BOUNDS FOR THE PHASE-SHIFTS OF MODIFIED COULOMB POTENTIALS

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In this paper we deduce bounds for the phase-shifts in the presence of the Coulomb potential, which, amongst other things, enables us to compute the energies or potential strengths for which these phase shifts become equal to $\pi/2$.

1. Introduction

Bounds for the phase-shifts of spherically symmetric potentials which have a short--range, i.e., which fall off faster than $(1/r)$ as $r \to \infty$ were recently obtained with useful deductions [1–3]. However, in several problems e.g., in the collisions of protons with protons or electrons with positive ions, we have to deal with modified Coulomb potentials, that is, those containing the Coulomb interaction together with a short-range component [4]. In the present paper, we shall try to obtain similar bounds for such modified Coulomb potentials. But in this case, considerable modification of the analysis is required.

2. The modified Coulomb potential

The radial Schrodinger equation reads,

$$\left[\frac{d^2}{dr^2} + K^2 - \frac{2\gamma K}{r} - U(r) - \frac{l(l+1)}{r^2}\right] U_l = 0,$$

$$u_l(r) \to r^{l+1} \quad \text{as} \quad r \to 0, \tag{1}$$

where $U(r)$ denotes the short-range part of the interaction, so that, $r^n U(r) \to 0$ as $r \to \infty$ for some $n > 1$. The asymptotic form of the solution can be taken to be [5],

$$u_l(r) \to B_l \exp(i\delta_l) [\sin(Kr - l\pi/2 - \gamma \log 2Kr + \sigma_l + \delta_l] \quad \text{as} \quad r \to \infty, \tag{2}$$

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with

$$B_l = (2\pi)^{-3/2}(1/K)(2l+1)i^l \exp(i\sigma_l).$$

In (2), the real quantity δ_l is the phase-shift due to the potential $U(r)$ in the presence of the Coulomb potential, and,

$$\sigma_l = \arg \Gamma(l+1+i\gamma).$$

Let $F_l(r; K)$ and $G_l(r; K)$ be respectively the regular and irregular spherical Coulomb wave functions, whose asymptotic behaviour is given by,

$$F_l(r; K) \to \sin(Kr - l\pi/2 - \gamma \log 2Kr + \sigma_l),$$

$$G_l(r; K) \to -\cos(Kr - l\pi/2 - \gamma \log 2Kr + \sigma_l), \quad \text{as} \quad r \to \infty. \tag{3}$$

$F_l(r; K)$ and $G_l(r; K)$ satisfy:

$$\left[\frac{d^2}{dr^2} + K^2 - \frac{2\gamma K}{r} - \frac{l(l+1)}{r^2}\right] w_l = 0. \tag{4}$$

Multiplying (1) by F_l and (4) by $u_l(r)$, then subtracting and integrating between 0 and R, we get:

$$u_l'(R)F_l(R) - F_l'(R)u_l(R) = \int_0^R U(r)u_l F_l(r; K)dr,$$

where we have used the fact that,

$$u_l'(0)F_l'(0) - F_l'(0)u_l(0) = 0$$

because, both u_l and $F_l \to$ Constant $\times (r^{l+1})$ as $r \to 0$.

We now let $R \to \infty$ and use the asymptotic forms of u_l and F_l as given in (2) and (3), to obtain,

$$KB_l \exp(i\delta_l) \sin \delta_l = -\int_0^\infty U(r)U_l F_l dr. \tag{5}$$

We shall next obtain an integral equation for u_l. For this, we adapt a well known technique [6].

We write,

$$u^l(r) = \alpha(r)F_l + \beta(r)G_l, \tag{6}$$

where we would like to choose $\alpha(r)$ and $\beta(r)$ such that,

$$\alpha'(r)F_l + \beta'(r)G_l = 0. \tag{7}$$

Remembering that $u_l(0) = 0 = F_l(0)$ and also comparing the asymptotic forms (2) and (3), we get,

$$\alpha(\infty) = B_l \exp(i\delta_l) \cos \delta_l, \quad \beta(0) = 0. \tag{8}$$

From (1), (6) and (7) we get,

$$\alpha'(r)F_l'+\beta'(r)G_l' = U(r)u_l.$$

Combining this with (7), we get,

$$\alpha'(r)\,(F_l'G_l-F_lG_l') = U(r)u_lG_l,$$

$$\beta'(r)\,(F_lG_l'-G_lF_l') = U(r)u_lF_l. \tag{9}$$

The Wronskian $F_lG_l'-G_lF_l' = K$, can be obtained from (3).
Integrating (9) and using the values of $\alpha(\infty)$ and $\beta(0)$ from (8), we get,

$$\alpha(r) = B_l\exp(i\delta_l)\cos\delta_l+\frac{1}{K}\int_r^\infty u_l(r')U(r')G_l(r')dr'$$

$$\beta(r) = \frac{1}{K}\int_0^r u_l(r')U(r')F_l(r')dr'.$$

Substituting these in (6), we get, finally,

$$u_l(r) = B_l\exp(i\delta_l)\cos\delta_lF_l(r)+\frac{F_l(r)}{K}\int_r^\infty u(r')u_l(r')G_l(r')dr'$$

$$+\frac{G_l(r)}{K}\int_0^r U(r')u_l(r')F_l(r')dr'. \tag{10}$$

Next in (1) we replace $U(r)$ by $\lambda U(r)$ to get

$$\left[\frac{d^2}{dr^2}+K^2-\frac{\gamma K}{r}-\lambda U(r)-\frac{l(l+1)}{r^2}\right]u_l(r;\lambda) = 0. \tag{11}$$

The phase-shift δ_l now depends on λ. We wish to show that:

$$KB_l^2\exp[2i\delta_l(\lambda)]\frac{\partial}{\partial\lambda}[\delta_l(\lambda)] = -\int_0^\infty U(r)\,[u_l(r;\lambda)]^2dr. \tag{12}$$

This is the analogue of a similar equation in the absence of the Coulomb potential [7]. (The equation is erroneously given in the reference [7]).

For this we need an equation similar to (11) with $\lambda+h$ in place of λ. Multiplying (11) by $u_l(r;\lambda+h)$ and the latter equation by $u_l(r;\lambda)$, subtracting, integrating between 0 and

∞ and invoking the forms of $u_l(r;\lambda)$ and $u_l(r;\lambda+h)$ when $r\to 0$ and $r\to\infty$ as given in (1) and (2), we get,

$$KB_l^2 \exp[i\delta_l(\lambda+h)+i\delta_l(\lambda)] \sin[\delta_l(\lambda+h)-\delta_l(\lambda)]$$
$$= -h\int_0^\infty U(r)u_l(r;\lambda)u_l(r;\lambda+h)dr,$$

whence, dividing by h and letting $h\to 0$ we get (12).

3. *The inequality*

For the potential $\lambda U(r)$, equation (5) reads,

$$KB_l \exp[i\delta_l(\lambda)] \sin \delta_l(\lambda) = -\lambda\int_0^\infty U(r)u_l(r;\lambda)F_l(r)dr. \tag{13}$$

Substituting in (13) the expression for $u_l(r)$ as given in (10) except that $\lambda U(r)$ replaces $U(r)$, we get finally,

$$K\tan\delta_l(\lambda) = -\lambda\int_0^\infty U(r)F_l^2(r)dr$$
$$-\lambda^2\int_0^\infty U(r)\frac{F_l(r)}{r}\left[F_l(r)\int_r^\infty U(r')F_l(r')G_l(r')dr'+G_l(r)\int_0^r U(r')F_l^2(r')dr'\right]dr+O(\lambda^3),$$

or,

$$K\tan\delta_l(\lambda) = -\lambda R_l-\lambda^2 S_l+O(\lambda^3), \tag{14}$$

where,

$$R_l \equiv \int_0^\infty U(r)F_l^2(r)dr,$$
$$S_l \equiv \int_0^\infty U(r)\frac{F_l(r)}{r}\left[F_l(r)\int_r^\infty U(r')F_l(r')G_l(r')dr'+G_l(r)\int_0^r U(r')F_l^2(r')dr'\right]dr. \tag{15}$$

Now, from (13), on using the Cauchy-Schwarz inequality, we get

$$K^2B_l^2\exp[2i\delta_l(\lambda)]\sin^2\delta_l(\lambda) \leqslant \lambda^2\int_0^\infty U(r)F_l^2dr\int_0^\infty U(r)\,[u_l(r;\lambda)]^2dr$$
$$= \lambda^2\int_0^\infty U(r)F_l^2dr\left\{-KB_l^2\exp[2i\delta_l(\lambda)]\frac{\partial}{\partial\lambda}[\delta_l(\lambda)]\right\},$$

on using (12). Whence we get,

$$1/\lambda^2 \leqslant (1/K)R_l \frac{\partial}{\partial\lambda}[\cot \delta_l(\lambda)].$$

On integrating with respect to λ when $0 < |\delta_l(\lambda)| < \pi$ in which case the integrand is continuous, we get,

$$[(1/\varepsilon)-(1/\lambda)] \leqslant (R_l/K)\,[\cot \delta_l(\lambda)-\cot \delta_l(\varepsilon)], \quad \text{or,}$$

$$(1/\varepsilon)+(R_l/K)\cot \delta_l(\varepsilon) \leqslant (1/\lambda)+(R_l/K)\cot \delta_l(\lambda). \tag{16}$$

On using (14), the left side of (16) becomes,

$$(1/\varepsilon)-\frac{R_l}{\varepsilon R_l+\varepsilon^2 S_l+O(\varepsilon^3)} \quad \text{which} \quad \to (S_l/R_l) \quad \text{as} \quad \varepsilon \to 0.$$

So, (16) now yields,

$$(1/\lambda)+(R_l/K)\,[\cot \delta_l(\lambda)] \geqslant (S_l/R_l).$$

$$(0 < |\delta_l(\lambda)| < \pi) \tag{17}$$

From (13) or (14), we can see that $\delta_l(\lambda) = 0$ when $\lambda = 0$, as is to be expected. We also note that $u_l(r;\lambda)$ is complex only through the normalization factor $B_l \exp(i\delta_l)$, as can be seen from (2). So, $u_l(r;\lambda)/\{B_l \exp[i\delta_l]\}$ is real. It follows from (12) that $\frac{\partial}{\partial\lambda}[\delta_l(\lambda)] \geqslant 0$ if $U(r) \leqslant 0$ everywhere, that is, if the potential is everywhere non-repulsive. As $\delta_l(0) = 0$, it follows that for $\lambda > 0$, $\delta_l(\lambda) \geqslant 0$. Also, in this case, from (15), $R_l < 0$.

Similarly if $U(r) \geqslant 0$, $\delta_l(\lambda) \leqslant 0$ for $\lambda > 0$ and R_l is also > 0. In either case, $-R_l \cot \delta_l(\lambda) = |R_l| \cot |\delta_l(\lambda)|$, and so from (17) we get,

$$(1/\lambda)-(S_l/R_l) \geqslant (1/K)\,|R_l| \cot |\delta_l(\lambda)|. \tag{18}$$

In particular, if $|\delta_l(\lambda)| \leqslant \pi/2$, then $\cot |\delta_l(\lambda)| > 0$ and we have,

$$\tan |\delta_l(\lambda)| \geqslant \frac{(1/K)\,|R_l|}{[(1/\lambda)-(S_l/R_l)]},$$

$$(|\delta_l(\lambda)| \leqslant \pi/2) \tag{19}$$

S_l and R_l are functions of known quantities only and are given by (15).

4. *Some deductions*

(*i*) From (18) we immediately deduce that if:
$|\delta_l(\lambda)| \leqslant \pi/2$, then $(1/\lambda) \geqslant (S_l/R_l)$ while, if, $(1/\lambda) \leqslant (S_l/R_l)$, then $|\delta_l(\lambda)| > \pi/2$.
(*ii*) For a modified Coulomb potential, it is known that [4]:

(A) Bound states occur for energies, $E_n = -2\pi^2 m(zz'e^2/h)^2(1/n')^2$, where, $n' = n-\mu_l(n)$, $n = 1, 2, 3 \ldots$; $\mu_l(n)$ is the quantum defect and for a pure Coulomb field, $\mu_l(n) = 0$

for all n and l. The quantum defect considered as a function of the energy K^2 can be extrapolated to positive energies, i.e., $\mu_l \equiv \mu_l(K^2)$, $K^2 > 0$ and is then given by

$$\cot [\pi\mu_l(K^2)] = \frac{\cot \delta_l}{1-\exp(\pi\beta/K)} \qquad (\beta = 2mzz'e^2/\hbar^2). \tag{20}$$

This relation is useful in calculating cross-sections for the collisions of electrons with positive ions.

(B) For low energy scattering, we have the analogue of the effective range formula:

$$c^2K \cot \delta_0 + \beta f(K) = -(1/a_c) + (1/2)K^2 r_0^c + O(K^4), \tag{21}$$

where

$$c^2 = \frac{2\pi\alpha}{\exp(2\pi\alpha)-1}, \quad \alpha = \beta/2K,$$

β as defined in (A) and

$$f(K) = -\Gamma - \log \alpha + \sum_s \frac{\alpha^2}{s(s^2+\alpha^2)},$$

Γ being Euler's constant. Equation (21) is useful in proton-proton scattering problems.

Now it follows from (19) that when $|\delta_l(\lambda)| \leqslant \pi/2$, for energies K^2 or potential strength λ such that,

$$(S_l/R_l) \approx (1/\lambda) \tag{22}$$

we have, $|\delta_l(\lambda)| \approx \pi/2$. When (22) is satisfied, (20) becomes,

$$\cot \pi\mu_l(K^2) = 0,$$

so that the quantum defect $\mu_l(K^2)$ can be calculated.

Similarly if (22) holds in the limit $K \to 0$ i.e., for low energies, then (21) simplifies to

$$\beta f(K) = -(1/a_c) + (1/2)K^2 r_0^c + O(K^4).$$

(*iii*) The scattering amplitude for a modified Coulomb potential is given by [5],

$$f(\theta) = f_c(\theta) + f_m(\theta),$$

where $f_c(\theta)$ is the known pure Coulomb amplitude and $f_m(\theta)$ is given by,

$$f_m(\theta) = (1/2iK) \sum_{l=0}^{\infty} \{(2l+1) \exp(2i\sigma_l) [\exp(2i\delta_l)-1] P_l(\cos\theta). \tag{23}$$

This shows that for energies K^2 or a potential strength, λ, such that $|\delta_l| \leqslant \pi/2$ (this being true in particular for high energies or large l when $\delta_l \approx 0$), if (22) holds then $|\delta_l| \approx \pi/2$ and the lth partial wave scattering dominates. Then (23) gives,

$$f_m(\theta) \approx -(1/iK)(2l+1) \exp(2i\sigma_l) P_l(\cos\theta).$$

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