

THE POLES OF THE S-MATRIX OF A RECTANGULAR POTENTIAL WELL OR BARRIER

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Abstract. To test the validity of current ideas on the poles of the S-matrix, a simple example is treated non-relativistic scattering by a spherically symmetric rectangular potential well (or barrier) The poles of the S-matrix associated with this problem, in the case of zero angular momentum, are determined, and their behaviour as a function of the well depth (barrier height) is discussed. Some results for higher angular momenta are also given The usual physical interpretation may be applied only to a very restricted class of poles Difficulties appear in the case of "short-lived decaying states". However, the present model leads to a connection between the limiting cases of strongly bound states in a deep well and of certain characteristic states attached to a "hard sphere" or to a perfect conductor (antenna). It is shown that some poles, previously described as "meaningless", give rise to important physical effects

1. Introduction

The general properties of the poles of the S-matrix have been the object of a great number of papers However, few attempts have been made to test and to illustrate these properties by determining all the poles of the S-matrix in concrete physical examples This has been done for the Coulomb potential, in this case, however, there are only purely imaginary poles, which correspond to bound states no complex ^{††} poles exist. To our knowledge, no example where complex poles occur has ever been completely treated

A simple example of this kind is the scattering of non-relativistic particles by a spherically symmetric rectangular potential well (or barrier) This example was considered in 1930 by Beck¹), who observed that, when the well depth decreases, the bound levels are "pushed" into the continuous spectrum, giving rise to "virtual" levels After the introduction of the S-matrix, the rectangular potential well was mentioned as an example in a paper by Møller²), where it is stated (incorrectly) that there are no complex poles in this case Complex poles were also disregarded in a later treatment of the problem by Schutzer³)

As will be shown in sect 3, the poles of the S-matrix associated with this

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^{††} We call a number complex if it has non-vanishing real and imaginary parts

problem, for angular momentum l = 0, may be completely determined Some results for higher angular momenta will be given in sect 4 The interest of this example is that it allows us to test the usual point of view on the poles of the S-matrix We have found several inexact statements in the literature, in fact, the whole problem of the physical interpretation of the poles of the S-matrix should be dealt with much more carefully than has usually been done hitherto

Let us summarize the usual point of view We shall restrict ourselves to the case of non-relativistic scattering by a central potential of finite radius In this case, as is well known, the S-matrix is a diagonal matrix, with elements

$$S_{l}(k) = \exp\left[2i\eta_{l}(k)\right],\tag{1}$$

where $\eta_l(k)$ is the phase-shift corresponding to the angular momentum l and wave number k In the cases in which we are interested, the analytic continuation of $S_l(k)$ in the complex k-plane is a meromorphic function. The following properties are generally ascribed to the poles of this function

(A) The poles are located either on the positive imaginary axis or in the lower half-plane 4,5)

(B) A pole on the positive imaginary axis, $k = i\kappa_n(\kappa_n > 0)$, corresponds to a bound state with energy $E_n = -(\hbar\kappa_n)^2/2m$, where *m* is the mass of the particle [†]

(C) Complex poles are usually interpreted either by means of so-called "quasi-stationary" or "virtual" states ^{8,9}) or in terms of resonance scattering ¹⁰) The first interpretation involves the analytic continuation of Schrödinger's wave function to "complex energies" A pole at the point $k = k' - i\kappa(\kappa > 0)$ is associated with the "complex energy"

$$W = E - \frac{1}{2} \imath \Gamma = (\hbar^2 / 2m) (k' - \imath \kappa)^2$$
⁽²⁾

If k' > 0, the corresponding "wave function" is said to represent a "decaying state", with decay constant Γ/\hbar and "energy" E (defined with an uncertainty given by Γ) Poles with k' < 0 are associated with "capture" processes. It is assumed, in both cases, that E > 0 (cf sect 52)

It is well known that a "complex-energy wave function" cannot be normalized, owing to its exponential increase with the distance (this is attributed to emission that took place "a long time ago" 9)) This difficulty is usually circumvented by interpreting a "complex-energy wave function" as an approximation to a wave packet that is a proper solution of Schrödinger's equation ^{11, 12}) It must be emphasized, however, that this approxima-

[†] If the scattering potential does not vanish rapidly enough at infinity, there may also exist "spurious" poles on the positive imaginary axis, which do not correspond to bound states 6 , ?)

tion rests upon the following assumptions (a) $|\Gamma| \ll E$, (b) $|\Gamma| \ll$ level spacing If these conditions are not fulfilled, it is very doubtful whether such an interpretation is possible (cf sect 52)

The interpretation of complex poles by means of resonance scattering associates (2) with a "Breit-Wigner peak" in the scattering cross-section, E gives the resonance energy and Γ is the half-width of the peak Besides conditions (a) and (b), it is assumed that the pole in question is a simple pole According to Hu¹⁰), this is always so if the scattering potential has a short range, i.e., if $k'a \ll 1$, where a is the radius of the potential

2. Formulation of the Problem

We shall consider the potential

$$V(r) = -V_0, r < a, V(r) = 0, r > a_r$$

where $V_0 > 0$ in the case of a well, and $V_0 < 0$ in the case of a barrier. It is convenient to introduce the following dimensionless parameters

$$\alpha = [2m(E+V_0)]^{\frac{1}{2}}a/\hbar, \qquad (3)$$

$$\beta = ka = (2mE)^{\frac{1}{2}}a/\hbar, \qquad (4)$$

$$\pm A^2 = V_0/\mathscr{E} \qquad (+ \text{ for a well, } - \text{ for a barrier}), \tag{5}$$

where E is the energy (taken, for the moment, to be real), and

$$\mathscr{E} = \hbar^2/(2ma^2) = E/\beta^2 \tag{6}$$

The parameters α and β correspond to the wave number inside and outside of the potential, respectively, \mathscr{E} is the energy of a particle for which ka = 1, A^2 is a well-depth (barrier-height) parameter. It follows from the above equations that

$$\alpha^2 = \beta^2 \pm A^2$$
 (+ for a well, - for a barrier) (7)

It follows from (1) and from the well-known expression for the phase-shift 13) that †

$$S_{l}(\beta) = -\frac{\beta \mathcal{J}_{l}(\alpha) h_{l}^{\prime(2)}(\beta) - \alpha \mathcal{J}_{l}^{\prime}(\alpha) h_{l}^{(2)}(\beta)}{\beta \mathcal{J}_{l}(\alpha) h_{l}^{\prime(1)}(\beta) - \alpha \mathcal{J}_{l}^{\prime}(\alpha) h_{l}^{(1)}(\beta)},$$
(8)

where $j_i(z)$ is the spherical Bessel function of the first kind, and $h_i^{(1)}(z)$, $h_i^{(2)}(z)$ are spherical Hankel functions of the first and second kinds, respectively ¹⁴)

To obtain the analytic continuation of $S_i(\beta)$, it suffices to consider (8) as a function of the complex variable $\beta = u + iv$ It follows from the properties of

[†] It is assumed in (8), as well as in subsequent expressions (unless otherwise stated), that, in accordance with (7), α has been replaced by $\pm (\beta^2 \pm A^2)^{\frac{1}{2}}$ (the sign of the square root is irrelevant)

the spherical Bessel functions that (8) is a meromorphic function of β , which satisfies the well-known relations

$$S_{\iota}(\beta)S_{\iota}(-\beta) = S_{\iota}(\beta)S_{\iota}^{*}(\beta^{*}) = 1$$
⁽⁹⁾

According to (9), if β is a pole of $S_{\iota}(\beta)$, so is $-\beta^*$, while $-\beta$ and β^* are zeros. Therefore, it suffices to determine the poles on the imaginary axis and in the right half-plane

3. The Case of Zero Angular Momentum

For l = 0, (8) becomes

$$S_0(\beta) = \exp(-2i\beta) (\alpha \cot \alpha + i\beta) (\alpha \cot \alpha - i\beta)^{-1}$$
(10)

The poles of $S_0(\beta)$ are the roots of the complex transcendental equation

$$\alpha \cot \alpha = \imath \beta \tag{11}$$

It can be shown, by considering the real and imaginary parts of (7) and (11), that property (A) of sect 1 is satisfied $S_0(\beta)$ cannot have any poles in the upper half-plane, except on the imaginary axis

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To determine the roots of (11), it is more convenient to work with the variable $\alpha = x + iy$ than with β Eliminating β from (7) and (11), we find

$$\alpha^{-1}\sin\alpha = \pm A^{-1} \tag{12}$$

The corresponding values of β are given by

$$\beta = \pm (\alpha^2 - A^2)^{\frac{1}{2}},\tag{13}$$

where the sign must be chosen in such a way that (11) is satisfied

The problem is now reduced to the determination of the roots of (12) as a function of the parameter A. This is carried out in appendix A Making use of (13) and of the results derived in appendix A, it is a simple matter to determine the poles of $S_0(\beta)$ in the β -plane. Some of these poles, together with the corresponding values of A, are shown in fig 1

For each given value of A, there exists an infinite number of poles When A varies, the poles describe certain paths in the β -plane (the curves in full line in fig 1) The poles corresponding to a given A may be numbered according to their limiting positions for $A \to 0$, thus, $\beta_n = u_n + iv_n$, where

$$\lim_{A\to 0}\beta_n=n\pi-i\infty \qquad (n=0,\,\pm 1,\,\pm 2,\,\,) \qquad (14)$$

The following abbreviations will be introduced for describing the poles a-poles (a = anti), for poles with $u_n = 0$, $v_n < 0$, b-poles (b = bound),

for poles with $u_n = 0$, $v_n > 0$, and c-poles (c = complex), for poles with $u_n \neq 0$, $v_n \neq 0$ The denomination "anti-pole" will be justified in sect 5.2

Let us describe the behaviour of the poles when A increases from 0 (free particles) to ∞ (infinitely deep well), beginning with the pole β_0 on the

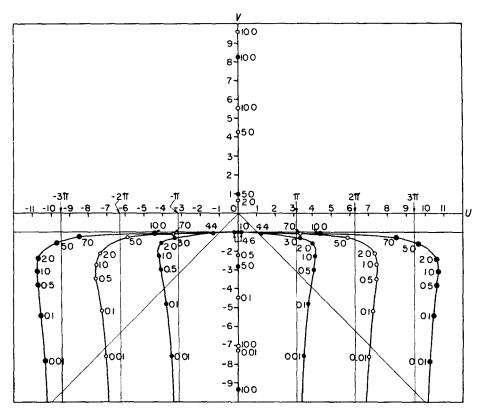
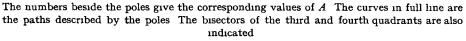


Fig 1 The poles β_n of $S_0(\beta)$ for a potential well $\Box n = 0$, $\odot n = \pm 1$ $\bigcirc n = \pm 2$ $\odot n = \pm 3$



imaginary axis For 0 < A < 1, β_0 corresponds to a root of (A3) (see appendix A), it is an a-pole, and it moves from $-i\infty$ to -i when A increases from 0 to 1 For A > 1, β_0 arises from a root of (A2) in the interval $0 < x < \pi$. According to (A4), when A increases from 1 to $\frac{1}{2}\pi$, β_0 is an a-pole, which moves from -i to the origin For $A > \frac{1}{2}\pi$, β_0 becomes a b-pole (first bound state), and it moves upwards from the origin to $i\infty$ when A increases from $\frac{1}{2}\pi$ to ∞

It must be pointed out that the origin itself is never a pole of $S_0(\beta)$, since

this would violate the unitarity condition In the present case, for $A = \frac{1}{2}\pi - \epsilon$, $|\epsilon| \ll 1$, we have, in the neighbourhood of the origin,

$$S_{0}(\beta) \approx -(\beta + \beta_{0})(\beta - \beta_{0})^{-1} \approx -(\beta - \frac{1}{2}i\pi\varepsilon)(\beta + \frac{1}{2}i\pi\varepsilon)^{-1} = -1 + i\pi\varepsilon(\beta + \frac{1}{2}i\pi\varepsilon)^{-1}, \quad (15)$$

so that the residue at $\beta = \beta_0$ vanishes when $\varepsilon \to 0$ This is due to the fact that $\beta_0^* = -\beta_0$, which is a zero of $S_0(\beta)$, approaches the origin simultaneously with β_0 Thus, the "conservation of the number of poles" fails to hold at the origin

Let us consider next a pair of poles, $\beta_{\pm n}$, with $n \ge 1$ For $0 < A < A_n$, where A_n is defined by (A7), β_n is a c-pole, which corresponds to the root α_n of (A1), and β_{-n} is the mirror image of β_n with respect to the imaginary axis The paths described by the first few pairs of poles are shown in fig 1 For $A \to 0$, β_n approaches asymptotically the straight line $u = n\pi$ When Aincreases, β_n moves upwards, until it approaches the straight line v = -1, and then it moves towards the imaginary axis When $A \to A_n$, β_n and β_{-n} approach, from opposite sides, the point $\beta = -i$, where they coalesce for $A = A_n$ The paths described by $\beta_{\pm n}$ are tangent to the straight line v = -1 at this point

Thus, for $A = A_n$, $S_0(\beta)$ has a double pole at the point $\beta = -i$ It may be easily verified that all other poles are simple poles. However, the existence of double poles $k = k' - i\kappa$, with k'a = 0, $\kappa a = 1$, contradicts Hu's statement, quoted at the end of sect 1 To explain this discrepancy, we notice that it is implicitly assumed in Hu's paper ¹⁰) (see his eqs. (32)—(33)) that $\kappa a \ll 1$, but, as shown by the present example, this need not be true

For $A > A_n$, the double pole at $\beta = -i$ splits into a pair of poles, which move in opposite directions along the imaginary axis We shall call the one which moves upwards β_n , and the one which moves downwards β_{-n} (this choice is, of course, entirely a matter of convention) Thus, β_{-n} is an a-pole, which moves from -i to $-i\infty$ when A increases from A_n to ∞ On the other hand, for $A_n < A < c_n$, where c_n is defined by (A6), β_n is an a-pole, which moves from -i to the origin For $A > c_n$, β_n becomes a b-pole, which moves from the origin to $i\infty$ when A increases from c_n to ∞ Thus, every pair of c-poles ultimately gives rise to an a-pole and a b-pole

An approximate analytical representation of the poles for $1 < A < A_n$ may easily be derived from (13), (A8) and (A11)—(A12) Let us notice, in particular, that, for $1 < A \ll A_n$, we have $\beta_n \approx x_n - iy_n$, where x_n , y_n are given by (A13) and (A14) The case $A \ll 1$ will be considered in sect 4.1

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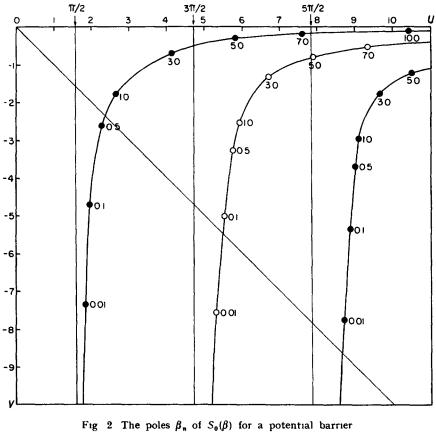
To carry out the transition from the potential well to the potential barrier, it suffices to replace A by iA in (12) and (13)

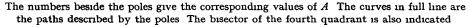
$$\alpha^{-1}\sin\alpha = \pm i A^{-1}, \tag{16}$$

$$\beta = \pm (\alpha^2 + A^2)^{\frac{1}{2}} \tag{17}$$

The roots of (16) are determined in appendix B, the poles of $S_0(\beta)$ in the β -plane then follow from (17) All of them are c-poles For each value of A, there is an infinite number of poles, $\beta_{\pm n} = \pm u_n + iv_n$, corresponding to the roots α_n of (16)

It suffices to consider the behaviour of the poles in the lower right quadrant The paths described by the first few poles as a function of A are shown in fig 2 We find that $\beta_n \to c_{n-1} - i\infty$ for $A \to 0$ When A increases,





 β_n moves upwards and away from the imaginary axis, tending to approach the real axis when A becomes very large In fact, when $A \gg \xi'_n$ (cf appendix B), we have, according to (17), (B9) and (B10),

$$\beta_n \approx A \left[1 + \frac{1}{2} (n\pi/A)^2 \right] - \imath z_n (n\pi/A) \left[1 + \frac{1}{2} (n\pi)^{-2} \right]$$
(18)

Thus, $u_n \to \infty$ and $v_n \to 0$ for $A \to \infty$ This means that $S_0(\beta)$ has no poles (at finite distance) in the limiting case of an impenetrable barrier ("hard sphere")

Notice that, for $1 < A \ll \xi'_n$, we have $\beta_n \approx x_n - iy_n$, where x_n , y_n are given by (B7) and (B8) The case $A \ll 1$ will be treated in sect. 41.

4. The Case of Higher Angular Momenta

The complete determination of the poles of $S_l(\beta)$ is more difficult for l > 0 than for l = 0 We shall restrict ourselves to a discussion of the general behaviour of "large" poles and to some special results for l = 1

41 GENERAL BEHAVIOUR OF "LARGE" POLES

A pole of $S_l(\beta)$ at $\beta = \beta_n = u_n - \iota w_n$, where $w_n = -v_n > 0$ (it suffices to consider $u_n \ge 0$), will be called a "large" pole if it fulfils the following conditions:

$$(1)|\beta_n| \gg A$$
, $(1)|\beta_n| \gg A^2$, $(11)|\beta_n| \gg l+1$, $(1v) \exp(w_n) \gg 1$ (19)

According to (5) and (6), (19) implies that $|E_n| \gg |V_0|$ and

$$|E_n| \gg l(l+1)\hbar^2/2ma^2$$

the height of the "centrifugal barrier". It is not surprising that, under these conditions, we find common features in the behaviour of the poles, as will be shown below

It follows from (8) and from the relationship

$$j_{l}(\beta)h_{l}^{\prime(1)}(\beta) - j_{l}^{\prime}(\beta)h_{l}^{(1)}(\beta) = i\beta^{-2}$$
(20)

that, in the free-particle limit $(A \rightarrow 0)$ we have, as it should be,

$$\lim_{A \to 0} S_{\iota}(\beta) = 1 \tag{21}$$

It may be expected, therefore, that the poles of $S_l(\beta)$ are rejected to infinity when $A \rightarrow 0$, so that there are only large poles for very small A

To determine the large poles of (8), we may, according to (1) and (ii), make the following approximations. $\alpha \approx \beta \pm A^2/(2\beta)$, $|A^2/\beta| \ll 1$. On the other hand, according to (11) and (1v), we may replace the spherical Bessel functions by their asymptotic expansions, neglecting terms in $\exp(-i\beta)$ in comparison with $\exp(i\beta)$. If this is done, we find that the large poles are approximately given by the equation

$$1 \pm (-1)^{i} \left[\frac{1}{2} A \beta^{-1} \exp(i\beta) \right]^{2} = 0 \quad (+ \text{ for a well, } -\text{ for a barrier})$$
(22)

In this approximation, therefore, the large poles of $S_l(\beta)$ for a potential well (barrier) with even l coincide with those for a potential barrier (well) with odd l

If we put

$$u_n = U_n + \varepsilon_n \qquad (0 \le \varepsilon_n < \frac{1}{2}\pi),$$
 (23)

where

 $U_n = \begin{cases} n\pi & \text{for a well with even } l \text{ or a barrier with odd } l, \\ (n-\frac{1}{2})\pi & \text{for a well with odd } l \text{ or a barrier with even } l, \end{cases}$ (24)

we find that (22) may be replaced, in both cases, by the pair of equations

$$\tan \varepsilon_n = u_n / w_n, \qquad (25)$$

$$\exp w_n = (2/A) (u_n^2 + w_n^2)^{\frac{1}{2}}$$
(26)

Neglecting ε_n in comparison with U_n , we get

$$\varepsilon_n = \tan^{-1}(U_n/w_n), \qquad (27)$$

$$w_n = \frac{1}{2} \log[(2U_n/A)^2 + (2w_n/A)^2] = f(w_n)$$
(28)

Eq (28) may be solved by iteration \dagger , taking

$$w_n^{(1)} = \log(2U_n/A)$$
 $(U_n \neq 0),$ (29)

$$w_n^{(r+1)} = f(w_n^{(r)}) \qquad (r = 1, 2, ...)$$
 (30)

In general, the third or fourth iteration already gives a very good approximation.

In particular, if $w_n^{(1)} \ll U_n$, which is certainly the case for A > 1,

$$w_n \approx \log (2U_n/A) + \frac{1}{2}U_n^{-2} [\log(2U_n/A)]^2 + ...,$$
 (31)

$$u_n \approx U_n + \frac{1}{2}\pi - U_n^{-1}w_n + \dots$$
 (32)

Equations (A13)-(A14) and (B7)-(B8) are particular cases of these results.

On the other hand, if $w_n^{(1)} \gg U_n$, which is the case for very small A, we find

$$w_n \approx L_1 + L_2 + L_2 L_1^{-1} + (L_2 - \frac{1}{2}L_2^2 + \frac{1}{2}U_n^2)L_1^{-2} + \quad , \tag{33}$$

$$u_n \approx U_n + U_n w_n^{-1} + \dots$$
 (34)

where

$$L_1 = \log(2/A), \qquad L_2 = \log\log(2/A).$$
 (35)

Notice that (33) remains valid if $u_n = U_n = 0$. It follows from (33) and (34) that

$$\lim_{A\to 0}\beta_n=U_n-\imath\infty,$$

which generalizes the results obtained for l = 0 Notice, in particular, that there is always an isolated (unpaired) pole on the imaginary axis in the first case of (24), but not in the second one

[†] A very similar equation has been discussed by de Bruijn¹⁵)

4.2 THE CASE l = 1

For l = 1, (8) becomes

$$S_{1}(\beta) = \exp(-2i\beta) (\alpha^{-1} \cot \alpha - \alpha^{-2} + \beta^{-2} + i\beta^{-1}) (\alpha^{-1} \cot \alpha - \alpha^{-2} + \beta^{-2} - i\beta^{-1})^{-1}$$
(36)

The poles of $S_1(\beta)$ are the roots of

$$\alpha^{-1}\cot\alpha - \alpha^{-2} + \beta^{-2} - \imath \beta^{-1} = 0$$
(37)

(a) The potential well

Let us consider first the poles on the imaginary axis, $\beta = iv$ No such poles exist for |v| > A For |v| < A, according to (7) and (37), they are given by the points of intersection of the curve

$$x^{-1}\cot x - x^{-2} = v^{-1} + v^{-2}, \qquad (38)$$

which has been drawn in full line in fig 3, with the family of circles

$$x^2 + v^2 = A^2, (39)$$

some of which have been drawn in dashed line in fig 3.

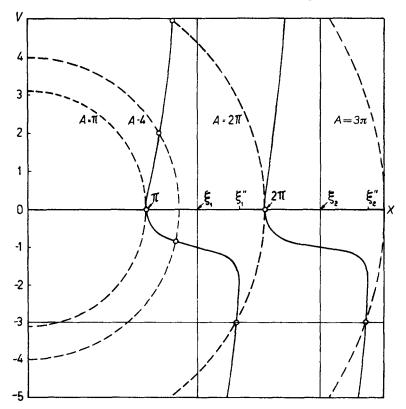


Fig 3 Determination of the purely imaginary poles of $S_1(\beta)$ for a potential well $-x^{-1} \cot x - x^{-2} = v^{-1} + v^{-2}, \quad ---x^2 + v^2 = A^2$ Notice that the intersections occur close to the straight line v = -3 for $A = 2\pi$ and $A = 3\pi$.

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The curve (38) is defined in the intervals $n\pi \leq x \leq {\xi''}_n (n = 1, 2, ...)$, where ${\xi''}_n$ is the *n*th positive root of the equation. $x^{-1} \cot x - x^{-2} = -\frac{1}{4}$. The straight lines $x = \xi_n$, where ξ_n is given by (A5), are vertical asymptotes

There are no poles on the imaginary axis for $A < \pi$ For $A = \pi$, (38)—(39) have a double root at v = 0 However, this is not a pole of $S_1(\beta)$ (cf sect 3 1) For $A > \pi$, this double root splits into a pair of roots, giving rise to an a-pole, which moves downwards for increasing A, and a b-pole (first bound p-state), which moves upwards when A increases A similar process takes place each time that A goes through an integral multiple of π

How do these poles appear on the imaginary axis? A comparison with the case l = 0 suggests that they must arise from the confluence of pairs of c-poles If this is true, there must be a pair of c-poles close to the origin whenever A approaches an integral multiple of π . In order to determine these poles, we shall make the following assumptions in (37)

$$0 < A(n\pi - A) = \delta_n \ll 1 \ (n = 1, 2, \dots), \tag{40}$$

$$|\beta| \ll A, \qquad |\beta|^2 \ll 2A.$$
 (41)

Under these conditions, (37) may be approximated by

$$\delta_n - \imath \delta_n \beta - \frac{3}{2} \beta^2 + \frac{1}{2} \imath \beta^3 = 0, \qquad (42)$$

neglecting terms of the order of $A^{-2}\beta^4$

The roots of (42) are

$$\begin{aligned} \beta_{\pm n} &= \pm (\frac{2}{3}\delta_n)^{\frac{1}{2}} - \imath (\frac{2}{9}\delta_n) + \mathcal{O}(\delta_n^{\frac{3}{2}}), \\ \beta' &= -3\imath + \frac{4}{9}\imath \delta_n + \mathcal{O}(\delta_n^{-2}) \end{aligned}$$

$$(43)$$

Notice that β_n and β_{-n} are approximate roots of (37), but this is only true for β' if it fulfils condition (41) Thus, β' is not an approximate root of (37) for n = 1 However, it may be shown that, for $n \ge 2$, there exists indeed an a-pole close to the point -3i For n = 2 and n = 3, this may be clearly seen in fig 3.

For $A \to n\pi$, the c-poles $\beta_{\pm n}$ approach the origin along a parabolic arc (with vertex at the origin) For $A > n\pi$, they dissociate into an a-pole and a b-pole

The behaviour of the poles differs from the behaviour for l = 0 in the following respects (1) according to sect 4 1, $\beta_n \rightarrow c_{n-1} - i\infty$ as $A \rightarrow 0$, therefore, there is no isolated pole on the imaginary axis, (2) the "joining-point" of the c-poles is at the origin (instead of the point $\beta = -i$)

(b) The potential barrier

In this case, according to sect 4.1, $\beta_n \to n\pi - i\infty$ as $A \to 0$, so that there is an isolated pole on the imaginary axis, $\beta_0 = iv_0$ When A increases from 0 to ∞ , β_0 moves upwards from $-i\infty$ to -i

As was the case for l = 0, the c-poles $\beta_{\pm n} = \pm u_n + iv_n$ $(n \ge 1)$ tend to approach the real axis for large values of A However, in contrast with the case l = 0, one pole remains at finite distance as $A \to \infty$, namely, the a-pole $\beta_0 = -i$

Generally, for any angular momentum l, l poles remain at finite distance in the limiting case of a "hard sphere". These poles are the roots of the equation

$$h_{l}^{(1)}(\beta) = 0 \tag{44}$$

The poles corresponding to the first few values of l are given in table 1¹⁶).

TABLE 1									
\mathbf{Th}	e p	oles	of	$S_i(\beta)$	for	a	"hard	sphere'	,
1 =	0	1			2			3	

	Ľ.	<u> </u>		0
β =	-	-1	$\pm \frac{1}{2}\sqrt{3-\frac{3}{2}}$	$-2 \ 26 \imath \\ \pm 1 \ 75 - 1 \ 87 \imath$

Notice that, in agreement with the results of sect 4 1, there are only pairs of c-poles for even l, whereas, for odd l, there is also an isolated a-pole.

By comparing the "hard sphere" with its electromagnetic counterpart, a perfect conductor, we find an interesting connection with antenna theory [†] In fact, the roots of (44), for $l \ge 1$, are also the characteristic values associated with the so-called magnetic modes of oscillation of a perfectly conducting sphere ¹⁸). These characteristic values are the poles of the S-matrix of the associated scattering problem.

5. Discussion

51 GENERAL PROPERTIES OF THE POLE DISTRIBUTION

The results obtained in the previous sections allow us to verify, in the present example, some general properties of the pole distribution for non-relativistic scattering by a central potential of finite range ^{††}:

(1) There is an infinite number of poles, but only a finite number of them lie on the imaginary axis 17, 18)

(2) For large *n*, the distance $|\beta_{n+1} - \beta_n|$ between two consecutive c-poles approaches the value π (see ref¹⁸)) This follows from sect 4 1

(3) The distance of the c-poles to the real axis increases logarithmically with n (see ref ¹⁸)) If we put $\beta_n = |\beta_n| \exp(-i\theta_n)$, we find, according to

 $[\]dagger$ The author is indebted to Prof G Beck for pointing out the connection between the antenna problem and the S-matrix We expect to treat this point more fully in a future paper, in collaboration

^{††} Properties (2) and (3) have been derived for the case of s-scattering ¹⁸)

sect. 41[†],

$$\sin \theta_n \approx (n\pi)^{-1} \log n \ (n \to \infty). \tag{45}$$

52 ON THE PHYSICAL INTERPRETATION OF THE POLES

According to Heitler and Hu⁹), almost all the poles of the S-matrix have a simple physical interpretation (namely, the interpretation that we have outlined in sect 1). In the non-relativistic case, the only "meaningless" poles would be those which are located in the region of the complex k-plane where the real part E of the "complex energy" (2) is negative, i e, below the bisectors of the third and fourth quadrants (cf fig 1 and fig 2).

Besides the fact that a continuous transition from these so-called meaningless poles to the so-called meaningful ones is possible (as shown by the present example), it must be pointed out that the interpretation of E as the approximate energy of a "decaying state" is certainly not valid if $|\Gamma/E| \gg 1$ Therefore, there seem to be no grounds for accepting the above criterion.

As we have mentioned in the introduction, the approximations involved in the usual interpretation of c-poles are based upon conditions (a) and (b) of sect 1 In the present example, these conditions are fulfilled only in a few cases (cf. fig 1 and fig 2) One of them is the case of the lowest-order poles for a very high barrier (which are given by (18) for l = 0) These poles correspond to virtual energy levels lying above the top of the barrier. The well-known analogy with optical interference phenomena in thin plates may be applied to them The "level width" may be estimated by the usual formula¹⁹)

$$\Gamma = \hbar T v_i / (2a), \tag{46}$$

where v_i is the "velocity" inside the potential and T is the "transmissivity" of the potential step

Eq (46) may also be applied to the lowest-order c-poles for a very deep potential well, provided $|\Gamma| \ll E$ In this case, it gives $\Gamma/\mathscr{E} \approx 4(E/\mathscr{E})^{\frac{1}{2}}$. This result is equivalent to the fact that the c-poles tend to approach the straight line v = -1 in the β -plane (cf fig. 2 and sect 3 1) The virtual levels of a well are much broader than those of a barrier of comparable range and transmissivity, this is due to the much larger value of v_i in the case of a well.

One runs into serious difficulties as soon as one tries to apply the usual interpretation in cases when the above-mentioned conditions are not fulfilled As the poles get farther away from the real axis, the corresponding resonance peaks in the scattering cross-section become broader and broader, tending to overlap in an inextricable way, until they merge into a slowly-

[†] Eq (45) should be compared with eq (19) of Regge's paper ¹⁸) ($\lambda = 0$ in our example). There are some errors in eqs (16)—(19) of that paper, in particular, a factor $2/\pi$ is missing in the second member of eqs (18) and (19) Notice that Regge's way of numbering the poles is different from ours, so that his n (in eq (19)) is equivalent to our $\frac{1}{2}n$

varying background, which is usually included in the so-called potential scattering

On the other hand, it is exceedingly doubtful whether these poles can be interpreted in terms of "decaying states". This is clearly seen when we consider the case of a very shallow well (or a very low barrier), in which all the poles are large poles (sect 4 1) If we build up a wave packet that is initially concentrated within the potential, in this case, it will propagate and spread practically in the same way as it would do in the case of free particles, and this process has nothing to do with exponential decay \dagger .

It has been shown by Regge $^{18, 21}$) that the asymptotic behaviour of the large poles depends very critically on the asymptotic behaviour of the potential Physically unimportant changes in the potential may completely modify the behaviour of the large poles, so that these poles cannot have much physical significance 21) This "hypersensitiveness" of the poles with respect to asymptotic conditions, which had previously been noticed in the case of "spurious" poles, is a very unwelcome feature of the S-matrix formalism

Let us now consider the poles on the negative imaginary axis (a-poles). The "energies" that formally correspond to them, according to (2), are real negative energies, just as in the case of bound states (b-poles) However, while the energy levels of the bound states are determined by the condition that the wave function at r = a may be smoothly joined to a *purely decreasing* exponential for r > a, the energies associated to a-poles are those for which the wave function at r = a may be smoothly joined to a *purely increasing* exponential for r > a. For this reason, we propose to call them *anti-levels*^{††}, and to call the associated poles *anti-poles*

In the case of a potential well with l = 0, the anti-level associated to the a-pole β_0 (sect 3 1) lies below the bottom of the well for 0 < A < 1, and within the well for $1 < A < \frac{1}{2}\pi$ All other anti-levels lie within the well, as may readily be verified, there is one anti-level between every pair of bound states.

Let us sum up It is convenient to classify the poles of the S-matrix into several (not sharply separated) groups They range all the way from those which are associated with well-defined physical concepts to those which seem to be no more than mathematical properties of the formalism The bound states belong to the first category The usual interpretation of c-poles may be applied to "long-lived decaying states", either for an attractive or for a repulsive potential However, it seems to be very difficult to give a precise and general formulation of the scattering problem in the case of "short-lived decaying states"

[†] A discussion of the exponential decay law has recently been given in a paper by Hohler²⁰)

^{††} They are sometimes called "virtual levels" (cf sect 5 3), but it seems to us that this is a most unfortunate terminology, since it is apt to suggest the idea of quasi-stationary states

The limiting case of a "hard sphere" is specially interesting In the related case of a perfect conductor, it is known that there exist certain characteristic states of the field, which are more or less strongly damped by radiation according to the shape of the conductor Our model indicates the existence of a connection between these "antenna states" and the other limiting case of strongly bound states in a deep well (cf the end of sect 42)

The large poles seem to have very little physical significance. It might be expected that the a-poles, which are "meaningless" in the usual interpretation, cannot have any physical importance. However, this is not true, as will be shown in the next section

53 THE LOW-ENERGY SCATTERING CROSS-SECTION

It will be shown in this section that some poles of the S-matrix that would be considered to be "meaningless" according to the usual interpretation (in particular, a-poles) may give rise to important physical effects in the low-energy scattering cross-section.

The scattering cross-section σ_l for angular momentum l is given by the well-known expression

$$\sigma_{l} = (2l+1)\pi a^{2}\beta^{-2}|1-S_{l}(\beta)|^{2}$$
(47)

(a) The case l = 0

Let us consider a potential well that is almost deep enough for the appearance of the first bound state, so that $A = \frac{1}{2}\pi - \varepsilon$, $0 < \varepsilon \ll 1$ According to (15), this implies the existence of an a-pole at $\beta = \beta_0 \approx -\frac{1}{2}i\pi\varepsilon$, and, according to (15) and (47),

$$\sigma_0 \approx 4\pi a^2 [\beta^2 + (\frac{1}{2}\pi\varepsilon)^2]^{-1}, \qquad (48)$$

so that the cross-section becomes very large as $\beta \rightarrow 0$ An a-pole very close to the origin gives rise to an anomalously large scattering cross-section at low energies

This behaviour is well known in the case of neutron-proton scattering It is usually interpreted in terms of a so-called virtual singlet state of the deuteron, the definition of which has occasioned some confusion in the literature There have been several attempts to define a "virtual level" at a small positive energy It must be stressed, in this connection, that, in the present example, all c-poles are far away from the origin for $A \approx \frac{1}{2}\pi$, as may readily be verified from fig 1 The definition by means of an a-pole of the S-matrix has been considered by several authors ^{22, 23, 24})

Let us follow the behaviour of the low-energy cross-section during the process which leads to the appearance of the next bound s-state $(A \rightarrow \frac{3}{2}\pi)$ In S-matrix language, this process corresponds to the transformation of the pair of c-poles $\beta_{\pm 1}$ into an a-pole and a b-pole (cf sect 31 and fig 1) It may be verified without difficulty that, as β_1 approaches the bisector of the fourth quadrant, the low-energy cross-section becomes very small ($\ll \pi a^2$) The value of A for which β_1 crosses the bisector practically coincides with the value $A = \pi \sqrt{2} \approx 4.44$, which marks the appearance of the first zero in the cross-section. This zero appears at the point $\beta = \frac{1}{2}\pi$, when Aincreases, it splits into a pair of zeros, one of which moves towards lower energies, while the other one moves towards higher energies. In fig. 4, the

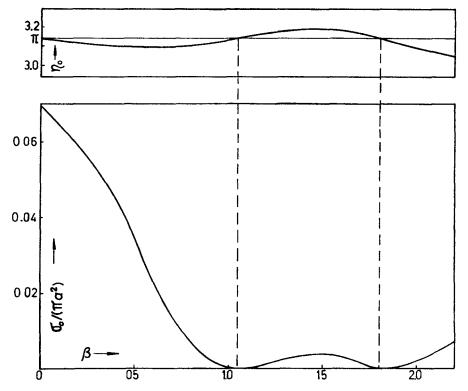


Fig 4 The ratio $\sigma_0/(\pi a^3)$ and the phase-shift η_0 as a function of β for a potential well with A = 4.46

ratio $\sigma_0/(\pi a^2)$ has been plotted as a function of β , for A = 4.46, together with the corresponding values of the phase-shift $\eta_0(\eta_0 = \pi$ at the zeros of the cross-section). A vanishing cross-section at low energy is well known in the theory of the Ramsauer-Townsend effect

For $A = \xi_1 \approx 4.49$, the zero-energy cross-section vanishes For $A > \xi_1$, the low-energy cross-section begins to increase For $A = A_1 \approx 4.61$, β_1 and β_{-1} coalesce at the point $\beta = -i$, giving rise to a pair of a-poles. The low-energy cross-section keeps increasing while one of these a-poles moves towards the origin, and it attains again very large values when the a-pole is very close to the origin $(A \rightarrow \frac{3}{2}\pi \approx 4.71)$

A similar process takes place before the appearance of other bound states. Thus, the typically quantal anomalies (very small or very large values) of the low-energy cross-section, which precede the appearance of a new bound state, are related to poles of the S-matrix that would be considered to be "meaningless" according to the usual interpretation

(b) The case l = 1

Let us consider a potential well that is almost deep enough for the appearance of a new bound p-state, so that (40) is satisfied In this case, as we have seen in sect 4 2, there exists a pair of c-poles, $\beta_{\pm n}$, given by (43), very close to the origin

To obtain the low-energy p-wave cross-section, we may employ (36) and (47), replacing the denominator of (36) by the first member of (42), and expanding $\exp(-2i\beta)$ in powers of β The result is †

$$\sigma_1/(12\pi a^2) \approx \beta^4 [(\frac{3}{2}\beta^2 - \delta_n)^2 + \beta^2 (\frac{1}{2}\beta^2 - \delta_n)^2]^{-1}$$
(49)

In the region

$$|\beta^2 - \frac{2}{3}\delta_n| \ll \frac{2}{3}\delta_n, \qquad (50)$$

eq (49) gives rise to a "Breit-Wigner peak" of half-width $(\frac{4}{3})(\frac{4}{3}\delta_n)^{\frac{3}{2}}$, centered at $\beta^2 = \frac{2}{3}\delta_n$ This agrees with the usual interpretation The existence of a sharp resonance in this case may be attributed to the "centrifugal barrier"

It might be expected that only the poles (and corresponding zeros) that are close to the origin would determine the behaviour of the low-energy cross-section If this were so, (36) could be replaced by

$$S_1(\beta) \approx \exp(-2i\beta)(\beta + \beta_n)(\beta + \beta_{-n})(\beta - \beta_n)^{-1}(\beta - \beta_{-n})^{-1}$$
(51)

Replacing (51) in (47), and taking into account (43), we get

$$\sigma_1/(12\pi a^2) \approx [(\beta^2 - \frac{2}{9}\delta_n)^2 + (\frac{2}{9}\delta_n)^2\beta^2][(\beta^2 - \frac{2}{3}\delta_n)^2 + \frac{4}{9}(\frac{2}{3}\delta_n)^3]^{-1}.$$
 (52)

Although this agrees with (49) in the region (50), it is by no means a good approximation outside of this region. In particular, (52) would give

$$\lim_{\beta \to 0} \left[\sigma_1 / (12\pi a^2) \right] = \begin{cases} \frac{1}{9} & \text{for } \delta_n \neq 0, \\ 1 & \text{for } \delta_n = 0, \end{cases}$$
(53)

whereas, according to $(49)^{\dagger\dagger}$,

$$\lim_{\beta \to 0} \left[\sigma_1 / (12\pi a^2) \right] = \begin{cases} 0 & \text{for } \delta_n \neq 0, \\ \frac{4}{9} & \text{for } \delta_n = 0. \end{cases}$$
(54)

[†] This differs from the result given by Schiff in eq. (19 30) of his book ²⁵) The discrepancy is due to the fact that Schiff fails to take into account terms of the order of $(ka)^2$ and $(ka)^4$ in the denominator of his eq. (19 27)

^{††} For $\delta_n = 0$, (54) does not agree with the result given in p 36 of Mott and Massey's book ¹³) This is due to an error in their eq. (39) a factor 2/(2n+1) should be inserted in the second member of that equation The difference between (52) and (49) is due to the omission of the root $\beta' \approx -3i$ of (43) from $S_1(\beta)$ According to sect. 42, β' is an a-pole for $n \geq 2$. In this case, therefore, the correct behaviour of the low-energy cross-section may only be obtained by taking into account the a-pole β' (together with the corresponding zero), even though it is far away from the origin This is another example of the physical effects that may be produced by an a-pole.

The author is greatly indebted to Prof G Beck for suggesting this problem and for many helpful discussions He is also grateful for the hospitality of the Technische Hogeschool at Eindhoven, where this work was written

Appendix

A THE ROOTS OF EQUATION (12)

Replacing $\alpha = x + iy$ in (12), and separating real and imaginary parts, we find the following three possibilities

$$\begin{array}{ll} x^{-1} \tan x = y^{-1} \tanh y & (I), \\ y = \cosh^{-1} |x/(A \sin x)| & (II), \end{array} (x \neq 0, \quad y \neq 0), \tag{A1}$$

$$\begin{aligned} x^{-1} \sin x &= \pm A^{-1}, \\ y &= 0, \end{aligned}$$
 (A2)

$$x = 0,$$

 $y^{-1} \sinh y = A^{-1}$ (A > 0) (A3)

The corresponding choice of sign in (13), in order to satisfy (11), is such that v < 0, in the case of (A1) and (A3), and such that

$$\operatorname{sgn} v = -\operatorname{sgn}(x \sin 2x) \tag{A4}$$

in the case of (A2), as may be easily proved.

Since the roots of (12) are symmetrical with respect to the x and y axes, we shall restrict ourselves to the first quadrant $(x \ge 0, y \ge 0)$ in the following discussion

There are no roots of (A3) for A > 1 For each value of A belonging to the interval 0-1, (A3) has one root, when A increases from 0 to 1, y decreases from ∞ to 0

The roots of (A1) and (A2) may be found by graphical means Equation (II) defines a family of curves depending on the parameter A. For each value of A, the roots of (A1) are given by the points of intersection of curves (II) and (I), whereas the roots of (A2) are given by the intersections of (II) with the real axis

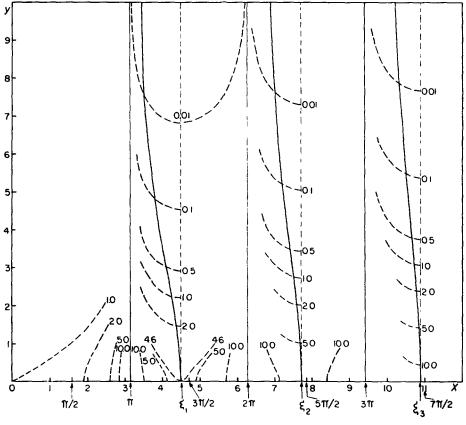
Curve (I) has been drawn in full line in fig 5. It is defined for $n\pi < x \leq \xi_n$ (n = 1, 2, 3, ...), where ξ_n is the *n*th positive root of the equation $\tan x = x$. For large *n*, we have

$$\xi_n \approx c_n - c_n^{-1} - \frac{2}{3}c_n^{-3} - \ldots$$
 (A5)

where

$$c_n = (n + \frac{1}{2})\pi \tag{A6}$$

Portions of curves (II) have been drawn in dashed line in fig 5, the corresponding values of A are also indicated



Let I_n be the interval $n\pi \leq x < (n+1)\pi$. In I_0 , curves (II) intersect the real axis only for $A \geq 1$ The corresponding root of (A2) increases from 0 to π when A increases from 1 to ∞ .

The following discussion applies to all the intervals I_n with $n \ge 1$ To illustrate the behaviour of curves (II) in I_n , a typical curve (A = 0.01 $\operatorname{In} I_1$ has been drawn in fig 5 Each curve (II) goes through a single minimum in I_n This point is located on the straight line $x = \xi_n$ When A increases, it moves downwards along this line, reaching the real axis for $A = A_n$, where

$$A_n = |\xi_n / \sin \xi_n| \approx c_n - \frac{1}{2}c_n^{-1} - \frac{7}{24}c_n^{-3} -$$
(A7)

It can easily be shown that, for every value of A between 0 and A_n , curves (I) and (II) intersect at one and only one point in I_n The corresponding root, $\alpha_n = x_n + iy_n$, moves downwards when A increases Notice that $\alpha_n \to n\pi + i\infty$ for $A \to 0$, and $\alpha_n \to \xi_n$ for $A \to A_n$.

For A > 1, an approximate analytical representation of α_n may be derived. Under this condition, the intersection occurs close to the minimum of (II), so that (II) may be approximated by

$$y_n \approx Y_n + \frac{1}{2}b_n(\xi_n - x_n)^2, \tag{A8}$$

where

$$Y_n = \cosh^{-1}|A_n/A|, \tag{A9}$$

$$b_n = y''(\xi_n) = [1 - (A/A_n)^2]^{-\frac{1}{2}}$$
(A10)

On the other hand, if we put $x_n = c_n - \delta_n$, (I) may be replaced by

$$(c_n\delta_n)^{-1} + c_n^{-2} + (c_n^{-2} - \frac{1}{3})c_n^{-1}\delta_n \approx Y_n^{-1} \tanh Y_n = (b_nY_n)^{-1},$$

from which we find, by iteration,

$$x_n \approx c_n \left\{ 1 - \left[\left(\frac{c_n^2}{b_n Y_n} - 1 \right) + \left(\frac{c_n^2}{3} - 1 \right) \left(\frac{c_n^2}{b_n Y_n} - 1 \right)^{-1} \right]^{-1} \right\}$$
(A11)

In the immediate neighbourhood of $A = A_n$, this may be replaced by $x_n \approx \xi_n - [1 - (b_n Y_n)^{-1}]\xi_n^{-1}$ (A12)

Equations (A8) and (A11)-(A12) give a very good approximation to the roots of (A1) when $1 < A < A_n$ In particular, for large *n*, i.e., for $1 < A \ll A_n$, we find

$$x_n \approx c_n - c_n^{-1} \log(2c_n/A) + ,$$
 (A13)

$$y_n \approx \log(2c_n/A) + \frac{1}{2}c_n^{-2} \{ [\log(2c_n/A) - 1]^2 - \frac{1}{2}A^2 - 1 \} + \dots$$
(A14)

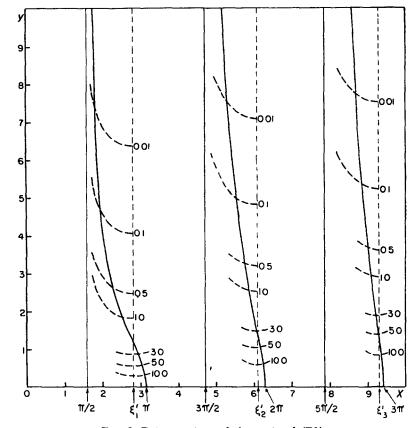
For $A = A_n$, we have $\alpha_n = \xi_n$ This is a double root of (12), which arises from the confluence of a root in the upper half-plane with a root in the lower half-plane For $A > A_n$, it splits into a pair of roots of (A2), which move in opposite directions when A increases, approaching the end-points of I_n when $A \to \infty$.

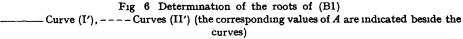
B THE ROOTS OF EQUATION (16)

Replacing $\alpha = x + iy$ in (16), and separating real and imaginary parts, we find that there are no solutions with x = 0 or y = 0. For $x \neq 0$, $y \neq 0$, we obtain

$$\begin{array}{l} x \tan x = -y \tanh y \quad (\mathrm{I}'), \\ y = \sinh^{-1}|x/(A \cos x)| \quad (\mathrm{II}') \end{array}$$
(B1)

The curve (I'), which is defined for $c_{n-1} < x \leq n\pi$ $(n \geq 1)$, has been drawn in full line in fig 6 Portions of curves (II') have been drawn in





dashed line, the corresponding values of A are indicated. In each interval $I'_n : c_{n-1} \leq x < c_n$, each curve (II') goes through a single minimum, located on the straight line $x = \xi'_n$, where ξ'_n is the *n*th positive root of the equation $\cot x = -x$ For large n,

$$\xi'_n \approx n\pi - (n\pi)^{-1} - \frac{2}{3}(n\pi)^{-3} - \dots$$
 (B2)

When A increases, the minimum of (II') moves downwards, approaching the real axis for $A \rightarrow \infty$

For every value of A, (I') and (II') intersect at one and only one point in

 I'_n The corresponding root of (16), $\alpha_n = x_n + \imath y_n$, moves downwards when A increases We find that $\alpha_n \to c_{n-1} + i\infty$ for $A \to 0$, and $\alpha_n \to n\pi$ for $A \to \infty$

The following formulae, the derivation of which is similar to that of (A8)—(A11), give a very good approximation to the roots when A > 1

$$x_n \approx n\pi - (n\pi)^{-1} b'_n Y'_n - (n\pi)^{-3} (b'_n Y'_n)^2 (1 - \frac{1}{3} b'_n Y'_n), \tag{B3}$$

$$y_n \approx Y'_n + \frac{1}{2} b'_n (\xi'_n - x_n)^2,$$
 (B4)

where

$$Y'_{n} = \sinh^{-1}z_{n}, \quad b'_{n} = (1+z_{n}^{-2})^{-\frac{1}{2}},$$
 (B5)

$$z_n = (1 + \xi_n'^2)^{\frac{1}{2}} / A \tag{B6}$$

In particular, for $1 < A \ll \xi'_n$, we have

 $x_n \approx n\pi - (n\pi)^{-1} \log(2n\pi/A) + ,$ (B7)

$$y_n \approx \log(2n\pi/A) + \frac{1}{2}(n\pi)^{-2} \{ [\log(2n\pi/A) - 1]^2 + \frac{1}{2}A^2 - 1 \} +$$
(B8)

On the other hand, for $A \gg \xi'_n(z_n \ll 1)$, we find

$$x_n \approx n\pi - (n\pi)^{-1} z_n^2 +$$
, (B9)

$$y_n \approx z_n + \frac{1}{2} (n\pi)^{-2} z_n +$$
 (B10)

Note added in proof It has been shown by Humblet (Mém in-8° Soc Roy Sc Liège 12 (1952) no 4) that the properties of the pole distribution which are mentioned in sect 5 l are valid for a very general class of potentials of finite range and for arbitrary values of the angular momentum Humblet has also given a thorough discussion of the asymptotic behaviour of large poles. The results given in sect 4 1 of the present paper are in complete agreement with his results The author wishes to thank Prof L Rosenfeld for bringing Humblet's paper to his attention

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