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ON THE DERIVATION OF THE NUCLEAR RESONANCE SCATTERING FORMULA

by

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ABSTRACT

In this thesis detailed calculations are given showing the equivalence of Siegert's derivation of the nuclear resonance scattering formula, and Hu's derivation of the same formula. Although at first glance it appears that Hu has given a solution to the problem using an entirely different formalism, we have shown that no matter what the final expression for the resonance scattering cross section may be, it must be the same in the case of Siegert's calculation and that of Ning Hu, provided, of course, that no more or less arbitrary approximations are introduced into the calculations.

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INTRODUCTION

There are several derivations of the Breit-Wigner dispersion formula for nuclear resonance scattering. These derivations can be divided into two groups: those using time-dependent wave functions, and those using time-independent wave functions. Among the derivations belonging to the latter group we mention, in particular, those by Siegert(1), Breit(2), Wigner(3), Feshbach and collaborators(4) ang Ning Hu(5).

Although the interdependence of the above derivations has been partly cleared up by the authors themselves, there are certain points which seem to require further investigation.

In this thesis detailed calculations are given of a critical comparison of Ning Hu's and Siegert's work. A critical investigation of Ning Hu's results seemed particularly desirable because his resonance scattering

(1) - Siegert - Physical Review, 56, 750, 1939
(2) - Breit - Physical Review, 58, 506, 1940
58,1068, 1940
(3) - Wigner - Physical Review, 70, 15, 1946
(4) - Feshbach, Peaslee, and Weisskopf - Physical Review, 71, 145, 1947
(5) - Ning Hu - Physical Review, 74, 131, 1948

formula differed from the usual one, and because the author himself attributed this difference to the fact that his "formulae rest on a much more solid basis than other theoretical derivations hitherto given". It turns out:

(a) that the difference is due to a trivial error in the calculation.

(b) that Ning Hu's derivation is exactly equivalent* to Siegert's derivation, which is, at first view, not obvious.

After our work had been completed a brief "Erratum" was published by Ning Hu in Physical Review[6] in which he concedes more or less statement (a) and retracts his above quoted sentence. However, he does not make any new statement about the relation of his derivation to the previously published ones.

In Section I of this thesis we shall give a brief outline of the calculations presented by Siegert and Hu together with a short note on some general properties of the "scattering matrix" used by Ning Hu in his calculation. The equivalence of Siegert's derivation and Hu's derivation is proved in Section II. In Section III we discuss more explicitly the relation of Hu's expression for the "scattering matrix" to Siegert's formulae.

* - By stating that Hu's derivation is exactly equivalent to Siegert's, we do not say that Hu's paper does not go beyond Siegert's results in other respects. This is so even if we ignore the fact that Hu's calculation is made for arbitrary l (angular momentum), whereas Siegert confines his attention to the case $l = 0$.

(6) - Ning Hu - Physical Review - 75, 1449, 1949

ON THE DERIVATION OF THE NUCLEAR RESONANCE SCATTERING FORMULA

I - PRELIMINARY CONSIDERATIONS

In this section we confine our attention to those aspects of Siegert's and Hu's calculations which are of direct interest in Sections II and III. For convenience we have also added a short note on some general properties of the "scattering matrix".

(1) Siegert's Calculation

If ψ is the solution of the radial part of the Schroedinger Wave Equation for the case $l = 0$, where l is the angular momentum of the incident particle, then $\phi_e = r\psi$ must be a solution of the equation

$$\frac{\hbar^2}{2m}\phi_e'' + (E - V)\phi_e = 0 \quad \ldots\ldots\ldots\ldots \quad (1)$$

where the primes on ϕ_e denote differentiation with respect to r,

E is the energy of the incident particle

and $V = V(r)$ for $r < a$

$V = 0$ for $r > a$

where a may be regarded as the "nuclear radius".

The asymptotic solution of the wave equation may be written as

$$\phi_e = \frac{I}{k} \sin kr + R e^{ikr} \ldots\ldots\ldots\ldots \quad (2)$$

where R and I are functions of k and

$$k^2 = 2mE/\hbar^2 \ldots\ldots\ldots\ldots\ldots\ldots \quad (3)$$

The scattering cross section is then given by

$$\sigma = 4\pi \left| R/I \right|^2 \ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

R/I may be expressed in terms of the wave function, ϕ_e, evaluated at the nuclear radius, a,

$$R/I = \frac{\phi_e(a) \cos ka - \phi_e'(a) \sin ka / k}{\phi_e'(a) - ik\phi_e(a)} e^{-ika} \quad (5)$$

The author then looks for singularities of the cross section arising from the vanishing of the denominator. The eigenvalues of the wave equation and hence the energy values for which the denominator vanishes, are given by the solutions of the equation

$$\frac{\hbar^2}{2m} \phi_n'' + (W_n - V) \phi_n = 0 \ldots\ldots\ldots\ldots \quad (6)$$

with the boundary conditions

$$\left.\begin{array}{l} \phi_n = 0 \text{ at } r = 0 \\ \phi_n' - ik_n\phi_n = 0 \text{ at } r = a \end{array}\right) \ldots\ldots\ldots\ldots \quad (7)$$

where $\phi_n(r)$ is the wave function corresponding to the energy W_n of the compound nucleus characterized by

$$k_n^2 = 2mW_n/\hbar^2 \ldots\ldots\ldots\ldots\ldots\ldots \quad (8)$$

To obtain R/I in the neighbourhood of a singularity, W_n, one multiplies equation (1) by ϕ_n and equation (6) by ϕ_e and on subtraction obtains

$$\frac{\hbar^2}{2m}(\phi_n''\phi_e - \phi_e''\phi_n) + (W_n - E)\phi_n\phi_e = 0 \quad \ldots\ldots\ldots (9)$$

Integrating (9) from 0 to a and using the boundary conditions (7), the author obtains

$$\phi_e'(a) - ik\phi_e(a) = \frac{(W_n - E)}{\frac{\hbar^2}{2m}\phi_n(a)}\left(\int_0^a \phi_n\phi_e dr + i\,\frac{\phi_e(a)\phi_n(a)}{k + k_n}\right). \quad (10)$$

Now assuming the eigenvalue W_n is not degenerate, then in the limit as $E \rightarrow W_n$, $\phi_e \rightarrow \phi_n$

$$\phi_e'(a) - ik\phi_e(a) \rightarrow \frac{(W_n - E)}{\frac{\hbar^2}{2m}\phi_n(a)}\left(\int_0^a \phi_n^2 dr + i\,\frac{\phi_n^2(a)}{2k_n}\right). \ldots (11)$$

For the numerator of R/I we have in the limit as $E \rightarrow W_n$

$$\phi_e(a)\cos ka - \phi_e'(a)\sin ka/k \rightarrow$$
$$\phi_n(a)(\cos k_n a - i\sin k_n a)$$
$$= \phi_n(a)\, e^{-ik_n a} \quad \ldots\ldots\ldots\ldots\ldots\ldots (12)$$

Thus in the limit, R/I becomes

$$R/I = \frac{1}{W_n - E}\,\frac{\hbar^2/2m\,\phi_n^2(a)\,e^{-2ik_n a}}{\int_0^a \phi_n^2 dr + i\,\frac{\phi_n^2(a)}{2k_n}} + f(E). \ldots (13)$$

where f(E) is a regular function in the surrounding of W_n and gives rise to the "potential scattering".

In order to express the scattering cross section in more familiar terms, Siegert derives, from the Schroedinger Wave

Equation, (1), and its complex conjugate, the relation

$$\frac{\hbar^2}{2m}\left|\phi_n(a)\right|^2 = \frac{\gamma_n}{k_n + k_n^*}\int_0^a \left|\phi_n\right|^2 dr \quad . \; . \; . \; . \; . \; . \; . \; . \qquad (14)$$

where $W_n = E_n - i\frac{\gamma_n}{2}$ . . . . (15)

with E_n and γ_n both real.

Now for sufficiently small values of γ_n we can multiply ϕ_n by a suitable constant, A, of modulus one, so as to make $A\phi_n$ real near $r = a$. Then if we assume that the major contribution to the integral in the denominator of (13) occurs for r very nearly equal to a, we may write

$$\int_0^a A^2\phi_n^2 dr = \int_0^a \left|\phi_n\right|^2 dr \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \qquad (16)$$

$$A\phi_n(a) \doteq \left|\phi_n(a)\right| e^{i(k_n a + \delta_n/2)} \quad . \; . \; . \; . \; . \; . \; . \qquad (17)$$

where δ_n is a phase determined entirely from the properties of the compound state.

This assumption means that the nuclear eigenfunction takes on values appreciably different from zero, only near the nuclear radius. The validity of such an assumption is, of course, questionable.

From equations (13), (16), and (17) it follows that

$$R/I = \frac{1}{W_n - E}\;\frac{\hbar^2/2m\;\left|\phi_n(a)\right|^2 e^{i\delta_n}}{\int_0^a\left|\phi_n\right|^2 dr + i\,\frac{\left|\phi_n(a)\right|^2}{2k_n}\, e^{2i(k_n a + \delta_n/2)}} + f(E) \qquad (18)$$

and by virtue of equation (14) the second term in the denominator is very much less than the first and hence one obtains the well known one level formula

$$\sigma = 4\pi \left| \frac{\gamma_n}{(E_n - E) - i\frac{\gamma_n}{2}} \cdot \frac{e^{i\delta_n}}{k_n + k_n^*} + f(E) \right|^2 \quad .. \quad (19)$$

That the eigenvalues and eigenfunctions given by the boundary condition characterize a long lived compound nucleus may be shown by the following arguement: If the levels are narrow, and therefore the escape of a particle from the nucleus is a rare event, then the state of the compound nucleus will undergo very little change if we prevent the escape of the particle altogether. It is obvious that (7) is equivalent to preventing the escape of the particle, since in the limit as $k \rightarrow k_n$, $I \rightarrow 0$, and hence we have no stream of incident particles. Therefore, there can be no scattered beam, so that there actually are no particles escaping from the nucleus.

(2) Some General Properties of the Scattering Matrix

The "scattering matrix", originally introduced by Wheeler[7], has been used by several authors - Wheeler, Wigner, Breit, Heisenberg, and others. The first three named physicists have used the matrix only to solve collision problems. Heisenberg, however, has attempted, through use of the "S-Matrix", to set up a future, divergence free, theory of elementary particles. According to his idea

(7) - Wheeler, Physical Review, 52, 1107, 1937

the "S" function should play a role in the future theory analogous to the part played by the Hamiltonian in the present quantum theory. It has been shown by Heisenberg, Kramers, Møller, and others, that from the "scattering matrix" one may obtain all observable quantities. However, in obtaining the energy levels of the system from the "scattering matrix", one must proceed with the utmost caution, since for a long range potential we are led, in some cases, to redundant energy values.(8)

The relation of the "scattering matrix" (which in the considered case reduces to a single element) to the asymptotic form of the wave function is as follows: Consider a non-relativistic particle in a central field of force. The Schroedinger Wave Equation is, in this case,

$$\frac{1}{r}\frac{d^2(r\psi)}{dr^2} + k^2\psi - \frac{\ell(\ell+1)}{r^2}\psi + V(r)\psi = 0 \quad . \; . \; (20)$$

where ℓ is the angular momentum of the particle. If we set $\phi = r\psi$, then the asymptotic solution of the wave equation is given by

$$\phi = \sin\left(kr + \eta_\ell(k)\right) \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; (21)$$

where $\eta_\ell(k)$ is the phase shift due to the interaction potential.

Equation (21) may be rewritten, aside from a factor, as

$$\phi \simeq e^{-ikr} - S_\ell(k)\, e^{ikr} \quad . \; . \; . \; . \; . \; . \; . \; . \; (22)$$

where $S_\ell(k) = e^{2i\eta_\ell(k)}$ . . . . (23)

is the "scattering matrix".

(8) Jost, Helvetica Physica Acta, 20, 256, 1947 - In this paper Jost discusses the conditions under which redundant energy values may occur.

Since $\eta_\ell(k)$ is a real and odd function of k - this is readily seen from equations (20) and (21) - we have the relations

$$S(k)S(-k) = 1 \quad \ldots\ldots\ldots\ldots \quad (24)$$

$$S(k)S^*(k) = 1 \quad \ldots\ldots\ldots\ldots \quad (25)$$

For the case $\ell = 0$, the expression for the scattering cross section of the particle by the central field of force follows immediately from equation (22):

$$\sigma = 4\pi \left| \frac{S(k) - 1}{2ik} \right|^2 \quad \ldots\ldots\ldots\ldots \quad (26)$$

According to the suggestion of Kramers and Heisenberg, we may continue the wave equation, and hence the "S" function, into the complex "k-plane". The stationary states of the system are then given by the negative imaginairy values of k which make S(k) = 0. In this case, ϕ, defined by (22) becomes

$$\phi \simeq e^{-|k_n| r} - S_\ell(-i|k_n|)\, e^{|k_n| r} \quad .$$

and if $S(-i|k_n|) = 0$, ϕ certainly satisfies the condition necessary for it to represent a closed state (provided ϕ does not vanish identically).

There are, of course, many other general properties of the "scattering matrix" which could be quoted, however, since this thesis deals only with a non-relativistic scattering problem, further general considerations will not be necessary.

(3) - <u>Hu's Calculation</u>

As Hu has pointed out, if the S function has simple poles, it follows that we may write for S(k)

$$S(k) \;=\; \frac{(k - k_n^*)(k + k_n)}{(k - k_n)(k + k_n^*)} + f(k) \quad . \; . \; . \quad (27)$$

where $k = k_n$ is a singularity of S(k) and is related to the nuclear energy level, W_n, by $W_n = \frac{\hbar^2}{2m} k_n^2 = E_n - i\frac{\gamma_n}{2}$

and f(k) is a regular function of k.

Substituting (27) into (26) one obtains the usual one level formula

$$\sigma = 4\pi \left| \frac{\gamma_n}{(E_n - E) - i\frac{\gamma_n}{2}} \cdot \frac{1}{k_n + k_n^*} + f(k) \right|^2 \quad (28)$$

which is the same as Siegert's formula, equation (19).

That S(k), in a certain approximation, has the above form may be shown as follows: From equation (24) one sees that if $k = -K$ is a pole of the "S" function, then $k = K$ is a zero of S(k). Now if we can show that $(dS/dk)_{k = K} \neq 0$, it follows at once that the singularity of the "S" function at $k = -K$ is a pole of the first order.

Consider the asymptotic form of the wave function*

$$\phi = b(e^{-ikr} - S(k)\, e^{ikr}) \quad . \; . \; . \; . \; . \; . \; . \; . \; . \quad (29)$$

where <u>b</u> is a function of k

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* We have here slightly generalized Hu's calculation, in that he assumes b = 1 from the start.

Now if $k = K$ is a zero of $S(k)$, then

$$\phi_K = b_K e^{-iKr}$$

By substitution of (29) into the expression

$$\left(\frac{d}{dk}\left\{\phi\left[(d\phi/dr) + ik\phi\right]\right\}\right)_{k = K} =$$

$$\phi_K(d^2\phi/dk\,dr)_{k = K} + i\,\phi_K^2 + iK\phi_K(d\phi/dk)_{k = K}$$

one easily shows that

$$-2iKb_K^2(dS/dk)_{k = K} = \phi_K(d^2\phi/dk\,dr)_{k = K} - (d\phi_K/dr)(d\phi/dk)_{k=K}$$

$$+ i\,\phi_K^2 \quad \ldots\ldots\ldots\ldots \quad (30)$$

Now from consideration of the Schroedinger Wave Equation it follows that

$$ib_K^2(dS/dk)_{k = K} = \int_0^a \phi_K^2 dr - \frac{i}{2K}\,\phi_K^2(a) \quad \ldots \quad (31)$$

where $r = a$ is the range of the potential, $V(r)$.

If $\phi_K(r)$ is very nearly real at $r = a$ and in a neighbourhood thereof, and if the major contribution to the integral in (31) occurs in this region, then $(dS/dk)_{k = K}$ cannot equal zero. Thus the pole of $S(k)$ at $k = -K$ must be of the first order. From equations (24), (25), and the conclusion drawn from the above, it follows that indeed $S(k)$ has the form given by (27).

It is worth while to point out that the assumption under which Ning Hu's resonance scattering formula holds is identical with that under which Siegert's holds. (Compare above discussion with comments connected with equations (16) and (17) in Siegert's derivation.)

II - Proof of the Equivalence of Siegert's and Ning Hu's Derivations

For the sake of simplicity we confine our attention to the case $l = 0$, where l is the angular momentum of the incident particle. If we denote by σ_S the scattering cross section given by Siegert and σ_H the scattering cross section given by Hu, we have, as stated in the previous section

$$\sigma_S = 4\pi \left| R/I \right|^2 \quad \text{(32-a)}$$

$$\sigma_H = 4\pi \left| \frac{S(k) - 1}{2ik} \right|^2 \quad \text{(32-b)}$$

In order to find the resonance maxima of the cross section, both authors look, as we have seen, for singularities of the right hand side of (32) as a function of complex k. Evidently the resonance part of the cross section will be, in both cases, exactly the same if the moduli of the residues of $R(k)/I(k)$ and of $S(k)/2ik$ are equal, provided the singularities of these two expressions are poles of the first order.

Now both authors assume that the behaviour of the incident particle "inside" the nucleus is described by the equation

$$\frac{\hbar^2}{2m} \phi_n'' + (W_n - V)\,\phi_n = 0 \quad \text{(33)}$$

where $\phi_n(r)$ is the wave function corresponding to an energy of the compound nucleus, characterized by

$$k_n^2 = 2mW_n/\hbar^2 \quad \text{(34)}$$

and they both assume that

$$\phi_n(r) \simeq b_n e^{ik_n r} \quad \text{for } r = a \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \quad (35)$$

where <u>a</u> is the "nuclear radius", and b_n is a complex amplitude.

It is thus almost obvious that the residues are indeed equal. The formal proof of this equality is as follows:

From the relation $S(k)S(-k) = 1$, one derives, on the assumption that the pole of $S(k)$ at $k = k_n$ is of the first order, the relation

$$\text{Residue } S(k)_{k = k_n} = -1/(dS/dk)_{k = -k_n} \; . \; . \quad (36)$$

That this equation is valid is easily seen from the following arguement: If $k = k_n$ is a pole of $S(k)$, we may expand $S(k)$ in a Laurent series about $k = k_n$, valid at least in the neighbourhood of the pole

$$S(k) = \frac{a_{-1}}{(k - k_n)} + a + a_1(k - k_n) + \ldots\ldots \quad (37)$$

Now if $k = k_{\cdot}$ is a zero fo $S(k)$, then we may expand $S(k)$ in a Taylor series about $k = k_{\cdot}$, valid in the neighbourhood of $k_{\cdot}$

$$S(k) = a_1'(k - k_{\cdot}) + a_2'(k - k_{\cdot})^2 + \ldots\ldots\ldots \quad (38)$$

By virtue of (24), if $k = k_n$ is a singularity of $S(k)$, then certainly $k = -k_n$ is a zero of $S(k)$. Thus we may rewrite (38) as

$$S(k) = a_1'(k + k_n) + a_2'(k + k_n)^2 + \ldots\ldots\ldots \quad (39)$$

with k in (39) equal to -k in (37). Thus from (24), (37), (39), and the remark just made, we have

$$S(k)S(-k) = -a_{-1}a_1' + (-aa_1' + a_{-1}a_2')(k - k_n) + \ldots\ldots \quad (40)$$

Now since this holds in a neighbourhood of $k = k_n$, it must also hold at the point k_n itself. We have, therefore,

$$a_{-1}a_1' = -1 \quad \ldots\ldots\ldots\ldots \quad (41)$$

But $a_1' = (dS/dk)_{k=-k_n}$, and since a_{-1} is equal to residue $S(k)_{k=k_n}$, equation (36) follows.

$$\text{Thus Residue } S(k)/2ik = -\frac{1}{\left(\frac{dS}{dk}\right)_{k=-k_n}} \cdot \frac{1}{2ik} \quad (42)$$

On the other hand, from equation (13) of our outline of Siegert's calculation and equation (35) of this section it follows, on the same assumption

$$\text{Residue } R/I = -\frac{b_n^2}{\int_0^\infty \phi_n^2 dr + i\frac{\phi_n^2(a)}{2k_n}} \cdot \frac{1}{2k} \quad \ldots\ldots \quad (43)$$

Now since the Schroedinger operator is even in k, it is obvious from equation (31) that

$$ib_n^2(dS/dk)_{k=-k_n} = \phi_n^2 dr + i\frac{\phi_n^2(a)}{2k_n} \quad \ldots \quad (44)$$

Thus by substituting (44) into (43) and comparing the resulting equation with (42), one sees that the two residues are indeed equal.

We have thus shown that whatever the final expression for the resonance scattering cross section may be, it must be the same in the case of Siegert's calculation and that of Ning Hu, provided, of course, that no more or less arbitrary approximations are introduced into the calculations.

Actually, as was stated in Section I, both Siegert and Ning Hu do introduce certain approximations, but the approximations are identical in both cases, so that the final result is the same, if we correct the trivial error in Ning Hu's calculation, which we have mentioned in the introduction.

III - A Further Discussion of the Relation between Siegert's Formulae and those of Ning Hu

In view of the arguement presented in Section II it is certainly evident that Siegert's derivation and Hu's derivation are fully equivalent. However, we can make the interdependence of these two derivations even more explicit in the following simple manner.

We may rewrite the singular part of equation (18) of our summary of Siegert's paper as

$$R/I = \frac{1}{k_n^2 - k^2} \cdot \frac{|\phi_n(a)|^2 e^{i\delta_n}}{\int_0^\infty |\phi_n|^2 dr + i\frac{|\phi_n(a)|^2}{2k_n} e^{2i(k_n a + \frac{\delta_n}{2})}} \tag{45}$$

Now making an approximation identical to that made in obtaining (19) from (18) - i.e. that ϕ_n is very nearly real in the region of major contribution to the integral in the denominator of (45) - we see that the second term in the denominator is very much less that the first. Thus combining (45) with (14), one obtains

$$R/I = 2m/\hbar^2 \frac{\gamma_n}{(k_n^2 - k^2)} \cdot \frac{e^{i\delta_n}}{(k_n + k_n^*)} \quad \ldots . \tag{46}$$

and from (15) one sees that

$$k_n^{*2} - k_n^2 = i\gamma_n 2m/\hbar^2 \quad \ldots\ldots\ldots\ldots \quad (47)$$

Thus (46) becomes

$$R/I = -\frac{ie^{i\delta_n}(k_n^* - k_n)}{k_n^2 - k^2} \quad \ldots\ldots\ldots\ldots \quad (48)$$

Now

$$2k\left|R/I\right| = \left|\frac{2k(k_n - k_n^*)}{(k^2 - k_n^2)}\right| \quad \ldots\ldots\ldots\ldots \quad (49)$$

and since

$$2k(k_n - k_n^*) = (k + k_n)(k - k_n^*) - (k + k_n^*)(k - k_n) \quad (50)$$

and

$$\left|(k - k_n)(k + k_n)\right| = \left|(k - k_n)(k + k_n^*)\right| \quad \ldots\ldots \quad (51)$$

then

$$2k\left|R/I\right| = \left|\frac{(k + k_n)(k - k_n^*) - (k + k_n^*)(k - k_n)}{(k - k_n)(k + k_n^*)}\right|$$

$$= \left|\frac{(k + k_n)(k - k_n^*)}{(k - k_n)(k + k_n^*)} - 1\right| \quad \ldots\ldots \quad (52)$$

Now it follows from (32) that

$$2k\left|R/I\right| = \left|S(k) - 1\right| \quad \ldots\ldots\ldots\ldots \quad (53)$$

We see, therefore, that Ning Hu's expression (27) for S(k)

$$S(k) = \frac{(k - k_n^*)(k + k_n)}{(k + k_n^*)(k - k_n)}$$

is indeed compatible with equation (52) which was here derived from Siegert's theory without any arbitrary assumption.

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