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Analytic expressions for phase shifts in partially screened Coulomb potentials with ionic long range Coulomb tails

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Abstract. Analytic expressions for the high energy phase shifts of an electron moving in a partially screened spherically symmetric potential corresponding to an atomic ion have been obtained using methods developed previously for phase shifts in neutral atom potentials. Comparison with numerical calculation shows that the ionic phase shift formula is accurate in the case of a self-consistent potential of the Hermann-Skillman type, provided the electron energy is large and the angular momentum is small. The effect of the ionic tail on the phase shift (as compared with the short-range case) becomes substantial at lower energies, higher ionicities or larger angular momenta. It is concluded that use of neutral atom high energy analytic phase shift expressions is justified even in the presence of ionic tails.

1. Introduction

In previous work (Bechler and Pratt 1983, 1985) we have obtained analytic expressions for the high energy phase shifts in a screened Coulomb short-range potential of the type

$$V(r) = -ag(\lambda r)/r \quad (1)$$

where $a = Z\alpha$ with Z being the atomic number and α the fine structure constant. Here λ is a small parameter characterising the screening in the sense that λ^{-1} characterises the dimensions of an atom. For short-range potentials the function $g(\lambda r)$ falls off to zero for $r \rightarrow \infty$. Assuming further that λ is small, i.e. λ^{-1} large compared to the electron Compton wavelength, we represented the potential in the interior of an atom by the first few terms of the expansion (McEneaney *et al* 1976a, b)

$$g(\lambda r) = \sum_n \tilde{V}_n(\lambda r)^n. \quad (2)$$

We were then able to obtain expressions for high energy phase shifts in such a potential in terms of an expansion in λ and in inverse electron momentum, which also included certain quadrature integrals over the potential characterising its global properties.

Our purpose here is to examine how these expressions for the phase shifts are modified if the assumption of a short-range potential is relaxed. We begin by briefly reviewing and summarising our procedure in the short-range case in order to make the nature of the subsequent modification intelligible.

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2. Summary of the short-range case

It has been shown that small distance properties of bound and continuum wavefunctions of given angular momentum l are well described by small distance properties of the potential (i.e. by V_n) in the case where the energy of the state (positive or negative) is large in magnitude and the angular momentum is not large (McEannan *et al* 1976a, b). For bound states, large energy corresponds to the binding energies of inner shell electrons of medium and higher Z atoms, whereas in the case of continuum electrons the energy should be such that $\nu = a/p < 1$. In addition to wavefunction shapes, bound-state energies and bound and continuum normalisations could also be determined as analytic expressions in each order in an expansion in λ with the use of the expansion (2).

However, small distance properties of the potential are not sufficient to determine (even at small distances) the full three-dimensional scattering wavefunction ψ_p characterised by a given value of the asymptotic linear momentum p (Bechler *et al* 1979). To identify, even for small distances, the particular solutions of the Schrödinger equation in three dimensions which satisfies the scattering boundary conditions requires the use of some large distance information about the potential. We have recently found (Bechler and Pratt 1983, 1985) that it is possible to link the needed information about the small and large distance regions through use of the iterated eikonal expansion of the full continuum wavefunction ψ_p . Writing the wavefunction in the form

$$\psi_p(\mathbf{r}) = \exp(i\mathbf{p} \cdot \mathbf{r})\phi_p(\mathbf{r}) \quad (3)$$

one gets the following equation for $\phi_p(\mathbf{r})$:

$$(-ip\partial/\partial z + V(\mathbf{r}))\phi_p(\mathbf{r}) = \frac{1}{2}\nabla^2\phi_p(\mathbf{r}). \quad (4)$$

The leading term in the iterated eikonal expansion is given by the eikonal approximation of Glauber (1959) and corresponds to the solution of (4) with zero right-hand side and with the boundary condition

$$\phi_p(\mathbf{r}) \xrightarrow{z \rightarrow -\infty} 1. \quad (5)$$

(Momentum p has been assumed parallel to the z axis.) The eikonal approximation for ϕ_p has the form

$$\phi_p^{\text{eik}}(\mathbf{r}) = \exp\left(-\frac{i}{p} \int_{-\infty}^z V(\boldsymbol{\rho} + \hat{p}z') dz'\right) \quad (6)$$

where $\boldsymbol{\rho}$ is the radius vector in the plane orthogonal to p . The next terms in the iterated eikonal expansion can be obtained by iteration of an integral equation for $\phi_p(\mathbf{r})$, equivalent to the partial differential equation (4) together with the boundary condition (5):

$$\phi_p(\mathbf{r}) = \phi_p^{\text{eik}}(\mathbf{r}) + \int_{-\infty}^z dz' \exp\left(-\frac{i}{p} \int_{z'}^z V(\boldsymbol{\rho} + \hat{p}z_1) dz_1\right) \frac{1}{2}\nabla'^2\phi_p(\mathbf{r}). \quad (7)$$

We have shown (Bechler and Pratt 1983, 1985) that the iterated eikonal, a valid expansion of the full scattering wavefunction ψ_p for complex momenta, may also be used to determine ψ_p at short distances and for real momenta. From the small distance expansion of this iterated eikonal of large complex momentum, the scattering wavefunction at small distances and real p is determined by continuation in p . The

screened Coulomb phase shifts, which are the coefficients (phases) of the radial solution of definite angular momentum in the partial wave expansion of ψ_p , can then be identified by comparing partial wave projections of ψ_p with the radial wavefunctions found previously (McEneaney *et al* 1976a, b).

The phase shifts are given by the formula (Bechler and Pratt 1983, 1985)

$$\begin{aligned} \delta_l(p) = & \delta_{cl}(p) + \nu[\ln(2p/\lambda) + \bar{b}_0] - \nu^3 \bar{V}_1 \ln(2p/\lambda) - \frac{1}{2}\nu^3 \bar{\beta}_0 \\ & + \nu^3 l(l+1) \{ \frac{1}{2} \bar{V}_2 [\ln(2p/\lambda) + 1] + \bar{b}_1 \} \\ & + \frac{1}{4}\nu^3 \bar{V}_2 + \text{Re } \psi(l+1 - i\nu) \nu^3 [\bar{V}_1 - \frac{1}{2} \bar{V}_2 l(l+1)] \end{aligned} \quad (8)$$

where

$$\begin{aligned} \bar{V}_i &= (\lambda/a)^i V_i & \bar{b}_0 &= - \int_0^\infty dy (\ln y) g'(y) \\ \bar{\beta}_0 &= - \frac{\lambda}{a} \int_0^\infty dy (\ln y) (d^2/dy^2) [g(y)]^2 \\ \bar{b}_1 &= - \frac{1}{4} \left(\frac{\lambda}{a} \right)^2 \int_0^\infty dy (\ln y) (d^3/dy^3) g(y). \end{aligned} \quad (9)$$

Here δ_{cl} is the point-Coulomb phase shift,

$$\delta_{cl} = \arg \Gamma(l+1 - i\nu) \quad (10)$$

ψ is the logarithmic derivative of Euler's Γ function and $\nu = a/p$.

3. Phase shifts for a potential with a Coulombic tail

We now want to use a similar procedure to find the phase shifts for a partially screened potential which is Coulombic (i.e. corresponds to nuclear and ionic charges respectively) both at small and large distances. We can characterise this potential as

$$V(r) = -ah(\lambda r)/r \quad (11)$$

where $h(0) = 1$ and $h(\lambda r) \rightarrow_{r \rightarrow \infty} Z_i/Z$, where Z_i is the ionic charge. For small λ the function $h(\lambda r)$ can be expanded according to equation (2) in the same way as in the short-range case.

Due to the long-range character of the ionic potential the eikonal expansion (6) is incorrect (and in fact would lead to a divergent eikonal phase), since it no longer corresponds to the correct boundary condition on the scattering wavefunction. The eikonal expression will be modified in such a way that it accounts correctly for the Coulomb phase at infinity. The boundary condition (5) has to be replaced by

$$\phi_p(\mathbf{r}) \xrightarrow{z \rightarrow -\infty} \exp[-i\nu_i \ln p(r-z)] \quad (12)$$

where $\nu_i = Z_i \alpha/p$. This boundary condition corresponds to the usual asymptotic Coulomb phase function of the scattering wavefunction in a Coulomb potential:

$$\psi_p(\mathbf{r}) \xrightarrow{r \rightarrow \infty} \exp[i\mathbf{p} \cdot \mathbf{r} - i\nu_i \ln p(r-z)] + \text{spherical wave.} \quad (13)$$

Note that we have assumed that the Coulomb phase function at infinity is the same for a potential with a Coulombic tail as for a corresponding point-Coulomb potential,

i.e. small distance properties of the potential do not influence the asymptotic Coulomb phase function. While commonly used (Starace 1982) this assumption may not necessarily be obvious. In the pure Coulomb case the asymptotic behaviour (12) is associated with the unique solution of the differential equation:

$$\psi_p^{\text{Coulomb}}(\mathbf{r}) = N \exp(i\mathbf{p} \cdot \mathbf{r}) M(i\nu_i, 1; ip(r-z)) \quad (14)$$

where M is the regular confluent hypergeometric function which satisfies the requirements of regularity at the origin and boundary condition at infinity corresponding to (modified) plane wave and outgoing (modified) spherical wave (Messiah 1961). On the other hand, for a potential with a Coulombic tail (and non-Coulombic at finite distances) the wavefunction is a solution of the point-Coulomb equation only at large r and therefore, looking at the asymptotic form of the wavefunction, we do not need to impose the regularity condition. For this reason the variety of physically acceptable solutions in the asymptotic region is now much wider than in the point-Coulomb case and it is not therefore *a priori* obvious that the distorting phase is in both cases the same.

To show that, at least for the plane wave part of the asymptotic wavefunction, the standard distorting phase function of the point-Coulomb case is required, note first that the only asymptotic solutions which are physically acceptable can depend only on $p(r-z)$ and not on the second parabolic variable $p(r+z)$. This means that the asymptotic form of the wavefunction, which is physically acceptable, looks like

$$\psi_{\text{asymptotic}} \sim \alpha \psi(i\nu_i, 1; ip(r-z)) + \beta M(i\nu_i, 1; ip(r-z)) \quad (15)$$

where $\psi(a, b; x)$ is the irregular solution of the confluent hypergeometric equation. Another solution, asymptotically equal to a (distorted) plane wave plus a (distorted) spherical wave, would be

$$\psi_{\text{asymptotic}} \sim a \psi(i\nu_i, 1, -ip(r+z)) + \beta M(i\nu_i, 1; ip(r-z)). \quad (16)$$

This choice would however lead to a plane wave asymptotic behaviour with a distorting phase function singular along the negative z semi-axis. This asymptotic behaviour is not physically acceptable since it corresponds to a singular incident wave, whereas one wishes the incident wave (corresponding to plane wave along the negative z semi-axis is the stationary picture of scattering) to be regular. One should therefore choose (15) rather than (16) and then, independent of the relative magnitude of the coefficients α and β , the wavefunction is asymptotically equal to (Bateman and Erdelyi 1953)

$$\psi_p \xrightarrow{r \rightarrow \infty} \exp[ipz - i\nu_i \ln p(r-z)] + \text{distorted spherical wave} \quad (17)$$

which shows that (12) is the correct boundary condition for $\phi_p(\mathbf{r})$. We can intuitively understand this result as saying that an incoming flux at asymptotic distances is sensitive only to the asymptotic long-range potential but has no way to know whether that potential changes at small distances.

We can now use the general procedure described previously (Bechler and Pratt 1985) to find the phase shifts in an ionic screened potential corresponding to an atomic ion with charge Z_i . The difference from that paper is due to the different form of the eikonal wavefunction. The solution of the eikonal equation, for a long-range potential behaving as $-Z_i\alpha/r$ for large distances, and satisfying the boundary condition (12), is

$$\phi_p^{\text{eik}}(\mathbf{r}) = \exp\left(-\frac{i}{p} \int_{-\infty}^z U(\rho + \bar{p}z') dz' + i \frac{Z_i\alpha}{p} \int_{z_0}^z \frac{dz'}{r'}\right) \quad (18)$$

where $U = V + Z_i\alpha/r$ and $z_0 = (p^2\rho^2 - 1)/2p$. Note that the first integral in this expression is convergent, since the long distance tail has been subtracted from $V(r)$.

In a similar way as for the short-range screened Coulomb potential we find the full continuum wavefunction ψ_p at small distances and, projecting ψ_p on partial waves, we can then determine the phase shifts. The expression for the phase shifts δ_l has the same form as (8), except that there is an additional l -independent term connected with the long-range character of the ionic potential. The formula for the ionic phase shift is

$$\begin{aligned} \delta_l(p) = & \delta_{cl}(p) + \nu[\ln(2p/\lambda) + \bar{b}_0] - \nu_i \ln(2p/\lambda) - \nu^3 \bar{V}_1 \ln(2p/\lambda) \\ & - \frac{1}{2}\nu^3 \bar{\beta}_0 + \nu^3 l(l+1) \left\{ \frac{1}{2} \bar{V}_2 [\ln(2p/\lambda) + 1] + \bar{b}_1 \right\} + \frac{1}{4}\nu^3 \bar{V}_2 \\ & + \text{Re } \psi(l+1 - i\nu) \nu^3 \left[\bar{V}_1 - \frac{1}{2} \bar{V}_2 l(l+1) \right] \end{aligned} \quad (19)$$

where \bar{b}_0 , $\bar{\beta}_0$ and \bar{b} are given by (9) with $g(y)$ replaced by $h(y)$, and the point-Coulomb phase δ_{cl} in (19) has to be calculated for the nuclear charge Z , i.e. it is given by (10).

We can see that expressions (19) and (8) are of the same form except for the additional l -independent term $\nu_i \ln(2p/\lambda)$ in the ionic case, which contributes to the divergent part of the phase when $\lambda \rightarrow 0$. Note that the divergent part of the phase when $\lambda \rightarrow 0$ is now equal to

$$\delta_{\text{divergent}} = (\nu - \nu_i) \ln(2p/\lambda) \quad (20)$$

whereas in the short-range case it was $\nu \ln(2p/\lambda)$. To understand the form of the divergent contribution for the ionic potential we have to look at formula (18), in which the long-range potential V was split into the short-range part

$$U(r) = -\frac{a}{r} \left(h(\lambda r) - \frac{Z_i}{Z} \right) \quad (21)$$

and the long-range Coulomb contribution $Z_i\alpha/r$, independent of λ . In the limit $\lambda \rightarrow 0$ the short-range potential U goes to the Coulomb potential of a charge $Z - Z_i$ and this is the charge which determines the behaviour of the phase when $\lambda \rightarrow 0$. The divergent part of the phase shift is determined by the short-range part of the potential (strictly speaking by its $\lambda = 0$ limit); the long-range contribution $Z_i\alpha/r$ in (22) does not contribute to the divergent phase since it is independent of λ .

Since our phase shift formulae for the short- and long-range potentials differ only by an l -independent term, expressions for the relative phases (e.g. $\delta_l - \delta_0$) look the same in both cases. In principle, this does not mean that at the same energies and angular momenta relative phases in both cases have the same values, since short and long distance potentials will be in general characterised by different values of \bar{b}_1 , even if their short-range characteristics (i.e. $\bar{V}_i - r$) are the same. We may expect, however, that at low angular momenta and high energies, the differences between relative phases for short- and long-range potentials with the same short-range parameters should not be large, i.e. that the effect of a Coulombic tail on the relative phases is negligible. Only at low energies or large angular momenta (or both) can the long-range tail of a potential play a role.

An example of a commonly used long-range potential having the same short distance characteristics as a certain short-range potential is provided by a screened potential with the Latter tail switched on at some distance r_0 (Latter 1955). This potential has

the form (11) with

$$h(\lambda r) = \begin{cases} g(\lambda r) & r < r_0 \\ Z_i/Z & r > r_0 \end{cases} \quad (22)$$

where $g(\lambda r)$ is the screening factor of the short-range potential (1) and r_0 has to be chosen in such a way that

$$g(\lambda r_0) = Z_i/Z \quad (23)$$

i.e. that our long-range potential is continuous. We may write $h(y)$ as

$$h(y) = \theta(y_0 - y)g(y) + \theta(y - y_0)Z_i/Z \quad (24)$$

where θ is the step function and $y_0 = \lambda r_0$. The difference between the phase shifts in the short-range (s) and ionic (i) cases can now be easily found:

$$\begin{aligned} \delta_i^s(p) - \delta_i^i(p) &= \nu_i \ln 2p/\lambda + \frac{\lambda}{a} \nu^3 \frac{Z_i}{Z} g'(y_0) \ln y_0 \\ &\quad - \frac{1}{4} \left(\frac{\lambda}{a} \right)^2 \nu^3 l(l+1) g''(y_0) \ln y_0 \\ &\quad + \int_{y_0}^{\infty} dy \ln y \left[-\nu g'(y) + \frac{1}{2} \frac{\lambda}{a} \nu^3 \frac{d^2 g^2}{dy^2} - \frac{1}{4} \left(\frac{\lambda}{a} \right)^2 \nu^3 l(l+1) \frac{d^3 g}{dy^3} \right]. \end{aligned} \quad (25)$$

Integrating by parts we obtain

$$\begin{aligned} \delta_i^s(p) - \delta_i^i(p) &= \nu_i \ln(2pr_0) - \int_{y_0}^{\infty} \frac{dy}{y} \left[-\nu g(y) + \frac{1}{2} \frac{\lambda}{a} \nu^3 \frac{dg^2}{dy^2} \right. \\ &\quad \left. - \frac{1}{4} \left(\frac{\lambda}{a} \right)^2 \nu^3 l(l+1) \frac{d^2 g}{dy^2} \right]. \end{aligned} \quad (26)$$

Whereas the differences between δ_i^s and δ_i^i can be, in general, large due to the terms independent of l in (26), the relative phases will not be very different from each other. Denoting $\delta_i - \delta_0 \equiv \Delta_i$ we obtain from (26)

$$\Delta_i^s(p) - \Delta_i^i(p) = \frac{1}{4} \left(\frac{\lambda}{a} \right)^2 \nu^3 l(l+1) \int_{y_0}^{\infty} \frac{1}{y} g''(y) dy. \quad (27)$$

At higher energies, i.e. when ν is smaller than one, this quantity will be small, since it is proportional to $(\lambda/a)^2$, which in our perturbative scheme has to be small, and also since the integration in (31) is over a region in which the screening factor $g(y)$ and its derivatives are small. Only at sufficiently low energies, and/or high angular momenta, may one expect larger differences between the short- and long-range cases. However, as we shall see in the next section, these are energies for which our perturbative approach to the phase shifts cannot be applied. We conclude that in most situations where APT results may be used, the use of neutral atom prediction is justified even if ionic tails are present.

4. Discussion of the results

In this section we discuss various features of our expression for the ionic phase shifts. To get an idea how much the ionic tail matters we calculated the ratio of $\Delta_l^s - \Delta_l^l$ (formula (27)) to Δ_l^s , for the Yukawa potential with and without a Latter tail. The results are summarised in table 1. We see that, except for large ionicities and low energies, the effect of the long-range tail on the relative phases is minor. For $Z = 13$, for instance, the difference between short- and long-range relative phases reaches 10% for ionicity equal to 8 at electron energy $E = 1$ keV. In general, the effect of the Coulombic tail on relative phases can be seen at low energies—basically, these are energies at which our perturbative scheme is not applicable ($\nu \leq 1$)—or at high ionicities. For large angular momenta one can expect deviations from the short-range case also at higher energies. In general, the ionic tail effects are unimportant in situations for which APT predictions can be justified, and hence (except perhaps in situations of high ionicity) it is sufficient to use neutral atom APT predictions.

Table 1. Relative differences of the phase shifts in short- and long-range potentials. The table shows the ratios $(\Delta_l^s - \Delta_l^l)/\Delta_l^s$, where Δ_l^s and Δ_l^l are relative phases $\delta_l - \delta_0$ for short- and long-range cases, respectively. The short-range potential is the Yukawa potential and for the long-range case we took the Yukawa potential with a Latter tail.

| Z | E (keV) | l | Ionicity | | | |
|----|----------------------|---|------------|------------|------------|---------|
| | | | 1 | 3 | 8 | 20 |
| 13 | 1 ($\nu = 1.58$) | 1 | -0.0016 | -0.0070 | -0.0385 | |
| | | 2 | -0.0028 | -0.0127 | -0.0696 | |
| | | 3 | -0.0043 | -0.0198 | -0.1087 | |
| | 3 ($\nu = 0.88$) | 1 | -0.0004 | -0.0020 | -0.0106 | |
| | | 2 | -0.0008 | -0.0037 | -0.0204 | |
| | | 6 | -0.0035 | -0.0160 | -0.0882 | |
| | 10 ($\nu = 0.48$) | 1 | -0.0002 | -0.0004 | -0.0028 | |
| | | 4 | -0.0005 | -0.0025 | -0.0139 | |
| | | 8 | -0.0016 | -0.0072 | -0.0395 | |
| 36 | 10 ($\nu = 1.33$) | 1 | $<10^{-4}$ | -0.0003 | -0.0013 | -0.0059 |
| | | 4 | -0.0002 | -0.0014 | -0.0054 | -0.0248 |
| | | 8 | -0.0005 | -0.0037 | -0.0146 | -0.0679 |
| | 100 ($\nu = 0.42$) | 1 | $<10^{-4}$ | $<10^{-4}$ | $<10^{-4}$ | -0.0005 |
| | | 4 | $<10^{-4}$ | -0.0001 | -0.0005 | -0.0021 |
| | | 8 | -0.0001 | -0.0004 | -0.0013 | -0.0060 |
| | | | Ionicity | | | |
| | | | 1 | 3 | 6 | 60 |
| 79 | 3 ($\nu = 5.32$) | 1 | -0.0005 | -0.0017 | -0.0061 | -0.1773 |
| | | 4 | -0.0011 | -0.0043 | -0.0152 | -0.4432 |
| | | 8 | -0.0017 | -0.0068 | -0.0244 | -0.7126 |
| | 30 ($\nu = 1.68$) | 1 | $<10^{-4}$ | $<10^{-4}$ | -0.0003 | -0.0080 |
| | | 4 | $<10^{-4}$ | -0.0003 | -0.0011 | -0.0313 |
| | | 8 | -0.0002 | -0.0008 | -0.0029 | -0.0833 |
| | 100 ($\nu = 0.92$) | 1 | $<10^{-4}$ | $<10^{-4}$ | $<10^{-4}$ | -0.0019 |
| | | 4 | $<10^{-4}$ | $<10^{-4}$ | -0.0003 | -0.0082 |
| | | 8 | $<10^{-4}$ | -0.0002 | -0.0008 | -0.0225 |

In table 2 we give the comparison of our analytic relative phases $\delta_l - \delta_0$ with the results of a numerical calculation for the self-consistent Hermann-Skillman potential with $Z_i = 1$. We used an analytic model of the screened ionic potential (McEnean *et al* 1976a),

$$V(r) = -(a/r)[Z^{-1} + \zeta \exp(-\mu_1 r) + (1 - \zeta - Z^{-1}) \exp(-\mu_2 r)]. \quad (28)$$

for which

$$h(y) = Z^{-1} + \zeta \exp(-\nu_1 y) + (1 - \zeta - Z^{-1}) \exp(-\nu_2 y) \quad (29)$$

where $\nu_i = \mu_i/\lambda$. We used the Thomas-Fermi expression for λ , i.e. $\lambda = 1.13\alpha Z^{1/3}$ and we took the values of μ_1 , μ_2 and ζ from McEnean *et al* (1976a). Comparison with numerical results is shown for $Z = 13, 36$ and 79 at various values of energy and angular momentum. As expected, APT gives better results at higher energies and lower angular

Table 2. Analytic and numerical relative phases for the self-consistent Hermann-Skillman potential with a Latter tail.

| Z | E (keV) | l | $\delta_l - \delta_0$ | | | |
|----|----------------------|----|-----------------------|-----------|---------|-----|
| | | | Analytic | Numerical | % error | |
| 13 | 3 ($\nu = 0.88$) | 1 | -0.725 | -0.771 | 6 | |
| | | 2 | -1.284 | -1.186 | 8 | |
| | | 3 | -1.249 | -1.441 | 10 | |
| | | 4 | -1.315 | -1.613 | 18 | |
| | 10 ($\nu = 0.48$) | 1 | -0.451 | -0.459 | 1.7 | |
| | | 2 | -0.674 | -0.694 | 2.8 | |
| | | 4 | -0.897 | -0.952 | 5.8 | |
| | | 6 | -0.989 | -1.098 | 9.9 | |
| | 30 ($\nu = 0.28$) | 1 | -0.271 | -0.273 | 0.7 | |
| | | 2 | -0.406 | -0.410 | 0.9 | |
| | | 4 | -0.554 | -0.566 | 2.1 | |
| | | 6 | -0.636 | -0.659 | 3.4 | |
| 36 | 10 ($\nu = 1.33$) | 10 | -0.714 | -0.771 | 7.4 | |
| | | 1 | -0.935 | -0.999 | 6.4 | |
| | | 2 | -1.463 | -1.612 | 9.2 | |
| | | 4 | -1.891 | -2.303 | 17.0 | |
| | 30 ($\nu = 0.77$) | 1 | -0.666 | -0.679 | 1.9 | |
| | | 2 | -1.021 | -1.050 | 2.7 | |
| | | 4 | -1.388 | -1.468 | 5.4 | |
| | | 6 | -1.548 | -1.711 | 9.5 | |
| | 100 ($\nu = 0.42$) | 1 | -0.401 | -0.403 | 0.5 | |
| | | 2 | -0.606 | -0.611 | 0.8 | |
| | | 4 | -0.835 | -0.848 | 1.5 | |
| | | 6 | -0.964 | -0.992 | 2.8 | |
| 79 | 30 ($\nu = 1.68$) | 10 | -1.096 | -1.167 | 6.0 | |
| | | 1 | -1.047 | -1.110 | 5.4 | |
| | | 2 | -1.711 | -1.854 | 7.7 | |
| | | 4 | -2.376 | -2.756 | 13.7 | |
| | 100 ($\nu = 0.92$) | 1 | -0.759 | -0.769 | 1.3 | |
| | | 2 | -1.188 | -1.211 | 1.8 | |
| | | 4 | -1.664 | -1.725 | 3.5 | |
| | | 6 | -1.910 | -2.032 | 6.0 | |
| | | | 8 | -2.036 | -2.243 | 9.2 |

momenta, i.e. in the region where screening effects are expected to be smaller. With increasing atomic number the lowest energies at which APT results for the phase shifts can be applied also increase since, to be able to use APT in the continuum case, one must in general have $\nu = a/p < 1$.

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