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Analytic Solution for the Bound-State Wave Functions of the Exponentially Screened Coulomb Potential

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A new method is described to obtain a sequence of wave functions and energy eigenvalues which converge rapidly to the exact bound state of the Schrödinger equation for the exponentially screened Coulomb potential.

The importance of screened Coulomb potentials in solid-state and in plasma physics has been recognized for a long time.[1] The purpose of this paper is to discuss a new method to obtain the bound-state wave functions and energy eigenvalues of the radial Schrödinger equation for potentials whose screening factor falls off exponentially. A sequence of wave functions and energy eigenvalues are derived which converge rapidly to the exact bound-state solution. It will be shown that for weak screening, i.e., when the characteristic screening length is large compared to the Bohr radius, the sequence approaches the Coulomb wave functions. For simplicity, we restrict our main discussion to zero angular momentum states, but the extension of our method to finite angular momentum is straightforward.

The radial Schrödinger equation for the s-wave bound states $u(x)$ of the screened Coulomb potential takes the form

$$\left(\frac{d^2}{dx^2}+g\frac{e^{-x}}{x}-k^2\right)u(x)=0\ , \tag{1}$$

where the radial distance x is given in units of a screening radius λ. The coupling constant $g=2Z\lambda/a_0$, where Z is the Coulomb charge and $a_0=\hbar^2/me^2$ is the Bohr radius, and the binding energy $E=(Z^2e^4m/2\hbar^2)(2k/g)^2$. Asymptotically the solutions of Eq. (1) have the form

$$u(x)=fe^{-kx}+he^{kx}\ , \tag{2}$$

where f and h are constants. We are interested in the particular solutions which vanish at the origin and have the property that $h=0$; these are the bound states, and the corresponding discrete values of k give the energy eigenvalues.

The first step in our method of solution is to transform the differential Schrödinger equation into two coupled integral equations which incorporate these boundary conditions. If we let f and h become functions of x as well as of k and g in order that Eq. (2) be valid for all values of x, we find that f and h satisfy the coupled linear integral equations

$$f(x)=-\frac{1}{2k}\left(1-g\int_0^x\frac{e^{-x'}}{x'}u(x')e^{+kx'}dx'\right)\ , \tag{3}$$

$$h(x)=\frac{1}{2k}\left(1-g\int_0^x\frac{e^{-x'}}{x'}u(x')e^{-kx'}dx'\right)\ . \tag{4}$$

In Eqs. (3) and (4), the wave function u [Eq. (2)] has been normalized by the condition that for small x, $u\sim x$.

The second step is to introduce a sequence of wave functions $u^{(n)}(x)$ of the form

$$u^{(n)}(x)=\phi^{(n)}(x)e^{-kx}, \tag{5}$$

where $\phi^{(n)}(x)$ is an expansion in powers of e^{-x} up to order n; i.e.,

$$\phi^{(n)}(x)=\sum_{r=0}^{r=n}a_r^{(n)}e^{-rx}\ . \tag{6}$$

The usefulness of the expansion, Eqs. (5) and (6), is threefold: (i) For small values of x, it corresponds to a power-series expansion of x up to x^n and therefore can be used to solve the Schrödinger equation for analytic potentials by standard techniques. (ii) For large values of x, $\phi^{(n)}$ approaches a constant value $a_0^{(n)}$ corresponding to the correct asymptotic behavior of the exact solution. (iii) For large x, the integrals appearing in Eqs. (3) and (4) can be carried out analytically. This will be important when we impose the condition that solutions of Eqs. (4) and (5) correspond to bound states. This expansion has also been used in variational solutions by Hulthén and Laurikainen,[2] and it leads to a Taylor-series expansion of the wave function in the variable $y=e^{-x}-1$.

Let c_s be the coefficients of the Taylor-series expansion of $u(x)e^{kx}/x$ in x, which satisfy the recurrence relation

$$c_s=\frac{1}{s(s+1)}\left((2ks-g)c_{s-1}-g\sum_{j=1}^{j=s-1}\frac{(-)^j}{j!}c_{s-j-1}\right)\ . \tag{7}$$

Then the requirement that for small x Eqs. (5) and (6) correspond to this expansion to order x^n implies that for $s=1, 2, \ldots, n$,

$$c_{s-1}=\sum_{r=0}^{r=n} \frac{(-r)^s}{s!} a_r^{(n)} , \tag{8}$$

while for $s=0$ this sum vanishes.

Solving Eq. (8) for $a_r^{(n)}$, we obtain

$$a_r^{(n)} = \frac{(-)^r}{r!\,(n-r)!} \sum_{s=1}^{s=n} s!\, b_{r,s}^{(n)} c_{s-1} . \tag{9}$$

The matrix element $b_{r,s}^{(n)}$ in Eq. (9) is given by the sum of all possible products of $n-s$ distinct integers between 0 and n excluding the integer r, while $b_{r,n}^{(n)}=1$. A convenient procedure to evaluate $b_{r,s}^{(n)}$ when n is a large integer is given by the recurrence relations

$$b_{r,s}^{(n)} = (n-r) b_{r,s}^{(n-1)} + \alpha_s^{(n)} , \tag{10}$$

$$\alpha_s^{(n)} = (n-1)\alpha_s^{(n-1)} + \alpha_{s-1}^{(n-1)} \tag{11}$$

for $r=0$ to n and $s=1$ to $n-1$, while

$$b_{r,n}^{(n)} = \alpha_n^{(n)} = 1 \text{ and } \alpha_0^{(n)} = 0 . \tag{12}$$

The final step in our procedure is to substitute the expansion for u [Eqs. (5) and (6)] in Eq. (4) and to impose the asymptotic condition for bound states that $h(\infty)=0$. We then obtain the eigenvalue equation

$$\sum_{m=0}^{m=n} a_m^{(m)} f_m(k) = \frac{1}{g} , \tag{13}$$

where

$$f_m(k) = (-)^m \sum_{r=0}^{r=m} \frac{(-)^{r+1} m!}{r!\,(m-r)!} \ln(2k+r+1) .$$

It can be readily verified that the left-hand side of Eq. (13) is a polynomial in g of order n. The roots of this polynomial are functions of k; the smallest root corresponds to the ground state, the next root to the first excited level, etc. We have evaluated these roots for several values of k between 0 and 10 and for $n=2, 3, \ldots, 20$ and found that g converges rapidly towards the solution. As an example, we give in Table I the values of g for $n=2-5$ for the ground-state energies E given by Rogers, Graboske, and Harwood[1] from numerical integrations of Eq. (1). Comparison with their results show complete agreement except for the two smallest values of E, where convergence to the fourth decimal place has not been reached at $n=5$. For $E=0$ we find that g has increased monotonically to $g=1.679\,74$ at $n=20$.

TABLE I. Values of the coupling constant g for selected values of E and n for the ground state.

E(Ry)	$n=2$	$n=3$	$n=4$	$n=5$	Rogers *et al.*[a]
0	1.6795	1.6724	1.6762	1.6777	1.6798
0.020 57	2.0048	1.9935	1.9971	1.9983	2.0
0.1351	2.8138	2.7954	2.7984	2.7993	2.8
0.2962	4.0193	3.9966	3.9990	3.9994	4.0
0.4737	6.0214	5.9981	5.9998	6.0000	6.0
0.5818	8.0201	7.9983	7.9996	7.9997	8.0
0.6536	10.019	9.9999	9.9998	9.9999	10.0
0.7424	14.015	13.999	14.000	14.000	14.0
0.8141	20.012	19.999	20.000	20.000	20.0

[a] Reference 1.

Applying the recurrence relations, Eqs. (10)–(12), to $\phi^{(n)}(x)$ we find that

$$\phi^{(n)}(x) - \phi^{(n-1)}(x) = (e^{-x}-1)^n a_n^{(n)} , \tag{14}$$

where $a_n^{(n)}$ is the last coefficient[3] of the expansion ϕ_n, [Eq. (6)]. We have calculated $a_n^{(n)}$ from Eq. (9) for all integers n from 2 to 20 at the roots of Eq. (14) and found that $a_n^{(n)}$ decreases monotonically in magnitude and alternates in sign between consecutive values of n, except at the smaller values of n. As an illustration, we show in Fig. 1 the function $\phi^{(n)}(x)$ for the third excited state with energy $E=0$. Substituting Eq. (5) in Eq. (3), we have also verified that $a_0^{(n)}$ approaches $f^{(n)}(\infty)$.

It is straightforward to show that in the weak-screening limit the wave function given by Eqs. (5)

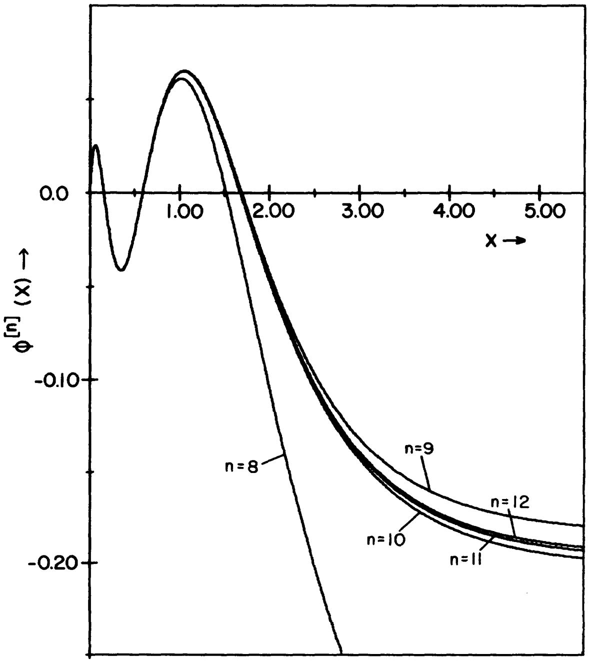

FIG. 1. The wave function for the third excited level of the screened exponential Coulomb potential with the critical coupling constant $g=25.33$ and $E=k=0$, for $n=8-12$.

and (6) approaches the exact s-wave Coulomb bound states. For large values of k the important contribution of $\phi^{(n)}(x)$ is in the range $0<x\lesssim 1/k$, and this becomes the domain where the power-series expansion in x is valid. If we set $g=2kn$ in the recurrence relation for c_s [Eq. (8)] and keep only the dominant contributions for large k and $s=1, 2, \ldots, n-1$, we obtain

$$c_s \approx \frac{(-)^s(2k)^s}{s!\,(s+1)!}\,\frac{(n-1)!}{(n-s-1)!}\,. \tag{15}$$

These are essentially the coefficients of the associated Laguerre polynomials L_n^1 which determine the s-wave Coulomb bound states. Furthermore, we verify that our ansatz for g approaches the solution of the eigenvalue problem for large k. In this limit we find that Eq. (13) takes the form

$$\sum_{s=0}^{s=n-1} \frac{s!\,c_s}{(2k)^{s+1}} \simeq \frac{1}{g}\,, \tag{16}$$

and substituting Eq. (15) for c_s in Eq. (16), we obtain again $g=2kn$.

For the case of finite angular momentum l, we replace the exponential functions $e^{\pm kx}$ in Eqs. (2)–(6) by the Hankel functions of order l, and proceed in the same manner as in the $l=0$ case. The details will be discussed in a subsequent publication.

We have applied this method successfully also to other short-range potentials. In particular, for the exponential potential we find that for $0\leqslant k\leqslant 4$ and $n=8$ the eigenvalues g have converged to the first zero of the Bessel function $J_{2k}(x)$ at $x=2\sqrt{g}$ to four decimal places.

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[1] F. J. Rogers, H. C. Graboske, Jr., and D. J. Harwood, Phys. Rev. A 1, 1577 (1970); earlier references to calculations of bound states of the screened Coulomb potential can be found in this work. In addition to this list, we should mention the analytic investigations of R. Jost [Helv. Phys. Acta 20, 256 (1947)] and A. Martin [Nuovo Cimento 14, 403 (1959)].

[2] L. Hulthén and K. V. Laurikainen, Rev. Mod. Phys. 23, 1 (1951).

[3] For fixed values of k and g, the coefficients $a_n^{(n)}$ correspond to the Taylor series expansion coefficients of $u(x)e^{kx}$ in powers of $(e^{-x}-1)$, and satisfy the condition $\sum_{m=1}^{m=n}(-)^m a_m^{(m)}=a_0^{(n)}$. The convergence of $a_0^{(n)}$ for large n is obtained if, and only if, k and g satisfy the eigenvalue condition [Eq. (13)]. While for $l=0$, the coefficients $a_n^{(n)}$ could also be obtained directly from a recurrence relation derived from the Schrödinger equation in the variable $(e^{-x}-1)$, this relation cannot be extended to the case $l\neq 0$.