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Exact results on scattering by the potential $ae^{-\lambda r}/r$ with $\lambda = +0$

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Abstract. A new, non-perturbative, coordinate space method is formulated to calculate the full and partial wave amplitudes for the potential $ae^{-\lambda r}/r$ with $\lambda = +0$. The basic ingredients are a plausible use of the point Coulomb wave function up to moderate distances and a Wronskian identity to take care of the large distance behaviour of integrands.

Keywords. Screened Coulomb; amplitude; phase shift.

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1. Introduction

As is well known (Merzbacher 1962; Schiff 1968; Taylor 1974) the problem of quantum mechanical scattering by the 'point' Coulomb potential

$$V^{I}(r) = a/r, \qquad a = \text{constant} \tag{1}$$

has many unusual features. For example, the phase of the wave function develops a logarithmic distortion even at infinite distances, the conventional perturbation expansion breaks down, the differential cross-section becomes infinite in the forward direction, the on-shell full and partial wave amplitudes are both supposedly expressible (Merzbacher 1962; Schiff 1968) in closed form as

$$\text{full} \quad : \quad \frac{-2\beta k}{q^2}\exp[i\beta\log(4k^2/q^2)+2i\Delta_0] \tag{2a}$$

$$\text{partial:} \quad [\exp(2i\Delta_L)-1]/2ik \tag{2b}$$

but the partial wave Legendre series does not converge (Taylor 1974) in the usual sense, etc. Here k is the magnitude of the relative momentum, θ the centre of mass scattering angle, μ the reduced mass, $\beta = \mu a/k$ the Sommerfeld parameter, $\Delta_L = \arg\Gamma(L+1+i\beta)$ a real number corresponding to the Lth partial wave, and

$$q^2 = (\mathbf{k}-\mathbf{p})^2 = 2k^2(1-\cos\theta) \tag{3}$$

is the square of the momentum transfer from the initial free state $|\mathbf{k}\rangle$ to the final free state $|\mathbf{p}\rangle$ (units $\hbar = c = 1$). Equations (2a) and (2b) cannot be connected to each other by a strict $P_L(\cos\theta)$ projection.

The above problems caused by the long-range nature of (1) can be overcome and the whole issue rendered mathematically precise by introducing the 'screened' Coulomb field (Dalitz 1951; Weinberg 1965; Semon and Taylor (1976, 1977)

$$V(r) = ae^{-\lambda r}/r, \qquad \lambda \to +0 \tag{4}$$

where the screening parameter (photon mass) λ tends to zero at the end of the calculation. For finite λ the solution of the Schrödinger equation corresponding to the *Yukawa* form (4) is not known and approximation schemes (such as the Born series and eikonal treatment) have been employed in the past. Indeed by performing explicitly the relevant momentum-space integrals Dalitz (1951) has conjectured that the non-relativistic Born series generated by (4) can be summed up to all orders in the coupling constant β so as to yield a new amplitude (labelled by the superscript D) in the non-forward directions as

$$f^{D}(k, \theta) = \frac{-2\beta k}{q^2} \exp\left[i\beta \log\frac{\lambda^2}{q^2}\right] + 0\left(\frac{\lambda}{q}\right), \quad \theta > 0 \tag{5}$$

Two important features of the Dalitz amplitude (5) are worth mentioning: the first Born approximation of the point Coulomb field has been effectively multiplied by a log-divergent unitary phase factor so that the Rutherford cross-sections produced by (2a) and (5) exactly coincide; and the correction terms on the right-hand-side of (5) go smoothly to zero with λ in contrast to the relativistic case in which additional IR-finite terms (Yennie *et al* 1961) do survive. Unfortunately, the derivation of (5) has at least four unsatisfactory characteristics: (i) The treatment is perturbative in spirit and the evaluation of the individual momentum space integrals in high orders is quite tedious in practice. (ii) A natural logical prescription to handle the singularity at $q = 0$ is not available in (5). (iii) The corresponding expression for the partial wave amplitude $f_L(k)$ in terms of the formal matrix element of the potential has not been given by Dalitz (1951) so that the exact phase shift δ_L produced by the field (4) remains unknown. (iv) The question of computing $f_L(k)$ through a $P_L(\cos\theta)$ projection of (5) also remains unanswered in the literature.

It may be remarked that significant progress in tackling items (i) and (iii) above has been achieved by Semen and Taylor (1976, 1977) who have applied the semiclassical eikonal approximation to the screened Coulomb potential (4). They have confirmed that the full 3-dimensional eikonal amplitude also has the peculiar phase factor present in $f^{D}(k, \theta)$ above, and the eikonal phase shift is simply given by

$$\delta_L^{\text{eik}} = \beta \log kb + \beta\gamma + \beta \log(\lambda/2k) \tag{6}$$

where $b = (L + \frac{1}{2})/k$ is the impact parameter and γ the Euler constant. However, it is not known in what way the inferences drawn in the work of Semon and Taylor will be modified if the assumptions behind the eikonal approach are relaxed.

This paper provides a new, non-perturbative, mathematical answer to items (i)–(iii) mentioned above, leaving item (iv) for a future communication. For the sake of ready reference § 2 summarizes relevant formulae corresponding to the point Coulomb case, the integral representations of the wave functions $\psi^{\prime}(\mathbf{y})$ and $\psi^{\prime}_L(y)$ being crucial for our purpose where $\mathbf{y} = k\mathbf{r}$. In § 3 a plausibility argument is given as to why the wave function $\psi(\mathbf{y})$ and amplitude $f(k, \theta)$ for the screened potential (4) can be generated through the conventional Lippmann-Schwinger formalism by inserting the point Coulomb quantities within the integrands. Three central lemmas then lead to the evaluation of $f(k, \theta)$ and $f_L(k)$ in the *closed* form; it is found that $f(k, \theta)$ is the same as

$f^D(k, \theta)$ (cf. (5)) with q^2 replaced by $q^2 + \lambda^2$ at all angles while the phase shift δ_L becomes a straight generalization of the form (6). The plausibility argument of §3 is made rigorous in §4 through a fourth lemma which proves why the contribution from the large y domain of integration *cannot* alter any of the above findings. Finally, §5 summarizes the main conclusions of the paper.

2. Pure Coulomb quantities

The regular scattering solution to the 3-dimensional Schrödinger equation for (1) is expressible (Schiff 1968) in terms of the confluent hypergeometric function M, or a suitable integral representation (Abramowitz and Stegun 1970) thereof, as

$$\psi^I(\mathbf{y}) = \exp(i\hat{k}\cdot\mathbf{y})M(-i\beta, 1, iy - i\hat{k}\cdot\mathbf{y}) \tag{7}$$
$$= \int_0^1 \mathrm{d}u\, g(u)\exp[iyu + i\hat{k}\cdot\mathbf{y}(1-u)]$$

where $\hat{k}$ is a unit vector along the direction of the incident beam, and

$$\mathbf{y} = k\mathbf{r},\; g(u) = \frac{u^{-i\beta-1}(1-u)^{i\beta}}{\Gamma(-i\beta)\Gamma(1+i\beta)} \tag{8}$$

In order to guarantee convergence of the integral over u in (1) we can take $0 < \mathrm{Im}\,\beta < 1$ in the beginning but set $\mathrm{Im}\,\beta = +0$ at the end. If we expand

$$\psi^I(\mathbf{y}) = \sum_{L=0}^{\infty} i^L(2L+1)\psi^I_L(y)P_L(\cos\theta_y) \tag{9}$$

then the radial wave function can also be expressed (Schiff 1968) in terms of a confluent (Abramowitz and Stegun 1970) hypergeometric M as

$$\psi^I_L(y) = c_L y^L \exp(-iy)M(L+1-i\beta, 2L+2, 2iy)$$
$$= \int_0^1 \mathrm{d}u\, g_L(u)(2y)^L \exp[iy(2u-1)] \tag{10}$$

where

$$c_L = 2^L\Gamma(L+1+i\beta)/[\Gamma(2L+2)\Gamma(1+i\beta)]$$
$$g_L(u) = u^{L-i\beta}(1-u)^{L+i\beta}/[\Gamma(1+i\beta)\Gamma(L+1-i\beta)] \tag{11}$$

Note that throughout $0 < y < \infty$ one has

$$\arg\psi^I_L(y) = \arg c_L = \Delta_L - \Delta_0 \tag{12}$$

We also need the asymptotic behaviour for $y \gg L + \frac{1}{2}$:

$$\psi^I_L(y) \xrightarrow[y\to\infty]{} \frac{1}{2i}[\exp(2i(\Delta_L - \Delta_0))N^*(y)h_L^+(y) - N(y)h_L^-(y)] \tag{13}$$

with $h_L^{\pm}(y) = n_L(y) \pm ij_L(y)$ = spherical Hankel function,

$$N(y) = \exp(\beta\pi/2 + i\beta\log 2y)/\Gamma(1+i\beta) \tag{14}$$

The numbers β and Δ_L were defined just before (3).

3. The screened Coulomb case

Given any positive λ however small, (4) represents a Yukawa potential for which the standard Lippmann-Schwinger form

$$\psi(\mathbf{y}) = \exp(i\hat{k}\cdot\mathbf{y}) + \int d^3y' G^0(\mathbf{y},\mathbf{y}')U(y')\psi(\mathbf{y}') \tag{15}$$

holds at all points . Here the free coordinate-space Green's function G^0 and reduced potential U are defined by

$$\begin{aligned} G^0(\mathbf{y},\mathbf{y}') &= -\exp(i|\mathbf{y}-\mathbf{y}'|)/(4\pi|\mathbf{y}-\mathbf{y}'|) \\ U(y) &= 2\mu V(r)/k^2 = 2\beta\exp(-\tilde{\lambda}y)/y \\ \tilde{\lambda} &= \lambda/k \ll 1 \end{aligned} \tag{16}$$

We now give a crucial 'plausibility argument' which shows why the desired quantities corresponding to the screened Coulomb case can be deduced from the knowledge (7)–(14) of the point Coulomb problem. Let us start by observing that, to within terms of relative order $\tilde{\lambda}y$, the interactions (1) and (4) essentially coincide in the region $0 \leqslant r \ll \lambda^{-1}$, *i.e.*, $0 \leqslant y \ll \tilde{\lambda}^{-1}$ implying that their regular Schrödinger solutions must become proportional to each-other in the said domain:

$$\psi(\mathbf{y}) = A\psi^I(\mathbf{y})[1 + 0(\tilde{\lambda}y)], \qquad 0 \leqslant y \leqslant y_0$$

with $\quad 1 \ll y_0 \ll 1/\tilde{\lambda} \qquad (17)$

Here A is a proportionality constant and the choice of the demarcation point y_0 is somewhat arbitrary (*e.g.* taking $y_0 = 10^{-3}/\tilde{\lambda}$ causes an error of not more than 0·1 % in the first line of (17)). Of course, in the region $y \gg y_0$ the solution $\psi(\mathbf{y})$ may become substantially different from the pure Coulomb value $A\psi^I(\mathbf{y})$. Luckily, as will be proved in § 4 this *cannot* change any result obtained in the present section.

Next, we observe that for small or moderate $y < y_0$ and due to the exponentially damped nature of $U(y')$ the integral on the right-hand-side of (15) should get most contribution from the integration domain $y' < \tilde{\lambda}^{-1}$, *i.e.*, the choice (17) of $\psi(\mathbf{y})$ should satisfy the two sides of (15). This plausible criterion will now be used to fix the coefficient A.

Lemma 1 To within terms of relative order $\tilde{\lambda}$ the normalization constant A is given by

$$A = (i\lambda/2k)^{i\beta} = \exp[-\beta\pi/2 + i\beta\log(\lambda/2k)] \tag{18}$$

Proof Substitution of (17) into (15) gives the following condition at the origin $\mathbf{y} = \mathbf{0}$:

$$\psi(\mathbf{0}) = A = 1 + \int d^3y' \left\{\frac{-e^{iy'}}{4\pi y'}\right\} U(y')A\psi^I(\mathbf{y}') \tag{19a}$$

Dropping the prime over y, recalling the value of $U(y)$ from (16), and employing the integral representation (7) of $\psi^I(\mathbf{y})$ we rewrite (19a) as

$$A = 1 - A2\beta\int_0^1 du\, g(u) X_1(u), \quad \text{say, with} \tag{19b}$$

$$\begin{aligned} X_1(u) &= \int d^3y \frac{1}{4\pi y^2}\exp[-\tilde{\lambda}y + i(1+u)y + i(1-u)\hat{k}\cdot\mathbf{y}] \\ &= \frac{1}{2i(1-u)}\log\left\{1 + \frac{2i(1-u)}{\tilde{\lambda}-2i}\right\} \end{aligned} \tag{20}$$

In simplifying $X_1(u)$ the polar axis of y space was taken along $\hat{k}$ and the radial integral performed using the standard tables (Gradshteyn and Ryzhik 1973). In (20) let us expand the log in a convergent power series, insert back into (19b), and carry out the integration term-by-term with the help of the definition (8) of $g(u)$. The resulting series is readily summed up and the value of A solved from (19b) as

$$A = [(\tilde{\lambda} - 2i)/\tilde{\lambda}]^{-i\beta}$$

which proves lemma (18) in the limit $\tilde{\lambda} = \lambda/k \to 0$.

Having determined A let us proceed to derive the primary result of this paper stated in the form of the next proposition.

Lemma 2 To within terms of relative order $\tilde{\lambda}$ the complete 3-dimensional scattering amplitude for the potential (4) is obtained from

$$f(k, \theta) = \frac{-2\beta k}{q^2 + \lambda^2} \exp\left\{ i\beta \log\left(\frac{\lambda^2}{q^2 + \lambda^2}\right)\right\} \tag{21}$$

Proof Recalling the notation of (3) we start from

$$kf(k, \theta) = -(2\mu k/4\pi)\langle \mathbf{p}|V|\psi\rangle \tag{22a}$$

Once again, since most contribution to the integral should come from the region $r < \lambda^{-1}$ it is plausible to replace ψ by $A\psi^I$ in view of (17). Use of (7) then converts (22a) into

$$kf(k, \theta) = -2\beta A \int_0^1 \mathrm{d}u\, g(u) X_2(u), \quad \text{with} \tag{22b}$$

$$X_2(u) = \int \mathrm{d}^3 y \frac{1}{4\pi y} \exp[-\tilde{\lambda} y + iuy - i\hat{p}\cdot \mathbf{y} + i(1-u)\hat{k}\cdot \mathbf{y}]$$
$$= k^2/[(q^2 + \lambda^2)(1 - Ju)] \tag{23}$$

where $J = (q^2 + 2ik\lambda)/(q^2 + \lambda^2)$. In performing the $\mathrm{d}^3 y$ integration we have taken the polar axis along $(1-u)\hat{k} - \hat{p}$. Using (23) along with standard tables (Gradshteyn and Ryzhik 1973) we can simplify (22b) as

$$kf(k, \theta) = -2\beta A k^2 (1 - J)^{i\beta}/(q^2 + \lambda^2)$$

which establishes the lemma (21) because A is known from (18).

The next proposition deals with the evaluation of the amplitude corresponding to a given orbital angular momentum.

Lemma 3 To within terms of relative order λ the partial wave amplitude generated by (4) reads

$$f_L(k) = [\exp(2i\delta_L) - 1]/2ik;\ \delta_L = \Delta_L - \Delta_0 + \beta \log(\lambda/2k) \tag{24}$$

Proof (for s-wave). Since the algebra for general L is rather tedious we present here the proof for the $L = 0$ case. By definition

$$kf_0(k) = -\int_0^\infty \mathrm{d}y\, y^2 j_0(y) U(y) \psi_0(y) \tag{25a}$$

From (17) we can replace $\psi_0(y)$ by $A\psi_0^I(y)$ and make an appeal to the integral representation (10) so as to get

$$kf_0(k) = \frac{-2\beta A}{2i}\int_0^1 \mathrm{d}u\, g_0(u) X_3(u), \quad \text{with} \tag{25b}$$

$$X_3(u) = \int_0^\infty \mathrm{d}y [\exp(iy) - \exp(-iy)] \exp(-\tilde{\lambda}y + i(2u-1)y)$$
$$= 1/[\tilde{\lambda} - 2iu] - 1/[\tilde{\lambda} + 2i(1-u)] \tag{26}$$

Inserting this value in (25b) and carrying out the u integration (Gradshteyn and Ryzhik 1973) yields

$$kf_0(k) = \frac{-A}{2i}[(i\tilde{\lambda}/2)^{-i\beta} - (-i\tilde{\lambda}/2)^{i\beta}], \quad L = 0$$

which agrees with lemma (24) because A is known from (18). This completes our calculation of the various observable quantities based on the plausibility argument (17).

4. Large y integration region

A major source of trouble in the above derivations may be expected to arise from the fact that when $y \gg y_0$ the unknown solution of the Yukawa potential (4) will not be proportional to the known solution of the Coulomb problem (1) so that the integrands appearing in (15) (22a) and (25a) become unknown for $y > y_0$. That this does not pose any real difficulty is shown in the following proposition.

Lemma 4 Even if $\psi(\mathbf{y}) - A\psi^I(\mathbf{y})$ is non-vanishing for $y > y_0$ the results of lemmas 1–3 remain unaffected to within terms of relative order $\tilde{\lambda}$ or $1/y_0$ if A has the precise value (18).

Proof We recall that the right-hand-side of (19a) was obtained *via* the replacement of $\psi(\mathbf{y}')$ by $A\psi^I(\mathbf{y}')$. Therefore, dropping the prime over y, the validity of (19a) will remain intact if we can demonstrate that the correction term

$$Z = \int \frac{\mathrm{d}^3 y}{4\pi} \frac{\exp(iy)}{y} U(y)[\psi(\mathbf{y}) - A\psi^I(\mathbf{y})] \tag{27}$$

vanishes. Upon angular integration in (27) we pick up the s-wave ($L = 0$) component of ψ and ψ^I while the equality (17) guarantees that the lower limit of radial integration becomes y_0. Furthermore, the term involving $\psi_0(y)$ can be handled through a Wronkian (notation W) identity as (cf. equation (13))

$$\int_{y_0}^\infty \mathrm{d}y\, y^2 h_0^+(y) U(y) \psi_0(y) = [W(yh_0^+, y\psi_0)]_{y_0}^\infty$$
$$= 1 - AN(y_0) + 0(\tilde{\lambda}) \tag{28}$$

while the term involving $\psi_0^I(y)$ can be explicitly integrated using the large y behaviour (13), (14) of the radial Coulomb functions:

$$A\int_{y_0}^\infty \mathrm{d}y\, y^2 h_0^+(y) U(y) \psi_0^I(y)$$
$$= A[(i\tilde{\lambda}/2)^{-i\beta} - N(y_0)] + 0(1/y_0) \tag{29}$$

Subtracting (29) from (28) we find that the quantity Z vanishes if A has the value (18). Similarly for the correction terms to be added to the right-hand-sides of (22b) and (25b).

5. Summary and conclusions

It was pointed out in § 1 that the theoretical treatment of scattering by the screened Coulomb field (4) raises many mathematical questions which deserve serious attention. The present paper aims at answering some of these issues and the salient features of the work may be summarized as follows:

(i) Our derivation of lemmas 1–4 is *non-perturbative* in spirit and the handling of various coordinate space integrals is straightforward unlike the momentum space Born series method of Dalitz (1951). Further, all our findings become *exact* in the limit $\tilde{\lambda} = \lambda/k \rightarrow 0$ in contrast to the lowest order eikonal approach of Semon and Taylor (1976, 1977)

(ii) Using the pure Coulomb wave function itself we are able to deduce the *full* screened Coulomb amplitude $f(k, \theta)$ (cf. (21) which agrees with the Dalitz result $f^D(k, \theta)$ (cf. (5)) except that q^2 gets replaced by $q^2 + \lambda^2$ at *all* angles. The fact that $\psi - A\psi^I$ may be non-zero for large y causes no difficulty as shown by the vanishing of the correction Z (cf. (27)).

(iii) The corresponding *partial* wave amplitude $f_L(k)$ is also obtainable analytically (cf. (24)) and the phase shift δ_L has a close analogy with the result (6) of Semon and Taylor (1976, 1977).

(iv) An interesting question is whether the validity of $f_L(k)$ in (24) can be checked by taking a straight $P_L(\cos\theta)$ projection of $f(k, \theta)$ in (21). The answer is in the *affirmative* but the proof will be published elsewhere.

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