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Resonance Method in Scattering Theory*

By

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This article was originally meant to precede a second article [1], where now definitions and notations used here are described in more detail. This part will here be cut down to a minimum.

The aim of the investigations is to replace the ordinary treatment of the scattering problem by an indirect one. This can be done by providing the scattering potential with an adjustable numerical factor which is used as an eigenvalue parameter of a discrete eigenvalue problem.

The term "resonance method" simply alludes to the structure of the formulae.

AUTHOR

1. Introduction

It is well known that in scattering problems an incoming plane wave of particles can be separated into waves of different angular momentum, S-, P- and D-waves, etc., and that each wave may be treated separately. The quantity governing the properties of the scattered wave is called the asymptotic phase or phase shift and is usually denoted by δ or η. Here we shall denote it by $\xi_l(k)$ with indications of its dependence on l and k, the azimuthal quantum number and the momentum k or energy k^2. Since for simplicity we are here dealing only with S-waves, $l=0$, we may simplify the notation into $\xi(k)$ or ξ_k, and when possible simply ξ.

The scattering problem is given by a differential equation

$$\left\{\frac{d^2}{dr^2}+k^2+AU(r)\right\}y=0 \tag{1}$$

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with the boundary condition $y(0)=0$. The function $AU(r)$ is the perturbing or scattering potential, however of opposite sign, so that $-AU(r)$ is the true potential energy. If the solution has the asymptotic form $y(r) \rightarrow \sin(kr+\xi)$ as $r \rightarrow \infty$, ξ is the asymptotic phase.

If the potential function does not allow for an elementary solution the problem is usually not easily solved directly, even though a number of variational methods (L. Hulthén, J. Schwinger, etc.) have been developed to serve the purpose fairly satisfactorily.

In this investigation we shall try an indirect method, using the potential strength A as a variable eigenvalue parameter, whereas k is so fixed that is corresponds to a negative energy state. If $k=i\varkappa$ the energy is $-\varkappa^2$. So it is also for $k=-i\varkappa$, but we shall distinguish between the two values so that the asymptotic solutions $e^{\mp\varkappa r}$ corresponds to $e^{\pm ikr}$. This means that k-values corresponding to bound states are always on the positive imaginary k-axis.

In order not to meet with particular difficulties we shall take $U(r)$ to be positive all the way. Then the eigenvalues of A are discrete eigenvalues which are usually somewhat easier obtained than the asymptotic phase itself by direct means. The calculation of an infinite number of eigenvalues $A=A_n, n=1,2,\ldots,$ is not a serious obstacle because as $n \rightarrow \infty$ asymptotic values are usually fairly easily found.

The method was first presented at a meeting of the Norwegian Physical Society in Trondheim, May 1956, and subsequently published [2] as a preprint, which because of several misprints was republished a long time afterwards in our Institute Reports [3].

As the investigation is presented here it is not much different from the institute report, even though former more complete. It was considered to use the notations introduced mainly by Jost and Kohn [6] (see references in ref. [8]) and adopted in recent works [4]. This was finally rejected because of some inconveniences and because of the uncertainty as to whether they are going to be the final ones [5].

2. Definitions and Notations

We shall consider two particular solutions of eq. (1), $u(\pm k, r)$, as our principal solutions. They are defined by their asymptotic values

$$u(\pm k, r) \rightarrow e^{\pm ikr} \quad \text{as} \quad r \rightarrow \infty, \tag{2}$$

and hence correspond to the Jost and Kohn functions $f(\mp k, r)$. They also differ from the notation of Ref. 3 where the exponentials are considered split off such that there $u(\pm k, r)\to 1$. For real k the two functions are conjugate and may be denoted by the shorter symbols u and u^*. In the case of complex k the shorter notation u may still be used. In particular for $k=i\varkappa$, $u(k,r)=u(i\varkappa,r)\to e^{-\varkappa r}$ and hence it is u which has to be used in the eigenvalue equation

$$\left\{\frac{d^2}{dr^2}-\varkappa^2+AU(r)\right\}u=0. \tag{3}$$

If we define by $$u(\pm k, r)\, e^{\pm i\xi}=y_2\pm iy_1, \tag{4}$$

a second set of independent solutions

$$\left.\begin{aligned} y_1(r)&=\frac{1}{2i}\{ue^{i\xi}-u^*e^{-i\xi}\}\\ y_2(r)&=\tfrac{1}{2}\{ue^{i\xi}+u^*e^{-i\xi}\}\end{aligned}\right\} \tag{4 a}$$

it is seen that requiring $u(k,0)\,e^{i\xi}$ real means $y_1(0)=0$. Using the abbreviations $u(\pm k,0)=u(\pm k)$ we have

$$\left.\begin{aligned} u(k)=|u(k)|\,e^{-i\xi},\quad u(-k)=|u(k)|\,e^{i\xi},\\ e^{2i\xi}=\frac{u(-k)}{u(k)}.\end{aligned}\right\} \tag{5}$$

$u(\pm k, r)$ may conveniently be called amplitude functions and $u(\pm k)$ asymptotic amplitudes.

The Wronskians of the two sets of functions, defined as $W\{y,z\}=y'z-yz'$, are seen to be

$$W\{u,u^*\}=2ik,\quad W\{y_1,y_2\}=k. \tag{6}$$

It follows from (4) and (6) that asymptotic values at $r=0$ are

$$y_2(0)=|u(k)|,\quad y_1(r)\to\frac{kr}{|u(k)|}\quad \text{as}\quad r\to 0. \tag{7}$$

3. Solutions by the Theory of Eigenvalues

Provided $U(r)$ positive in the region $0\leqslant r\leqslant\infty$, eq. (3) has an infinity of positive eigenvalues $A_n(\varkappa)$, $n=1,2,\dots,\infty$. In the case of $U(r)\to Ce^{-\alpha r}$ as $r\to\infty$, $e^{-\alpha r}$ may be used for a new independent variable transforming the fundamental region into a finite region $0\leqslant e^{-\alpha r}\leqslant 1$, from which it may be concluded that the eigenvalues increase quadratically with n.

We now consider $u(k)$ a function of A. Since $u(k,0)=u(k)$ is bound to be zero for any k producing a closed state eigenfunction we must have

$$u(i\varkappa)=\prod_{n=1}^{\infty}\left[1-\frac{A}{A_n(\varkappa)}\right], \tag{8}$$

its value for $A=0$ being unity. Provided the $A_n(\varkappa)$ are known for all real values of $\varkappa$ and, moreover, may be taken to be analytical functions of $\varkappa$

$$u(k)=\prod_{n=1}^{\infty}\left[1-\frac{A}{A_n(-ik)}\right], \tag{8 a}$$

$$u(-k)=\prod_{n=1}^{\infty}\left[1-\frac{A}{A_n(ik)}\right], \tag{8 b}$$

and

$$\xi=\frac{1}{2i}\sum_{n=1}\log\frac{1-A/A_n(ik)}{1-A/A_n(-ik)}. \tag{9}$$

4. Zeros and Infinities of the Asymptotic Amplitudes

If the parameter A fixing the magnitude of the scattering potential is given the zeros of $u(i\varkappa)$ are found from the equation

$$A_n(\varkappa)=A. \tag{10}$$

The $A_n(\varkappa)$ increase monotonically with $\varkappa$ for positive real $\varkappa$. Therefore, if

$$A_m(0)\leqslant A\leqslant A_{m+1}(0) \tag{10 a}$$

there will be a positive $\varkappa$-value for which $A_m(\varkappa)=A$, and there will be another and higher $\varkappa$-value for which $A_{m-1}(\varkappa)=A$, and so on, the number of positive $\varkappa$-values which are zeros of $u(i\varkappa)$ becoming m. In the k-plane these zeros $k=i\varkappa$ are all on the positive imaginary k-axis.

In the case of an exponentially decreasing potential of the asymptotic form $e^{-\alpha r}, x=e^{-\alpha r}$ may be used for a new independent variable in a limited region $0\leqslant x\leqslant 1$. If $U(r)$ is positive all the way it is found that asymptotically $A_n(\varkappa)$ is a quadratic function in n. Since $A_n(\varkappa)$ increases with $\varkappa$ it must have the asymptotic form

$$A_n(\varkappa)=c(n+a\varkappa)(n+b\varkappa) \tag{10 b}$$

with $a,b\geqslant 0$. For larger n therefore $u(i\varkappa)$ will have a double set of negative $\varkappa$-zeros corresponding to a double set of k-zeros on the negative imaginary axis. In the case of a or b being zero, there is only one such set, the other one being skipped away to infinity. The result hence is a finite number of zeros of $u(k)$ on the positive imaginary axis, the number depending on the magnitude of A, and an infinite number on the negative imaginary k-axis.

Similarly the condition for $u(k)$ becoming infinitely large is

$$A_n(\varkappa)=0. \tag{11}$$

From (10 b) we see that asymptotically the corresponding $\varkappa$-values are negative and the k-values on the negative imaginary axis. Moreover, the infinities are simple poles except in the case of $a=b$.

Similarly, $u(-k)$ has a limited number of zeros on the negative imaginary k-axis, all other zeros and poles being on the positive imaginary axis. The poles of $u(-k)$ are by some authors called redundant zeros of $S(-k)=e^{-2i\xi}$ $=u(k)/u(-k)$.

5. Exemplifications

Example 1. $$U(r)=\lambda(\lambda+1)\alpha^2(1-\mathrm{tgh}^2\,\alpha r). \tag{12}$$

This is a particularly nice example, an Eckhardt potential decreasing asymptotically as $e^{-2\alpha r}$ and with a flat bottom of the symmetric true potential $-U(r)$, i.e., $U(-r)=U(r)$. For this reason the transformed equation (3)

$$\left\{\frac{d}{dx}(1-x^2)\frac{d}{dx}-\frac{(\varkappa/\alpha)^2}{1-x^2}+\lambda(\lambda+1)\right\}y=0 \tag{13}$$

with
$$x=\mathrm{tgh}\,\alpha r \tag{13 a}$$

becomes extremely simple with symmetric and antisymmetric solutions in x or r, of which only the antisymmetric ones fulfil the requirement $y(0)=0$. Hence, using

$$A=\lambda(\lambda+1) \tag{13 b}$$

for eigenvalue parameter its eigenvalues are

$$A_n(\varkappa)=\left(2n-1+\frac{\varkappa}{\alpha}\right)\left(2n+\frac{\varkappa}{\alpha}\right)\quad(n=1,2,\ldots,\infty). \tag{13 c}$$

The double set of poles are at $\varkappa_m=-m\alpha$ and, hence, the poles of $u(k)$ at

$$k_m=-im\alpha\quad(m=1,2,\ldots,\infty). \tag{13 d}$$

The double set of zeros of $u(k)$ as obtained from eq. (10) are at $\varkappa=-\alpha(2n-1-\lambda)$ and $\varkappa=-(2n+\lambda)$, or

$$k_n=-i\alpha(2n-1-\lambda),\quad k_n'=-i\alpha(2n+\lambda)\quad(n=1,2,\ldots,\infty). \tag{13 c}$$

If $1\leqslant\lambda\leqslant 3$ there is one zero, and if $2m-1\leqslant\lambda\leqslant 2m+1$ there are m zeros on the positive imaginary k-axis, all other zeros being on the negative side.

The asymptotic amplitude $u(k)$ therefore must be

$$u(k)=\frac{\left(-\frac{ik}{2\alpha}-\frac{1}{2}\right)!\left(-\frac{ik}{2\alpha}\right)!}{\left(-\frac{ik}{2\alpha}-\frac{\lambda+1}{2}\right)!\left(-\frac{ik}{2\alpha}+\frac{\lambda}{2}\right)!} \tag{14}$$

since the gamma functions of the nominator are accounting for the poles and those of the denominator for the zeros, and finally for $A=0$, $\lambda=0$, its value is 1. By the duplication formula of the gamma function it may also be written

$$u(k)=\frac{2^{ik/\alpha}\left(-\frac{ik}{\alpha}\right)!\,(-\frac{1}{2})!}{\left(-\frac{ik}{2\alpha}-\frac{\lambda+1}{2}\right)!\left(-\frac{ik}{2\alpha}+\frac{\lambda}{2}\right)!}. \tag{14 a}$$

In varying λ the situation is: At $\lambda=0$ the zeros and poles are accurately cancelling. As λ increases the poles are kept fixed, whereas one set of the zeros are creeping up, the other down. For integral λ there is a particular degeneration, the zeros and poles again cancelling except for some few of them on either side, for instance,

$$\left.\begin{aligned}
&\lambda=1,\ u(k)=\frac{k}{k+i\alpha}, && \lambda=2,\ u(k)=\frac{k-i\alpha}{k+2i\alpha},\\
&\lambda=3,\ u(k)=\frac{k(k-2i\alpha)}{(k+i\alpha)(k+3i\alpha)}, && \lambda=4,\ u(k)=\frac{(k-i\alpha)(k-3i\alpha)}{(k+2i\alpha)(k+4i\alpha)},
\end{aligned}\right\} \tag{14 b}$$

from which the law for the distribution of zeros and poles in the degenerate case is easily seen.

The amplitude function $u(k,r)$ is of course easily found in the ordinary way as expressed in powers of $\frac{1}{2}(1-\operatorname{tgh}\alpha r)$ or $(1-\operatorname{tgh}^2\alpha r)$. It may be given in three useful forms, namely,

$$\exp\left(-\frac{ik}{\alpha}r\right)u(k,r)=F\left(-\lambda,\lambda+1,1-\frac{ik}{\alpha},\frac{1-\operatorname{tgh}\alpha r}{2}\right), \tag{15}$$

$$\exp\left(\frac{ik}{\alpha}r\right)u(k,r)=\left(\frac{1-\operatorname{tgh}\alpha r}{2}\right)^{-ik/\alpha}F\left(-\lambda-\frac{ik}{\alpha},\lambda+1-\frac{ik}{\alpha},1-\frac{ik}{\alpha},\frac{1-\operatorname{tgh}\alpha r}{2}\right), \tag{15 a}$$

$$\begin{aligned}&\exp\left(\frac{ik}{\alpha}r\right)u(k,r)\\ &\quad=\left(\frac{1-\operatorname{tgh}\alpha r}{2}\right)^{-ik/\alpha}F\left(-\frac{\lambda}{2}-\frac{ik}{2},\frac{\lambda+1}{2}-\frac{ik}{2\alpha},1-\frac{ik}{\alpha},1-\operatorname{tgh}^2\alpha r\right).\end{aligned} \tag{15 b}$$

Putting $r=0$ in (15 b) and using the formula

$$F(a,b,c,1)=\frac{(c-1)!\,(c-1-a-b)!}{(c-1-a)!\,(c-1-b)!} \tag{15 c}$$

we obtain the asymptotic amplitude in the form (14 a).

Example 2.
$$U(r)=\frac{4\lambda^2\alpha^2 e^{-2\alpha r}}{1-e^{-2\alpha r}}. \tag{16}$$

This is a most interesting potential similar to the Yukawa in having a pole at the origin. It is also more definite in its results than the above Eckhardt potential of Example 1. Putting

$$A=\lambda^2, \quad x=e^{-2\alpha r}, \quad k=i\varkappa, \tag{16 a}$$

we have the eigenvalue equation

$$\left\{(1-x)\frac{d}{dx}x\frac{d}{dx}-\frac{\varkappa^2}{4\alpha^2}\frac{1-x}{x}+A\right\}u=0. \tag{17}$$

Noting the asymptotic factors

$$1-e^{-2\alpha r}=1-x \quad \text{and} \quad e^{ikr}=x^{\varkappa/2\alpha} \tag{17 a}$$

to be split off before expanding u in a power series it is not hard to see that the eigenvalues of A are

$$A_n(\varkappa)=\left(n+\frac{\varkappa}{2\alpha}\right)^2-\left(\frac{\varkappa}{2\alpha}\right)^2=n\left(n+\frac{\varkappa}{\alpha}\right) \quad (n=1,2,\ldots,\infty). \tag{17 b}$$

Consulting eq. (11), we see that there is now only one set of poles, $\varkappa=-n\alpha$, or

$$k_n=-in\alpha \quad (n=1,2,\ldots,\infty). \tag{17 c}$$

According to eq. (10) the zeros are found from

$$n\left(n+\frac{\varkappa}{\alpha}\right)=\lambda^2, \tag{17 d}$$

which gives
$$\varkappa=\alpha\left(\frac{\lambda^2}{n}-n\right), \quad k_n=i\alpha\left(\frac{\lambda^2}{n}-n\right). \tag{17 e}$$

Again we see there are only a few zeros on the positive imaginary axis giving bound eigenstates. The rest, infinite in number, are on the negative side, as are also the poles. There is, however, no general degeneration. Even in the case of integral λ cancelling of zeros and poles occurs only accidentally, even though their asymptotic distributions as $n\to\infty$ have the same density.

For the purpose of expressing $u(k)$ by means of gamma functions eq. (17 d) should rather have been solved with respect to n. We therefore write it in the form

$$\left(n+\frac{\varkappa}{2\alpha}+l\right)\left(n+\frac{\varkappa}{2\alpha}-l\right)=0,\quad l^2=\lambda^2+\left(\frac{\varkappa}{2\alpha}\right)^2=\lambda^2+\left(\frac{ik}{2\alpha}\right)^2, \tag{17 f}$$

from which we easily obtain the asymptotic amplitude

$$u(k)=\frac{\left(-\frac{ik}{\alpha}\right)!}{\left(-\frac{ik}{2\alpha}+l\right)!\left(-\frac{ik}{2\alpha}-l\right)!} \tag{18}$$

Since for $A=0$, $\lambda=0$, $l=ik/2\alpha$, it follows that $u(k)=1$. The zeros of $u(k)$ are all obtained from the second gamma function of the denominator by putting

$$-\frac{ik}{2\alpha}-l=-n \quad (n=1,2,\ldots,\infty), \tag{18 a}$$

which on squaring l gives (17 d) and (17 e).

If in this example we go the ordinary way our amplitude function is found to be

$$u(k,r)=e^{ikr}F\left(-\frac{ik}{2\alpha}-l,\ -\frac{ik}{2\alpha}+l,\ 1-\frac{ik}{\alpha},\ e^{-2\alpha r}\right), \tag{18 b}$$

which, using (15 c), gives $u(k)$ in the form of eq. (18).

6. Application to a Potential with a Singularity at the Origin

The singularity of $U(r)$ in Example 2 does not change the origin into a singular point of the wave equation. For that purpose a double-pole of $U(r)$ is needed, and as an example we shall study the potential function

$$U(r)=-\mu(\mu+1)\frac{1-\mathrm{tgh}^2 r}{\mathrm{tgh}^2 r}+A(1-\mathrm{tgh}^2 r). \tag{19}$$

The most interesting feature of this potential is that if we choose

$$A=(\lambda+\mu)(\lambda+1+\mu) \tag{19 a}$$

the energy levels of the bound states are the same for all μ and depend only on λ. The potential is well known from the theory of molecular potentials [7] under the name of the Pöschl–Teller [8] potential, however written in quite a different form. In molecular theory it may be thought of as a modification of the Morse potential which gives the same energy levels, however a different variation of the rotational constant or mean interatomic distance with the vibrational quantum number. This modification is, however, for most diatomic molecules the opposite of what is wanted when starting with a Morse potential, for which reason the Pöschl–Teller potential did not prove to be of much use in molecular theory.

Introducing in the wave equation the new variables

$$x = \mathrm{tgh}\, r, \quad k = i\varkappa, \tag{19 b}$$

it becomes
$$\left\{\frac{d}{dx}(1-x^2)\frac{d}{dx} - \frac{\mu(\mu+1)}{x^2} - \frac{\varkappa^2}{1-x^2} + A\right\} y = 0. \tag{20}$$

This again may be transformed into

$$\left\{(1-x^2)\frac{d^2}{dx^2} - (2+2\varkappa)\,x\frac{d}{dx} + 2(\mu+1)\frac{1-x^2}{x^2}\frac{d}{dx} \right.$$
$$\left. - (\varkappa+\mu+1)(\varkappa+\mu+2) + A\right\} x^{-\mu-1}\left(\frac{1-x^2}{4}\right)^{-\varkappa/2} y = 0, \tag{20 a}$$

and finally with the new variable

$$\eta = 1 - x^2 = 1 - \mathrm{tgh}^2 r \tag{20 b}$$

into the hypergeometric equation

$$\left\{\eta(1-\eta)\frac{d^2}{d\eta^2} + \left[\varkappa + 1 - \left(\varkappa + \frac{5}{2} + \mu\right)\eta\right]\frac{d}{d\eta} - \frac{1}{4}\left[\left(\varkappa + \frac{3}{2} + \mu\right)^2 - \left(A + \frac{1}{4}\right)\right]\right\} v = 0, \tag{20 c}$$

$$y = \mathrm{tgh}^{\mu+1} r \left(\frac{1-\mathrm{tgh}^2 r}{4}\right)^{\varkappa/2} v. \tag{20 d}$$

The solutions v of this equation are polynomials of degree $n-1$, $n = 1, 2, \ldots, \infty$, provided

$$A = A_n(\varkappa) = (2n - \tfrac{1}{2} + \varkappa + \mu)^2 - \tfrac{1}{4} = (2n - 1 + \varkappa + \mu)(2n + \varkappa + \mu). \tag{20 e}$$

Equating this expression with (19 a) we find the $\varkappa$-values

$$\varkappa = \lambda + 1 - 2n, \quad \varkappa = -(\lambda + 2\mu + 2n) \tag{21}$$

for which $y(0) = 0$. For negative $\varkappa$-values, however, the asymptotic value as $r \to \infty$ is $y(r) \to e^{|\varkappa| r}$ and hence must be rejected as a bound state function.

In order to be able to discuss the scattering properties of our potential (19) from the same viewpoint as in Examples 1 and 2 we must redefine the amplitude functions $u(\pm k, r)$ and asymptotic amplitudes. Again we choose solution $y_1(r)$ and $y_2(r)$ of eq. (20) with the properties

$$y_1(r) \rightarrow \sin(kr+\xi), \quad y_2(r) \rightarrow \cos(kr+\xi) \quad (r \rightarrow \infty), \tag{22}$$

with the boundary condition $y_1(0)=0$. Owing to the singularity of the endpoint $r=0$ of the domain of integration this means that the two functions have the asymptotic forms

$$y_1(r) \rightarrow c_1 r^{\mu+1}, \quad y_2(r) \rightarrow c_2 r^{-\mu} \quad (r \rightarrow 0). \tag{22 a}$$

As before, the amplitude function should have the asymptotic values $u(\pm k, r) \rightarrow e^{\pm ikr}$; however, in order that the asymptotic amplitudes be finite, we must now choose

$$u(k, r) = \mathrm{tgh}^{\mu} r (y_2 + iy_1) \tag{22 b}$$

or

$$\left.\begin{aligned} y_1(r) &= \mathrm{tgh}^{-\mu} r \cdot \frac{1}{2i} [ue^{i\xi} - u^* e^{-i\xi}], \\ y_2(r) &= \mathrm{tgh}^{-\mu r} \cdot \tfrac{1}{2} [ue^{i\xi} + u^* e^{-i\xi}]. \end{aligned}\right\} \tag{22 c}$$

The condition $y_1(0)=0$ now determines the phase shift formally as before

$$e^{2i\xi} = \frac{u(-k)}{u(k)}, \tag{22 d}$$

however, for $A=0$ we have no more $\xi=0$ or $u(k)=1$. Therefore formula (8 a) is fallible, which means that, although the zeros of $u(k)$ can be found from (10), the infinities of $u(k)$ are not given by (11). The poles of $u(k)$, as might erroneously be concluded from (20 e), are not $k=-i(\mu+n)$ but as in Examples 1 and 2 still

$$k = -in \quad (n = 1, 2, \ldots, \infty). \tag{22 e}$$

This requires an explanation. Assume the potential $U(r)$ to have the asymptotic form $e^{-2\alpha r}$ or for simplicity e^{-2r} as above and take $e^{-2\alpha r}$ or rather $x=e^{-2r}$ as a new independent variable. Then for $r=\infty$ or $x=0$ the wave equation has a regular singularity with initial forms of the solution

$$x^{\pm \varkappa/2} = e^{\mp \varkappa r} = e^{\pm ikr}. \tag{23}$$

Therefore, as $\varkappa$ approaches an integer n, the solution beginning with $x^{-\varkappa/2}$ will have $x^{n-\varkappa/2}$ and higher terms with coefficients of the order of magnitude $1/(\varkappa-n)$, i.e., the solution has poles in $\varkappa=n$, and this means that $u(k)$ has poles in $k=-in$ as stated in (22 e).

The former general formula (8 a) should therefore be replaced by

$$u(i\varkappa)=\prod_{n=1}^{\infty}\frac{A_n(\varkappa)-A}{(2n-1+\varkappa)(2n+\varkappa)}C(n), \tag{23 a}$$

where $C(n)$, if needed, is some converging factor independent of $\varkappa$. Introducing A and $A_n(\varkappa)$ from (19 a) and (20 c) the result is

$$u(i\varkappa)=\prod_{n=1}^{\infty}\frac{\left(\frac{\varkappa}{2}+\frac{\lambda}{2}+\mu+n\right)\left(\frac{\varkappa}{2}-\frac{\lambda+1}{2}+n\right)}{\left(\frac{\varkappa}{2}+n\right)\left(\frac{\varkappa}{2}-\frac{1}{2}+n\right)}\left(1+\frac{1}{n}\right)^{-\mu}, \tag{23 b}$$

where $C(n)$ has been chosen so that according to the Gauss product formula the $u(i\varkappa)$ can be expressed by gamma functions, namely,

$$u(i\varkappa)=\frac{\left(\frac{\varkappa}{2}\right)!\left(\frac{\varkappa}{2}-\frac{1}{2}\right)!}{\left(\frac{\varkappa}{2}+\frac{\lambda}{2}+\mu\right)!\left(\frac{\varkappa}{2}-\frac{\lambda+1}{2}\right)!}. \tag{23 c}$$

From $k=i\varkappa$, $\varkappa=-ik$, and using the gamma function duplication formula,

$$u(k)=\frac{2^{ik}(-ik)!\,(-\frac{1}{2})!}{\left(-\frac{ik}{2}+\frac{\lambda}{2}+\mu\right)!\left(-\frac{ik}{2}-\frac{\lambda+1}{2}\right)!}. \tag{24}$$

This result may be checked by the ordinary method of obtaining $u(k,r)$ and $u(k)$, using the differential equation (20 c) in which $\mu+1$ is replaced by $-\mu$,

$$\left\{\eta(1-\eta)\frac{d^2}{d\eta^2}+\left[\varkappa+1-\left(\varkappa+\frac{3}{2}-\mu\right)\eta\right]\frac{d}{d\eta}-\frac{1}{4}\left[(\varkappa+\tfrac{1}{2}-\mu)^2-\left(A+\frac{1}{4}\right)\right]\right\}v=0, \tag{25}$$

$$y=\mathrm{tgh}^{-\mu}r\left(\frac{1-\mathrm{tgh}^2 r}{4}\right)^{\varkappa/2}v. \tag{25 a}$$

Introducing A from (19 a) it is found that

$$v=F\left(\frac{\varkappa}{2}-\frac{\lambda}{2}-\mu,\frac{\varkappa}{2}+\frac{\lambda+1}{2},\varkappa+1,1-\mathrm{tgh}^2 r\right). \tag{25 b}$$

Since
$$\left(\frac{1-\mathrm{tgh}^2 r}{4}\right)^{\varkappa/2}=\left(\frac{1+\mathrm{tgh}\,r}{2}\right)^{\varkappa}e^{-\varkappa r} \tag{25 c}$$

it means that $y\,\mathrm{tgh}^{\mu}r$ has the correct asymptotic form and that we may write

$u(k, r)$

$$= \left(\frac{1+\operatorname{tgh} r}{2}\right)^{-ik} F\left(-\frac{ik}{2}-\frac{\lambda}{2}-\mu,\quad -\frac{ik}{2}+\frac{\lambda+1}{2},\quad -ik+1, 1-\operatorname{tgh}^2 r\right) \tag{25 d}$$

with the result (24) using (15 c) for $F(a, b, c, 1)$.

On comparing (24) with (14 a) for $\alpha = 1$ we see that the bound states, as determined by the second gamma function of the denominator, are exactly the same, whereas there is a difference in the asymptotic phase shift amounting to

$$\Delta\xi = \arg\left(\frac{ik}{2}+\frac{\lambda}{2}\right)! - \arg\left(\frac{ik}{2}+\frac{\lambda}{2}+\mu\right)!. \tag{26}$$

For integral μ this means a decrease of

$$\Delta\xi = -\operatorname{arctg}\frac{k}{\lambda+2} - \operatorname{arctg}\frac{k}{\lambda+4} - \ldots - \operatorname{arctg}\frac{k}{\lambda+2\mu}, \tag{26 a}$$

which vanishes as $k \to 0$. As $k \to \infty$, however, it approaches the value $\Delta\xi = -\frac{1}{2}\mu\pi$, similar to the asymptotic values

$$\sqrt{\frac{\pi r}{2}}\, J_{u+\frac{1}{2}}(r) \to \sin\left(r - \mu\frac{\pi}{2}\right). \tag{26 b}$$

It is of some interest to compare potentials of the type (19) themselves for different μ-values. Beginning with $\mu = 0$ the maximum depth is at $r = 0$ and is $\lambda(\lambda+1)$. If μ is not too small we make the convenient, however insignificant, change of writing

$$U(r) = \left[-\frac{(u+\frac{1}{2})^2}{\operatorname{tgh}^2 r} + (\lambda+\mu+\tfrac{1}{2})^2\right](1-\operatorname{tgh}^2 r). \tag{27}$$

The maximum depth is then found to be

$$U(r_0) = \lambda^2 \tag{27 a}$$

at the distance r_0 from the origin given by

$$\operatorname{tgh}^2 r_0 = \frac{\mu+\frac{1}{2}}{\lambda+\mu+\frac{1}{2}} \approx 4e^{-2r_0}. \tag{27 b}$$

Using
$$1-\operatorname{tgh}^2 r = \frac{4e^{-2r}}{(1+e^{-2r})^2} = 4e^{-2r} - 8e^{-4r} + \ldots, \tag{27 c}$$

$$\frac{1-\operatorname{tgh}^2 r}{\operatorname{tgh}^2 r} = \frac{4e^{-2r}}{(1-e^{-2r})^2} = 4e^{-2r} + 8e^{-4r} + \ldots, \tag{27 d}$$

we find to the relative order of magnitude $\lambda^2/(\lambda+\mu+\frac{1}{2})^2$,

$$U(r) = 2\lambda^2 e^{-2(r-r_0)} - \lambda^2 e^{-4(r-r_0)} - \frac{3}{\lambda+\mu+\frac{1}{2}}\left(e^{-2(r-r_0)} - e^{-4(r-r_0)}\right), \quad (27\,\mathrm{e})$$

i.e. the potential is approaching the Morse potential.

If in a similar manner we try to generalize the potential of Example 2 by an additional term with a double pole at $r=0$ no coinciding sets of bound states are obtained.

7. Calculation of the Potential $U(r)$ from the Phase Shift for Infinitesimal Perturbations

If in eq. (9) we take A to be small, then to the first order in A

$$\xi = \frac{A}{2i}\sum_{n=1}^{\infty}\left\{\frac{1}{A_n(-ik)} - \frac{1}{A_n(ik)}\right\}, \quad (28)$$

or

$$\dot{\xi} = \frac{1}{2i}\sum_{n=1}^{\infty}\left\{\frac{1}{A_n(-ik)} - \frac{1}{A_n(ik)}\right\}, \quad (28\,\mathrm{a})$$

if for brevity we write

$$\dot{\xi} = \left(\frac{\partial \xi}{\partial A}\right)_{A=0}. \quad (28\,\mathrm{b})$$

On the other hand, writing the wave equation of the former $y_1(r)$ in the form

$$\left\{\frac{d^2}{dr^2} + k^2 + AU(r)\right\} y_1(r) = 0 \quad (29)$$

and combining it with the equation for sin kr, we find

$$k \sin \xi = A\int_0^\infty U(r)\, y_1(r) \sin kr\, dr. \quad (29\,\mathrm{a})$$

As $A \to 0$, $y(r) \to \sin kr$ and $\sin \xi \to \xi$. Hence

$$\dot{\xi} = \frac{1}{k}\int_0^\infty U(r) \sin^2 kr\, dr = \int_0^\infty F(r) \sin 2kr\, dr, \quad (29\,\mathrm{b})$$

and this equation can readily be converted into

$$F(r) = \frac{4}{\pi}\int_0^\infty \dot{\xi} \sin 2kr\, dk, \quad U(r) = -F'(r), \quad F(r) = \int_r^\infty U(r)\, dr. \quad (29\,\mathrm{c})$$

Take now the potential

$$U(r) = \frac{4e^{-2r}}{1-e^{-2r}} \quad (30)$$

of Example 2, eq. (16), putting for simplicity $\alpha=1$, we have from (17 b) $A_n(\varkappa)=n(n+\varkappa)$ and from (28 a)

$$\xi=\frac{1}{2i}\sum_{n=1}^{\infty}\left\{\frac{1}{n(n-ik)}-\frac{1}{n(n+ik)}\right\}. \tag{30 a}$$

From (29 c), transforming half of the integral into the region $-\infty\leqslant k\leqslant 0$, we obtain

$$F(r)=-\frac{1}{\pi}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\left\{\frac{1}{n(n-ik)}-\frac{1}{n(n+ik)}\right\}e^{2ikr}\,dk. \tag{30 b}$$

Closing the path of integration in the upper half plane and contracting it into circles around the poles $k=in$ of the second term, the result is

$$F(r)=2\sum_{n=1}^{\infty}\frac{1}{n}e^{-2nr}=2\log\frac{1}{1-e^{-2r}}, \tag{30 c}$$

$$-F'(r)=U(r)=\frac{4e^{-2r}}{1-e^{-2r}}. \tag{30 d}$$

Similarly, in the case of Example 1 with $\alpha=1$ and

$$U(r)=1-\mathrm{tgh}^2 r,\quad A_n(\varkappa)=(2n-1+\varkappa)(2n+\varkappa), \tag{31}$$

$$F(r)=-\frac{1}{\pi}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\left\{\frac{1}{(2n-1-ik)(2n-ik)}-\frac{1}{(2n-1+ik)(2n+ik)}\right\}e^{2ikr}\,dk \tag{31 a}$$

For the latter term in the bracket we write

$$\frac{1}{[k-(2n-1)i][k-2ni]}=-\frac{1}{i}\left[\frac{1}{k-(2n-1)\,i}-\frac{1}{k-2ni}\right] \tag{31 b}$$

and, on proceeding as above, we obtain

$$F(r)=2\sum_{n=1}^{\infty}(-1)^{n-1}e^{-2nr}=\frac{2e^{-2r}}{1+e^{-2r}}=1-\mathrm{tgh}\,r, \tag{31 c}$$

$$-F'(r)=1-\mathrm{tgh}^2\,r=U(r). \tag{31 d}$$

8. Derivation of the Coulomb Phase Shift by Confluence

In the case of a pure Coulomb potential it is well known that the solutions of the wave equation are confluent hypergeometric functions, which may fairly easily be studied directly. If we write

$$U(r)=\frac{2}{r} \tag{32}$$

for the standard potential function, using $AU(r)$ in the wave equation, it is seen, however, that it can be obtained from

$$AU(r)=\frac{4\lambda^2\alpha^2 e^{-2\alpha r}}{1-\ e^{-2\alpha r}}=\frac{4A\alpha\, e^{-2\alpha r}}{1-e^{-2\alpha r}} \tag{32 a}$$

by putting $\qquad \lambda^2=\dfrac{\mathrm{A}}{\alpha}$ and making $\quad \alpha\to 0.$ (32 b)

In this way we are able to use all results from the former treatment of the potential in Example 2.

The apparently hardest point to settle in this way is the occurrence of the r-dependent part of the phase shift $(A/k)\log\, 2kr$. But this is in the Coulomb case obtained as an asymptotic part of the solution of the equation

$$\left\{\frac{d^2}{dr^2}+2ik\frac{d}{dr}+\frac{2A}{r}\right\}u\, e^{-ikr}=0 \tag{32 c}$$

using only the two last terms, which gives $u\,e^{-ikr}\sim i(A/k)\log r$.

The amplitude function $u(k, r)$ may therefore be defined by its asymptotic value

$$u(k, r)\to e^{i(kr+A/k\,\log\, 2kr)}\quad (r\to\infty), \tag{33}$$

and the asymptotic amplitudes as before by $u(\pm k)=u(\pm k, 0)$. Then writing

$$y_1(r)=\frac{1}{2i}\{u(k,r)\,e^{i\xi}-u(-k,r)\,e^{-i\xi}\}, \tag{33 a}$$

$$y_1(r)\to\sin(kr+(A/k)\log 2kr+\xi)\quad \text{as}\quad r\to\infty. \tag{33 b}$$

Requiring $y(0)=0$ we obtain as before the r-independent part of the phase shift as

$$e^{2i\xi}=\frac{u(-k)}{u(k)},\quad \xi=\frac{1}{2i}\log\frac{u(-k)}{u(k)}. \tag{33 c}$$

It should be noted that the argument kr in the logarithm is suggested in a natural way by introducing the variable kr, which also leads to A/k as a natural constant of the equation. The factor 2 in the logarithm must, however, be justified separately.

Using the equation

$$\left\{\frac{d^2}{dr^2}+2ik\frac{d}{dr}+\frac{4A\alpha\, e^{-2\alpha r}}{1-e^{-2\alpha r}}\right\}u\, e^{-ikr}=0 \tag{34}$$

in a similar manner as (32 c) we may argue that the asymptotic factor

$$\left[\frac{2k(1-e^{-2\alpha r})}{2\alpha}\right]^{iA/k} \to (2kr)^{iA/k} \quad \text{as} \quad \alpha \to 0, \tag{34 a}$$

as obtained from the two last terms of eq. (34) should be taken into the asymptotic expression for $u(k, r)$.

As long as we are dealing with finite α the factor $1-e^{-2\alpha r}$ is 1 as $r \to \infty$, so it means that we have multiplied our former $u(k, r)$, and hence also $u(k)$, by $(k/\alpha)^{iA/k}$. We therefore have to change expression (18) into

$$u(k) = \lim_{\alpha \to 0} \frac{\left(-\frac{ik}{\alpha}\right)! \left(\frac{k}{\alpha}\right)^{iA/k}}{\left(-\frac{ik}{2\alpha}+l\right)! \left(-\frac{ik}{2\alpha}-l\right)!}, \quad l = \sqrt{\frac{A}{\alpha}+\left(\frac{ik}{2\alpha}\right)^2}. \tag{34 b}$$

As $\alpha \to 0$ we find
$$l = \frac{ik}{2\alpha} + \frac{A}{ik} \tag{34 c}$$

and
$$u(k) = \frac{1}{\left(\frac{A}{ik}\right)!} \lim_{\alpha \to 0} \frac{\left(-\frac{ik}{\alpha}\right)! \left(\frac{k}{\alpha}\right)^{iA/k}}{\left(-\frac{ik}{\alpha}-\frac{iA}{k}\right)!}. \tag{34 d}$$

From Stirling's formulae for asymptotic values of gamma functions it is found that for large n, $n!/(n+\varepsilon)! = n^{-\varepsilon}$. Hence

$$u(k) = \frac{i^{iA/k}}{(A/ik)!} = \frac{\exp\left(-\frac{\pi}{2}\frac{A}{k}\right)}{\left(\frac{A}{ik}\right)!}, \tag{35}$$

and
$$\xi = -\arg u(k) = -\arg \left(\frac{iA}{k}\right)!. \tag{35 a}$$

9. The Coulomb Scattering by the Resonance Method

The Coulomb potential $U(r) = 2/r$ has an infinity of bound states,

$$E_n = k_n^2 = -\varkappa_n^2 = -\frac{1}{n^2} \quad (n = 1, 2, \ldots, \infty). \tag{36}$$

Take $k = i\varkappa$ to be given and A an eigenvalue parameter, the equation

$$\left\{\frac{d^2}{dr^2} - \varkappa^2 + \frac{2A}{r}\right\} y = 0 \tag{37}$$

has the eigenvalues $\quad A_n = n\varkappa \quad (n = 1, 2, \ldots, \infty)$ (37 a)

and the eigenfunctions

$$y_n(r) = e^{-\varkappa r} \sum_{\nu=1}^{n} \binom{n-1}{\nu-1} (-2\varkappa r)^\nu \frac{n!}{\nu!} \tag{37 b}$$

with the asymptotic values

$$y_n(0) = 0, \quad y_n(r) \to e^{-\varkappa r}(-2\varkappa r)^n. \tag{37 c}$$

Replacing now $\varkappa$ by ik and n by $A/\varkappa = iA/k$ we define $u(k, r)$ to be the corresponding solution with the asymptotic value

$$u(k, r) \to e^{i(kr + (A/k)\log 2kr)}, \tag{38}$$

dropping the factor

$$i^{(iA/k)} = \exp\left(i\frac{\pi}{2} \cdot i\frac{A}{k}\right) = \exp\left(-\frac{\pi}{2}\frac{A}{k}\right). \tag{38 a}$$

As usual we define two real solutions of the wave equation

$$\left\{\frac{d^2}{dr^2} + k^2 + \frac{2A}{r}\right\} y = 0 \tag{39}$$

by $$y_1 = \frac{1}{2i}\{u(k, r)\, e^{i\xi} - u(-k, r)\, e^{-i\xi}\} \to \sin\left(kr + \frac{A}{k}\log 2kr + \xi\right) \tag{39 a}$$

$$y_2 = \tfrac{1}{2}\{u(k, r)\, e^{i\xi} + u(-k, r)\, e^{-i\xi}\} \to \cos\left(kr + \frac{A}{k}\log 2kr + \xi\right) \tag{39 b}$$

and obtain from the boundary condition $y_1(0) = 0$

$$e^{2i\xi} = \frac{u(-k)}{u(k)}, \quad u(k) = u(k, 0). \tag{39 c}$$

The bound states require $u(k) = 0$ for some positive imaginary k. It follows that $u(k)$ must be expressible as an infinite product containing the factors $1 - A/A_n(-ik)$.

It is clear also that $u(k)$ has no poles, contrary to the case of an exponential potential. The poles of $u(k)$ in eq. (34), for instance, which are $k = -in\alpha$, are creeping upwards in direction of the origin as $\alpha \to 0$. Moreover, according to (17 e) and (32 b) they are killed by the half-set of zeros, $n = (A/\alpha)^{\frac{1}{2}} + m$, $k = -i(A\alpha)^{\frac{1}{2}} - im\alpha$, which as $\alpha \to 0$ have the same distribution $k = -im\alpha$. The other half-set of zeros, $n < A/\alpha^{\frac{1}{2}}$, are all of them above the origin. As $\alpha \to 0$ they become infinite in number and are distributed as

$$k_n = iA/n. \tag{39 d}$$

Since $u(k)$ has only zeros and no infinities we need not worry about the converging factors in the above-mentioned infinite product but may write at once

$$u(k)=\frac{C\left(\frac{A}{k}\right)}{\left(\frac{A}{ik}\right)!}, \tag{40}$$

since from
$$\frac{A}{ik}=-n \quad (n=1,2,\ldots,\infty), \tag{40 a}$$

we obtain all zeros of (39 d). Unknown is still the factor $C(A/k)$, which from the transformation properties of the wave equation, is seen to be a function of A/k.

Now the absolute value $|u(k)|$ is easily found from

$$y_2(0)=|u(k)|, \quad y(r\to 0)=\frac{kr}{|u(k)|}, \tag{40 b}$$

which follows as before from (39 b) and the unaltered value k of the Wronskian. On the other hand, the asymptotic value of (37 b) as $r\to 0$ is

$$y_n(r\to 0)=2ikr\cdot n!=2ikr\cdot\left(\frac{iA}{k}\right)! \tag{40 c}$$

and this has to be divided by $2i$ from (39 a), by $\exp(-\frac{1}{2}\pi A/k)$ from (38 a), and finally multiplied by

$$e^{i\xi}=\frac{u(-k)}{|u(k)|}=\frac{\left|\left(i\frac{A}{k}\right)!\right|}{\left(\frac{iA}{k}\right)!} \tag{40 d}$$

from eq. (40). Hence

$$y(r\to 0)=kr\cdot\exp\left(\frac{\pi}{2}\frac{A}{k}\right)\left|\left(i\frac{A}{k}\right)!\right|, \tag{40 e}$$

which gives from (40 b)

$$|u(k)|=\frac{\exp(-\frac{1}{2}\pi A/k)}{\left|\left(i\frac{A}{k}\right)!\right|} \tag{40 f}$$

Hence $C(A/k)=\exp(-\frac{1}{2}\pi A/k)$ and (40) and (35) are in accordance also with respect to the numerical factor.

The phase shift is independent of this real factor and could have been given from (40) without additional considerations as

$$\xi = -\arg\left(\frac{iA}{k}\right)! = -Im \log\left(\frac{iA}{k}\right)! \tag{41}$$

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