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On the calculation of phase shifts produced by complex potentials

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A formula for the complex phase shift, pertaining to the one-turning-point scattering problem with a complex potential, is given in a general form based on a kind of arbitrary-order phase-integral approximation. The accuracy of the formula is illustrated by application to a real Coulomb potential supplemented by an imaginary potential term proportional to $1/r^2$. For that case the arbitrary-order phase-integral expression for the complex phase shift is evaluated in a closed, analytical form, which displays the simplicity and accuracy of the higher-order corrections.

I. INTRODUCTION

Complex potentials are extensively used in scattering theory to describe inelastic, absorptive processes, for instance in molecular-beam experiments (see Ref. 1 and references given therein) and in heavy-ion collision theory.[2-7] In the extensive literature on singular potentials, many authors have in recent years considered complex coupling constants.[8-11] Since the wavelength associated with the relative motion of the colliding particles is in many cases small compared to the dimensions of the region in which the interaction is appreciable, the conditions are favorable for the use of semiclassical methods for the calculation of phase shifts.

The justification of the extension of the JWKB expression for the phase shift to the case of complex potentials is, in the literature, usually taken for granted, and generalized formulas are merely written down. In the case of weak absorption, the complex phase shift is often expanded with respect to the absorptive, imaginary part of the potential, and only the linear term is retained, which yields, of course, a strongly oversimplified picture of the phenomena involved. In the review article by Koeling and Malfliet,[3] the generalization of the JWKB formula for the phase shift to allow for complex potentials is discussed on the basis of Feynman's path-integral method, and in Ref. 11 the phase shift for the case of inverse-power, singular potentials with complex coupling constant, is derived along the same lines followed by Goldberger and Watson[12] in the derivation of the JWKB phase shift for real potentials.

While a merit of the semiclassical treatment of absorptive processes is that it provides necessary physical insight, such a treatment often yields only a qualitative description and is hence too crude. In heavy-ion collision theory, the possibility of improving the accuracy by including higher-order corrections to the complex phase shift has been considered occasionally but not systematically. A correction to the semiclassical phase shift was derived by Malfliet (see pp. 10–12 in Ref. 4) who, neglecting the imaginary part of the potential, arrived at the same correction as obtained by Rosen and Yennie[13] by a different approach.

In the present paper, attention is drawn to the fact that the phase-integral method developed by N. Fröman and P. O. Fröman is applicable to the case of complex potentials also. For a general background of the method we refer to Refs. 14–17 and pp. 126–131 in Ref. 18. A detailed documentation of the advantages of the higher-order phase-integral approximations used in the method *versus* the usual higher-order JWKB approximations is given in Ref. 19. Assuming that there is only one complex turning point to be taken into account, we derive in Sec. II the arbitrary-order phase-integral formula for the complex phase shift.

In Sec. III we illustrate the role of an absorptive potential by considering a real Coulomb potential supplemented by an imaginary potential term proportional to $1/r^2$. The integrals occurring in the phase-shift formula can then be evaluated analytically. The resultant closed analytical expression for the complex phase shift displays the simplicity of the higher-order corrections. The great increase in accuracy obtainable when higher-order approximations are used is illustrated numerically, and the inherent property of the approximations to break down at very high orders is shown as well.

II. ARBITRARY-ORDER PHASE-INTEGRAL FORMULA FOR THE PHASE SHIFT FOR THE CASE WHEN THERE IS ONE TURNING POINT TO BE TAKEN INTO ACCOUNT

Using standard notations, we write the radial Schrödinger equation as

$$\frac{d^2u}{dr^2} + Q^2(l\,;\,r)u = 0\,. \tag{1a}$$

with

$$Q^2(l\,;r)=k^2-\frac{2m}{\hbar^2}V(r)-\frac{l(l+1)}{r^2}\,, \tag{1b}$$

where the potential $V(r)$ may be complex. If certain conditions are fulfilled (see, e.g., Chap. 11 in Ref. 14), the boundary condition $u(0)=0$ selects a solution $u_l(r)$ of the differential equation (1a) and (1b), which is unique except for an arbitrary constant factor. We shall here include the case of a potential with a Coulombic behavior when $r\to\infty$. If the Coulomb term in the right-hand member of (1b) is $-2k\eta/r$, the solution $u_l(r)$ is (except for a constant factor) represented by the asymptotic formula (see, e.g., Chap. III, subsec. 6 in Ref. 20)

$$u_l(r)\sim\sin[kr-\eta\ln(2kr)-\tfrac{1}{2}l\pi+\delta_l]\,,\quad r\to\infty\,, \tag{2}$$

where δ_l is the phase shift. For the case of a potential, which tends to zero faster than $1/r$ when $r\to\infty$, the term $-\eta\ln(2kr)$ in (2) should merely be omitted.

We shall choose the function $Q_{\text{mod}}{}^2$, introduced in Ref. 17 and on pp. 126–131 in Ref. 18, such that the phase-integral approximations are valid also when r tends to zero, which is achieved if we set

$$\begin{aligned}Q_{\text{mod}}{}^2(l\,;r)&=Q^2(l\,;r)-\frac{1}{4r^2}\\&=k^2-\frac{2m}{\hbar^2}V(r)-\frac{(l+\frac{1}{2})^2}{r^2}\,.\end{aligned} \tag{3}$$

For the phase-integral approximation of the order $2N+1$, we have

$$q(l\,;r)=Q_{\text{mod}}(l\,;r)\sum_{n=0}^{N}Y_{2n}\,, \tag{4}$$

where the first few functions Y_{2n} are

$$Y_0=1\,, \tag{5a}$$

$$Y_2=\tfrac{1}{2}\epsilon_0\,, \tag{5b}$$

$$Y_4=-\tfrac{1}{8}\epsilon_0{}^2+\text{a term which contributes to } u_l(r) \text{ for finite values of } r \text{ but does not contribute to the complex phase shift}\,, \tag{5c}$$

with

$$\epsilon_0=\frac{Q^2-Q_{\text{mod}}{}^2}{Q_{\text{mod}}{}^2}+\frac{1}{16Q_{\text{mod}}{}^6}\left[5\left(\frac{dQ_{\text{mod}}{}^2}{dr}\right)^2-4Q_{\text{mod}}{}^2\frac{d^2Q_{\text{mod}}{}^2}{dr^2}\right]. \tag{6}$$

Explicit expressions for Y_{2n} up to Y_8 are given in Ref. 21 and up to Y_{20} in Ref. 22.

With the aid of the connection formula given by Eq. (21) in Ref. 16, and with due regard to the generalization described in Ref. 17 and on pp. 126–131 in Ref. 18, the formula for the phase shift pertaining to a real potential and a one-turning-point scattering problem is readily obtained in any order of approximation. It is a straightforward procedure to generalize the derivation of the connection formula in question to apply to that case in which one is dealing with a complex transition point and is making a connection from a certain Stokes's line emerging from that transition point to the anti-Stokes's line which continues the Stokes's line on the other side of the transition point [see Eq. (5.16) and Sec. 10 in Ref. 23]. With the aid of this connection formula, the general arbitrary-order phase-shift formula applying to a complex potential and to the case in which only one complex turning point r_0 is to be taken into account can be obtained as follows. The behavior of the wave function $u_l(r)$ in the vicinity of $r=0$ determines (except for a constant factor) the phase-integral expression for $u_l(r)$ on a Stokes's line emerging from r_0 and passing close to the origin. Hence, according to the above-mentioned generalized connection formula, i.e., Eq. (5.16) in Ref. 23, the phase-integral expression for $u_l(r)$ on the anti-Stokes's line that continues the Stokes's line on the other side of the transition point r_0 becomes

$$u_l(r)=k^{1/2}q^{-1/2}(l\,;r)\sin\left[\tfrac{1}{2}\int_\Gamma q(l\,;r)dr+\tfrac{1}{4}\pi\right], \tag{7}$$

apart from a constant factor. In the limit $r=\infty$, the contour Γ is an infinite, nonclosed loop starting at $+\infty-i0$, encircling in the negative sense the complex zero r_0 of $Q_{\text{mod}}{}^2(l\,;r)$, and ending at $+\infty+i0$, as shown schematically in Fig. 1.

Comparing (7) and (2), we obtain the following approximate formula for the phase shift:

$$\delta_l=\lim_{r\to\infty}\left[\tfrac{1}{2}\int_\Gamma q(l\,;r)dr-kr+\eta\ln(2kr)+\tfrac{1}{2}(l+\tfrac{1}{2})\pi\right]. \tag{8}$$

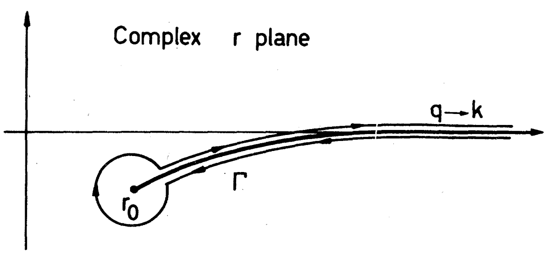

FIG. 1. Schematic drawing of the path of integration Γ encircling the complex zero r_0 of $Q_{\text{mod}}{}^2(l;r)$. The point r_0 lies in the fourth quadrant since $V(r)$ contains a negative imaginary part. The heavy line emerging from r_0 indicates a cut. The phase of q is chosen such that $q\to k\,(>0)$ when $r\to+\infty+i\,0$.

For $N=0$ [and with the term $\eta\ln(2kr)$ omitted], we recognize (8) as the usual first-order JWKB expression for the phase shift [see, e.g., Eq. (11.45) in Ref. 14], the extension of which, to the case of complex potentials, usually is taken for granted without justification in the literature.

III. APPLICATION OF THE FORMULA FOR THE PHASE SHIFT TO A PARTICULAR POTENTIAL

To illustrate the role of an absorptive potential, Broglia *et al.*[2] considered the special case of a particle moving in a purely imaginary potential corresponding to $V(r)=-ib\hbar^2/(2mr^2)$ in (1b). The Schrödinger equation for this case can be solved analytically in terms of Bessel functions of complex order, and the complex phase shift can be obtained from the asymptotic form of the solution. Just as in the case of a real potential proportional to $1/r^2$, already the first-order JWKB formula yields the complex phase shift exactly, and hence the potential in question is not useful for our present purpose of studying the accuracy, in successive orders of approximation, of the phase-integral expression for the complex phase shift.

For the purpose of studying the effect of the higher-order corrections to the phase shift, we shall consider a real, repulsive Coulomb potential, supplemented by the above-mentioned imaginary potential. For this model, the radial Schrödinger equation (1a) and (1b) becomes

$$\frac{d^2u}{dr^2}+\left[k^2-\frac{2k\eta}{r}-\frac{l(l+1)-ib}{r^2}\right]u=0\,, \tag{9}$$

and it is a straightforward procedure to calculate the function $q(l\,;r)$ in (8) with the aid of Eqs. (4)–(6). The evaluation of the integral over Γ in (8) is also straightforward but tedious. Therefore, without entering into any details, we give only the resulting phase-integral expression for the complex phase shift in the $(2N+1)$th-order approximation, which can be written as

$$\delta_l=\sum_{n=0}^{N}\delta_l^{(2n+1)}\,, \tag{10}$$

where

TABLE I. Phase shifts for states with $l=1$ in the complex potential $V(r)=\hbar^2(2k\eta/r-ib/r^2)/(2m)$, where η and b are dimensionless parameters. The phase-integral values are obtained from formula (10) with (10a) and (10b), and the exact values are obtained from formula (12). For $b=0.25$, a few values obtained in very high orders of approximation (23, 25, 27, 61) are given to illustrate the approach to optimal order, subsequent deterioration, and final breakdown of the phase-integral approximations.

	Order of	$\eta=0.5$		$\eta=1$		$\eta=4$	
b	approximation	Real part	Imag. part	Real part	Imag. part	Real part	Imag. part
0.25	1	0.210	0.104 0	0.47	0.081 9	3.626	0.029 9
	3	0.217 8	0.104 81	0.482 9	0.082 84	3.635 43	0.030 022
	5	0.217 27	0.104 72	0.482 47	0.082 799	3.635 444 6	0.030 024 06
	7	0.217 34	0.104 741	0.482 476	0.082 796	3.635 444 51	0.030 024 100 4
	9	0.217 322	0.104 736 0	0.482 483	0.082 799	3.635 444 489	0.030 024 101 2
	11	0.217 325 95	0.104 735 7	0.482 479 7	0.082 798 4	3.635 444 487 2	0.030 024 101 05
	13	0.217 329	0.104 740	0.482 479 6	0.082 797 5	3.635 444 487 096	0.030 024 101 006
	23	0.217 34	0.105 2	0.482 46	0.082 82	3.635 444 487 106 8	0.030 024 100 995 74
	25	0.216 4	0.101	0.482 40	0.082 6	3.635 444 487 106 6	0.030 024 100 995 90
	27	0.225	0.12	0.483 1	0.083 2	3.635 444 487 106 21	0.030 024 100 995 91
	61	···	···	···	···	3.635 443 9	0.030 024 4
	exact	0.217 325 90	0.104 736 76	0.482 480 4	0.082 798 3	3.635 444 487 106 17	0.030 024 100 995 71
1	1	0.178	0.410	0.45	0.325	3.625	0.119 6
	3	0.185 1	0.413 2	0.464 2	0.328 7	3.634 36	0.120 06
	5	0.184 76	0.412 96	0.463 79	0.328 585	3.634 377 0	0.120 071 7
	7	0.184 795	0.413 01	0.463 808 9	0.328 581	3.634 376 78	0.120 071 903
	9	0.184 787	0.412 996	0.463 809 0	0.328 589	3.634 376 757	0.120 071 905
	11	0.184 791	0.413 001	0.463 807	0.328 585	3.634 376 755 3	0.120 071 904 2
	13	0.184 785	0.413 000 30	0.463 810	0.328 585 7	3.634 376 755 14	0.120 071 904 04
	exact	0.184 788 99	0.413 000 23	0.463 808 1	0.328 586 3	3.634 376 755 18	0.120 071 904 00
4	1	−0.165	1.438	0 .232	1.199	3.609	0.477
	3	−0.163 05	1.441 9	0.237 19	1.205 6	3.617 484 1	0.478 72
	5	−0.162 99	1.441 745	0.237 184	1.205 33	3.617 484 3	0.478 747 5
	7	−0.163 003	1.441 749 9	0.237 178	1.205 347	3.617 483 53	0.478 747 71
	9	−0.163 000 4	1.441 751 6	0.237 179 4	1.205 343 1	3.617 483 497	0.478 747 669
	11	−0.163 000 77	1.441 750 5	0.237 178 8	1.205 344 6	3.617 483 498 7	0.478 747 662 9
	13	−0.163 001 0	1.441 751 1	0.237 179 3	1.205 343 7	3.617 483 499 84	0.478 747 662 9
	exact	−0.163 000 79	1.441 750 87	0.237 179 0	1.205 344 1	3.617 483 499 88	0.478 747 663 19

$$\delta_l^{(1)} = \tfrac{1}{2}\pi\{l + \tfrac{1}{2} - [(l+\tfrac{1}{2})^2 - ib]^{1/2}\} - \eta + \tfrac{1}{2}i\{[(l+\tfrac{1}{2})^2 - ib]^{1/2} - i\eta\}\ln\{[(l+\tfrac{1}{2})^2 - ib]^{1/2} - i\eta\}$$
$$- \tfrac{1}{2}i\{[(l+\tfrac{1}{2})^2 - ib]^{1/2} + i\eta\}\ln\{[(l+\tfrac{1}{2})^2 - ib]^{1/2} + i\eta\}, \qquad (10a)$$

$$\delta_l^{(2n+1)} = \frac{(1-2^{1-2n})|B_{2n}|}{4n(2n-1)}\left(\frac{1}{\{\eta + i[(l+\frac{1}{2})^2 - ib]^{1/2}\}^{2n-1}} + \frac{1}{\{\eta - i[(l+\frac{1}{2})^2 - ib]^{1/2}\}^{2n-1}}\right)$$
$$= \frac{(1-2^{1-2n})|B_{2n}|}{2n(2n-1)[\eta^2 + (l+\frac{1}{2})^2 - ib]^{2n-1}} \sum_{j=0}^{n-1} \binom{2n-1}{2j} [ib - (l+\tfrac{1}{2})^2]^j \eta^{2n-2j-1}, \quad n > 0, \qquad (10b)$$

and B_{2n} are the Bernouilli numbers.[24]

Since Eq. (9) has the form of a Coulomb wave equation with a complex angular momentum quantum number (see, e.g., Eq. (14.1.1) in Ref. 24 with $\rho = kr$ and $L = -\frac{1}{2} + [(l+\frac{1}{2})^2 - ib]^{1/2}$), we can easily obtain a formula for the exact wave function and hence for the exact phase shift. Using Eqs. (14.1.3) and (13.5.1) in Ref. 24, we thus obtain, for large values of r, the asymptotic formula for the regular solution $u_l(r)$,

$$u_l(r) \sim \sin\left(kr - \eta\ln(2kr) + \tfrac{1}{4}\pi - \tfrac{1}{2}\pi[(l+\tfrac{1}{2})^2 - ib]^{1/2} + \tfrac{1}{2}i\ln\frac{\Gamma(\frac{1}{2} + [(l+\frac{1}{2})^2 - ib]^{1/2} - i\eta)}{\Gamma(\frac{1}{2} + [(l+\frac{1}{2})^2 - ib]^{1/2} + i\eta)}\right), \qquad (11)$$

apart from a constant factor. Comparing (11) and (2), we obtain the exact value of the complex phase shift

$$(\delta_l)_{\text{exact}} = \tfrac{1}{2}\pi\{l + \tfrac{1}{2} - [(l+\tfrac{1}{2})^2 - ib]^{1/2}\} + \tfrac{1}{2}i\ln\frac{\Gamma(\frac{1}{2} + [(l+\frac{1}{2})^2 - ib]^{1/2} - i\eta)}{\Gamma(\frac{1}{2} + [(l+\frac{1}{2})^2 - ib]^{1/2} + i\eta)}. \qquad (12)$$

It is immediately seen that for $\eta = 0$ the phase-integral expression (10) with (10a) and (10b) for the phase shift becomes identical with the exact expression (12).

For given values of η and b a numerical comparison between the exact formula (12) and the phase-integral formula (10) with (10a) and (10b) shows that the accuracy of the phase-integral values of δ_l increases as l increases. In Table I it is illustrated that already for $l = 1$ a very high accuracy is obtainable, when higher-order phase-integral approximations are used. However, if we go beyond an optimal order, the approximation deteriorates and eventually breaks down for sufficiently high orders of approximation. The optimal order of approximation becomes higher with increasing values of η and l. In practice one hardly ever goes to such high orders, and for many practical purposes it is sufficient to use the formula for δ_l in the first-order approximation, but even then the first few higher-order approximations are useful, since they give information about the error involved.

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