25				
		4	10	18	8	12				
		6	9	13	7	11				
		8	8	13	6	10				
79		100	0	12	22	8	16	1.7	28.3	10.0
			1	10	20	7	14			
			2	5	17	6	11			
	4		7	11	6	9				
	6		7	10	5	8				
	8		6	10	4	7				

L shell, our third-order expression for the normalization is generally good to better than 5% for intermediate Z . For high Z , the relative error is on the order of 1%. Except at very high Z , including only the terms through third order in our expansion is not sufficient to determine the M -shell normalization. Again, this situation may improve somewhat if we consider higher orders in λ .

In the continuum case, our results are summarized in Tables VI–VIII. Again, we consider $Z = 13, 36, \text{ and } 79$, in order to cover the range of low to high atomic numbers, for both the Yukawa and HS potentials. In Table VI, we present results for continuum shapes. For convenience, we give the values of the radial distances $R_{\max}(\epsilon)$ (in Compton wavelengths) at which the relative error ϵ of our analytic expression compared to the exact numerical result reaches 0.1% and 1.0%. Because

both the continuum radial wave function itself and the difference between numerical and analytic results may have many nodes, we define the relative error at the point r as follows:

$$\epsilon(r) = \left(\frac{|\psi_{\text{num}}(r) - \psi_{\text{an}}(r)|}{(|\psi_{\text{num}}(r)|)_{\text{envelope}}} \right)_{\text{envelope}}, \quad (122)$$

where the envelope is given by linear interpolation between maxima. This expression for the relative error is simple to evaluate numerically and gives a result which is essentially monotonic in r . In addition, it gives a more accurate characterization of the validity of our results than would the simple form (120), as we have determined by a detailed comparison of our analytic results with the exact numerical values. In the continuum case, from Table VI we see that for energies on the order of the K -shell binding energy above threshold, our analytic expression for radial

TABLE VII. Continuum normalizations for the Yukawa and HS potentials as a function of T , l , and Z . For comparison we also give the point Coulomb results.

Potential	Z	T (keV)	l	Continuum normalizations			Fractional error			
				Numerical	Analytic	Point Coulomb	Analytic	Point Coulomb		
Yukawa	13	3	0	2.346(0)	2.347(0)	2.350(0)	0.000 26	0.0018		
			1	1.027(-1)	1.027(-1)	1.128(-1)	0.000 30	0.099		
			2	2.147(-3)	2.135(-3)	2.669(-3)	0.0055	0.24		
		10	0	1.773(0)	1.773(0)	1.780(0)	0.000 00	0.0040		
			1	1.249(-1)	1.249(-1)	1.302(-1)	0.000 01	0.042		
			2	4.875(-3)	4.874(-3)	5.297(-3)	0.000 21	0.087		
		30	4	2.863(-6)	2.808(-6)	3.356(-6)	0.019	0.17		
			0	1.448(0)	1.448(0)	1.453(0)	0.000 00	0.0032		
			1	1.692(-1)	1.692(-1)	1.722(-1)	0.000 00	0.017		
			2	1.154(-2)	1.154(-2)	1.191(-2)	0.000 03	0.032		
			4	2.106(-5)	2.102(-5)	2.235(-5)	0.0019	0.061		
			6	1.691(-8)	1.658(-8)	1.840(-8)	0.019	0.088		
	36	30	0	2.201(0)	2.201(0)	2.204(0)	0.000 00	0.0012		
			1	3.047(-1)	3.047(-1)	3.172(-1)	0.000 00	0.041		
			2	2.124(-2)	2.124(-2)	2.328(-2)	0.000 08	0.096		
			4	3.754(-5)	3.722(-5)	4.559(-5)	0.0086	0.21		
		100	0	1.683(0)	1.683(0)	1.686(0)	0.000 00	0.0016		
			1	3.747(-1)	3.747(-1)	3.813(-1)	0.000 00	0.018		
			2	4.710(-2)	4.710(-2)	4.874(-2)	0.000 01	0.035		
			4	2.875(-4)	2.873(-4)	3.075(-4)	0.000 66	0.069		
			6	7.673(-7)	7.619(-7)	8.465(-7)	0.0070	0.10		
			79	100	0	2.409(0)	2.409(0)	2.410(0)	0.000 00	0.000 45
					1	6.638(-1)	6.638(-1)	6.834(-1)	0.000 00	0.030
					2	8.764(-2)	8.764(-2)	9.415(-2)	0.000 02	0.074
4	5.340(-4)	5.329(-4)			6.279(-4)	0.0021	0.18			
6	1.379(-6)	1.349(-6)	1.768(-6)	0.022	0.28					
HS	13	3	0	2.346(0)	2.348(0)	2.350(0)	0.000 57	0.0018		
			1	1.032(-1)	1.033(-1)	1.128(-1)	0.0014	0.093		
			2	2.147(-3)	2.135(-3)	2.669(-3)	0.0055	0.24		
		10	0	1.773(0)	1.773(0)	1.780(0)	0.000 00	0.0040		
			1	1.251(-1)	1.251(-1)	1.302(-1)	0.000 03	0.041		
			2	4.897(-3)	4.895(-3)	5.297(-3)	0.000 40	0.082		
		30	4	2.897(-6)	2.797(-6)	3.356(-6)	0.035	0.16		
			0	1.448(0)	1.448(0)	1.453(0)	0.000 00	0.0032		
			1	1.693(-1)	1.693(-1)	1.722(-1)	0.000 00	0.017		
			2	1.155(-2)	1.155(-2)	1.191(-2)	0.000 05	0.031		
			4	2.113(-5)	2.106(-5)	2.235(-5)	0.0034	0.058		
			6	1.701(-8)	1.644(-8)	1.840(-8)	0.033	0.081		
	36	30	0	2.201(0)	2.201(0)	2.204(0)	0.000 00	0.0012		
			1	3.039(-1)	3.040(-1)	3.172(-1)	0.000 03	0.044		
			2	2.115(-2)	2.115(-2)	2.328(-2)	0.000 25	0.10		
			4	3.745(-5)	3.644(-5)	4.559(-5)	0.027	0.22		
		100	0	1.682(0)	1.682(0)	1.686(0)	0.000 00	0.0022		
			1	3.743(-1)	3.743(-1)	3.813(-1)	0.000 00	0.019		
			2	4.702(-2)	4.701(-2)	4.874(-2)	0.000 02	0.037		
			4	2.868(-4)	2.862(-4)	3.075(-4)	0.0019	0.072		
			6	7.658(-7)	7.510(-7)	8.465(-7)	0.019	0.11		
			79	100	0	2.409(0)	2.409(0)	2.410(0)	0.000 00	0.000 38
					1	6.616(-1)	6.616(-1)	6.834(-1)	0.000 01	0.033
					2	8.702(-2)	8.701(-2)	9.415(-2)	0.000 07	0.082
4	5.279(-4)	5.236(-4)			6.279(-4)	0.0083	0.19			
6	1.365(-6)	1.250(-6)	1.768(-6)	0.084	0.30					

TABLE VIII. Phase shifts for the Yukawa and HS potentials as a function of T , l , and Z . For the exterior contribution to the phase shift we use $r_0 = \frac{1}{2} |k_c|^{-1}$.

Z	T (keV)	l	Yukawa phase shifts			HS phase shifts			
			Numerical	Analytic	Fractional error	Numerical	Analytic	Fractional error	
13	3	0	2.1459	2.1807	-0.016	2.1102	2.1783	-0.032	
		1	1.3705	1.3487	0.016	1.3420	1.3440	-0.0015	
		2	0.9497	0.7976	0.16				
	10	0	1.4589	1.4764	-0.012	1.4217	1.4401	-0.013	
		1	0.9995	1.0118	-0.012	0.9639	0.9769	-0.013	
		2	0.7644	0.7671	-0.0036	0.7305	0.7333	-0.0039	
		4	0.5037	0.4744	0.058	0.4723	0.4424	-0.063	
	30	0	0.9911	0.9980	-0.0070	0.9590	0.9655	-0.0067	
		1	0.7185	0.7245	-0.0084	0.6868	0.6923	-0.0080	
		2	0.5813	0.5856	-0.0074	0.5501	0.5538	-0.0066	
		4	0.4249	0.4235	0.0033	0.3946	0.3921	0.0063	
		6	0.3310	0.3212	0.030	0.3014	0.2902	0.037	
36	30	0	2.4414	2.4583	-0.0069	2.4845	2.5187	-0.014	
		1	1.7632	1.7744	-0.0063	1.8068	1.8342	-0.015	
		2	1.3883	1.3887	-0.00029	1.4348	1.4499	-0.011	
		4	0.9577	0.9217	0.038	1.0121	0.9880	0.024	
	100	0	1.6033	1.6105	-0.0045	1.6200	1.6295	-0.0059	
		1	1.2006	1.2070	-0.0053	1.2174	1.2259	-0.0070	
		2	0.9924	0.9972	-0.0049	1.0100	1.0167	-0.0067	
		4	0.7515	0.7511	0.00045	0.7711	0.7722	-0.0013	
	6	0.6044	0.5962	0.014	0.6264	0.6191	0.012		
		100	0	3.1818	3.1935	-0.0037	3.2758	3.3113	0.012
			1	2.4144	2.4227	-0.0034	2.5075	2.5388	-0.012
			2	1.9702	1.9721	-0.00096	2.0650	2.0887	-0.012
4	1.4436		1.4238	0.014	1.5458	1.5451	0.00047		
6	1.1237		1.0717	0.046	1.2349	1.2153	0.016		

wave-function shapes is accurate to better than 1% over nearly the entire interior of the atom, and improves with increasing energy. For fixed energy, the value of $R_{\max}(\epsilon)$ decreases somewhat as l is increased. However, even for relatively high angular momenta our results are accurate over most of the interior region. It is interesting to note (cf. Figs. 3 and 4) that the phase of our continuum radial wave function is nearly exactly that of the numerical wave function. It is the amplitude which begins to account for the difference between our analytic results and the numerical values at distances near the edge of the atom. This is because of the additional powers of r which appear in the asymptotic form (46) and may be traced to the failure of our expansion of the potential at large r . For reference, we also give in Table VI the values (in Compton wavelengths) of the Bohr radius ($=a^{-1}$), the Thomas-Fermi radius ($=\lambda^{-1}$), and the de Broglie wavelength of the electron ($=\hbar^{-1}$) for the corresponding energy.

In Table VII, we compare continuum normalizations in our theory with exact numerical results and with the point Coulomb values for the same Z .

For energies on the order of the K -shell binding energy above threshold, for $l \leq 8$, our results, in general, are accurate to better than 1%, and improve with increasing energy. For a given element at fixed energy, the accuracy of our results decreases as l increases. Even for these higher partial waves, however, we see that our expression for the screened continuum normalization represents a considerable improvement over the point Coulomb values.

Finally, in Table VIII we give a comparison of our results for screened Coulomb phase shifts with exact numerical values. For the exterior phase $\phi(k_c)$ we use the expression (88) in the Yukawa case, whereas for the HS potential we use the form (89). In each case, we set $r_0 = \frac{1}{2} |k_c|^{-1}$. We see that for sufficiently high energies our results are accurate to better than 1%. Because of the specific form of our expression (102) for the phase shifts, our results may improve slightly as l increases for low partial waves. For higher values of the angular momentum, however, our analytic expression will become less accurate as l increases. At low energy, the major part of the

screened S -wave phase shift stems from the exterior phase $\phi(k_c)$. As l increases, for fixed energy $\phi(k_c)$ is essentially constant while the interior phase increases in magnitude. For the higher partial waves, the interior and exterior phases become comparable in magnitude. As the energy is increased, both the interior and exterior phases decrease in magnitude. Because of the large magnitude of the nonanalytic part of the screened Coulomb phase shift, it is not possible to compare the screened and point Coulomb results directly.

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- ¹R. H. Pratt and H. K. Tseng, *Phys. Rev. A* **5**, 1063 (1972).
- ²I. M. Band, L. A. Sliv, and M. B. Trzhaskovskaya, Institute of Technical Physics Report No. 262, 1970 (unpublished) (Order No. 1314, 21/IV).
- ³H. K. Tseng and R. H. Pratt, *Phys. Rev. A* **4**, 1835 (1971); **6**, 2049 (1973).
- ⁴H. K. Tseng and R. H. Pratt, *Phys. Rev. A* **7**, 1423 (1973).
- ⁵J. W. Cooper, *Phys. Rev. A* **9**, 2236 (1974).
- ⁶See, for example, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1955).
- ⁷L. L. Foldy, *Phys. Rev.* **111**, 1093 (1958).
- ⁸M. J. Seaton, *Mon. Not. R. Astron. Soc.* **118**, 504 (1958).
- ⁹The phase shifts also have a contribution which is non-analytic in λ .
- ¹⁰For an introduction, see J. Kleinert, *Lectures in Theoretical Physics*, edited by A. O. Barut and W. E. Brittin (Gordon and Breach, New York, 1968), Vol. X B, p. 427, and references therein.
- ¹¹A. I. Sherstnyuk, *Zh. Eksp. Teor. Fiz.* **62**, 1238 (1972) [*Sov. Phys.-JETP* **35**, 655 (1972)].
- ¹²(a) M. Bednář, *Ann. Phys. (N.Y.)* **75**, 305 (1973); (b) A. E. S. Green, D. L. Sellin, and A. S. Zachor, *Phys. Rev.* **184**, 1 (1969); D. D. Doda, R. H. Garvey, and A. E. S. Green, *Phys. Rev. A* **12**, 712 (1975); (c) E. J. McGuire, *Phys. Rev.* **161**, 51 (1967); **175**, 20 (1968); (d) U. Fano, C. E. Theodosiov, and J. L. Dehmer, *Rev. Mod. Phys.* **48**, 49 (1976).
- ¹³B. I. Dunlap and L. Armstrong, Jr., *Phys. Rev. A* **6**, 1370 (1972).
- ¹⁴C. S. Lam and Y. P. Varshui, *Phys. Rev. A* **6**, 1391 (1972).
- ¹⁵C. S. Lam and Y. P. Varshui, *Phys. Rev. A* **4**, 1875 (1971).
- ¹⁶F. J. Rogers, H. C. Graboske, and D. J. Harwood, *Phys. Rev. A* **1**, 1577 (1970).
- ¹⁷S. D. Oh and R. H. Pratt, *Bull. Am. Phys. Soc.* **20**, 680 (1975).
- ¹⁸V. Florescu, J. McEannan, and R. H. Pratt, *Bull. Am. Phys. Soc.* **20**, 101 (1975).
- ¹⁹M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Nat. Bur. Stand., U.S. GPO, 1964).
- ²⁰Note that we cannot choose C_2 such that this asymptotic behavior is cancelled, since $U(x)$ and the last term of (13) are linearly independent.
- ²¹For sufficiently low values of T , T_c may become complex and our formalism breaks down. This is because the effective expansion parameter is $a\lambda/T$ in the continuum case, so that for $T \approx a\lambda$, our expansions no longer converge.
- ²²With this substitution, the bound-state poles of the scattering amplitude will appear only on an unphysical sheet. Thus there will be no bound states corresponding to our continuum wave function in this case. For a repulsive potential, we thus obtain the continuum solution by analytic continuation from the solution for an attractive potential.
- ²³This particular form of the energy shift was not considered by Pratt and Tseng, Ref. 1. They did, however, find significant improvement using only the first-order shift, $\delta T = -\lambda V_1 a$.
- ²⁴The requirement that $R(r)$ be finite at infinity for bound states is not a boundary condition, *per se*, but an eigenvalue problem. It imposes a condition on one of the parameters of the differential equation which is reflected in the behavior of the wave function.
- ²⁵Theorem of Poincaré: If a differential equation depends holomorphically on a parameter and the boundary conditions are independent of that parameter, then the solutions of the equation are holomorphic functions of the parameter.
- ²⁶A. G. Sitenko, *Lectures in Scattering Theory* (Pergamon, New York, 1971), Chap. 7.
- ²⁷Note, this is the same normalization as that used in Ref. 1.
- ²⁸*Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill, New York, 1953).
- ²⁹To first order in λ , we can see explicitly that $\phi(k_c) = -\phi(-k_c)$ from the fact that we must obtain the correct Coulomb solution in zeroth order.
- ³⁰We note that with these two linearly independent solutions we could also construct the radial screened Coulomb Green's functions.
- ³¹J. R. Taylor, *Nuovo Cimento B* **23**, 313 (1974).
- ³²In this form (101) our expression for the bound-state normalization resembles the Fermi-Dirac formula.
- ³³H. K. Tseng and A. Ron (University of Pittsburgh, Report 6985207-24) (unpublished).
- ³⁴F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N.J., 1963).
- ³⁵J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill, New York, 1960), Vol. II.
- ³⁶Herman and Skillman use the latter approximation to

ensure that their screened potential has the correct asymptotic point Coulomb form corresponding to a unit charge.

³⁷It is doubtful that the HS potentials themselves are accurate to better than 1%.

³⁸In fact, we note that neglecting exchange, V_2 must be identically zero. In the Slater approximation to ex-

change, the second derivative of $U(r)$ is negative for $0 \leq r \leq 3$ Compton wavelengths, and then becomes positive. In our fits to the HS potentials, however, we find that generally $V_2 \approx +\frac{1}{2}$.

³⁹R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), pp. 421, 422.