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High-energy expansions for the phase shifts in screened Coulomb potentials

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A high-energy expansion is obtained for nonrelativistic phase shifts in a screened Coulomb potential, expressing their difference from the corresponding point Coulomb phase shifts as quadrature integrals over the potential. The result exhibits the role of small- and large-distance regions of the potential in determining these phase shifts.

We wish to report high-energy expansions for nonrelativistic phase shifts in screened Coulomb potentials $V(r)$. We characterize screening by a function g, with $rV \equiv -ag$, $a \equiv Ze^2$, $g(0)=1$, and $g(\infty)=0$, with units $\hbar = m_e = c = 1$. We assume we may take $g = g(\lambda r)$, with λ a small parameter (λ^{-1} large compared to the electron Compton wavelength) characterizing the screening of the nuclear charge, and we assume the potential in the interior of the atom is well represented by the first few terms of a power series expansion in λr: $g = \sum_n V_n(\lambda r)^n$, $V_0 \equiv 1$. The Yukawa and Hulthén potentials are analytic examples; a Herman-Skillman potential may be fit to such a form. [Here $g(\lambda r)$ should be understood as corresponding to a *smoothed* potential, omitting, for example, shell structure effects, in order that a few terms in an expansion in integral powers suffice; such a smoothed potential is quite adequate to obtain energy levels and wave functions close to those of a more accurate potential.] We have previously found[1,2] that small-distance properties of bound and continuum wave functions of given angular momentum l are well determined by the small-distance properties of the smoother potential (by the V_n), including also bound-state energies and bound- and continuum-state normalizations in the case that the energy of the state (positive or negative) is large in magnitude and the angular momentum is not large. Our results here complete this discussion by showing to what extent the phase shifts at high energy are also determined from the short-distance properties of the potential. With these results it should be possible to obtain analytic expansions for bound-free angular distributions, just as before such expressions were obtained for total cross sections.

Our result for the phase shift $\delta_l(p)$, as a function of angular momentum l and momentum p, expressed relative to the corresponding point Coulomb phase shift $\delta_{Cl}(p) = \arg(\Gamma(l+1-i\nu))$, keeping terms through p^{-3} (i.e., through r^3 in a small-r expansion, and making no expansion in λ, but collecting terms by order in $\lambda/a \simeq 1/Z^{2/3}$), is

$$\begin{aligned}\delta_l(p) - \delta_{Cl}(p) = {} & \nu(\ln 2p/\lambda + b_0) - \nu^3(\overline{V}_1 \ln 2p/\lambda + \tfrac{1}{2}\overline{\beta}_0) + \nu^3 l(l+1)(\tfrac{1}{2}\overline{V}_2 \ln 2p/\lambda + \overline{b}_1 + \tfrac{1}{2}\overline{V}_2) \\ & + \tfrac{1}{4}\nu^3\overline{V}_2 + \nu^3 \operatorname{Re}\psi(l+1)[\overline{V}_1 - \tfrac{1}{2}\overline{V}_2 l(l+1)] \ ,\end{aligned} \tag{1}$$

where $\nu = a/p$, ψ is the logarithmic derivative of the Γ function, $V_n \equiv (\lambda/a)^n V_n$, and

$$\begin{aligned} b_0 &= -\int_0^\infty dx\, g'(x) \ln x \ , \\ \overline{b}_1 &= -\tfrac{1}{4}(\lambda/a)^2 \int_0^\infty dx\, g'''(x) \ln x \ , \\ \overline{\beta}_0 &= -(\lambda/a) \int_0^\infty dx \frac{d^2}{dx^2}[g(x)]^2 \ln x \ . \end{aligned} \tag{2}$$

The well-known term[3] $\nu \ln 2p/\lambda$ reflects the infinite phase difference as one approaches the Coulomb potential as the limit of a screened potential; Taylor's result includes the portion of Eq. (1) of order ν. The three coefficients $b_0, \overline{b}_1, \overline{\beta}_0$ are not determined from the first V_n and represent larger-distance information about the atomic potential. We shall examine the significance of other aspects of this result subsequently.

We will give the derivation of this result, which is fairly lengthy, elsewhere.[4] In summary, our procedure is (1) to obtain an iterated eikonal wave function of complex momentum, (2) to use the iterated eikonal to reconstruct the small-distance behavior of the solution of the three-dimensional Schrödinger equation characterized by an incoming plane wave and outgoing scattered spherical wave, and (3) to read out the phase shifts from the coefficients in the partial-wave decomposition of the three-dimensional wave function. We had previously obtained[5] the small-distance behavior of the general solution of the Schrödinger equation in three dimensions, well behaved at the origin, in a screened Coulomb potential characterized by g, and also the partial-wave decomposition of the general solution. However, we did not have a way to pick out the particular scattering solution (equivalent to determining the phase shifts), since our solution was only valid at small distances, not in the asymptotic region where the boundary condition is applied which usually determines the scattering wave solution. We now see the eikonal wave function, valid for large p, as providing a bridge between small- and large-distance properties, since it can be determined from quadrature integrals (which do involve large-distance properties of the potential) in the small-distance region and, therefore (in the large p case), can be used to identify the correct particular three-dimensional solution. To go beyond order p^{-1} one must iterate the eikonal, and the further results can also be obtained in quadrature. However, for real p the iteration is in fact not justified, as is illustrated by the failure to produce terms of an asymptotic spherical wave character. The problem is avoided by considering complex p, for which the spherical terms are exponentially small for large p, and then returning to real p only after having constructed the desired three-dimensional solution. The issue is related to the Stokes phenomena.[6]

Several checks of our expansion for screened Coulomb phase shifts are available. In the case of the Hulthén potential $V(r)=-a(e^{\lambda r}-1)^{-1}$, the exact analytic result for the s-wave case is known.[7] In the large-p limit it becomes (through order p^{-3})

$$\delta_0^{\text{Hulthén}}-\delta_{Co}\simeq -\tfrac{1}{2}(\lambda/a)\nu^3\,\mathrm{Re}\psi(1-i\nu) + [\nu+\tfrac{1}{2}(\lambda/a)\nu^3]\ln 2p/\lambda - \tfrac{1}{4}(\lambda/a)\nu^3+\tfrac{1}{48}(\lambda/a)^2\nu^3 \ . \tag{3}$$

With use of the results for this potential

$$\overline{V}_1=-\tfrac{1}{2},\quad \overline{V}_2=\tfrac{1}{12},\quad b_0=0,\quad \overline{\beta}_0=\tfrac{1}{2}(\lambda/a) \tag{4}$$

in Eq. (1), Eq. (3) is indeed obtained. Another test of the s-wave phase shifts is provided by Puff's quadratures[8] (rewritten in our units),

$$\delta_0(p)=-\frac{1}{p}\int_0^\infty V(r)\,dr-\frac{1}{p^3}\left(\tfrac{1}{4}V'(0)+\tfrac{1}{2}\int_0^\infty V^2(r)\,dr\right) \ , \tag{5}$$

for potentials finite at the origin. However, if we work with the *difference* of two screened Coulomb potentials g having the same V_1, the result (5) becomes

$$\delta^a-\delta^b=-\frac{1}{p}\int_0^\infty (V^a-V^b)\,dr-\frac{1}{4p^3}[V^a-V^b]'\Big|_0 -\frac{1}{2p^3}\int_0^\infty [(V^a)^2-(V^b)^2]\,dr \ , \tag{6}$$

while Eq. (1) gives

$$-\frac{a}{k}\int_0^\infty dx\,\ln x\,[g^a-g^b]'+\frac{1}{2}\frac{\lambda}{a}\left(\frac{a}{k}\right)^3\int dx\,\ln x\frac{d^2}{dx^2}[(g^a)^2-(g^b)^2]+\frac{1}{4}\left(\frac{\lambda}{a}\right)^2\left(\frac{a}{k}\right)^3[V_2^a-V_2^b] \ . \tag{7}$$

Integrating by parts, we verify that these two expressions are identical. As a third check we have made comparisons with numerical calculations of Yukawa phase shifts; the agreement is good over the range of elements and energies for which $\nu\lesssim 0.5$ for l as great as 6.

For many purposes the phase information of interest is the *relative* phase, say $\delta_l-\delta_0$. Our expression for this relative phase is very simple:

$$(\delta-\delta_C)\big|_0^l=\nu^3 l(l+1)\left(\frac{1}{2}\overline{V}_2\ln\frac{2P}{\lambda}+\overline{b}_1+\frac{1}{2}\overline{V}_2-\frac{1}{2}\overline{V}_2\,\mathrm{Re}\psi(l)\right)+\nu^3\overline{V}_1\,\mathrm{Re}[\psi(l+1)-\psi(1)] \ . \tag{8}$$

It is also known[9] that, in general, a screened Coulomb wave function is closest in shape to a Coulomb wave function of shifted energy, corresponding to the analytic shift between screened and Coulomb energies,

$$E=E_C+\tfrac{1}{2}a^2\{-2\overline{V}_1+\overline{V}_2[3\nu^2+l(l+1)]\} \ . \tag{9}$$

In this form the expression for the phases is indeed also very simple:

$$\overline{\Delta}_l\equiv\delta_l(p)-\delta_l(p_C)=\nu_C\ln\frac{2p_C}{\lambda}-\overline{V}_1\nu_C^3+\nu\overline{b}_0-\tfrac{1}{2}\nu_C^3\overline{\beta}_0+\overline{V}_2\nu_C^3[l(l+1)+\tfrac{1}{4}]+\nu_C^3 l(l+1)\overline{b}_1 \ . \tag{10}$$

Expressing Δ_l as a function of p we may finally write in the most compact form

$$\overline{\Delta}_l-\overline{\Delta}_0=\nu^3 l(l+1)[\tfrac{1}{2}\overline{V}_2(\ln 2p/\lambda+1)]+\overline{b}_1 \ . \tag{11}$$

All dependence on $\mathrm{Re}\psi$ has now disappeared. We note that there are additional terms beyond $\nu\ln 2p/\lambda$ which are not analytic as $\lambda\rightarrow 0$, although these further terms all vanish in the limit. Further, these terms are not just part of an overall phase, but they also enter the phase-shift differences of Eq. (8).

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