Monotonic properties of the shift and penetration factors

Carl R. Brune*

Edwards Accelerator Laboratory, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, USA

Gerald M. Hale† and Mark W. Paris‡

T-2 Nuclear & Particle Physics, Astrophysics, & Cosmology Theoretical Division, Los Alamos National Laboratory Los Alamos, New Mexico 87545, USA

(Received 22 August 2017; published 5 February 2018)

We study derivatives of the shift and penetration factors of collision theory with respect to energy, angular momentum, and charge. Definitive results for the signs of these derivatives are found for the repulsive Coulomb case. In particular, we find that the derivative of the shift factor with respect to energy is positive for the repulsive Coulomb case, a long anticipated but heretofore unproven result. These results are closely connected to the properties of the sum of squares of the regular and irregular Coulomb functions; we also present investigations of this quantity.

DOI: 10.1103/PhysRevC.97.024603

I. INTRODUCTION

The shift and penetration factors occur in the theoretical description of nuclear, atomic, and molecular scattering and reactions, particularly in R-matrix descriptions of such processes [1,2]. These quantities are defined to be the real and imaginary parts of the logarithmic radial derivative of the outgoing Coulomb function, as given below by Eq. (5). They play a central role in determining how physical quantities, such as cross sections and resonance widths, depend upon energy, angular momentum, and charge.

This study is motivated by a desire to understand the sign of the energy derivative of the shift factor for the repulsive Coulomb case, as is applicable to the study of nuclear reactions. This sign has important implications for the relationship between the R-matrix parameters describing a level and its observed width, as discussed by Lane and Thomas [1, Sec. XII.3, pp. 327–328]. The sign is also important for establishing the uniqueness of the alternative R-matrix parametrization given by Brune [3]. We will elaborate on these points further in the Conclusions, Sec. VII. While this sign appears to be positive in practice, a general proof for positive energies is lacking and several authors have commented on this point [1–3]. Lane and Thomas did show that it is positive for negative energies [1, Eq. (A.29), p. 351], for positive energies in the JWKB approximation [1, Eq. (A.19), p. 350], and they also gave a heuristic argument that it should be positive below the Coulomb and/or angular momentum barriers [1, Eq. (A.32), p. 352]. It is also straightforward to show that this sign is positive in the limits of zero radius, infinite radius, zero energy, and infinite energy (see Appendices C and D).

We have succeeding in proving that the energy derivative of the shift factor is always positive for the repulsive Coulomb case. We report results for the sign of the derivatives of the shift and penetration factors, as well as the related amplitude and phase, with respect to energy, angular momentum, and charge. The results are obtained using the phase-amplitude parametrization of the Coulomb functions and a little-known Nicholson-type integral representation for the sum of squares of the regular and irregular Coulomb functions. We also find that almost none of the results are generally valid in the attractive Coulomb case.

This paper is organized as follows. We first review the relevant properties of the Coulomb functions and then derive derive the monotonicity results, with discussion and conclusions following. Appendices include information on the theory of monotonic functions, further properties of Coulomb functions, and additional integral relations for the energy derivative of the shift factor.

II. OVERVIEW OF COULOMB FUNCTIONS

A. Definitions

In terms of physical parameters, a Coulomb function u satisfies

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2}+\frac{Z_1Z_2q^2}{r}u+\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}u=Eu, \qquad (1)$$

where $r \geqslant 0$ is the radial coordinate, E is the energy, $\hbar^2/\mu$ is a positive constant, $Z_1Z_2q^2/r$ is the Coulomb potential, and $\hbar^2\ell(\ell+1)/(2\mu r^2)$ is an effective potential corresponding to the centrifugal or angular momentum barrier. The quantity ℓ is the angular momentum quantum number and is a nonnegative integer in physical applications, but unless otherwise indicated we will consider it to be a nonnegative continuous real parameter. The quantity $Z_1Z_2q^2$ is the constant charge factor that is positive for a repulsive Coulomb field, zero in the neutral case,

*brune@ohio.edu
†ghale@lanl.gov
‡mparis@lanl.gov

and negative otherwise. We will also assume $E > 0$, unless otherwise indicated. In terms of the dimensionless parameters ρ and η, we have $u(\ell,\eta,\rho)$ and this equation becomes

$$u'' + \left[1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]u = 0, \tag{2}$$

where $\rho = kr$, $k = \sqrt{2\mu E/\hbar^2}$, $\eta k = Z_1 Z_2 q^2 \mu/\hbar^2$, and $' \equiv d/d\rho$. The outgoing $u = H_\ell^+$ and incoming $u = H_\ell^-$ solutions are given, respectively, by

$$H_\ell^+ = G_\ell + iF_\ell \quad \text{and} \tag{3a}$$

$$H_\ell^- = G_\ell - iF_\ell, \tag{3b}$$

where $G_\ell(\eta,\rho) \equiv G_\ell$ and $F_\ell(\eta,\rho) \equiv F_\ell$ are the irregular and regular Coulomb functions, respectively.

The logarithmic derivative of the outgoing solution is given by

$$L_\ell \equiv \frac{r}{H_\ell^+}\frac{dH_\ell^+}{dr} = \rho\frac{H_\ell^{+\prime}}{H_\ell^+}, \tag{4}$$

with the real and imaginary parts defined to be

$$L_\ell \equiv S_\ell + iP_\ell, \tag{5}$$

where S_ℓ and P_ℓ are the shift and penetration factors, respectively. Note that for for $E \leqslant 0$ we have $P_\ell = 0$. It is also customary to define the asymptotic phase

$$\theta_\ell = \rho - \eta\log(2\rho) - \tfrac{1}{2}\ell\pi + \sigma_\ell, \tag{6}$$

where σ_ℓ is the Coulomb phase shift defined in Appendix B. We also define the energy derivative ∂E which is understood to be taken at fixed radius (i.e., with the product $\eta\rho$ fixed):

$$\frac{\partial}{\partial E} = \frac{2\mu r^2}{\hbar^2}\left(\frac{1}{2\rho}\frac{\partial}{\partial\rho} - \frac{\eta}{2\rho^2}\frac{\partial}{\partial\eta}\right) \tag{7a}$$

$$= \frac{\rho}{2E}\left(\frac{\partial}{\partial\rho} - \frac{\eta}{\rho}\frac{\partial}{\partial\eta}\right). \tag{7b}$$

B. Amplitude and phase

It is possible to parametrize the Coulomb functions in terms of an amplitude (or modulus) A_ℓ and phase ϕ_ℓ [1,4–6]:

$$A_\ell = \left(F_\ell^2 + G_\ell^2\right)^{1/2}, \tag{8}$$

$$\phi_\ell = \tan^{-1} F_\ell/G_\ell, \tag{9}$$

$$H_\ell^\pm = A_\ell \exp(\pm i\phi_\ell), \tag{10}$$

$$P_\ell = \frac{\rho}{A_\ell^2}, \quad \text{and} \tag{11}$$

$$S_\ell = \frac{\rho A_\ell'}{A_\ell} = \frac{\rho\left(A_\ell^2\right)'}{2A_\ell^2}, \tag{12}$$

where the Wronskian relation

$$H_\ell^+ H_\ell^{-\prime} - H_\ell^{+\prime} H_\ell^- = -2i \tag{13}$$

has been used to derive Eq. (11) from Eq. (5). The amplitude and phase obey the following differential equations:

$$A_\ell'' + \left[1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]A_\ell - A_\ell^{-3} = 0 \quad \text{and} \tag{14}$$

$$\phi_\ell' = A_\ell^{-2}. \tag{15}$$

In this work we make extensive use of square of A_ℓ and we will refer to A_ℓ^2 as "the amplitude." A differential equation satisfied by A_ℓ^2 is discussed in Sec. VIC.

Thomas derived an integral representation for A_ℓ^2 that is useful for establishing its monotonic properties [1, p. 350], [6]:

$$A_\ell^2 = 2\rho\int_0^\infty dz\, e^{-2\rho z}\, Q(z), \quad \text{where} \tag{16a}$$

$$Q(z) = \exp(2\eta\tan^{-1} z)(1+z^2)^\ell \times {}_2F_1\left(-\ell - i\eta, -\ell + i\eta, 1; \frac{z^2}{1+z^2}\right) \tag{16b}$$

$$= \exp(2\eta\tan^{-1} z)(1+z^2)^{i\eta} \times {}_2F_1(\ell + 1 + i\eta, -\ell + i\eta, 1; -z^2). \tag{16c}$$

The equivalence of the two expressions for $Q(z)$ results from Pfaff and Euler transformations of the hypergeometric function. This formula is also given in Hull and Breit [7, Eq. (12.5), p. 440], but one of the factors of $-i\eta$ in their hypergeometric function must be reversed in sign to agree with Eq. (16b).

Expressions such as Eq. (16) are known as *Nicholson-type integrals*; further discussion is provided below in Sec. VIC. This equation appears to have been overlooked for over half a century, but it is very useful in the present context. The formula is based on a result given by Erdélyi [8] that expresses the product of two Whittaker functions as a Laplace transform, which is applicable since we also have

$$A_\ell^2 = H_\ell^+ H_\ell^- = e^{\pi\eta}\, W_{-i\eta,\ell+1/2}(-2i\rho)\, W_{i\eta,\ell+1/2}(2i\rho), \tag{17}$$

where W is the Whittaker function.

The particular hypergeometric function in Eq. (16b) may be defined via

$$t = \frac{z^2}{1+z^2}, \tag{18a}$$

$${}_2F_1(-\ell - i\eta, -\ell + i\eta, 1; t) \equiv F(t) = \sum_{n=0}^{\infty} d_n t^n, \tag{18b}$$

$$d_0 = 1, \quad \text{and} \tag{18c}$$

$$d_{n+1} = d_n\frac{\eta^2 + (n-\ell)^2}{(n+1)^2}, \tag{18d}$$

which is absolutely convergent for $|t| \leqslant 1$. We also note that $F(t)$ is real, positive, and monotonically increasing between $F(0) = 1$ and

$$F(1) = \frac{2^{2\ell} e^{-\pi\eta}}{C_\ell^2(\eta)(2\ell+1)^2\Gamma(2\ell+1)}, \tag{19}$$

where $C_\ell(\eta)$ is defined in Appendix C. The function $Q(z)$ is likewise positive for $0 \leqslant z < \infty$. The integral representation of Erdélyi and the positivity of the integrand in certain circumstances are also remarked upon by Buchholz [9, p. 89, Eq. (10a)].

Equation (16a) may be integrated by parts to yield [1,6]

$$A_\ell^2 = 1 + \int_0^\infty dz\, e^{-2\rho z} \frac{dQ}{dz}. \tag{20}$$

Further integrations by parts would yield an asymptotic expansion for A_ℓ^2 in terms of inverse powers of ρ. We also have

$$\frac{1}{Q}\frac{dQ}{dz} = \frac{2(\eta + \ell z)}{1+z^2} + \frac{1}{F(t)}\frac{dF(t)}{dt}\frac{dt}{dz}, \tag{21a}$$

$$\frac{dF(t)}{dt} = \sum_{n=1}^{\infty} n d_n t^{n-1}, \quad \text{and} \tag{21b}$$

$$\frac{dt}{dz} = \frac{2z}{(1+z^2)^2}. \tag{21c}$$

Considering only the repulsive Coulomb case ($\eta > 0$), we clearly have $dQ/dz > 0$, and hence $A_\ell^2 > 1$. By differentiating Eq. (20) with respect to ρ, one can see that $(A_\ell^2)' < 0$ and consequently $S_\ell < 0$ [1,6]. Further differentiation shows that all derivatives of A_ℓ^2 have well-defined sign:

$$0 < (-1)^n \left(\frac{d}{d\rho}\right)^n A_\ell^2 < \infty \qquad n = 1,2,3,\ldots \tag{22}$$

This result shows that A_ℓ^2 is a *completely monotonic* (CM) function of ρ. Many of the conclusions reached in this paper follow from this fact and are proven rather easily using the machinery of CM functions. Some properties of CM functions are discussed in Sec. A 2 of the Appendix; additional details are available in the review article of Miller and Samko [10].

Using Eqs. (16a) and (16b), Prosser and Biedenharn [6] showed that $\partial(A_\ell^2)/\partial\eta > 0$; noting that

$$\frac{\partial P_\ell}{\partial E} = \frac{\rho}{2E}\left[\frac{A_\ell^2 - \rho(A_\ell^2)' + \eta\frac{\partial A_\ell^2}{\partial \eta}}{A_\ell^4}\right], \tag{23}$$

it is clear that $\partial P_\ell/\partial E > 0$. These authors went on to show that $\partial S_\ell/\partial\eta < 0$. However, it does not appear to be feasible to extend their approach to determine the sign of $\partial S_\ell/\partial E$.

Some additional properties of the Coulomb functions are discussed in Appendices B–D. It should be noted that S_ℓ is *not* monotonic in ρ: from the formulas given in Appendix C it is clear that S_ℓ' is negative for $\rho \to 0$ and positive for $\rho \to \infty$.

III. ENERGY DERIVATIVE OF *L*

Using the differential equation with two different solutions O_1 and O_2 with outgoing wave boundary conditions (i.e., $O \propto H^+$) corresponding to energies E_1 and E_2 in Eq. (1), one can show that

$$-\frac{\hbar^2}{2\mu}\frac{d}{dr}\left[\frac{O_1 O_2}{r}(L_2 - L_1)\right] = (E_2 - E_1) O_1 O_2. \tag{24}$$

Note that the ℓ (angular momentum label) subscripts will be suppressed from this point forward in this paper. Upon integrating from $r = a$ to b with $a < b$ this becomes

$$-\frac{\hbar^2}{2\mu}\left[\frac{O_1 O_2}{r}(L_2 - L_1)\right]_a^b = (E_2 - E_1)\int_a^b O_1 O_2\, dr. \tag{25}$$

In the limit that $O_2 \to O_1$, this becomes

$$-\frac{\hbar^2}{2\mu}\left[\frac{O^2}{r}\frac{\partial L}{\partial E}\right]_a^b = \int_a^b O^2\, dr, \tag{26}$$

where ∂E is taken at fixed radius as discussed above. For bound states ($E < 0$), O is proportional to the exponentially decaying Whittaker function and one can take $b \to \infty$ with the surface term at $r = b$ in the left-hand side of Eq. (26) vanishing; see also Lane and Thomas [1, Eq. (A.29), p. 351]:

$$\frac{\hbar^2}{2\mu}\left[\frac{O^2}{r}\frac{\partial L}{\partial E}\right]_a = \int_a^\infty O^2\, dr. \tag{27}$$

Since $O(r)/O(a)$ is real, it follows that $\partial S/\partial E$ is positive for $E < 0$ [1].

It is not immediately obvious how to extend this result to positive energies because $O(r)/O(a)$ is nonzero and oscillating for large r and it is also necessarily a complex quantity. We attempted to find an integral expression with a positive-definite integrand, analogous to Eq. (27). These efforts were not successful; some of the results found are given in Appendix E. We show here a successful approach to proving $\partial S/\partial E > 0$ for the repulsive Coulomb case, using an integral expression with an integrand that oscillates in sign with properties that allow a definitive sign for the integral to be deduced.

Adopting $O = H^+ = A\exp(i\phi)$ and changing the integration variable from r to ρ, we can write Eq. (26) in terms of the amplitude and phase

$$-E\left[e^{2i\phi}\frac{A^2}{\rho}\frac{\partial L}{\partial E}\right]_{\rho_a}^{\rho_b} = \int_{\rho_a}^{\rho_b} A^2 e^{2i\phi}\, d\rho. \tag{28}$$

We next change the integration variable to ψ, noting that ψ is a monotonically increasing function of ρ:

$$\psi \equiv 2[\phi(\rho) - \phi(\rho_a)], \tag{29}$$

$$\psi' = 2A^{-2}, \tag{30}$$

$$\psi_b = 2[\phi(\rho_b) - \phi(\rho_a)], \quad \text{and} \tag{31}$$

$$-E\left[e^{i\psi}\frac{A^2}{\rho}\frac{\partial L}{\partial E}\right]_0^{\psi_b} = \frac{1}{2}\int_0^{\psi_b} A^4 e^{i\psi}\, d\psi, \tag{32}$$

where Eq. (30) follows from Eq. (15). Using

$$\frac{d(A^4)}{d\psi} = \frac{2A^2(A^2)'}{\psi'} = A^4(A^2)', \tag{33}$$

we can integrate by parts to find

$$\left[e^{i\psi}\left(-E\frac{A^2}{\rho}\frac{\partial L}{\partial E} + \frac{i}{2}A^4\right)\right]_0^{\psi_b} = \frac{i}{2}\int_0^{\psi_b} A^4(A^2)' e^{i\psi}\, d\psi. \tag{34}$$

Considering the large-ρ behavior of the Coulomb quantities given in Tables III and IV of Appendix C, one can now take $\psi_b \to \infty$ as $A^4(A^2)' \sim -\eta/\rho^2$ and the integral is absolutely convergent:

$$\left[E\frac{A^2}{\rho}\frac{\partial L}{\partial E}-\frac{i}{2}A^4\right]_{\rho_a}=\frac{i}{2}\int_0^\infty A^4(A^2)'e^{i\psi}\,d\psi. \quad (35)$$

Taking the real part of this expression yields

$$E\left[\frac{A^2}{\rho}\frac{\partial S}{\partial E}\right]_{\rho_a}=-\frac{1}{2}\int_0^\infty A^4(A^2)'\sin(\psi)\,d\psi. \quad (36)$$

Our strategy will be to use the fact that A^2 is a CM function of ρ (see Secs. II B and A 2) to prove that certain integrals, such as the one appearing in Eq. (36), have definite sign. Since A^4 is the product of two CM functions (i.e., $A^2\times A^2$) it is also CM. Furthermore, we have

$$\left(-\frac{d}{d\psi}\right)^n A^4=\left(-\frac{A^2}{2}\frac{d}{d\rho}\right)^n A^4>0$$
$$n=1,2,3,\ldots \quad (37)$$

and thus A^4 is also a CM when considered as a function of ψ. The quantity

$$-\frac{dA^4}{d\psi}=-A^4(A^2)' \quad (38)$$

appearing in the right-hand side of Eq. (36), which is the negative of Eq. (33), is thus a CM function of ψ. In particular, the fact that this quantity is positive and monotonically decreasing allows one to conclude that the right-hand side of Eq. (36) is positive using reasoning given in Appendix A. To summarize, the definite integral from zero to infinity of a CM function multiplied by the sine or cosine function is positive, provided the integral converges. We thus finally have

$$E\left[\frac{A^2}{\rho}\frac{\partial S}{\partial E}\right]_{\rho_a}=-\frac{1}{2}\int_0^\infty A^4(A^2)'\sin(\psi)\,d\psi>0, \quad (39)$$

and we can conclude that $\partial S/\partial E$ is indeed always positive for $E>0$ and a repulsive Coulomb field.

This method can also provide information about $\partial P/\partial E$. Starting from Eq. (32) and choosing b such that

$$\psi_b=\psi_n=2\pi n \qquad n=1,2,3,\ldots \quad (40)$$

the range of integration becomes an integer multiple of the period of $e^{i\psi}$ and the surface terms are simplified since $e^{i\psi_n}=1$:

$$-E\left[\frac{A^2}{\rho}\frac{\partial L}{\partial E}\right]_0^{\psi_n}=\frac{1}{2}\int_0^{\psi_n}A^4e^{i\psi}\,d\psi. \quad (41)$$

Taking imaginary part, we have

$$E\left[\frac{A^2}{\rho}\frac{\partial P}{\partial E}\right]_{\rho_a}=\frac{1}{2}\int_0^{\psi_n}A^4\sin(\psi)\,d\psi+E\left[\frac{A^2}{\rho}\frac{\partial P}{\partial E}\right]_{\rho_n}, \quad (42)$$

where $\rho_n=\rho_b$ when $\psi_b=\psi_n$. We cannot take $n\to\infty$ in this case since $A^4\sim 1$ for large ρ (at least without employing a regularization procedure), but it is sufficient to consider n to be very large such that the asymptotic expansions of the Coulomb functions are applicable (see Tables III and IV in Appendix C):

$$E\left[\frac{A^2}{\rho}\frac{\partial P}{\partial E}\right]_{\rho_a}=\frac{1}{2}\int_0^{\psi_n}A^4\sin(\psi)\,d\psi$$
$$+\frac{1}{2}\left(1+\frac{2\eta}{\rho_n}+\cdots\right). \quad (43)$$

Since A^4 is a CM function of ψ, we observe that both terms on the right-hand side of Eq. (43) are positive and we can conclude that $\partial P/\partial E>0$ (which has been derived previously using a different method [6]). In fact, we can do better because the surface term is nonzero as $\rho_n\to\infty$:

$$\frac{\partial P}{\partial E}>\frac{\rho}{2EA^2}. \quad (44)$$

It is also interesting to consider further integrations by parts. Since

$$\int e^{\alpha x}f\,dx=\sum_{k=0}^m(-1)^k\frac{e^{\alpha x}}{\alpha^{k+1}}\frac{d^kf}{dx^k}$$
$$+(-1)^{m+1}\int\frac{e^{\alpha x}}{\alpha^{m+1}}\frac{d^{m+1}f}{dx^{m+1}}\,dx \quad (45)$$

for $m=0,1,2,\ldots$, Eq. (35) generalizes to

$$\left[2E\frac{A^2}{\rho}\frac{\partial L}{\partial E}\right]_{\rho_a}=\left[\sum_{k=0}^m i^{k+1}\left(\frac{d}{d\psi}\right)^k A^4\right]_{\rho_a}$$
$$+i^{m+1}\int_0^\infty e^{i\psi}\left(\frac{d}{d\psi}\right)^{m+1}A^4\,d\psi. \quad (46)$$

Setting $m=1$ provides

$$\left[2E\frac{A^2}{\rho}\frac{\partial L}{\partial E}\right]_{\rho_a}=\left[iA^4-\frac{d(A^4)}{d\psi}\right]_{\rho_a}-\int_0^\infty e^{i\psi}\frac{d^2(A^4)}{d\psi^2}\,d\psi, \quad (47)$$

and then taking the imaginary part gives

$$\left[2E\frac{A^2}{\rho}\frac{\partial P}{\partial E}-A^4\right]_{\rho_a}=-\int_0^\infty\sin(\psi)\frac{d^2(A^4)}{d\psi^2}\,d\psi. \quad (48)$$

Since the right-hand side of this equation must be negative, it provides an upper-limit constraint on $\partial P/\partial E$:

$$\frac{\partial P}{\partial E}<\frac{\rho}{2E}A^2, \quad (49)$$

This result could also be deduced from the imaginary part of Eq. (35). Taking the real part of Eq. (47) yields

$$\left[2E\frac{A^2}{\rho}\frac{\partial S}{\partial E}+\frac{d(A^4)}{d\psi}\right]_{\rho_a}=-\int_0^\infty\cos(\psi)\frac{d^2(A^4)}{d\psi^2}\,d\psi. \quad (50)$$

Since the right-hand side of this equation must be negative, this implies

$$\frac{\partial S}{\partial E}<-\frac{\rho}{2EA^2}\left[\frac{d(A^4)}{d\psi}\right]_{\rho_a}=-\frac{\rho}{2E}A^2(A^2)'. \quad (51)$$

The results of this section are summarized in the first two lines of Table I.

TABLE I. Summary of the result of Secs. III and IV for the variation of S and P with E, ℓ, and η. The second column is deduced from the first using Eqs. (11) and (12).

$0 < \frac{\partial S}{\partial E} < -\frac{\rho A^2 (A^2)'}{2E}$	$0 < \frac{\partial S}{\partial E} < -\frac{\rho^2 S}{E P^2}$
$\frac{\rho}{2EA^2} < \frac{\partial P}{\partial E} < \frac{\rho A^2}{2E}$	$\frac{P}{2E} < \frac{\partial P}{\partial E} < \frac{\rho^2}{2EP}$
$(2\ell+1)\frac{A^4}{\rho^2}\left[\frac{\rho (A^2)'}{2A^2} - \frac{1}{2}\right] < \frac{\partial S}{\partial \ell} < 0$	$\frac{2\ell+1}{P^2}\left(S - \frac{1}{2}\right) < \frac{\partial S}{\partial \ell} < 0$
$-\frac{(2\ell+1)A^2}{2\rho} < \frac{\partial P}{\partial \ell} < 0$	$-\frac{2\ell+1}{2P} < \frac{\partial P}{\partial \ell} < 0$
$\frac{2A^4}{\rho}\left[\frac{\rho (A^2)'}{2A^2} - \frac{1}{4}\right] < \frac{\partial S}{\partial \eta} < 0$	$\frac{2\rho}{P^2}\left(S - \frac{1}{4}\right) < \frac{\partial S}{\partial \eta} < 0$
$-A^2 < \frac{\partial P}{\partial \eta} < 0$	$-\frac{\rho}{P} < \frac{\partial P}{\partial \eta} < 0$

IV. VARIATION OF L WITH ANGULAR MOMENTUM AND CHARGE

It is also interesting and feasible with the above approach to investigate the variation of L with the angular momentum ℓ and charge. On page 414 of their article, Prosser and Biedenharn [6] stated that $\partial(A^2)/\partial\ell > 0$ (and consequently also $\partial P/\partial \ell < 0$) based on Eqs. (16a) and (16b) of the present paper, but it is not clear how they arrived at that conclusion. The other statements made by the authors in that paragraph follow simply from the properties of $Q(z)$, but this one does not. Assuming that $Q(z)$ is defined by Eq. (16b), $\partial(A^2)/\partial\ell > 0$ is true provided that $\partial F(t)/\partial \ell > 0$, where $F(t)$ is the hypergeometric function defined by Eq. (18). However, it is not always the case that $\partial F(t)/\partial\ell > 0$. Ref. [6] was unable to find a result for $\partial S/\partial \ell$.

Using Eq. (2) with two different solutions O_1 and O_2 corresponding to angular momenta l_1 and l_2 but with the same energy, one finds

$$\frac{d}{d\rho}\left[\frac{O_1 O_2}{\rho}(L_2 - L_1)\right] = (\ell_1 + \ell_2 + 1)(\ell_2 - \ell_1)\frac{O_1 O_2}{\rho^2}. \tag{52}$$

Integrating and taking $O_2 \to O_1$ (considering ℓ to be a continuous parameter) leads to

$$\left[\frac{O^2}{\rho}\frac{\partial L}{\partial \ell}\right]_{\rho_a}^{\rho_b} = (2\ell+1)\int_{\rho_a}^{\rho_b}\frac{O^2}{\rho^2}\,d\rho. \tag{53}$$

One can now take $\rho_b \to \infty$ and proceed as before:

$$\frac{2}{2\ell+1}\left[\frac{A^2}{\rho}\frac{\partial L}{\partial \ell}\right]_{\rho_a} = -\int_0^\infty \frac{A^4 e^{i\psi}}{\rho^2}\,d\psi. \tag{54}$$

Noting that ρ^{-2} is a CM function of ρ, and that hence A^4/ρ^2 is likewise CM, we have

$$\left(-\frac{d}{d\psi}\right)^n \frac{A^4}{\rho^2} = \left(-\frac{A^2}{2}\frac{d}{d\rho}\right)^n \frac{A^4}{\rho^2} > 0$$
$$n = 1,2,3,\dots, \tag{55}$$

and we can conclude immediately that

$$\frac{\partial S}{\partial \ell} < 0 \quad \text{and} \quad \frac{\partial P}{\partial \ell} < 0, \tag{56}$$

using the methods of Appendix A. Integrating Eq. (54) by parts twice yields

$$\frac{2}{2\ell+1}\left[\frac{A^2}{\rho}\frac{\partial L}{\partial \ell}\right]_{\rho_a} = \left[-i\frac{A^4}{\rho^2} + \frac{A^6}{\rho^3}\left(\frac{\rho(A^2)'}{A^2} - 1\right)\right]_{\rho_a} + \int_0^\infty \frac{d^2}{d\psi^2}\left(\frac{A^4}{\rho^2}\right)e^{i\psi}\,d\rho, \tag{57}$$

which shows

$$\frac{\partial S}{\partial \ell} > (2\ell+1)\frac{A^4}{\rho^2}\left[\frac{\rho(A^2)'}{2A^2} - \frac{1}{2}\right] \tag{58}$$

and

$$\frac{\partial P}{\partial \ell} > -\frac{(2\ell+1)A^2}{2\rho}. \tag{59}$$

The variation of L with charge can be studied using this procedure via the Coulomb parameter η. This results in

$$\frac{d}{d\rho}\left[\frac{O_1 O_2}{\rho}(L_2 - L_1)\right] = 2(\eta_2 - \eta_1)\frac{O_1 O_2}{\rho}. \tag{60}$$

Upon integrating and taking $O_2 \to O_1$,

$$\left[\frac{O^2}{\rho}\frac{\partial L}{\partial \eta}\right]_{\rho_a}^{\rho_b} = 2\int_{\rho_a}^{\rho_b}\frac{O^2}{\rho}\,d\rho. \tag{61}$$

Proceeding as above, we have

$$\left[\frac{A^2}{\rho}\frac{\partial L}{\partial \eta}\right]_{\rho_a} = -\int_0^\infty \frac{A^4 e^{i\psi}}{\rho}\,d\psi. \tag{62}$$

Noting that ρ^{-1} is a CM function of ρ and thus

$$\left(-\frac{d}{d\psi}\right)^n \frac{A^4}{\rho} = \left(-\frac{A^2}{2}\frac{d}{d\rho}\right)^n \frac{A^4}{\rho} > 0,$$
$$n = 1,2,3,\dots, \tag{63}$$

we conclude

$$\frac{\partial S}{\partial \eta} < 0 \quad \text{and} \quad \frac{\partial P}{\partial \eta} < 0, \tag{64}$$

confirming the findings of Ref. [6]. Integrating Eq. (62) by parts twice yields

$$\left[\frac{A^2}{\rho}\frac{\partial L}{\partial \eta}\right]_{\rho_a} = \left[-i\frac{A^4}{\rho} + \frac{A^6}{2\rho^2}\left(\frac{2\rho(A^2)'}{A^2} - 1\right)\right]_{\rho_a} + \int_0^\infty \frac{d^2}{d\psi^2}\left(\frac{A^4}{\rho}\right)e^{i\psi}\,d\rho, \tag{65}$$

which shows

$$\frac{\partial S}{\partial \eta} > \frac{2A^4}{\rho}\left[\frac{\rho(A^2)'}{2A^2} - \frac{1}{4}\right] \tag{66}$$

and

$$\frac{\partial P}{\partial \eta} > -A^2. \tag{67}$$

The results of this section are summarized in Table I.

V. VARIATION OF THE AMPLITUDE AND PHASE WITH E, ℓ, AND η

It is also expected that the amplitude and phase depend monotonically on E, ℓ, and η. Noting $P = \rho/A^2$, the variations of squared amplitude A^2 with ℓ and η are easily found to be opposite of those already derived for P: $\partial A^2/\partial\ell > 0$ and $\partial A^2/\partial\eta > 0$. The latter result can also be shown by differentiating Eq. (16a) with $Q(z)$ given by Eq. (16b) [6]. For the energy variation of the amplitude, we have using Eq. (7)

$$\frac{\partial A^2}{\partial E} = \frac{\rho}{2E}\left[(A^2)' - \frac{\eta}{\rho}\frac{\partial A^2}{\partial \eta}\right]. \tag{68}$$

Since $(A^2)' < 0$ and $\partial A^2/\partial\eta > 0$, we can also conclude that $\partial A^2/\partial E < 0$.

The variation of the phase ϕ with these parameters can also be related to those for P. Noting that

$$\frac{d\phi}{dr} = \frac{P}{r} \quad \text{and hence} \quad [\phi]_a = \int_0^a \frac{P}{r}\,dr, \tag{69}$$

we have

$$\left[\frac{\partial\phi}{\partial X}\right]_a = \int_0^a \frac{\partial P}{\partial X}\frac{dr}{r}, \tag{70}$$

where $X = E$, ℓ, or η, and the variation of ϕ with these parameters is seen to be in the same direction as it is for P. Note that in the case of $\ell = 0$ for $\partial\phi/\partial\ell$ the integrand has a logarithmic singularity as $r \to 0$, but the integral is still convergent. The results of this section are summarized in Table II.

VI. DISCUSSION

We have limited our consideration to the repulsive Coulomb field ($\eta > 0$) in this work. In this section we will briefly consider the attractive Coulomb field and then in more detail the neutral case. We next provide further discussion of the amplitude A^2, followed by a brief review of negative energies. In Fig. 1 we show shift factor $S(E)$ for the repulsive, neutral, and attractive cases ($Z_1Z_2 = 1$, 0, and -1, respectively). We have also assumed $\ell = 0$, q to be the fundamental charge, μ to be the nucleon-nucleon reduced mass, and a radius of 2 fm. The repulsive case shows the expected results: $S < 0$ and $\partial S/\partial E > 0$ for all energies.

A. The attractive Coulomb case

In the case of an attractive Coulomb field, the amplitude A^2 is no longer guaranteed to be a CM function of ρ because according to Eq. (21) dQ/dz is not necessarily positive. Consequently, very few of the results from the repulsive case

TABLE II. Summary of the result of Sec. V.

$\frac{\partial A^2}{\partial E} < 0$	$\frac{\partial A^2}{\partial \ell} > 0$	$\frac{\partial A^2}{\partial \eta} > 0$
$\frac{\partial \phi}{\partial E} > 0$	$\frac{\partial \phi}{\partial \ell} < 0$	$\frac{\partial \phi}{\partial \eta} < 0$

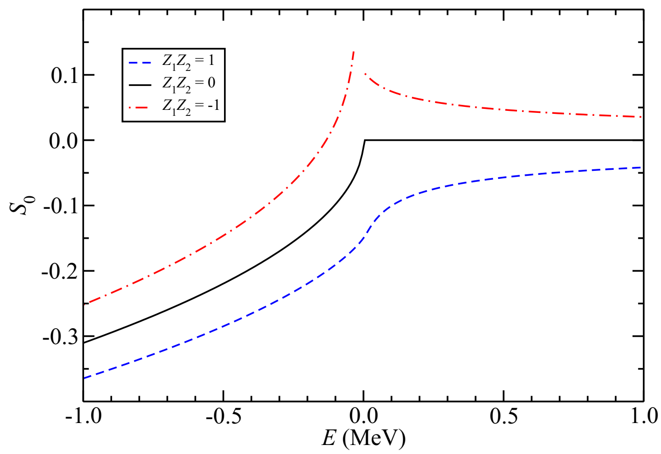

FIG. 1. The $\ell = 0$ shift factor versus energy for the repulsive (blue dashed curve), uncharged (black solid curve), and attractive (red dot-dashed curve) cases. Additional details are provided in the text.

are generally valid for $\eta < 0$. We can conclude that $A^2 > 0$ and hence $P > 0$ from Eqs. (16a) and (16b). For the particular case with $\ell = 0$ plotted in Fig. 1, it can be seen that $\partial S/\partial E < 0$ for $E > 0$.

B. The neutral case

In the neutral or uncharged case, we have $\eta = 0$ and the amplitude is given by

$$A^2 = \frac{\pi}{2}\rho\left[J^2_{\ell+1/2}(\rho) + Y^2_{\ell+1/2}(\rho)\right], \tag{71}$$

where J and Y are the regular and irregular Bessel functions. It is convenient in this case to use form of $Q(z)$ given by Eq. (16c), which becomes

$$Q(z) = {}_2F_1(-\ell,\ell+1,1;-z^2). \tag{72}$$

Following Prosser and Biedenharn [6, Eq. (16a)] may then be integrated termwise to yield

$$A^2 = {}_3F_0\left(-\ell,\ell+1,\tfrac{1}{2};-\rho^{-2}\right), \tag{73}$$

where ${}_3F_0$ is a generalized hypergeometric function, and it is assumed that both hypergeometric functions may be represented by their canonical power series. If ℓ is a nonnegative integer (the case for physical problems), then the hypergemeotric functions in Eqs. (72) and (73) are represented by series that terminate and there are no questions of convergence. Otherwise, the ${}_2F_1$ in Eq. (72) cannot be represented by its series when $z > 1$ and the series for ${}_3F_0$ in Eq. (73) is a nonconvergent asymptotic expansion, equivalent to Eq. 13.75(1) of Watson [11, p. 449].

Alternatively, one may utilize the fact that Eq. (72) is a representation of the Legendre function $\tilde{P}_\ell$ (a polynomial if ℓ is a nonnegative integer) [12, Eq. 15.4.16, p. 562]

$${}_2F_1(-\ell,\ell+1,1;-z^2) = \tilde{P}_\ell(1+2z^2), \tag{74}$$

to write

$$A^2 = 2\rho\int_0^\infty dz\, e^{-2\rho z}\tilde{P}_\ell(1+2z^2). \tag{75}$$

This is a known integral representation for Eq. (71) deduced by Hartman [13, Eq. (11.6), p. 588] using a different approach.

In the neutral case, the monotonicity results are essentially unchanged from the repulsive charge case, since $dQ/dz \geqslant 0$ [see Eq. (21)]. Note that $dQ/dz = 0$ only occurs when $\ell = 0$, in which case we have $Q = 1$ and $A^2 = 1$, which leads to $P = \rho$, $S = 0$, and $\phi = \rho$ for $E > 0$. This shift factor is plotted in Fig. 1. In this case, the monotonicity properties are trivial may be deduced by inspection. In particular, we note that $\partial S/\partial E = 0$ for $\ell = 0$ and positive energy.

C. Further discussion of the amplitude A^2

Our finding that $A^2 = F_\ell^2 + G_\ell^2$ is CM for the case of a repulsive Coulomb field is a generalization of the result that $\rho[J_\nu^2(\rho) + Y_\nu^2(\rho)]$ is CM [14]. The key to proving that A^2 is CM is the Laplace transform representation given by Eq. (16). Integral representations for the sum of squares of linearly independent solutions to an ordinary second-order differential equation, such as Eq. (16), are known as *Nicholson-type integrals* and may considered to be generalizations of $\sin^2\rho + \cos^2\rho = 1$. These representations are often useful for establishing monotonicity properties of special functions [14–16], as has been the case in the present work.

Hartman [13,17] has studied the differential equation

$$u'' + [c + s(\rho)]u = 0, \tag{76}$$

where c is a positive constant and $s \to 0$ as $\rho \to \infty$. He has shown that there are always solutions x and y to Eq. (76) with unit Wronskian such that the generalized amplitude $A^2 = x^2 + y^2 \to 1$ as $\rho \to \infty$ and, if $-s(\rho)$ is CM, the generalized amplitude A^2 is CM. Since Eq. (2) is of this form with both the repulsive Coulomb potential and the centrifugal barrier making CM contributions to $-s(\rho)$, this provides an alternate proof that A^2 is CM for the repulsive Coulomb case. It is also clear from this perspective that we are unable to draw general conclusions regarding the monotonicity of A^2 for an attractive Coulomb potential.

We finish the discussion of the amplitude by deriving its asymptotic expansion for large ρ. Leading asymptotic expansions for A have been given by Hull and Breit [7] that lack general formulas for the coefficients. The asymptotic expansion for A^2 turns out to be considerably simpler. If u and v are solutions of Eq. (2), their product $w = uv$ satisfies the Appell equation, a third-order homogeneous linear differential equation [13, p. 560, Eq. (2.23)], which in our case reads

$$w''' + 4\left[1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]w' + 2\left[\frac{2\eta}{\rho^2} + \frac{2\ell(\ell+1)}{\rho^3}\right]w = 0. \tag{77}$$

Any linear combinations of such solutions, including $A^2 = F_\ell^2 + G_\ell^2$, is likewise a solution of Eq. (77). Assuming an expansion of the form

$$A^2 \sim \sum_{k=0}^{\infty} \frac{a_k}{\rho^k} \tag{78a}$$

with $a_0 = 1$ and substituting into Eq. (77) leads to the following result for the coefficients:

$$a_0 = 1, \tag{78b}$$

$$a_1 = \eta, \quad \text{and} \quad \text{for} \quad k \geqslant 1 \tag{78c}$$

$$a_{k+1} = \eta\frac{2k+1}{k+1}a_k + \frac{k(2\ell+k+1)(2\ell-k+1)}{4(k+1)}a_{k-1}. \tag{78d}$$

Considering that any solution of Eq. (77) must be a linear combination of F_ℓ^2, G_ℓ^2, and $F_\ell G_\ell$ and the leading asymptotic expansions of these possibilities, it is clear that Eq. (78) is in fact the asymptotic expansion of A^2. If $\eta = 0$ (i.e., the neutral case), the expansion only contains even terms and is equivalent to Eq. (73). If ℓ is also a nonnegative integer (the case for physical problems), the series terminates. Equation (78) is the generalization to the Coulomb case of the asymptotic series for $J_\nu^2 + Y_\nu^2$ given by Eq. 13.75(1) of Watson [11, p. 449].

D. Negative energies

In the case of negative energies, the Coulomb functions satisfy

$$u'' + \left[-1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]u = 0, \tag{79}$$

where $\rho = kr$, $k = \sqrt{-2\mu E/\hbar^2}$, $\eta k = Z_1 Z_2 q^2 \mu/\hbar^2$, and $' \equiv d/d\rho$. We will consider the solution given by the exponentially-decaying Whittaker function $W_{-\eta,\ell+1/2}(2\rho) \equiv W$ and the shift factor that is given for negative energies by

$$S = \rho\frac{W'}{W}. \tag{80}$$

Adapting Eqs. (27), (53), and (61) to negative energies, we have

$$\left[\frac{W^2}{\rho}\frac{\partial S}{\partial E}\right]_{\rho_a} = -\frac{1}{E}\int_{\rho_a}^{\infty} W^2\, d\rho, \tag{81}$$

$$\left[\frac{W^2}{\rho}\frac{\partial S}{\partial \ell}\right]_{\rho_a} = -(2\ell+1)\int_{\rho_a}^{\infty} \frac{W^2}{\rho^2}\, d\rho, \quad \text{and} \tag{82}$$

$$\left[\frac{W^2}{\rho}\frac{\partial S}{\partial \eta}\right]_{\rho_a} = -2\int_{\rho_a}^{\infty} \frac{W^2}{\rho}\, d\rho. \tag{83}$$

These equations show $\partial S/\partial E > 0$, $\partial S/\partial \ell < 0$, and $\partial S/\partial \eta < 0$ for negative energies, regardless of whether the Coulomb potential is repulsive, attractive, or zero. These results have been noted previously—see the discussion of Eq. (27) above regarding $\partial S/\partial E$ and Prosser and Biedenharn [6, Sec. IV]. Also, all of the shift factors plotted in Fig. 1 are consistent with $\partial S/\partial E > 0$ for $E < 0$. One should be aware that, for the attractive Coulomb case, the shift factor has singularities for slightly negative energies due to zeros of the Whittaker function.

In the absence of the Coulomb potential, the negative-energy solutions are modified Bessel functions. Goldstein and Thaler [18] showed that an amplitude and phase parametrization can be implemented in this situation. Here, the solutions depend exponentially on the "phase," as opposed to the sinusoidal dependence used for positive energies. Presumably, this description could be extended to include the Coulomb potential and describe the negative-energy Whittaker function solutions.

VII. CONCLUSIONS

We have studied the derivatives of the shift and penetration factors, as well as the related amplitude and phase, with respect to energy, angular momentum, and charge. For the cases of neutral or repulsive Coulomb fields, we find definitive results for the signs of these quantities, as summarized in Tables I and II. In particularly, we have succeeded in proving $\partial S/\partial E > 0$, a result that has been long thought to be true, but for which a general proof was lacking.

The fact that $\partial S/\partial E > 0$ for positive energies and a repulsive or neutral Coulomb field has implications for the R-matrix description of nuclear reactions. When relating R-matrix reduced width amplitudes to physical quantities, one is presented with the factor

$$N^{-1} = 1 + \sum_c \gamma_{\lambda c}^2 \frac{\partial S_c}{\partial E}, \tag{84}$$

where c is the channel label and $\gamma_{\lambda c}$ are the reduced width amplitudes. For an unbound state in the one-level approximation, the observed partial width is given by Lane and Thomas [1, Eqs. (3.5) and (3.6), p. 327],

$$\Gamma_{\lambda c} = 2N P_c \gamma_{\lambda c}^2. \tag{85}$$

The Thomas approximation [19] has been employed here, which assumes that $S_c(E)$ may be replaced by its first-order Taylor series. Knowledge that $\partial S/\partial E > 0$ ensures that $N > 0$ and that the observed partial width is nonnegative, a requirement for a physically reasonable partial width. In the case of a bound level, the factor N defined by Eq. (84) also arises. In this situation, N changes the normalization volume of the wave function from inside the channel surfaces to all space [1, Sec. IV.7, p. 280; Eqs. (A.29) and (A.30), p. 351]. For this case, N was already known to be positive. The description of the physical properties of bound and unbound levels may be unified by considering the complex poles of the scattering matrix [20]. In this approach, a similar normalization factor containing $\partial L/\partial E$ naturally appears in the residues of the scattering matrix poles. If the level is narrow such that the pole is near the real energy axis, this normalizaton factor becomes equivalent to Eq. (84) in the one-level approximation. Although less fundamental than partial widths defined via the residues of the poles of the scattering matrix, Eqs. (84) and (85) may serve as a practical definition of the observed partial width in R-matrix theory.

Brune [3] has given an alternative parametrization of R-matrix theory that utilizes level energies and reduced width amplitudes that are more closely connected to the observed resonance energies and partial widths than in the standard parametrization [1]. The present result that $\partial S/\partial E > 0$ is sufficient to prove that the alternative parameters have a one-to-one relationship to the standard parameters and ensures that the alternative parametrization is well defined and fully equivalent to the standard parametrization. Further information on this point is provided by Eq. (45) of Ref. [3] and that equation's surrounding discussion.

The results given in this paper follow from the Nicholson-type integral representation of the amplitude A^2 given by Eq. (16). When the Coulomb field is repulsive or absent, we find that A^2 is a CM function of ρ, which leads to definitive monotonicity properties for the shift and penetration factors. Considering the work of Hartman [13,17] on the theory of differential equations, it is apparent that any central potential that is a CM function of radius will give analogous results. To be explicit, a CM potential is necessarily repulsive and monotonically decreasing with radius, with the signs of higher derivatives prescribed according to Eq. (A5). An attractive potential cannot be CM and almost none of the conclusions of this paper apply in this case.

ACKNOWLEDGMENTS

This work was carried out under the auspices of the U.S. Department of Energy, under Grants No. DE-FG02-88ER40387 and No. DE-NA0002905 at Ohio University and Grant No. DE-AC52-06NA25396 at Los Alamos National Laboratory.

APPENDIX A: SOME RESULTS CONCERNING MONOTONIC FUNCTIONS

We summarize here some aspects of monotonic functions that are of use in this paper.

1. Integrals of the type $\int_0^{2\pi m} f(x)\sin(x)\,dx$

Consider the integral

$$I = \int_0^{2\pi} f(x)\sin(x)\,dx, \tag{A1}$$

where $f(x) > 0$ and $f'(x) < 0$ for $x > 0$. The integral can be split and rewritten as an integral from 0 to π:

$$I = \int_0^{\pi} f(x)\sin(x)\,dx + \int_{\pi}^{2\pi} f(x)\sin(x)\,dx \tag{A2}$$

$$= \int_0^{\pi} [f(x) - f(x+\pi)]\sin(x)\,dx. \tag{A3}$$

Since the conditions on $f(x)$ imply $f(x) - f(x+\pi) > 0$ and $\sin(x) > 0$ for $0 < x < \pi$, we can conclude that $I > 0$. The same result holds if the integration range is extended by an integer multiple m of 2π:

$$\int_0^{2\pi m} f(x)\sin(x)\,dx > 0 \quad m = 1,2,3,\ldots, \tag{A4}$$

including for $m \to \infty$, provided the integral converges. Note that an analogous conclusion *cannot* in general be drawn for $\int_0^{2\pi} f(x)\cos(x)\,dx$, but in may be possible to draw conclusions using integration by parts—depending on the sign of $f''(x)$ (see Sec. A 2 below).

2. Completely monotonic functions

A function $f(x)$ is said to be *completely monotonic* (CM) if

$$0 \leqslant (-1)^n \left(\frac{d}{dx}\right)^n f(x) < \infty \tag{A5}$$

for all $x > 0$ and $n = 0,1,2,\ldots$ The properties of CM functions are reviewed in Ref. [10]. Besides the definition, the feature of CM functions that is particularly useful for this work the fact that the product of two CM functions is also a CM function. A consequence of this property that we will utilize is that

$$h(x) = \left[-g(x)\frac{d}{dx}\right]^n f(x) \qquad n = 0,1,2,\ldots \tag{A6}$$

is a CM function if $f(x)$ and $g(x)$ are CM. The definition Eq. (A5) allows $f(x)$ to be a non-negative constant; we exclude this case which eliminates the possibility that $(d/dx)^n f(x)$ in Eq. (A5) can be zero [14, Appendix I, p. 71-72].

We now consider a CM $f(x)$ and integrals over $0 < x < 2\pi m$ where $m = 1,2,3,\ldots$ Using the results of Sec. A 1, we can immediately conclude that

$$\int_0^{2\pi m} f(x)\sin(x)\,dx > 0. \tag{A7}$$

We now also have an analogous result for the cosine integral:

$$\begin{aligned}\int_0^{2\pi m} & f(x)\cos(x)\,dx \\ &= [f(x)\sin(x)]_0^{2\pi m} - \int_0^{2\pi m}\frac{df}{dx}\sin(x)\,dx \qquad \text{(A8)}\\ &= -\int_0^{2\pi m}\frac{df}{dx}\sin(x)\,dx \qquad \text{(A9)}\\ &> 0, \qquad \text{(A10)}\end{aligned}$$

where the assumption that the original integral is convergent allows one to conclude the surface term vanishes and we have used the fact that $-df/dx$ is a CM function. Similar reasoning has been used in Ref. [21] to derive sufficient conditions for a Fourier sine or cosine transform to be positive.

APPENDIX B: COULOMB PHASE SHIFT AND $h(\eta)$

The Coulomb phase shift σ_ℓ is defined by

$$e^{2i\sigma_\ell} = \frac{\Gamma(1+\ell+i\eta)}{\Gamma(1+\ell-i\eta)} = \frac{(\ell+i\eta)\ldots(1+i\eta)}{(\ell-i\eta)\ldots(1-i\eta)}e^{2i\sigma_0}, \tag{B1}$$

with the derivative of σ_ℓ is given by

$$\frac{d\sigma_\ell}{d\eta} = \frac{1}{2}[\Psi(1+\ell+i\eta)+\Psi(1+\ell-i\eta)], \tag{B2}$$

$$\frac{d\sigma_{\ell>0}}{d\eta} = \frac{d\sigma_0}{d\eta} + \sum_{m=1}^{\ell}\frac{m}{m^2+\eta^2}, \tag{B3}$$

$$\frac{d\sigma_0}{d\eta} = \frac{1}{2}[\Psi(1+i\eta)+\Psi(1-i\eta)], \quad \text{and} \tag{B4}$$

$$\equiv h(\eta) + \log(\eta), \tag{B5}$$

where Ψ is the digamma function. Note that the final part of Eq. (B1) and Eq. (B3) are only applicable when ℓ is a nonnegative integer. Equation (B5) serves to define, for a repulsive Coulomb field, the auxiliary function $h(\eta)$ that also arises in the series expansion of the irregular Coulomb functions and in effective range theory [22–24]. Note that $h(\eta)$ is real when η is real and positive and that it is also given by [22,23]

$$h(\eta) = -\log\eta - \gamma + \eta^2\sum_{k=1}^{\infty}\frac{1}{k(k^2+\eta^2)}, \tag{B6}$$

where $\gamma = 0.57721566\ldots$ is Euler's constant.

It appears that $h(\eta)$ is a completely monotonic function of η, but we have been unable to prove this. Using Eq. (6.3.21) of Abramowitz and Stegun [12, p. 259] and the properties of the digamma function, we have found the following representation for $h(\eta)$:

$$h(\eta) = I_1(\eta) + I_2(\eta) + e^{-\pi\eta}I_3(\eta), \quad \text{where} \tag{B7a}$$

$$I_1(\eta) = \int_0^{\pi}\left[\frac{1}{t} - \frac{1}{2\tan(t/2)}\right]e^{-\eta t}\,dt, \tag{B7b}$$

$$I_2(\eta) = \int_{\pi}^{\infty}\frac{e^{-\eta t}}{t}\,dt, \quad \text{and} \tag{B7c}$$

$$I_3(\eta) = \int_0^{\pi}\frac{1}{2\tan(t/2)}\frac{\sinh(\eta t)}{\sinh(\eta\pi)}\,dt \tag{B7d}$$

that is sufficient to demonstrate that

$$h(\eta) > 0 \quad \text{and} \quad \frac{dh}{d\eta} < 0 \tag{B8}$$

for the repulsive Coulomb field. These results are useful for determining the sign of the energy derivative of σ_ℓ and/or $h(\eta)$ in this work. To the best of our knowledge, these results regarding the monotonic properties of σ_ℓ and $h(\eta)$ have not been noted previously. Finally, we note that for $\eta \to \infty$ we have asymptotically [12, Eq. (6.3.19), p. 259]

$$h(\eta) \sim \frac{1}{12\eta^2} + \frac{1}{120\eta^4} + \cdots, \tag{B9}$$

which is consistent with the Eq. (B8).

APPENDIX C: LIMITING FORMS FOR SMALL AND LARGE ρ

We present in Table III the leading behavior of the various Coulomb quantities used in this work for $\rho \to 0$ and $\rho \to \infty$, considering η to be constant. The small-ρ forms are deduced starting from Eqs. (14.1.3)–(14.1.23) of Abramowitz and Stegun [12, pp. 539–540], with the Gamow factor defined to be

$$C_\ell(\eta) = \frac{2^\ell e^{-\pi\eta/2}[\Gamma(\ell+1+i\eta)\Gamma(\ell+1-i\eta)]^{1/2}}{\Gamma(2\ell+2)}. \tag{C1}$$

To extract $\partial S_\ell/\partial E$ as ρ (or the radius) goes to zero, it is necessary to consider the expansion of S_ℓ beyond the leading term given in Table III. For ℓ a nonnegative integer, this results in

$$S_\ell = \begin{cases} 2\eta\rho[\log(2\eta\rho) + 2\gamma + h(\eta)] + \ldots & \ell = 0 \\ -\ell - \frac{\eta\rho}{\ell} + \frac{1+(\eta/\ell)^2}{2\ell-1}\rho^2 + \ldots & \ell > 0 \end{cases}, \tag{C2}$$

where γ and $h(\eta)$ are defined in Appendix B. The resulting expressions for the energy dependence of the shift factor in the

TABLE III. Limiting forms of various Coulomb quantities for small and large ρ. The complete asymptotic expansion of A_ℓ^2 for large ρ is given in the text by Eq. (78). A refined small-ρ expansion for S_ℓ is given in the text by Eq. (C2).

Quantity	$\rho \to 0$	$\rho \to \infty$
H_ℓ^+	$[\rho^\ell(2\ell+1)C_\ell(\eta)]^{-1} + \dots + i[\rho^{\ell+1}C_\ell(\eta) + \dots]$	$\exp(i\theta_\ell)\left[1 + \frac{\eta}{2\rho} + i\frac{\eta^2+\ell(\ell+1)}{2\rho} + \cdots\right]$
A_ℓ^2	$[\rho^\ell(2\ell+1)C_\ell(\eta)]^{-2} + \cdots$	$1 + \frac{\eta}{\rho} + \frac{3\eta^2+\ell(\ell+1)}{2\rho^2} + \cdots$
ϕ_ℓ	$\rho^{2\ell+1}(2\ell+1)C_\ell^2(\eta) + \cdots$	$\theta_\ell + \frac{\eta^2+\ell(\ell+1)}{2\rho} + \cdots$
P_ℓ	$\rho^{2\ell+1}[(2\ell+1)C_\ell(\eta)]^2 + \cdots$	$\rho - \eta - \frac{\eta^2+\ell(\ell+1)}{2\rho} + \cdots$
S_ℓ	$-\ell + \cdots$	$-\frac{\eta}{2\rho} - \frac{2\eta^2+\ell(\ell+1)}{2\rho^2} + \cdots$

$\rho \to 0$ limit (with η fixed) are

$$\frac{\partial S_\ell}{\partial E} = \begin{cases} -\frac{\eta^2\rho}{E}\frac{dh}{d\eta} + \dots & \ell = 0 \\ \frac{2\mu r^2}{\hbar^2(2\ell-1)} + \dots & \ell > 0 \end{cases}. \tag{C3}$$

As discussed in Appendix B, $dh/d\eta < 0$, and consequently $\partial S_\ell/\partial E > 0$ in this limit. It is also interesting to note that for $\ell > 0$ the quantity $\partial S_\ell/\partial E$ is independent of the energy and Coulomb field for sufficiently small radii.

The large-ρ forms are deduced from asymptotic expansions given by Eqs. (14.5.1)–(14.5.9) of Ref. [12, pp. 539–540]. Energy derivatives of some the Coulomb quantities were determined for the large-ρ limit and are given in Table IV. They are useful for evaluating the surface terms of integrals that arise in this work. In addition, one can see that $\partial S_\ell/\partial E > 0$ in the large-ρ limit.

APPENDIX D: LIMITING FORMS FOR SMALL AND LARGE E

We will first consider the case of large energies at fixed radius, where $\rho \to \infty$ and $\eta \to 0$. Since the asymptotic formulas for large ρ are still valid when η is small, the high-energy limits can be calculated using the $\rho \to \infty$ formulas located in Tables III and IV of Appendix C.

For considering the low-energy limit at fixed radius, the expansions in terms of modified Bessel functions and inverse powers of η^2 are appropriate [25,26]. We will focus our attention on the shift factor, as the penetration factor has been thoroughly covered elsewhere [1,27]. In this limit, it is convenient to use the energy-independent radial coordinate x_0:

$$x_0 = \sqrt{8\eta\rho} = \sqrt{8\alpha r}, \tag{D1}$$

where $\alpha = \eta k$ is likewise independent of energy. In the low-energy limit, we have $G_\ell \gg F_\ell$ and the shift factor at zero energy is given by the well-known result [1,6]

$$S_\ell = -\ell - \frac{x_0 K_{2\ell}(x_0)}{2K_{2\ell+1}(x_0)}, \tag{D2}$$

where K_ν are the irregular modified Bessel functions. The energy derivative of the shift factor can be found by considering the leading energy-dependent terms in the expansions of G_ℓ and G'_ℓ. The slope of the shift factor at zero energy is thus found:

$$\begin{aligned} \frac{\partial S_\ell}{\partial E} = {} & \frac{2\mu}{\hbar^2\alpha^2}\frac{x_0^3}{192[K_{2\ell+1}(x_0)]^2} \\ & \times \{6(\ell+1)[K_{2\ell+1}(x_0)K_{2\ell+2}(x_0) \\ & - K_{2\ell}(x_0)K_{2\ell+3}(x_0)] + x_0[K_{2\ell}(x_0)K_{2\ell+4}(x_0) \\ & - K_{2\ell+1}(x_0)K_{2\ell+3}(x_0)]\}. \end{aligned} \tag{D3}$$

Lane and Thomas [1, p. 351] have given in their Eq. (A.25) a similar expression, valid for $\ell = 0$ only, that is equivalent to our result in that case. It is not at all clear that $\partial S_\ell/\partial E$ as given by Eq. (D3) is positive. An alternative approach is to realize that at zero energy the wave function decays exponentially at large radii all the way out to ∞ (physically, the classical turning radius is infinite) and Eq. (27) can be used. This results in

$$\frac{\partial S_\ell}{\partial E} = \frac{2\mu}{\hbar^2\alpha^2}\frac{x_0^2}{32}\int_{x_0}^{\infty}\left[\frac{xK_{2\ell+1}(x)}{x_0K_{2\ell+1}(x_0)}\right]^2 x\,dx, \tag{D4}$$

which clearly shows $\partial S_\ell/\partial E > 0$ at zero energy. The equivalence of Eqs. (D3) and (D4) can be confirmed using differentiation and recurrence formulas. The small radius ($x_0 \to 0$) limits of these results, for ℓ a nonnegative integer, are

$$S_\ell = \begin{cases} \frac{x_0^2}{2}[\gamma + \log(x_0/2)] + \dots & \ell = 0 \\ -\ell - \frac{x_0^2}{8\ell} + \dots & \ell > 0 \end{cases} \tag{D5}$$

and

$$\frac{\partial S_\ell}{\partial E} = \frac{2\mu}{\hbar^2\alpha^2}\begin{cases} \frac{x_0^2}{48} + \dots & \ell = 0 \\ \frac{x_0^4}{64(2\ell-1)} + \dots & \ell > 0 \end{cases}, \tag{D6}$$

which are consistent with Eqs. (C2) and (C3) when the low-energy behavior of $h(\eta)$ is taken into consideration via Eq. (B9).

TABLE IV. Energy derivatives of some Coulomb quantities for large ρ.

$\frac{\partial A_\ell^2}{\partial E}$	$\sim \frac{\rho}{2E}\left[-\frac{2\eta}{\rho^2} - \frac{6\eta^2+\ell(\ell+1)}{\rho^3} + \dots\right]$
$\frac{\partial \phi_\ell}{\partial E}$	$\sim \frac{\rho}{2E}\left[1 + \frac{\eta}{\rho}\log(2\rho) - \frac{\eta}{\rho} - \frac{3\eta^2+\ell(\ell+1)}{2\rho^2} + \cdots\right] + \frac{\partial\sigma_\ell}{\partial E}$
$\frac{\partial P_\ell}{\partial E}$	$\sim \frac{\rho}{2E}\left[1 + \frac{\eta}{\rho} + \frac{3\eta^2+\ell(\ell+1)}{2\rho^2} + \cdots\right]$
$\frac{\partial S_\ell}{\partial E}$	$\sim \frac{\rho}{2E}\left[\frac{\eta}{\rho^2} + \frac{4\eta^2+\ell(\ell+1)}{\rho^3} + \cdots\right]$

APPENDIX E: ADDITIONAL INTEGRAL RELATIONS

Some integral expressions involving $\partial S/\partial E$ are given here. A general class of relations may be derived by multiplying through by an arbitrary function f before integrating to achieve Eq. (25). This procedure results in

$$-E\left[\frac{fO^2}{\rho}\frac{\partial L}{\partial E}\right]_{\rho_a}^{\rho_b} = \int_{\rho_a}^{\rho_b} O^2\left[f - \frac{E}{\rho}f'\frac{\partial L}{\partial E}\right]d\rho. \quad \text{(E1)}$$

One choice for f is

$$f = e^{-i\psi}, \quad \text{(E2)}$$

where ψ is defined by Eq. (29), such that $fO^2 = A^2$, $f' = -2if/A^2$, and

$$-E\left[\frac{A^2}{\rho}\frac{\partial L}{\partial E}\right]_{\rho_a}^{\rho_b} = \int_{\rho_a}^{\rho_b} A^2\left[1 + \frac{2i}{A^2}\frac{E}{\rho}\frac{\partial L}{\partial E}\right]d\rho. \quad \text{(E3)}$$

Taking the real part gives

$$-E\left[\frac{A^2}{\rho}\frac{\partial S}{\partial E}\right]_{\rho_a}^{\rho_b} = \int_{\rho_a}^{\rho_b}\left[A^2 - \frac{2E}{\rho}\frac{\partial P}{\partial E}\right]d\rho, \quad \text{(E4)}$$

and then letting $\rho_b \to \infty$ (noting that the integrand $\sim 1/\rho^3$ for large ρ) yields a relation for $\partial S/\partial E$:

$$E\left[\frac{A^2}{\rho}\frac{\partial S}{\partial E}\right]_{\rho_a} = \int_{\rho_a}^{\infty}\left[A^2 - \frac{2E}{\rho}\frac{\partial P}{\partial E}\right]d\rho. \quad \text{(E5)}$$

Interestingly, Eq. (49) ensures that the integrand in the right-hand side of this equation is positive. Alternatively, noting that

$$\frac{d\phi}{dr} = \frac{P}{r} \quad \text{and hence} \quad \frac{\partial}{\partial E}\left(\frac{d\phi}{dr}\right) = \frac{1}{r}\frac{\partial P}{\partial E}, \quad \text{(E6)}$$

the second term in the integrand of Eq. (E4) can be integrated to give

$$E\left[-\frac{A^2}{\rho}\frac{\partial S}{\partial E} + 2\frac{\partial\phi}{\partial E}\right]_{\rho_a}^{\rho_b} = \int_{\rho_a}^{\rho_b} A^2\, d\rho, \quad \text{(E7)}$$

which happens to be equivalent to Eq. (A.31) of Lane and Thomas [1, p. 352]. The leading asymptotic behavior of A^2 for large ρ can be subtracted

$$\left[-E\frac{A^2}{\rho}\frac{\partial S}{\partial E} + 2E\frac{\partial\phi}{\partial E} - \rho - \eta\log(2\rho)\right]_{\rho_a}^{\rho_b} = \int_{\rho_a}^{\rho_b}\left(A^2 - 1 - \frac{\eta}{\rho}\right)d\rho \quad \text{(E8)}$$

to allow $\rho_b \to \infty$ to be taken:

$$\left[E\frac{A^2}{\rho}\frac{\partial S}{\partial E} - 2E\left(\frac{\partial\phi}{\partial E} - \frac{\partial\sigma}{\partial E}\right) + \rho + \eta\log(2\rho) + \eta\right]_{\rho_a} = \int_{\rho_a}^{\infty}\left(A^2 - 1 - \frac{\eta}{\rho}\right)d\rho, \quad \text{(E9)}$$

where the asymptotic forms of the functions have been used to evaluate the surface terms at ∞.

It is also natural to investigate the integral relations arising from considering solutions O_1^* and O_2 with $O_2 \to O_1$. Assuming that $O = A\exp(i\phi)$ and multiplying through by an arbitrary function g before integrating yields:

$$-E\left[g\left(\frac{A^2}{\rho}\frac{\partial S}{\partial E} - 2\frac{\partial\phi}{\partial E}\right)\right]_{\rho_a}^{\rho_b} = \int_{\rho_a}^{\rho_b}\left[gA^2 - Eg'\left(\frac{A^2}{\rho}\frac{\partial S}{\partial E} - 2\frac{\partial\phi}{\partial E}\right)\right]d\rho. \quad \text{(E10)}$$

These relations are not independent of those derivable from Eq. (E1).

[1] A. M. Lane and R. G. Thomas, *R*-matrix theory of nuclear reactions, Rev. Mod. Phys. **30**, 257 (1958). There is a misprint in the third formula from the bottom of p. 350, column 1 (unnumbered): an equals sign should be placed between $(F^2 + G^2)/(2\rho)$ and the $\int$ symbol.

[2] P. Descouvemont and D. Baye, The *R*-matrix theory, Rep. Prog. Phys. **73**, 036301 (2010).

[3] C. R. Brune, Alternative parametrization of *R*-matrix theory, Phys. Rev. C **66**, 044611 (2002).

[4] John A. Wheeler, Wave functions for large arguments by the amplitude-phase method, Phys. Rev. **52**, 1123 (1937).

[5] R. M. Thaler and L. C. Biedenharn, A note on the calculation of Coulomb penetration and Coulomb wave functions, Nucl. Phys. **3**, 207 (1957).

[6] F. W. Prosser and L. C. Biedenharn, Some properties of the shift and penetration factors in nuclear reactions, Phys. Rev. **109**, 413 (1958). Note that this reference defines the shift factor S with the opposite sign compared to modern conventions. This paper also contains some errors. In Sec. III(c), Eq. (25) is incorrect [compare to Eq. (D5) of the present work], as is the statement that S cannot be monotonic in energy.

[7] M. H. Hull, Jr. and G. Breit, Coulomb wave functions, in *Nuclear Reactions II: Theory/Kernreaktionen II: Theorie* (Springer, Berlin/Heidelberg, 1959), p. 408. One of the factors of $-i\eta$ in the hypergeometric funtion in their Eq. (12.5) on p. 440 must be reversed in sign to agree with Eq. (16b) of the present work. Also, the $n = 5$ line of their Table 1 on p. 440 must contain an error because the asymptotic expansion of A_ℓ only consists of even terms when $\eta = 0$.

[8] A. Erdélyi, LXXV. Integral representations for products of Whittaker functions, London, Edinburgh Dublin Philos. Mag. J. Sci. **26**, 871 (1938).

[9] Herbert Buchholz, *The Confluent Hypergeometric Function*, Springer Tracts in Natural Philosophy, Vol. 15 (Springer-Verlag, Berlin, 1969).

[10] K. S. Miller and S. G. Samko, Completely monotonic functions, Integr. Trans. Spec. Funct. **12**, 389 (2001).

[11] G. N. Watson, *A Treatise on the Theory of Bessel Functions*, 2nd ed. (Cambridge University Press, Cambridge, 1944).
[12] M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions* (Dover Publications, New York, 1965).
[13] Philip Hartman, On differential equations, Volterra equations and the function $J_\mu^2 + Y_\mu^2$, Amer. J. Math. **95**, 553 (1973).
[14] Lee Lorch and Peter Szego, Higher monotonicity properties of certain Sturm-Liouville functions, Acta Math. **109**, 55 (1963).
[15] Loyal Durand, Product formulas and Nicholson-type integrals for Jacobi functions. I: Summary of results, SIAM J. Math. Anal. **9**, 76 (1978).
[16] M. E. Muldoon, On the zeros of some special functions: Differential equations and Nicholson-type formulas, in *Equadiff 6: Proceedings of the International Conference on Differential Equations and their Applications held in Brno, Czechoslovakia, Aug. 26–30, 1985*, edited by Jaromír Vosmanský and Miloš Zlámal (Springer, Berlin/Heidelberg, 1986), pp. 155–160.
[17] Philip Hartman, On differential equations and the function $J_\mu^2 + Y_\mu^2$, Amer. J. Math. **83**, 154 (1961).
[18] M. Goldstein and R. M. Thaler, Bessel functions for large arguments, Math. Comp. **12**, 18 (1958).
[19] R. G. Thomas, On the determination of reduced widths from the one-level dispersion formula, Phys. Rev. **81**, 148 (1951).
[20] G. M. Hale, Ronald E. Brown, and Nelson Jarmie, Pole Structure of the $J^\pi = 3/2^+$ Resonance in ^{5}He, Phys. Rev. Lett. **59**, 763 (1987).
[21] E.O. Tuck, On positivity of Fourier transforms, Bull. Austral. Math. Soc. **74**, 133 (2006).
[22] H. A. Bethe, Theory of the effective range in nuclear scattering, Phys. Rev. **76**, 38 (1949).
[23] J. David Jackson and John M. Blatt, The interpretation of low energy proton-proton scattering, Rev. Mod. Phys. **22**, 77 (1950).
[24] H. van Haeringen, T matrix and effective range function for Coulomb plus rational separable potentials especially for $l = 1$, J. Math. Phys. **18**, 927 (1977).
[25] Milton Abramowitz, Regular and irregular Coulomb wave functions expressed in terms of Bessel-Clifford functions, J. Math. Phys. **33**, 111 (1954).
[26] J. Humblet, Bessel function expansions of Coulomb wave functions, J. Math. Phys. **26**, 656 (1985).
[27] J. Humblet, W. A. Fowler, and B. A. Zimmerman, Approximate penetration factors for nuclear reactions of astrophysical interest, Astron. Astrophys. **177**, 317 (1987).