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Some remarks on effective range formulae in potential scattering

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Abstract

In this paper, we consider the radial Schrödinger equation with a real-valued potential having spherical symmetry, and we present alternative proofs of very recent results on the necessary, as well as sufficient, conditions on the decrease of the potential at infinity for the validity of effective range formulae in 3D in low energy potential scattering (Khuri *et al* 2008 arXiv:0812.4054v1. See theorem 1 below. This paper also contains a careful study of the 2D case, with some amazing new results). Our proofs are based on compact formulae for the phase shifts. The sufficiency conditions have been well known for a long time. But the necessity of the same conditions for potentials keeping a constant sign at large distances are new. All these conditions are established here for dimension 3 and for all angular momenta $\ell \ge 0$.

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1. Introduction

We consider potential scattering in three dimensions with a real, local and spherically symmetric potential V(r) [1–3]. V(r) is assumed to be real, and locally L^1 . The spherical symmetry allows us to consider separately each angular momentum state ℓ , and study the corresponding radial Schrödinger equation. We begin with the *S*-wave ($\ell = 0$) in order to see clearly the main points without algebraic complications. We therefore have the following approximation, called the effective range formula, for the *S*-wave phase shift $\delta_0(k)$ [1–3]

$$k \operatorname{cotg} \delta_0(k) \underset{k \text{ small}}{\cong} -\frac{1}{a_0} + \frac{1}{2} r_0 k^2, \tag{1}$$

where k, in appropriate units, is the momentum of the particle. This formula was found to be very useful in the past for low energy scatterings of particles, especially for nucleon–nucleon

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scattering. The conditions for the validity of (1) are not very stringent. In general, for having a decent scattering theory, and finite phase shifts $\delta_{\ell}(k)$, continuous and bounded for all $\ell \ge 0$, and all $k \ge 0$, one needs only [1–3]

$$rV(r) \in L^1(0,\infty). \tag{2}$$

In case it is necessary to have a faster decrease of V(r) at infinity, we usually formulate it by $r^{\alpha}V(r) \in L^{1}(1, \infty)$, with some appropriate α . Obviously, if (2) is satisfied, then $r^{\alpha}V(r)$ is L^{1} at the origin for all $\alpha \ge 1$. We use the notation $r^{\alpha}V(r) \in L^{1}(1, \infty)$ instead of $r^{\alpha}V(r) \in L^{1}(0, \infty)$ in order to emphasize the faster decrease at infinity than given by (2). Under condition (2), one has then, at most, a finite number *n* of bound states, and the Levinson theorem [1–3]

$$\begin{cases} \delta_0(0) - \delta_0(\infty) = n\pi \text{ if no resonance at } E = k^2 = 0, \\ \delta_0(0) - \delta_0(\infty) = n\pi + \frac{\pi}{2} \text{ a resonance at } E = 0. \end{cases}$$
(3)

Usually, one chooses $\delta_0(\infty) = 0$. In the case of a resonance at $E = 0, a_0$ becomes infinite. We shall assume (2) throughout this paper.

Whatever the number of bound states *n*, one has then [3, 4]

(a) for having a finite scattering length a_0 , it is sufficient to have also

$$r^2 V(r) \in L^1(1,\infty);$$
 (4)

(b) and for having a finite effective range r_0 it is sufficient to have

$$V(r) \sim r^{-s}, \qquad s > 5. \tag{5}$$

Remark 1. Assuming only (2), the phase shifts $\delta_{\ell}(k)$ are defined only for real values of k, and without extra conditions on the decrease of the potential at infinity, they cannot be extended to complex values of k. However, if one assumes also an exponential decrease at infinity: $e^{2\mu r}V(r) \in L^1(1, \infty)$, then the *S*-matrix $S_{\ell}(k) = \exp[2i\delta_{\ell}(k)]$ is meromorphic in $|\text{Im } k| < \mu$, and one can extend (1) in this strip of the *k*-plane, which may contain the lowest bound states $k_j = i\gamma_j$, $\gamma_j < \mu$. This is the case for neutron–proton scattering. We refer the reader to [3] for more details.

Very recently, the above conditions have been made more precise [11]. Their essential points can be summarized as follows:

Theorem 1. For the S-wave, with (2) and in the absence of a resonance at $E = k^2 = 0$, if the potential V(r) keeps a constant sign beyond some finite R, then for having a_0 finite, it is both necessary and sufficient to have also $r^2V(r) \in L^1(1, \infty)$. Then, in order to have also r_0 finite, it is again necessary and sufficient to have also $r^4V(r) \in L^1(1, \infty)$.

One may ask then what happens to the second term in (1) when $r^4V(r)$ is not L^1 at infinity? This also has been studied for $V(r) \sim r^{-s}$ at infinity [4], and shown by Khuri *et al* in examples.

Remark 2. If the effective range formula (1) is exact for all k, the corresponding potential is decreasing exponentially at infinity [5]. It corresponds to a Jost function analytic in the whole k-plane, with one zero and one pole.

The purpose of the present paper is to give a different proof of theorem 1, and generalize also to all angular momenta $\ell \ge 0$.

We end this introduction by quoting the following general theorem, which will be useful for our proofs:

Theorem 2 (Hille [6]). Consider the differential equation

$$\phi_0''(r) - V(r)\phi_0(r) = 0.$$
(6)

If $rV(r) \in L^1(0, \infty)$, this equation has a unique solution $\chi_0(r)$ such that

$$\lim_{r \to \infty} \chi_0(r) = 1, \qquad \lim_{r \to \infty} \chi'_0(r) = 0.$$
(7)

If V(r) is real, and ultimately keeps a constant sign, the condition on V is both necessary and sufficient for the existence of such a solution χ_0 . There is also a solution $\phi_0(r)$, non-unique (modulo the addition of $\alpha \chi_0(r)$), such that

$$\lim_{r \to \infty} \frac{\varphi_0(r)}{r} = 1, \qquad \lim_{r \to \infty} \phi'_0(r) = 1.$$
(8)

If V(r) has a faster decrease at infinity, satisfying also the condition $r^2V(r) \in L^1(1, \infty)$, then $\chi_0(r)$ satisfies

$$\lim_{r \to \infty} r \left[\chi_0(r) - 1 \right] = 0, \qquad \lim_{r \to \infty} r^2 \chi_0'(r) = 0, \tag{9}$$

and there exists a unique solution $\psi_0(r)$ such that

$$\lim_{r \to \infty} [\psi_0(r) - r] = 0, \qquad \lim_{r \to \infty} r[\psi'_0(r) - 1] = 0.$$
(10)

Again, if V(r) keeps a constant sign, the extra condition $r^2V(r) \in L^1(1, \infty)$ is both necessary as well as sufficient for the existence of such a solution ψ_0 .

Obviously, ϕ_0 and χ_0 , or ψ_0 and χ_0 , are two independent solutions of (6) since the Wronskians at $r = \infty$, are, according to (7), (8) and (10),

$$\phi_0'\chi_0 - \phi_0\chi_0' = \psi_0'\chi_0 - \psi_0\chi_0' = 1.$$
⁽¹¹⁾

Remark 3. In general, $\phi_0(0) \neq 0$, so that, the solution $\varphi_0(r)$, with $\varphi_0(0) = 0$, is a linear combination of the fundamental solutions ϕ_0 and χ_0

$$\varphi_0(r) = \alpha \phi_0(r) + \beta_0 \chi_0(r). \tag{12}$$

Because of (7), φ_0 obviously satisfies (8). If we have $r^2 V(r) \in L^1(1, \infty)$, then $\varphi_0 = \psi_0 + \alpha \chi_0$, and because of (9), φ_0 satisfies also (10). The solution ψ_0 being unique, the same is true for φ_0 . Note that $\varphi_0(r)$ is given by the solution of the Volterra integral equation (here we normalized it to $\varphi'_0(0) = 1!$)

$$\varphi_0(r) = r + \int_0^r (r-t)V(t)\varphi_0(t) \,\mathrm{d}t, \tag{13}$$

whereas $\chi_0(r)$ is the solution of

$$\chi_0(r) = 1 + \int_r^\infty (t - r) V(t) \chi_0(t) \,\mathrm{d}t.$$
(14)

In case V(r) is positive, it is obvious on these equations, and on the basis of (2) and (6), that

(a) $\varphi_0(r)$ is an increasing convex function of r. Also $\varphi'_0(r)$ is increasing, and therefore, $\varphi'_0(r) \ge 1$ for all r. Assuming now also $r^2 V(r) \in L^1(1, \infty)$, one has

$$\varphi_0'(\infty) = A < \infty, \qquad A = \int_0^\infty r V(r) \varphi_0(r) \,\mathrm{d}r, \tag{15}$$

as seen on (13)

(b) $\chi_0(r)$ is a positive, convex and decreasing function, with $\chi_0(\infty) = 1$.

2. Proof of Theorem 1

The proof is based on the single formula for the phase shift [7]

$$\delta_0(k) = -k \int_0^\infty \frac{\varphi^2(k, r)}{\varphi'^2(k, r) + k^2 \varphi^2(k, r)} V(r) \,\mathrm{d}r,\tag{16}$$

where one assumes $V(r) \ge 0$, φ being the reduced radial wavefunction, solution of [1–4]

$$\begin{cases} \varphi''(k,r) + k^2 \varphi(k,r) = V(r)\varphi(k,r), \\ r \in [0,\infty), \quad \varphi(k,0) = 0, \quad \varphi'(k,0) = 1. \end{cases}$$
(17)

In some sense, (16) is an absolute definition of the phase shift since, for potentials satisfying (2), one has, automatically, $\delta_0(\infty) = 0$. Note that, in (16), the normalization of φ is irrelevant. However, we keep the normalization $\varphi'(k, 0) = 1$ for convenience. The formula (16) is valid for all k > 0. One can prove, in fact, the following:

Theorem 3. ([7]). Under the conditions $V(r) \ge 0$ and $rV(r) \in L^1(0, \infty)$, the formula (16) is valid for all $k \ge 0$, $\delta_0(k)$ is a continuous and bounded function, and $\delta_0(\infty) = 0$. It is also differentiable for k > 0. In order to have also differentiability at k = 0, with a finite derivative $\delta'(0)$, it is sufficient to add $r^2V(r) \in L^1(1, \infty)$. In making $k \downarrow 0$ in (16), the integral diverges, according to theorem 2 of Hille, if we only have $rV(r) \in L^1(0, \infty)$. However, there is the factor k in front of it, and the net result is $\delta_0(0) = 0$.

Remark 4. If we make k = 0 in (16), the denominator becomes $\varphi'^2(0, r)$. If there are bound states, $\varphi(0, r)$ has, according to the nodal theorem [8], *n* zeros in $(0, \infty)$. Between these zeros, it has maxima and minima, and so the integral is meaningless. In case of a resonance at k = 0, one has $\varphi(0, \infty) = \text{constant}$, and $\varphi'(0, \infty) = 0$, and so, again, the breakdown of (16). If $V(r) \ge 0$, there are no bound states, and no resonance at $E = k^2 = 0$ [1–3, 5].

Finiteness of a_0 . Consider now

$$a_0 = \lim_{k \downarrow 0} \frac{-\delta_0(k)}{k} \equiv -\lim_{k \downarrow 0} \frac{\delta_0(k) - \delta_0(0)}{k} = -\delta'(k=0),$$
(18)

assuming $V(r) \ge 0$. Therefore, according to theorem 3 above, (2) and $r^2 V \in L^1(1, \infty)$ are sufficient to secure that $\delta'(0)$ is finite, that is, a_0 is finite. So, in essence, [7] contains already the proof of the old result that $r^2 V \in L^1(1, \infty) \Rightarrow a_0$ finite.

From (16), we also have

$$a_0 = \int_0^\infty V(r) \frac{\varphi_0^2(r)}{\varphi_0'^2(r)} \,\mathrm{d}r.$$
 (19)

Again, on the basis of theorem 2 of Hille, $r^2 V \in L^1(1, \infty)$ is also necessary to make a_0 finite. This completes the proof of the first part of theorem 1. Finally, let us remark that, using $\varphi_0'' = V \varphi_0$ in (19), and integrating by parts, we find $a_0 = \lim_{R \to \infty} \left(R - \frac{\varphi_0(R)}{\varphi_0'(R)}\right)$ also a known result. Finiteness of r_0 . We must first compare (1) with (16). From the well-known expansion of $\cot x$

$$\cot g x = \frac{1}{x} - 2x \left(\frac{1}{6} + \frac{x^2}{90} + \frac{x^4}{945} + \cdots \right),$$
(20)

and using (δ_0 is an odd function of k [1–3])

$$\delta_0(k) = n\pi - ka_0 + bk^3 + \cdots, \qquad k \ge 0, \tag{21}$$

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we find easily

$$r_0 = \frac{2}{3}a_0 - \frac{2b}{a_0^2}.$$
(22)

We assume now, of course, that a_0 is finite. It follows that the finiteness of r_0 and b are completely equivalent. We can therefore concentrate ourselves on (16). Combining (16) and (19), we find

$$b = \lim_{k \downarrow 0} \frac{\delta_0(k) + ka_0}{k^3}$$

=
$$\lim_{k \downarrow 0} \frac{1}{k^2} \int_0^\infty V(r) \frac{\varphi^2(k, r) \varphi_0'^2(r) - \varphi_0^2(r) \varphi'^2(k, r) - k^2 \varphi_0^2 \varphi^2}{\varphi'_0^2(\varphi'^2 + k^2 \varphi^2)} dr.$$
 (23)

Writing now $\varphi^2 \varphi'_0^2 - \varphi_0^2 \varphi'^2 = (\varphi \varphi'_0 - \varphi_0 \varphi')(\varphi \varphi'_0 + \varphi_0 \varphi')$, we get, from (17) and $\varphi''_0 = V \varphi_0$, that $(\varphi \varphi'_0 - \varphi_0 \varphi')' = k^2 \varphi \varphi_0$. Since, at r = 0, φ and φ_0 vanish, and their derivatives are one (remember (2) !), we find

$$\varphi(k,r)\varphi'_{0}(r) - \varphi_{0}(r)\varphi'(k,r) = k^{2} \int_{0}^{r} \varphi(k,t)\varphi_{0}(t) \,\mathrm{d}t.$$
(24)

Therefore, taking the limit in (23), we find

$$b = \int_0^\infty V(r) \left(\frac{2\varphi_0(r)\varphi'_0(r) \int_0^r \varphi_0^2(t) \, \mathrm{d}t - \varphi_0^4(r)}{\varphi'_0^4(r)} \right) \mathrm{d}r.$$
(25)

Now, from the asymptotic behaviour of $\varphi_0(r) \sim r$, and $\varphi'(r) \sim 1$, for $r \to \infty$, one sees immediately that the fraction in (25) behaves exactly as $-\frac{1}{3}r^4$. It follows that, for $V(r) \ge 0, b$ is finite if and only if $r^4V(r) \in L^1(0, \infty)$. The same conclusions hold therefore for r_0 . The net conclusion is:

Theorem 1'. If $V(r) \ge 0$, (2) and $r^2 V(r) \in L^1(1, \infty)$ are both necessary and sufficient for having a_0 finite. And for having also r_0 finite, it is both necessary and sufficient to have $r^4 V(r) \in L^1(0, \infty)$. We must now include bound states.

Bound states. We shall choose, as is usually done, $\delta_0(\infty) = 0$. If there are bound states of energies $-\gamma_j^2$, $\gamma_j > 0$, j = 1, ..., n, one has the Levinson theorem (3): $\delta(0) \equiv \delta(0) - \delta(\infty) = n\pi$. One can define then

$$\widetilde{\delta}_0(k) = \delta_0(k) - 2\sum_{j=1}^n \operatorname{Arctg} \frac{\gamma_j}{k}.$$
(26)

One has now, again, $\delta(\infty) = 0$, and $\delta(0) = \delta(0) - n\pi = 0$. Using the inverse problem theory of Gel'fand and Levitan [5], one can calculate the potential $\tilde{V}(r)$ corresponding to $\delta(k)$. If we write

$$V(r) = V(r) + \Delta V(r), \tag{27}$$

it can be shown that the additional potential $\Delta V(r)$ has the following asymptotic behaviour [5]:

$$\Delta V(r) \underset{r \to \infty}{=} -\sum_{j=1}^{n} C_j e^{-\gamma_j \cdot r}, \qquad (28)$$

where C_j are positive constants. $\Delta V(r)$ keeps therefore a negative sign for large values of r, and is fast decreasing. We assume, of course, that V(r) is not exponentially decreasing for,

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otherwise, there would be no problem, and a_0 and r_0 would be finite. So, for the purpose of theorem 4, V and \tilde{V} are equivalent. Since \tilde{V} has no bound states, or a resonance at E = 0 because of $\tilde{\delta}(0) = 0$, the theorem applies to $\tilde{\delta}(k)$. Now, as it is easily seen by using the known expansion

Arctg
$$x = \frac{\pi}{2} - \frac{1}{x} + \frac{1}{3x^3} + \cdots,$$
 (29)

the coefficients of the expansions of $\delta_0(k)$ and $\tilde{\delta}_0(k)$ for small k, (21), are related to each other by (remember that, for $\tilde{\delta}(k)$, n = 0 in (21))

$$\begin{cases} \widetilde{a}_0 = a_0 - 2\sum_j \frac{1}{\gamma_j}, \\ \widetilde{b} = b - 2\sum_j \frac{1}{\gamma_j^3}. \end{cases}$$

$$(30)$$

They differ by finite quantities, and this completes the proof of theorem 1.

If there is a resonance at E = 0, in the first term in the sum in (26) there is no factor 2, and one has $\delta(0) = \frac{\pi}{2} + (n-1)\pi$. In this case, as we said before (remark 4), $\varphi_0(\infty) = C$, $\varphi'_0(\infty) = 0$, and so $a_0 = \infty$.

3. Higher ℓ

The validity of the usual scattering theory leading to a continuous and bounded phase shift $\delta_{\ell}(k)$ is, as we said in the introduction, secured always by $rV(r) \in L^1(0, \infty)$. Under this condition, the generalization of (16) for $\ell > 0$ is [7]

$$\delta_{\ell}(k) = -k \int_{0}^{\infty} \frac{\varphi_{\ell}^{2}(k, r)}{\left[(u_{\ell}'\varphi_{\ell} - u_{\ell}\varphi_{\ell}')^{2} + (v_{\ell}'\varphi_{\ell} - v_{\ell}\varphi_{\ell}')^{2} \right]} V(r) \,\mathrm{d}r, \tag{31}$$

where $u_{\ell}(kr)$ and $v_{\ell}(kr)$ are appropriately normalized spherical Bessel and Neumann functions, and $\varphi_{\ell}(k, r)$ the solution of the reduced radial Schrödinger equation [1–4]

$$\begin{cases} \varphi_{\ell}''(k,r) + k^{2}\varphi_{\ell}(k,r) = \left[V(r) + \frac{\ell(\ell+1)}{r^{2}}\right]\varphi_{\ell}(k,r),\\ \varphi_{\ell}(k,r) = \frac{r^{\ell+1}}{r \to 0} \frac{r^{\ell+1}}{(2\ell+1)!!} + \cdots \end{cases}$$
(32)

The effective range formula becomes now [1–3]

$$k^{2\ell+1} \operatorname{cotg} \delta_{\ell}(k) = -\frac{1}{a_{\ell}} + \frac{1}{2}r_{\ell}k^{2} + \cdots$$
(33)

In order to continue further, one needs now the equivalent of theorem 2 in the presence of the centrifugal potential $\ell(\ell + 1)/r^2$. One can prove very easily, by mimicking the proofs of theorem 2 [6], that one has

Theorem 2'. Consider the equation

$$\phi_0''(r) - V(r)\phi_0(r) = \frac{\ell(\ell+1)}{r^2}\phi_0(r).$$
(6')

If $rV(r) \in L^1(0, \infty)$, this equation has a unique solution $\chi_0(r)$ such that

$$\lim_{r \to \infty} r^{\ell} \chi_0(r) = 1, \qquad \lim_{r \to \infty} (r^{\ell} \chi_0(r))' = 0.$$
(7')

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If V(r) is real, and ultimately keeps a constant sign, the condition on V(r) is both necessary and sufficient for the existence of $\chi_0(r)$. There is also a solution $\phi_0(r)$, non-unique (modulo the addition of $\alpha \chi_0(r)$), such that

$$\lim_{r \to \infty} r^{-\ell - 1} \phi_0(r) = 1, \qquad \lim_{r \to \infty} (r^{-\ell} \phi_0(r))' = 1.$$
(8')

If V(r) satisfies also the condition $r^2 V(r) \in L^1(0, \infty)$, then $r^{\ell} \chi_0(r)$ satisfies

$$\lim_{r \to \infty} r[r^{\ell} \chi_0(r) - 1] = 0, \qquad \lim_{r \to \infty} r^2 (r^{\ell} \chi_0(r))' = 0, \tag{9'}$$

and there exists a unique solution $\psi_0(r)$ such that

$$\lim_{r \to \infty} [r^{-\ell} \psi_0(r) - r] = 0, \qquad \lim_{r \to \infty} r[(r^{-\ell} \psi_0(r))' - 1] = 0.$$
(10')

The solutions ϕ_0 and χ_0 , or ψ_0 and χ_0 , are two independent solutions of (6'), and their Wronskians are

$$\phi_0'\chi_0 - \phi_0\chi_0' = \psi_0'\chi_0 - \psi_0\chi_0' = (2\ell + 1).$$
(11')

Again, if V(r) keeps a constant sign beyond some *R*, the condition $r^2V(r) \in L^1(1, \infty)$ is both necessary and sufficient for the existence of ψ_0 . In short, one gets theorem 2' from theorem 2 by replacing χ_0 by $r^{\ell}\chi_0$, and ϕ_0 and ψ_0 by $r^{-\ell}\phi_0$ and $r^{-\ell}\psi_0$, and changing the right-hand side of (11) to (11'). From these formulae (7')–(10'), one can immediately obtain the asymptotic properties of χ'_0 , ϕ'_0 and ψ'_0 themselves, to be used in (31).

The proofs are based on the Volterra integral equation for χ_0 and ϕ_0 [1, 9]

$$\begin{cases} \chi_0(r) = r^{-\ell} - \int_r^\infty \frac{r^{\ell+1} r'^{-\ell} - r^{-\ell} r'^{\ell+1}}{(2\ell+1)} V(r') \chi_0(r') \, \mathrm{d}r', \\ \phi_0(r) = r^{\ell+1} - \int_r^\infty \frac{r^{\ell+1} r'^{-\ell} - r^{-\ell} r'^{\ell+1}}{(2\ell+1)} V(r') \phi_0(r') \, \mathrm{d}r', \end{cases}$$
(34)

by iterating them, starting from the zero order solutions $r^{-\ell}$ and $r^{\ell+1}$, respectively, and mimicking exactly the proof of theorem 2 of [6]. We leave the details to the reader. It is quite standard.

One can then continue the analysis, as was done for the S-wave, and one finds:

Theorem 4. In the absence of a bound state at E = 0, if the potential satisfies (2) and keeps a constant sign for r > R, then: (a) for having a finite a_{ℓ} , it is necessary and sufficient to have $r^{2\ell+2}V(r) \in L^1(1, \infty)$; (b) the effective range r_{ℓ} is finite if and only if $r^{2\ell+4}V(r) \in L^1(1, \infty)$. In case there is a bound state at zero energy (for $\ell \ge 1$, it is a real bound state at E = 0, with an L^2 wavefunction, instead of being a resonance. It contributes by π to the Levinson theorem), the scattering length a_{ℓ} is infinite [1–3], as in the case of a resonance when $\ell = 0$. This is obvious on (30), when making $\gamma_1 \downarrow 0$.

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