Analytic phase shifts for truncated and screened Coulomb potentials

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For a special class of truncated and screened Coulomb potentials, some analyticity properties of the phase shifts are deduced as functions of β, the truncation and screening parameter. Use of these properties and scale transformations leads to analytic expressions for the phase shifts, which are valid in the region of small β.

I. INTRODUCTION

The scattering phase shifts are essential for the analysis of the interaction between particles. Apart from providing an expression for the collision cross sections, they serve as an important source of information[1,2] regarding the nature of the interaction in general, and the bound states and resonances in particular. For example, a negative phase shift near the threshold implies either a repulsive interaction or the existence of the bound states. They play a dominant role in probing the electronic configuration of the atoms, and an analysis of their properties is necessary for the understanding of the atomic structures.

For most of the potentials, the scattering phase shifts cannot be obtained in closed forms, an important exception being the Coulomb potential for which analytic phase shifts are available. It is usually the case that the phase shifts have to be evaluated numerically, or by making use of an approximation method such as a perturbational or a variational approach.[3] However, these calculations do not elucidate the analytic structure of the phase shifts.

Here, we analyze the analyticity properties of the phase shifts for truncated and screened Coulomb potentials, as functions of the truncation and screening parameter β. These analyticity properties give us useful information about the general behavior of the phase shifts. Indeed, since they are singular at $\beta=0$, a knowledge of their analyticity properties is essential for obtaining an analytic expression for $\delta_l(\beta)$, valid near $\beta=0$. Specifically, for the truncated Coulomb potentials which arise in the case of scattering by a nucleus of finite size, we consider a class of potentials

$$V_t(r) = -\frac{\lambda}{(r^n+\beta)^{1/n}}, \tag{1}$$

while for the screened Coulomb potentials we consider a class of potentials which have the form

$$V_s(r) = -\lambda\left(\frac{1}{r} - \frac{1}{(r^n+\beta)^{1/n}}\right), \tag{2}$$

where n is a positive integer. It is shown that the scattering phase shifts δ_l as functions of β, satisfy the Herglotz property and hence have no poles or algebraic branch-point singularities with negative powers in the complex cut plane $-\pi < \text{phase}\beta < \pi$. It is also argued that $\delta_l(\beta)$ have a branch point at $\beta=0$, which with the knowledge of the imaginary part of $\delta_l(\beta)$ near $\beta=0$, allows us to obtain their leading singular behavior at $\beta=0$. We also obtain the leading terms in the analytic part of $\delta_l(\beta)$, so that together with the singular part, we have expressions for $\delta_l(\beta)$, which are valid in the neighborhood of $\beta=0$. These results are discussed in detail for specific cases of potentials (1) and (2). They are compared with the known results[4] of potential (2) with $n=3$.

In our earlier work[5] we had exploited the analyticity in β to obtain expressions for the bound-state energies for small β. The extension of these considerations to the analysis of phase shifts enhances the utility of the analytical approach in solving potential problems. We begin with a derivation of some general results.

II. GENERAL CONSIDERATIONS

Consider a collision process described by the Hamiltonian (in atomic units)

$$H=\tfrac{1}{2}p^2+V(r). \tag{3}$$

The equation satisfied by $u_l(r)=rR_l(r)$, where R_l is the radial part of the wave function, is

$$\frac{d^2u_l(r)}{dr^2}+\left(k^2-2V(r)-\frac{l(l+1)}{r^2}\right)u_l(r)=0, \tag{4}$$

with

$$u_l(0)=0, \tag{5}$$

$$u_l(r)\to\frac{1}{k}\sin\left(kr-\frac{l\pi}{2}+\delta_l\right)\quad\text{for } r\to\infty, \tag{6}$$

and $k^2=2E$. We first obtain an expression for $\text{Im}\delta_l$ in terms of $\text{Im}V(r)$.

A. $\mathrm{Im}\delta_l(\beta)$

Multiply Eq. (4) by $u^*(r)$, subtract from the equation its complex conjugate and integrate by parts, to obtain

$$\left(u_l^*(r)\frac{du_l(r)}{dr}-u_l(r)\frac{du_l^*}{dr}\right)\Big|_0^\infty = 2\int_0^\infty u_l^*(r)u_l(r)[V(r)-V^*(r)]dr. \quad (7)$$

On using Eqs. (5) and (6), one gets

$$\sin[2i\,\mathrm{Im}\delta_l(\beta)] = -4ik\int_0^\infty |u_l(r)|^2\,\mathrm{Im}V(r)dr, \quad (8)$$

where the dependence of $\delta_l(\beta)$ on k is suppressed. This relation leads to the result

$$\mathrm{Im}\delta_l(\beta) \to -2k\int_0^\infty |u_l(r)|^2\,\mathrm{Im}V(r)dr, \quad (9)$$

for $k\to 0$ or for $\mathrm{Im}V(r)\to 0$. It also leads us to the Herglotz property for $\delta_l(\beta)$.

B. Herglotz property

It can be easily deduced that for the potentials $V_t(r)$ and $V_s(r)$ given in Eqs. (1) and (2), one has for $\lambda>0$,

$$\frac{\mathrm{Im}\,V_t(r)}{\mathrm{Im}\,\beta}>0, \quad (10)$$

$$\frac{\mathrm{Im}\,V_s(r)}{\mathrm{Im}\,\beta}<0, \quad (11)$$

in the complex cut plane $-\pi<\mathrm{phase}\beta<\pi$, but $\mathrm{Im}\beta\neq 0$. Therefore, we deduce from Eq. (8) that

$$\frac{\mathrm{Im}\delta_l(\beta)}{\mathrm{Im}\beta}<0 \quad \text{for } V_t(r) \quad (12)$$

and

$$\frac{\mathrm{Im}\delta_l(\beta)}{\mathrm{Im}\beta}>0 \quad \text{for } V_s(r) \quad (13)$$

in the complex cut plane $-\pi<\mathrm{phase}\beta<\pi$, $\mathrm{Im}\beta\neq 0$. Thus the phase shifts $\delta_l(\beta)$ [or $-\delta_l(\beta)$] satisfy the Herglotz property. This immediately implies an important result that $\delta_l(\beta)$ have no poles in the complex cut plane $-\pi<\mathrm{phase}\beta<\pi$, $\mathrm{Im}\beta\neq 0$, since a pole would dominate in its neighborhood and can have any phase depending on the direction of approach to the pole. Similar arguments also exclude algebraic branch-point singularities with negative powers. These results are similar to the corresponding properties for the bound-state energies.[5]

C. Real and positive β

Consider Eq. (4) for two real potentials

$$\frac{d^2u_l^{(1)}}{dr^2}+\left(k^2-2V_1(r)-\frac{l(l+1)}{r^2}\right)u_l^{(1)}=0, \quad (14)$$

$$\frac{d^2u_l^{(2)}}{dr^2}+\left(k^2-2V_2(r)-\frac{l(l+1)}{r^2}\right)u_l^{(2)}=0. \quad (15)$$

Multiply Eq. (14) by $u_l^{(2)}$ and Eq. (15) by $u_l^{(1)}$, and integrate the difference by parts to obtain

$$\left(u_l^{(2)}\frac{du_l^{(1)}}{dr}-u_l^{(1)}\frac{du_l^{(2)}}{dr}\right)\Big|_0^\infty = 2\int_0^\infty u_l^{(2)}u_l^{(1)}[V_1(r)-V_2(r)]dr. \quad (16)$$

Using Eqs. (5) and (6) one obtains

$$\sin(\delta_l^{(2)}-\delta_l^{(1)}) = 2k\int_0^\infty u_l^{(2)}u_l^{(1)}[V_1(r)-V_2(r)]dr. \quad (17)$$

We now take $V_1(r)$ and $V_2(r)$ to have the same form, but differ only in the values of the parameter β, say β_1 and β_2. Then taking the limit $\beta_1\to\beta_2$ one gets

$$\frac{\partial\delta_l(\beta)}{\partial\beta} = -2k\int_0^\infty (u_l)^2\frac{\partial V}{\partial\beta}dr. \quad (18)$$

This is analogous to the Feynman-Hellmann theorem for bound-state energies. In view of Eq. (6) we then deduce that $\partial\delta_l(\beta)/\partial\beta$ exists if

$$\int_0^\infty\left|\frac{\partial V}{\partial\beta}\right|dr<\infty. \quad (19)$$

The above condition is satisfied by the potentials $V_t(r)$ and $V_s(r)$ in Eqs. (1) and (2) for real and positive definite β. Therefore, one has the result that $\delta_l(\beta)$ are analytic for real and positive β in the sense that the first derivative exists in this region. Furthermore, it is observed that since $\partial V_t(r)/\partial\beta>0$ and $\partial V_s(r)/\partial\beta<0$, for $\beta>0$ and $\lambda>0$, $\delta_l(\beta)$ are monotonically decreasing functions for $V_t(r)$ and monotonically increasing functions for $V_s(r)$. It may also be noted that $\delta_l(\beta)$ are real for real and positive β, and have an imaginary part given by Eq. (8), for real but negative β. This suggests that $\delta_l(\beta)$ are singular at $\beta=0$.

D. Dispersion and relations

We have shown that $\delta_l(\beta)$ for potentials $V_t(r)$ and $V_s(r)$ have no poles or branch-point singularities with negative powers in the complex cut plane $-\pi<\mathrm{phase}\beta<\pi$. If this result is supplemented with the assumption, indeed a serious assumption, that milder singularities such as logarithmic singularities are absent or unimportant, one can write the dispersion relations,

$$\delta_l(\beta)=\sum_{i=0}^{N-1} c_i\beta^i+\frac{\beta^N}{\pi}\int_{-\infty}^{0}\frac{\mathrm{Im}\,\delta_l(\beta')}{\beta'^N(\beta'-\beta)}d\beta', \tag{20}$$

where c_i are the subtraction constants which would be dictated by the asymptotic behavior of $\mathrm{Im}\,\delta_l(\beta)$. Actually, our interest in the dispersion relations is primarily for separating out the leading singular behavior at $\beta=0$, which is unaffected by the contributions of singularities away from the origin as also by the possible need for subtractions.

E. Subtraction constants

When the subtraction constants are present, they dominate the behavior of $\delta_l(\beta)$ for $\beta\to 0$. They can be calculated perturbatively.

The behavior of $V_t(r)$ and $V_s(r)$ for large r is of the form

$$V(r)\to -\frac{\lambda_1}{r}+\frac{\lambda_3}{r^3}+\frac{\lambda_4}{r^4}+\cdots, \tag{21}$$

where $\lambda_1=\lambda$ for $V_t(r)$ but $\lambda_1=0$ for $V_s(r)$. Here we have not shown the $1/r^2$ term since it can be absorbed in the angular-momentum term. Then, the radial equation satisfied by the wave function correct to first order in λ_3 and λ_4 is

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+\left(k^2-\frac{l(l+1)}{r^2}+\frac{2\lambda_1}{r}\right)R=2\left(\frac{\lambda_3}{r^3}+\frac{\lambda_4}{r^4}\right)R^{(0)}, \tag{22}$$

with $R^{(0)}$ being the solution for $\lambda_3=\lambda_4=0$. Substituting

$$x=2ikr,\qquad R(r)=e^{-ikr}(2ikr)^lF(r), \tag{23}$$

leads to

$$x\frac{d^2F}{dx^2}+(2l+2-x)\frac{dF}{dx}-\left(l+1+\frac{i\lambda_1}{k}\right)F=\left(\frac{4ik\lambda_3}{x^2}-\frac{8k^2\lambda_4}{x^3}\right)M\left(l+1+\frac{i\lambda_1}{k},2l+2,x\right), \tag{24}$$

where M is the confluent hypergeometric function

$$M(a,b,x)=1+\frac{a}{b}\frac{x}{1!}+\frac{a(a+1)}{b(b+1)}\frac{x^2}{2!}+\cdots. \tag{25}$$

The solution to this equation is

$$F=M+4ik\lambda_3F_2-\frac{8k^2\lambda_4}{6-2b}\times\left[\frac{1}{x^2}M+\frac{2}{(1+b)}\left(\frac{1}{x}+\frac{1}{b}\right)M'+\frac{2a}{b(1+b)}F_1+\left(\frac{6a}{1+b}-2\right)F_2\right], \tag{26}$$

where

$$M'=\frac{dM}{dx},$$

$$F_1=\frac{1}{b-1}\left(M\ln x+\frac{dM}{da}+2\frac{dM}{db}\right), \tag{27}$$

$$F_2=\frac{1}{2-b}\left(\frac{1}{x}M+\frac{2}{b}M'+\frac{2a-b}{b}F_1\right), \tag{28}$$

and the M functions are evaluated for $a=l+1+i\lambda_1/k$ and $b=2l+2$. The solution (26) was found essentially by operating the operator P,

$$P=x\frac{d^2}{dx^2}+(2l+2-x)\frac{d}{dx}-\left(l+1+\frac{i\lambda_1}{k}\right), \tag{29}$$

on dM/dx, dM/da, dM/db, $M\ln x$, etc., and using the equations satisfied by them, i.e.,

$$P\frac{dM}{dx}=\frac{dM}{dx}-\frac{d^2M}{dx^2},$$

$$P\frac{dM}{da}=M,$$

$$P\frac{dM}{db}=-\frac{dM}{dx},$$

$$P(M\ln x)=2\frac{dM}{dx}+\left(\frac{b-1}{x}-1\right)M, \tag{30}$$

$$P\left(\frac{M}{x}\right)=\left(\frac{2-b}{x^2}+\frac{b-2a}{bx}\right)M-\frac{2}{b}\left(\frac{dM}{dx}-\frac{d^2M}{dx^2}\right),$$

$$P\left(\frac{M}{x^2}\right)=\left(\frac{6-2b}{x^3}+\frac{2b-4a}{bx^2}\right)M-\frac{4}{bx}\left(\frac{dM}{dx}-\frac{d^2M}{dx^2}\right),$$

$$P\left(\frac{1}{x}\frac{dM}{dx}\right)=\frac{(2-b-x)a}{bx^2}M+\left(\frac{2+2b-x}{bx}\right)\left(\frac{dM}{dx}-\frac{d^2M}{dx^2}\right).$$

Taking suitable combinations of these equations then yields the solution (26) to Eq. (24).

For calculating the phase shifts, one takes the asymptotic limit of Eq. (26) and identifies the phase shifts δ_l by requiring F to be of the form

$$F\underset{r\to\infty}{\simeq}\sin\left(kr+\frac{\lambda_1}{k}\ln(2kr)-\frac{l_0\pi}{2}+\delta_l\right), \tag{31}$$

where l_0 is the angular-momentum quantum number which would be different from l if an interaction of the form $1/r^2$ is included. One finally gets

$$\delta_l = \theta(l) - \frac{\pi}{2}(l - l_0) - 4k\lambda_3 B_3 - 8k^2\lambda_4 B_4 + \cdots, \quad (32)$$

where

$$\theta(l) = \arg\Gamma\left(l+1-\frac{i\lambda_1}{k}\right), \quad (33)$$

$$B_3 = \frac{1}{2l(2l+1)(2l+2)} \times\left[\frac{2\lambda_1}{K}\left(\frac{\pi}{2} - \frac{d}{dl}\theta(l)\right) + (2l+1)\right], \quad (34)$$

and

$$B_4 = \frac{1}{2(2l-1)2l(2l+1)(2l+2)(2l+3)}\left[\left(2l(2l+2) + \frac{12\lambda_1^2}{k^2}\right)\left(\frac{\pi}{2} - \frac{d}{dl}\theta(l)\right) + \frac{6\lambda_1}{k}(2l+1)\right]. \quad (35)$$

The terms in Eq. (32) will be identified with the subtraction constants in dispersion relations (20).

F. Scale transformations

Here we show by means of scale transformations, that the scattering phase shifts for potentials $V_t(r)$ and $V_s(r)$ given in Eqs. (1) and (2), are functions, effectively, of only one variable. To see this we write the potentials in Eqs. (1) and (2) as functions of λ and β, and subject Eq. (4) to a Symanzik scale transformation[6,7]

$$r \to wr. \quad (36)$$

The resulting equation is

$$\frac{d^2u_l}{dr^2} + \left(k^2w^2 - 2V_{t,s}(\lambda w, \beta w^{-n}, r) - \frac{l(l+1)}{r^2}\right)u_l = 0. \quad (37)$$

Since the phase shifts are the same for Eqs. (4) and (37), one obtains

$$\delta_l(k, \lambda, \beta) = \delta_l(kw, \lambda w, \beta w^{-n}). \quad (38)$$

Two specific values of λ will be of interest. If we take $w = 1/\lambda$, one has

$$\delta_l(k, \lambda, \beta) = \delta_l\left(\frac{k}{\lambda}, 1, \beta\lambda^n\right), \quad (39)$$

so that effectively one has a function only of k/λ and $\beta\lambda^n$. Alternatively one could take $w = \beta^{1/n}$ in which case we have

$$\delta_l(k, \lambda, \beta) = \delta_l(k\beta^{1/n}, \lambda\beta^{1/n}, 1). \quad (40)$$

This relation is also quite useful, especially for $\beta \to 0$ in which case we need to consider only the case of the effective strength $\lambda\beta^{1/n} \to 0$. In the following sections we apply the results of this section to specific examples of truncated and screened Coulomb potentials.

III. TRUNCATED COULOMB POTENTIAL

We consider two specific examples of truncated Coulomb potentials, to illustrate the method of approach. The two examples are

$$V_t^{\mathrm{I}}(r) = -\frac{1}{r+\beta} \quad (41)$$

and

$$V_t^{\mathrm{II}}(r) = -\frac{1}{(r^2+\beta)^{1/2}}, \quad (42)$$

where in view of relation (39) we have taken $\lambda = 1$.

A. Leading singular part of $\delta_l(\beta)$ near $\beta = 0$

For obtaining the singular part of $\delta_l(\beta)$ near $\beta = 0$, we use Eq. (9) for real, negative β. Since

$$\mathrm{Im}V_t^{\mathrm{I}}(r) = \pi\delta(r - |\beta|), \quad (43)$$

$$\mathrm{Im}V_t^{\mathrm{II}}(r) = \frac{1}{(|\beta| - r^2)^{1/2}}, \quad r < |\beta| \quad (44)$$

for β approaching the negative, real axis from above, and

$$u_l(r) \xrightarrow[\beta\to 0]{} \frac{1}{\Gamma(2l+2)}\Gamma\left(l+1+\frac{i}{k}\right)r(2kr)^l e^{\pi/2k} \times e^{-ikr}M\left(l+1+\frac{i}{k}, 2l+2, 2ikr\right), \quad (45)$$

we obtain

$$\mathrm{Im}\delta_l(\beta) \xrightarrow[\beta\to 0_-]{} -\frac{\pi}{|\Gamma(2l+2)|^2}\left|\Gamma\left(l+1+\frac{i}{k}\right)\right|^2 \times \beta^{2l+2}(2k)^{2l+1}e^{\pi/k}, \quad \text{for } V_t^{\mathrm{I}}(r) \quad (46)$$

and

$$\mathrm{Im}\delta_l(\beta) \xrightarrow[\beta\to 0_-]{} \frac{\pi}{2|\Gamma(2l+2)|^2}\left|\Gamma\left(l+1+\frac{i}{k}\right)\right|^2 \times \beta^{(l+1)}(2k)^{2l+1}e^{\pi/k}, \quad \text{for } V_t^{\mathrm{II}}(r). \quad (47)$$

On using the dispersion relations (20), one obtains for the leading singular term in $\delta_l(\beta)$

$$\delta_l^{\mathrm{sing}}(\beta) = -\frac{1}{|\Gamma(2l+2)|^2}\left|\Gamma\left(l+1+\frac{i}{k}\right)\right|^2(2k)^{2l+1} \times e^{(\pi/k)}\beta^{2l+2}\ln\beta, \quad \text{for } V_t^{\mathrm{I}}(r) \quad (48)$$

and

$$\delta_l^{\text{sing}}(\beta) = (-1)^l \frac{1}{2|\Gamma(2l+2)|^2}\left|\Gamma\left(l+1+\frac{i}{k}\right)\right|^2 (2k)^{2l+1} \times e^{(\pi/k)}\beta^{l+1}\ln\beta, \quad \text{for } V_t^{\text{II}}(r). \tag{49}$$

B. Leading analytic part of $\delta_l(\beta)$ near $\beta = 0$

For obtaining the leading analytic terms for $\delta_l(\beta)$ near $\beta = 0$, we expand the potential in powers of β:

$$V_t^{\text{I}}(r) = -\frac{1}{r} + \frac{\beta}{r^2} - \frac{\beta^2}{r^3} + \frac{\beta^3}{r^4} - \cdots, \tag{50}$$

$$V_t^{\text{II}}(r) = -\frac{1}{r} + \frac{\beta}{2r^3} - \cdots. \tag{51}$$

The β term in $V_t^{\text{I}}(r)$ is taken into account by redefining l as

$$l(l+1) = l_0(l_0+1) + 2\beta, \tag{52}$$

where l_0 is the angular-momentum quantum number, which gives

$$l = l_0 + \frac{2\beta}{2l_0+1} - \frac{4\beta^2}{(2l_0+1)^3} + \frac{16\beta^3}{(2l_0+1)^5} - \cdots. \tag{53}$$

The β^2 and β^3 terms in the potentials, are treated perturbatively as in Sec. II E, and the results are given by Eq. (32) with $\lambda_3 = -\beta^2$ and $\lambda_4 = \beta^3$, i.e.,

$$\delta_{l_0}^{\text{anal}}(\beta) = \theta(l) - \frac{\pi}{2}\left(\frac{2\beta}{2l_0+1} - \frac{4\beta^2}{(2l_0+1)^3} + \frac{16\beta^3}{(2l_0+1)^5}\right) + 4k\beta^2 B_3 - 8k^2\beta^3 B_4 + \cdots, \quad \text{for } V_t^{I}(r) \tag{54}$$

where $\theta(l)$ is given in Eq. (33), and B_3 and B_4 are obtained from Eqs. (34) and (35) with $\lambda_1 = 1$.

For $V_t^{\text{II}}(r)$, the β term is treated perturbatively as in Sec. II E, and the result is given by Eq. (32) with $\lambda_3 = \frac{1}{2}\beta$, $\lambda_4 = 0$, i.e.,

$$\delta_{l_0}^{\text{anal}}(\beta) = \theta(l_0) - 2k\beta B_3 + \cdots, \tag{55}$$

with $\theta(l_0)$ given by Eq. (33) and B_3 given by Eq. (34) with $\lambda_1 = 1$.

C. $\delta_l(\beta)$ near $\beta = 0$

Combining the results for the singular and analytic parts of $\delta_l(\beta)$, we get an expression which is valid near $\beta = 0$. For $V_t^{I}(r)$ one has

$$\delta_0(\beta) = \theta(2\beta) - \pi\beta - 2\beta^2(\ln\beta)ke^{\pi/k} \times \left|\Gamma\left(1+\frac{i}{k}\right)\right|^2 + O(\beta^2), \quad \text{for } l_0 = 0 \tag{56}$$

$$\delta_{l_0}(\beta) = \theta(l) - \frac{\pi}{2}(l-l_0) + 4k\beta^2 B_3 - 8k^2\beta^3 B_4 - \beta^{2l_0+2}(\ln\beta)B + O(\beta^4), \quad \text{for } l_0 \geqslant 1 \tag{57}$$

where $\theta(l)$ is given by Eq. (33), l is given by Eq. (53), B_3 and B_4 are given by Eqs. (34) and (35) with $\lambda_1 = 1$, and

$$B = \frac{1}{|\Gamma(2l+2)|^2}\left|\Gamma\left(l+1+\frac{i}{k}\right)\right|^2 (2k)^{2l+1} e^{\pi/k}. \tag{58}$$

Similarly for $V_t^{\text{II}}(r)$ we have

$$\delta_0(\beta) = \theta(0) + \beta(\ln\beta)ke^{\pi/k}\left|\Gamma\left(1+\frac{i}{k}\right)\right|^2 + O(\beta) \tag{59}$$

and

$$\delta_{l_0}(\beta) = \theta(l_0) - 2k\beta B_3 + (-1)^l \tfrac{1}{2}\beta^{l+1}(\ln\beta)B + O(\beta^2), \quad \text{for } l_0 > 0 \tag{60}$$

where as before, $\theta(l_0)$ is given by Eq. (33), B_3 is given by Eq. (34) with $\lambda_1 = 1$, and B is given by Eq. (58).

IV. SCREENED COULOMB POTENTIAL

We will consider two specific examples of screened Coulomb potentials

$$V_s^{\text{I}}(r) = -\frac{1}{r} + \frac{1}{r+\beta} \tag{61}$$

and

$$V_s^{\text{II}}(r) = -\frac{1}{r} + \frac{1}{(r^3+\beta)^{1/3}}, \tag{62}$$

where in view of Eq. (39) we have taken $\lambda = 1$.

A. Leading singular part of $\delta_l(\beta)$ near $\beta = 0$

In order to be able to use Eq. (9) one notes that for real negative β,

$$\text{Im}V_s^{\text{I}}(r) = -\pi\delta(r - |\beta|), \tag{63}$$

$$\text{Im}V_s^{\text{II}}(r) = -\frac{\sin\pi/3}{(|\beta| - r^3)^{1/3}}, \quad r < |\beta| \tag{64}$$

with β approaching the negative real axis from above, and

$$u_l(r) \xrightarrow[\beta\to 0]{} \frac{1}{\Gamma(2l+2)}\Gamma(l+1)r(2kr)^l \times e^{-ikr}M(l+1, 2l+2, 2ikr). \tag{65}$$

We then get from Eq. (9)

$$\text{Im}\delta_l(\beta) \xrightarrow[\beta\to 0_-]{} \frac{\pi}{|\Gamma(2l+2)|^2}|\Gamma(l+1)|^2 \times \beta^{2l+2}(2k)^{2l+1}, \quad \text{for } V_s^{I}(r) \tag{66}$$

and

$$\text{Im}\delta_l(\beta) \xrightarrow[\beta\to 0_-]{} \frac{(\sin\pi/3)}{|\Gamma(2l+2)|^2}|\Gamma(l+1)|^2 \times (2k)^{2l+1}\beta^{2(l+1)/3} I_l, \quad \text{for } V_s^{\text{II}}(r) \tag{67}$$

where

$$I_l=\int_0^1 \frac{x^{2l+2}}{(1-x^3)^{1/3}}dx\,. \tag{68}$$

On using dispersion relations (20) one gets the leading singular term in $\delta_l(\beta)$:

$$\delta_l^{\rm sing}(\beta)=\frac{1}{|\Gamma(2l+2)|^2}|\Gamma(l+1)|^2(2k)^{2l+1}\times\beta^{2l+2}\ln\beta,\quad \text{for } V_s^{\rm I}(r) \tag{69}$$

and

$$\delta_l^{\rm sing}(\beta)=\frac{1}{|\Gamma(2l+2)|^2}|\Gamma(l+1)|^2\times(2k)^{2l+1}I_lJ_l(\beta)\,,\quad \text{for } V_s^{\rm II}(r) \tag{70}$$

where

$$\begin{aligned}J_l(\beta)&=\beta^{2(l+1)/3},\quad \text{for } l=0,3,6\ldots\\ &=-\beta^{2(l+1)/3},\quad \text{for } l=1,4,7,\ldots\\ &=\frac{\sin\frac{1}{3}\pi}{\pi}\beta^{2(l+1)/3}\ln\beta,\quad \text{for } l=2,5,8,\ldots.\end{aligned} \tag{71}$$

B. Leading analytic part of $\delta_l(\beta)$ near $\beta=0$

For obtaining the leading analytic terms in $\delta_l(\beta)$ near $\beta=0$, the potential is expanded in powers of β:

$$V_s^{\rm I}(r)=-\frac{\beta}{r^2}+\frac{\beta^2}{r^3}-\frac{\beta^3}{r^4}+\cdots\,, \tag{72}$$

$$V_s^{\rm II}(r)=-\frac{\beta}{3r^4}+\cdots\,. \tag{73}$$

The β term in $V_s^{\rm I}(r)$ is taken into account by redefining it as

$$l(l+1)=l_0(l_0+1)-2\beta\,, \tag{74}$$

where l_0 is the angular-momentum quantum number, which gives

$$l=l_0-\frac{2\beta}{2l_0+1}-\frac{4\beta^2}{(2l_0+1)^3}-\frac{16\beta^3}{(2l_0+1)^5}-\cdots\,. \tag{75}$$

The β^2 and β^3 terms in the potentials are treated perturbatively as in Sec. II E, and the results are given by Eq. (32) with $\lambda_3=\beta^2$, $\lambda_4=-\beta^3$, and $\lambda_1=0$, i.e.,

$$\delta_{l_0}^{\rm anal}(\beta)=\frac{\pi}{2}\left(\frac{2\beta}{2l_0+1}+\frac{4\beta^2}{(2l_0+1)^3}+\frac{16\beta^3}{(2l_0+1)^5}\right)-4k\beta^2D_3+8k^2\beta^3D_4+\cdots,\quad \text{for } V_s^{\rm I}(r) \tag{76}$$

where

$$D_3=\frac{1}{2l(2l+2)}, \tag{77}$$

$$D_4=\frac{\pi}{4(2l-1)(2l+1)(2l+3)}. \tag{78}$$

For $V_s^{\rm II}(r)$, the β term is treated perturbatively as in Sec. II E, and the result is given by Eq. (32) with $\lambda_3=0$ and $\lambda_4=-\frac{1}{3}\beta$, i.e.,

$$\delta_{l_0}^{\rm anal}(\beta)=\tfrac{8}{3}k^2\beta D_4+\cdots\,, \tag{79}$$

where D_4 is given in Eq. (78).

C. $\delta_l(\beta)$ near $\beta=0$

We now combine the results for the leading singular and analytic parts of $\delta_l(\beta)$ to get an expression which is valid near $\beta=0$. For $V_s^{\rm I}(r)$ one obtains

$$\delta_0(\beta)=\pi\beta+2\beta^2(\ln\beta)k+O(\beta^2)\,, \tag{80}$$

$$\delta_{l_0}(\beta)=-\frac{\pi}{2}(l-l_0)-4k\beta^2D_3+8k^2\beta^3D_4+\beta^{2l_0+2}(\ln\beta)D+O(\beta^4)\quad \text{for } l_0>0 \tag{81}$$

where l is given by Eq. (75), D_3 and D_4 are given by Eqs. (77) and (78), and

$$D=\frac{1}{|\Gamma(2l+2)|^2}|\Gamma(l+1)|^2(2k)^{2l+1}\,. \tag{82}$$

Similarly, for $V_s^{\rm II}(r)$ we have

$$\delta_0(\beta)=k\beta^{2/3}+O(\beta) \tag{83}$$

and

$$\delta_l(\beta)=\tfrac{8}{3}k^2\beta D_4+I_lJ_l(\beta)D+O(\beta^2),\quad l>0 \tag{84}$$

where I_l is given by Eq. (68), $J_l(\beta)$ is given by Eq. (71), and D is given by Eq. (82).

V. COMMENTS

We have obtained analytic expressions for the scattering phase shifts for special classes of truncated and screened Coulomb potentials given in Eqs. (1) and (2), in the region near $\beta=0$, where β is the truncation or screening parameter. These expressions include the leading singular terms and the analytic terms which correspond to the subtraction constants in the dispersion relations. We end our discussion with a few comments.

(1) In the cases considered, the phase shifts have either logarithmic singularities or algebraic branch-point singularities at $\beta=0$.

(2) Though the detailed expressions for the phase shifts have been given for $\lambda=1$, the phase shifts for arbitrary values of λ can be obtained by using relation (39) which follows from the scale transformation.

(3) Truncated Coulomb potentials come into play for scattering by a finite charge distribution. In particular, for scattering by a uniform spherical charge distribution, the potential near $r=0$

is simple harmonic and is Coulombic for large r. Such a potential is well simulated by $V_t^{II}(r)$ given in Eq. (42).

(4) For the scattering of an electron by a polarizable atom, the potential for large r is given by

$$V(r) \to -\frac{\alpha/2}{r^4} \quad \text{for } r \to \infty . \tag{85}$$

For this case O'Malley *et al.*[4] have given expressions for the phase shifts for $k \to 0$. Since $V_s^{II}(r)$ has an asymptotic behavior

$$V_s^{II}(r) \to -\frac{\beta/3}{r^4} \quad \text{for } r \to \infty . \tag{86}$$

We compare our results for $\beta = \frac{3}{2}\alpha$, with those of O'Malley *et al.*[4] The results are in agreement for $l > 0$ and for $l = 0$, our expression (83) gives the leading approximation for the Scattering length. This is indeed an interesting coincidence since our results are valid for $\beta \to 0$ whereas those of O'Malley *et al.* are valid for $k \to 0$. However, it can be shown that in the limit of $k \to 0$, the terms which are higher order in β vanish and hence the two results are consistent. Thus the results of O'Malley *et al.*[4] for $\delta_l(\beta)$, $l > 0$ are not only valid for $k \to 0$, but also for finite k with $\beta \to 0$. It is interesting to note that the wave function we have obtained in Eq. (26) is different from the solution of O'Malley *et al.* in terms of Mathieu functions. This is because we treat the $1/r^4$ part of the potential perturbatively. However, both the solutions differ in their behavior near $r = 0$, from the behavior required for the solution to the potential $V_s^{II}(r)$ in Eq. (62).

(5) In the case of potentials for which the $r \to \infty$ behavior is dominated by terms smaller than $1/r^4$, Eq. (22) for obtaining the subtraction terms, needs to be modified. For example, if

$$V(r) = -\frac{1}{r} + \frac{1}{(r^5 + \beta)^{1/5}} \to -\frac{\beta}{5r^6}, \quad r \to \infty \tag{87}$$

the term on the right-hand side of Eq. (22) should be replaced by $-\frac{2}{5}\beta r^{-6} R^{(0)}$. The solutions to the equation are considerably more complicated now. However, the singular terms are still relatively simple and can be obtained from Eqs. (9) and (20). They become

$$\delta_l^{\text{sing}}(\beta) = \left| \frac{\Gamma(l+1)}{\Gamma(2l+2)} \right|^2 (2k)^{2l+1} I_l J_l(\beta) , \tag{88}$$

where

$$I_l = \int_0^1 \frac{x^{2l+2}}{(1-x^5)^{1/5}} dx$$

and

$$J_l(\beta) = \beta^{(2l+2)/5} \frac{\sin \pi/5}{\sin \frac{2}{5}\pi(l+1)} \quad \text{for } l \neq 4, 9, \ldots$$

$$= \frac{1}{\pi} \beta^{(2l+2)/5} \ln\beta \quad \text{for } l = 4, 9, \ldots .$$

For $l = 0$ and 1, this is the dominant term in the limit $\beta \to 0$, whereas for $l > 1$, the subtraction terms are more important.

(6) The explicit expressions for $\delta_l(\beta)$ allow us to calculate the Boltzman sum[8] of phase shifts. For example, for $V_s^{II}(r)$ the Boltzman sum G_B is

$$G_B \equiv \sum_l (2l+1)\delta_l = ka - \frac{2\pi}{9}\beta k^2 + \frac{2\pi}{3}\beta k^2 \sum_{l=1}^{\infty} \frac{1}{(2l-1)(2l+3)} + O(k^3), \tag{89}$$

where the first two terms are the contribution from the s wave with a being the scattering length.[4] It can then be shown that

$$G_B = ka + O(k^3), \tag{90}$$

which allows us to calculate G_B in terms only of the scattering length a to a good approximation.

(7) Finally we note that the analysis we have discussed can be applied to other forms of screened Coulomb potentials such as

$$V(r) = -\frac{\lambda}{r}\left(\frac{\beta}{r+\beta}\right)^n . \tag{91}$$

It is also applicable to partially screened Coulomb potentials of the type

$$V(r) = -\frac{\lambda_1}{r} + \frac{\lambda_2}{(r^n + \beta)^{1/n}}, \quad \lambda_2 < \lambda_1 \tag{92}$$

which might be relevant for the scattering of electrons by ionized atoms.

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