

Interpretation of the Virtual Level of the Deuteron

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I. INTRODUCTION

FROM the measurements of the cross section of low-energy neutron-proton scattering, it became evident to physicists^{1,2,3} in the early days that the interaction of the neutron and the proton is spin-dependent. According to these authors, there is a 1S state that plays a role in the theoretical formula for the 1S scattering similar to that played by the ground state of the deuteron for the 3S scattering. Experiments on the scattering of neutrons by *ortho*- and *para*-hydrogen have led to the conclusion that the 1S state is a virtual state having a negative binding energy.

While the bound state is a familiar concept in quantum mechanics, the true nature of the virtual state has been a subject of much discussion during the subsequent years, and various definitions of the virtual level of the deuteron have appeared in the literature. In view of the interest this subject has received, it is desirable to clarify the theoretical background of the definitions that have been proposed.

The object of this article is not to give a comprehensive exposition of the motives that led to the various definitions of the virtual level, but rather to elucidate some of the definitions from the viewpoint of the theory of S matrix (scattering matrix)⁴ and the theory of R (derivative) and Q matrices.⁵ After a brief general

review in Part II, we shall confine our attention to the following definitions: (1) definitions which are based on the analogy of the 1S virtual state with the 3S bound state, and which fit in a simple way into the theory of the S matrix; (2) a definition that identifies the 1S virtual level with the lowest 1S resonance level according to the theory of the R matrix. From a general formula connecting the S and R matrices, one can derive a simple connection between the two kinds of definitions. There have been scattered remarks on this subject in the literature. It is our purpose to give a connected account. It should be mentioned that the term "virtual level" has been given different meanings in the literature. In this article we use it only for the energy levels that form the basis of one-level representations of the low-energy neutron-proton 1S scattering cross section. As usual, we use the term "resonance level" for the energy levels that occur in resonance scattering and resonance reactions. It is beyond the scope of the present article to discuss in detail the theory of resonance, and we shall merely mention briefly the definitions of the resonance level that have been given in terms of the S , R , and Q matrices.

In dealing with the neutron-proton system we shall confine our attention to the central-force approximation and the S states. The matrix elements of the S , R , and Q matrices that concern us are simply functions of the momentum or energy of the relative motion of the two nucleons.

II. DEFINITIONS OF THE VIRTUAL LEVEL

A. Approximate Definition

The wave equation for the S states of the neutron-proton system is, for the center-of-mass frame of reference,

$$\left[-(d/dr)^2 + V(r)\right]u(r) = Eu(r). \quad (1)$$

Here r is the distance between the nucleons, E and $V(r)$ are the total energy and the potential energy, divided by the factor $\hbar^2/2m$, m being the reduced mass of the nucleons.^{5a} For the scattering problem, there is a continuous spectrum of energies $E_k = k^2$ extending from $k=0$ to $k=\infty$, and the wave Eq. (1) corresponding to an energy E_k is of the form

$$\left[(d/dr)^2 + k^2\right]u_k(r) = V(r)u_k(r). \quad (2)$$

The wave function $u_k(r)$ vanishes at $r=0$ and has the asymptotic expression

$$u_k(r) = \text{const} \sin[kr + \delta(k)] \quad (3)$$

^{5a} The quantity E will be referred to as energy for brevity.

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¹ The idea suggested by E. P. Wigner was developed by H. A. Bethe and R. F. Bacher, *Revs. Modern Phys.* **8**, 82 (1936); See also H. A. Bethe, *Elementary Nuclear Theory* (John Wiley and Sons, Inc., New York, 1947).

² E. Fermi, *Phys. Rev.* **48**, 570 (1935); *Ricerca sci.* **7**, No. II, 13 (1936); E. Amaldi and E. Fermi, *Phys. Rev.* **50**, 899 (1936).

³ J. Schwinger and E. Teller, *Phys. Rev.* **52**, 286 (1937).

⁴ J. A. Wheeler, *Phys. Rev.* **52**, 1107 (1937); W. Heisenberg, *Z. Physik* **120**, 513, 673 (1943); *Z. Naturforsch.* **1**, 608 (1946); C. Møller, *Kgl. Danske Videnskabs Selskab. Mat-fys. Medd.* **23**, No. 1 (1945); **22**, No. 19 (1946).

⁵ E. P. Wigner and L. Eisenbud, *Phys. Rev.* **72**, 29 (1947); T. Teichmann and E. P. Wigner, *Phys. Rev.* **87**, 123 (1952).

for large r , $\delta(k)$ being the phase shift. The scattering cross section is given by

$$\sigma(k) = 4\pi \sin^2[\delta(k)]/k^2 \quad (4)$$

or

$$\sigma(k) = 4\pi/k^2 \{1 + \cot^2[\delta(k)]\}. \quad (5)$$

At low energies we have approximately

$$\cot[\delta(k)] = -\alpha/k, \quad (6)$$

where

$$\alpha = -\lim_{k \rightarrow 0} k \cot[\delta(k)], \quad (7)$$

and therefore

$$\sigma(k) = 4\pi/(k^2 + \alpha^2). \quad (8)$$

The quantity α is the reciprocal of Fermi's scattering length.

The connection between the scattering cross section and the bound and virtual states arises from the following situation. It is known theoretically that the existence of a bound state for the deuteron depends on the sign of the scattering length. If $\alpha > 0$, there is a bound state whose energy is approximately $E_\alpha = -\alpha^2$. On the other hand, there is no bound state if $\alpha < 0$. These conclusions have been drawn from the mathematical scheme of wave mechanics.^{1,6} A simple derivation of these conclusions provided by the theory of the S matrix will be given in Sec. IIIB. The first of the above two possibilities holds for 3S . In this case the scattering cross section can be expressed in terms of the binding energy of the ground state of the deuteron according to the approximate formula

$$\sigma(k) = 4\pi/(E_k + |E_\alpha|). \quad (9)$$

In the case of 1S , the second possibility holds and there is no bound state. However, Eq. (9) is still valid if one introduces a virtual state whose energy is numerically equal to α^2 . It is customary to speak of a positive binding energy if the state is real, a negative binding energy if it is virtual.

B. Exact Definitions for the Square-Well Potential

The definition of the virtual level given above is approximate. Exact definitions have been given, without reference to the scattering formula, for the case of a nuclear potential having the shape of a square well,

$$V(r) = \begin{cases} -V_0 & (r < a) \\ 0 & (r > a). \end{cases} \quad (10)$$

As a preparation for our later general discussions we shall discuss some of these definitions that are better known.⁷

In the case of 3S , there is a bound state of energy

⁶ J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics*, (John Wiley and Sons, New York, 1952).

⁷ There is an extensive collection of definitions of the virtual level for the square-well potential in a recent article by O. Bergmann, *Acta Phys. Austriaca* **5**, 240 (1951).

$E_\gamma = -\gamma^2$. Its wave function for $r \geq a$ is

$$u(r) = \text{const exp}(-\gamma r) \quad (11)$$

with $\gamma > 0$. The continuity of $u(r)$ and its derivative at $r = a$ requires

$$(V_0 - \gamma^2)^{1/2} \cot[(V_0 - \gamma^2)^{1/2}a] = -\gamma. \quad (12)$$

The solutions of this equation have been discussed by Schiff⁸ and by Mott and Massey.⁹ There is only one solution of Eq. (12) for the deuteron because V_0 is only slightly larger than the critical value $(\pi/2a)^2$. Breit and his collaborators^{10,11} have expressed the scattering cross section in terms of k and γ . Their result is

$$\sigma(k) = [4\pi/(k^2 + \gamma^2)] [1 + (\gamma a) + G_2(\gamma a)^2 + G_3(\gamma a)^3 + \dots], \quad (13)$$

where the coefficients G_n are even functions of k and γ .

In the case of 1S , the value of V_0 is slightly smaller than $(\pi/2a)^2$. The value of γ that satisfies Eq. (12) is now negative and the wave function given by Eq. (11) is no longer permissible. It now becomes necessary to introduce a virtual level. The choice of reference 10 amounts to using Eq. (12) also for 1S , with the understanding that γ is negative, and the magnitude of the energy of the virtual level is defined to be γ^2 . This choice for the virtual level was designed to make the expansion expressed by Eq. (13) valid also for 1S . It appears natural from the viewpoint of the theory of the S matrix, as will be seen in Sec. IIIB.

A slightly different choice¹² is to define the energy of the virtual level as the positive energy $k^2 = \gamma^2$ for which

$$(d/dr)u_k(r)/u_k(r) = k \quad (r = a). \quad (14)$$

This leads to the condition

$$(V_0 + \gamma^2)^{1/2} \cot[(V_0 + \gamma^2)^{1/2}a] = \gamma \quad (\gamma > 0) \quad (15)$$

for the virtual level.

According to a general definition given by Hulthén,^{11,13} the virtual state is the positive-energy state k such that

$$\int_0^\infty [u_k(r)]^2 |V(r)| dr = \text{maximum}, \quad (16)$$

$u_k(r)$ being normalized in the energy scale. For the square-well potential, Eq. (16) reduces to

$$\int_0^a [u_k(r)]^2 dr = \text{maximum}. \quad (17)$$

⁸ L. I. Schiff, *Quantum Mechanics*, (McGraw-Hill Book Company, Inc., New York, 1949).

⁹ N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Oxford University Press, Oxford, 1949).

¹⁰ Breit, Thaxton, and Eisenbud, *Phys. Rev.* **55**, 1018 (1939); C. Kittel and G. Breit, *Phys. Rev.* **56**, 744 (1939).

¹¹ L. Rosenfeld, *Nuclear Physics* (Interscience Publishers, New York, 1949), Chap. 5.

¹² M. S. Plesset and F. W. Brown, *Proc. Natl. Acad. Sci. U. S. A.* **25**, 600 (1939).

¹³ L. Hulthén, *Arkiv. Mat. Astron. Fysik.* **29**, No. 1 (1942).

Flügge, Hückel,¹⁴ Wu, and Foley¹⁵ have shown that it is possible to take the lowest energy λ^2 satisfying the equation

$$\cot[(V_0 + \lambda^2)^{\frac{1}{2}}a] = 0 \quad (18)$$

to be the virtual level. Equation (18) is the condition for the derivative of $u_k(r)$ to vanish at $r=a$, $k=\lambda$. Treating k and λ as small quantities, these authors obtained the following formulas:

$$\sigma(k) = 4\pi(1 - \lambda^2 a^2) / [k^2 + (k^2 - \lambda^2)^2 a^2 / 4], \quad (19)$$

$$\sigma(k) = 4\pi / [k^2 + (k^2 + \lambda^2)^2 a^2 / 4]. \quad (20)$$

Equation (19) is the result of reference 14, including the correction factor $(1 - \lambda^2 a^2)$ given in their later publications. Equation (20) is the result of reference 15. These results are consistent with each other, as can be seen by transferring the factor $1 - \lambda^2 a^2$ in Eq. (19) from the numerator to the denominator and retaining only the first two terms in the expansion in powers of k^2 and λ^2 . The cross sections given by Eqs. (19) and (20) decrease monotonically with energy, but the ratio of $\sigma(k)$ to $4\pi/E_k$ has a maximum at $k=\lambda$ according to both formulas. For $k \ll \lambda$, Eq. (20) may be replaced by^{15a}

$$\sigma(k) = 4\pi / [k^2 + (a\lambda^2/2)^2]. \quad (21)$$

As will be seen in Sec. IVA, Eq. (18) is the condition for resonance levels adopted by many authors. Eisenbud¹⁶ has discussed the formula of Flügge and Hückel from this point of view. Eisenbud's energy of resonance includes, besides λ^2 , the level shift.

A similar formula has been derived by Schiff.⁸ For low energies Schiff's result reduces to

$$\sigma(k) = 4\pi / [k^2 + V_0 \cot^2(V_0 a^2)^{\frac{1}{2}}]. \quad (22)$$

This is the same as Eq. (21), since

$$\begin{aligned} (V_0 a^2)^{\frac{1}{2}} \cot(V_0 a^2)^{\frac{1}{2}} \\ = [(\pi/2)^2 - \lambda^2 a^2]^{\frac{1}{2}} \cot[(\pi/2)^2 - \lambda^2 a^2]^{\frac{1}{2}} \\ = \frac{1}{2} \lambda^2 a^2 \end{aligned} \quad (23)$$

for small λ . The case of resonance at zero energy occurs when $V_0 = (\pi/2a)^2$ and $\lambda = 0$. The use of Eq. (18) for the virtual level has also been discussed in reference 12 and by Bohm.¹⁷

The condition for resonance levels expressed by Eq. (18) may also be written in the more general form

$$\cot[ka + \delta(k)] = 0 \quad (k = \lambda). \quad (24)$$

¹⁴ S. Flügge and E. Hückel, *Phys. Rev.* **73**, 520 (1948); E. Hückel, *Z. Naturforsch.* **3**, 134, 308 (1948).

¹⁵ T. Y. Wu and H. M. Foley, *Phys. Rev.* **73**, 1117 (1948).

^{15a} Comparison of Eq. (21) with the lowest approximation for Eq. (13) gives

$$\gamma^2 = (a\lambda^2/2)^2, \quad (21a)$$

which is a special case of a formula to be given in Sec. IVB. Since $(a\lambda)^2$ is of the order 0.2, the ratio γ^2/λ^2 is of the order 1/20. Numerical values given in the literature are about 0.06 Mev for the energy γ^2 and 0.9–1.9 Mev for the energy λ^2 .

¹⁶ L. Eisenbud, *Phys. Rev.* **73**, 1407 (1948).

¹⁷ D. Bohm, *Quantum Theory* (Prentice Hall, Inc., New York, 1951), p. 262.

A different condition for the resonance levels has been adopted by Sexl¹⁸ and Bergmann,⁷ namely

$$\cot[\delta(k)] = 0. \quad (25)$$

This condition will be discussed in Sec. IVA.

For the same square-well potential, the condition for the decaying states is

$$(V_0 + k_c^2)^{\frac{1}{2}} \cot[(V_0 + k_c^2)^{\frac{1}{2}}a] = ik_c, \quad (26)$$

where k_c is a complex number. The general condition corresponding to Eq. (26) will be given in Sec. IIIB.

C. The Theory of Effective Range

The theory of effective range developed by Schwinger,¹⁹ Blatt and Jackson,²⁰ and Bethe and Longmire²¹ is an improvement on the approximate treatment of Sec. IIA. In the shape-independent approximation for low-energy 3S scattering, the phase shift is given by

$$k \cot[\delta(k)] = -\alpha + \frac{1}{2} r_0 k^2 \quad (27)$$

or

$$k \cot[\delta(k)] = -\gamma + \frac{1}{2} r_0 (\gamma^2 + k^2). \quad (28)$$

Here α is the reciprocal of the scattering length, r_0 is a constant known as the effective range, γ is connected with the binding energy and wave function of the bound state according to the relations $E_\gamma = -\gamma^2$ and $u(r) = \text{const exp}(-\gamma r)$ for large r . The relation between α and γ is given by the equations

$$\gamma(1 - \frac{1}{2} \gamma r_0) = \alpha, \quad (29)$$

$$\gamma = [1 - (1 - 2\alpha r_0)^{\frac{1}{2}}] / r_0. \quad (30)$$

The observed values of α , γ , r_0 and $1 - 2\alpha r_0$ are all positive. Substitution of Eqs. (27) and (28) into Eq. (5) gives

$$\sigma(k) = 4\pi / [k^2 + (-\alpha + \frac{1}{2} r_0 k^2)^2], \quad (31)$$

$$\sigma(k) = 4\pi / (k^2 + \gamma^2) [1 - \gamma r_0 + (k^2 + \gamma^2) r_0^2 / 4], \quad (32)$$

respectively. Equation (32) gives the connection between σ and the binding energy γ^2 .

In the case of the 1S scattering, Eqs. (27) and (31) hold with the appropriate values for α and r_0 . The numbers r_0 and $1 - 2\alpha r_0$ are still positive, but α is now negative and so, by Eq. (30), γ is also negative. Hence there is no bound state. However, Eqs. (28), (29), (30), and (32) remain mathematically valid. As pointed out in references 20, 21, one can introduce a virtual level whose energy is numerically equal to γ^2 . Equation (32) gives now the connection between σ and the virtual state instead of the bound state. Blatt and Jackson have discussed this question from the viewpoint of the theory of the S matrix. We shall give a more detailed discussion in Sec. IIID.

¹⁸ T. Sexl, *Z. Physik.* **115**, 571 (1940).

¹⁹ J. Schwinger, *Lecture Notes on Nuclear Physics* (Harvard, Cambridge, 1947).

²⁰ J. M. Blatt and J. D. Jackson, *Phys. Rev.* **76**, 18 (1949).

²¹ H. A. Bethe, *Phys. Rev.* **76**, 38 (1949); H. A. Bethe and C. Longmire, *Phys. Rev.* **77**, 647 (1950).

III. THE VIRTUAL LEVEL ACCORDING TO THE THEORY OF THE S MATRIX

A. The Functions S and f

The matrix elements of the S matrix for the S states having a particular value of spin are represented by the function

$$S(k) = \exp[2i\delta(k)]. \quad (33)$$

From Eq. (33) we obtain

$$S(k) = \{\cot[\delta(k)] + i\} / \{\cot[\delta(k)] - i\}, \quad (34)$$

and

$$\cot[\delta(k)] = i[S(k) + 1] / [S(k) - 1]. \quad (35)$$

Because of Eq. (33), Eq. (4) may be written as

$$\sigma(k) = (\pi/k^2) |S(k) - 1|^2. \quad (36)$$

The function $S(k)$ can be expressed in terms of the functions $f(\pm k)$.²²⁻²⁴ These functions are the values of $f(\pm k, r)$ at $r=0$, where $f(\pm k, r)$ are two linearly independent solutions of Eq. (2) specified by the asymptotic behavior

$$\lim_{r \rightarrow \infty} f(\pm k, r) \exp(\pm ikr) = 1. \quad (37)$$

The solutions $f(\pm k, r)$ are complex conjugate of each other, and satisfy the relation

$$f(k, r)(d/dr)f(-k, r) - f(-k, r)(d/dr)f(k, r) = 2ik. \quad (38)$$

Hence for $k \neq 0$ there is no solution $f(\pm k, r)$ that vanishes at $r=0$. The solution of Eq. (2) that satisfies the requirement for a wave function at $r=0$ must be a linear combination of the form

$$u_k(r) = \text{const}[f(k)f(-k, r) - f(-k)f(k, r)]. \quad (39)$$

Comparing Eq. (3) with the asymptotic expression of $u_k(r)$ given by Eq. (39), we find

$$S(k) = f(k)/f(-k). \quad (40)$$

On account of the relation

$$f(k)^* = f(-k), \quad (41)$$

one can write

$$\delta(k) = \arg[f(k)]. \quad (42)$$

It can be shown that $f(\infty) = 1$. Hence one can set $\delta(\infty) = 0$.

The functions $f(\pm k)$ and $S(k)$ are defined above for $0 \leq k < \infty$, but may be extended by analytic continuation to the complex plane. It has been shown by Jost and Bargmann that, if

$$\int_0^\infty r |V(r)| dr < \infty, \quad (43)$$

then $f(k)$ is regular in the region $\text{Im } k < 0$ and continuous on the real axis. In the region $\text{Im } k > 0$, the analytic continuation of $f(k)$ exists in the problems we shall be concerned with, but it has, in general, singularities. The generalization of Eq. (41) for complex values of k is

$$f(k^*)^* = f(-k). \quad (41)^*$$

If the potential energy satisfies the equation

$$\int_0^\infty \exp(2\kappa r) |V(r)| dr < \infty \quad (\kappa > 0), \quad (44)$$

then the function $f(k)$ is regular in region $\text{Im } k < \kappa$.

Levinson²⁵ has shown that, for potentials satisfying the condition

$$\int_0^\infty r^2 |V(r)| dr < \infty, \quad (45)$$

the phase shift at $k = +0$ is connected with the number of bound states m by the relation

$$\left. \begin{aligned} \delta(+0) &= m\pi & \text{if } f(0) \neq 0, \\ \delta(+0) &= (m + \frac{1}{2})\pi & \text{if } f(0) = 0. \end{aligned} \right\} \quad (46)$$

Hence $S(0) = \pm 1$ for the two cases.

B. Bound, Virtual, and Decaying States

While the function $f(k)$ does not vanish for any real nonvanishing k , it may have imaginary zeros. Corresponding to any real number γ that satisfies the equation

$$f(-i\gamma) = 0 \quad (47)$$

there is a solution $f(-i\gamma, r)$ of Eq. (1) that vanishes at $r=0$ and varies as $\exp(-\gamma r)$ for large r , with $E = -\gamma^2$. If γ is positive, the function $f(-i\gamma, r)$ satisfies the requirements for the wave function of a bound state. On the other hand, a negative γ does not correspond to a bound state.

As a result of Eq. (40), any γ that satisfies Eq. (47) often satisfies also the equations

$$S(-i\gamma) = 0, \quad (48)$$

$$S(i\gamma) = \infty, \quad (49)$$

and vice versa. The connection between the bound states and the zeros and poles of $S(k)$ was first observed by Kramers.⁴ Subsequent investigations have shown that there are exceptions.^{22,23} For Eq. (47) does not necessarily imply Eqs. (48), (49) if

$$f(i\gamma) = 0, \quad (50)$$

while Eqs. (48), (49) do not necessarily imply Eq. (47) if

$$f(i\gamma) = \infty. \quad (51)$$

Thus Kramers' relation should be more precisely stated as follows: Eq. (47) is equivalent to Eqs. (48), (49) if

²⁵ N. Levinson, Kgl. Danske Videnskab Selskab Math-fys. Medd. **25**, No. 9 (1949).

²² R. Jost, Helv. Phys. Acta **20**, 256 (1947); R. Jost and W. Kohn, Phys. Rev. **87**, 977 (1952); Kgl. Danske Videnskab Selskab Mat-fys. Medd. **27**, No. 9 (1953).

²³ V. Bargmann, Phys. Rev. **75**, 301 (1949); Revs. Modern Phys. **21**, 488 (1949).

²⁴ J. Meixner, Z. Naturforsch., **3**, 75 (1948).

$f(i\gamma)$ is neither zero nor infinite. Otherwise there may be zeros of f and S that do not coincide.

A negative imaginary zero of $S(k)$ that is not a zero of $f(k)$ has been referred to as redundant or false zero in the literature. Since $f(k)$ is regular in the region $\text{Im } k < 0$, a number γ that satisfies Eq. (51) must be positive. If Eq. (44) holds, there is no solution of Eq. (51) for $\gamma < \kappa$ and therefore no redundant zero in the region $-\kappa < \text{Im } k < 0$. An example of $f(k)$ that satisfies both Eq. (47) and Eq. (50), but not Eqs. (48), (49), has recently been given by Jost and Kohn.

The connection between the existence of a bound state and the sign of the scattering length mentioned in Sec. IIA follows immediately if $f(k)$ is regular and has one and only one simple zero $-i\gamma$ near the origin, so that

$$f(k) = \text{const } (k + i\gamma) \quad (52)$$

in this neighborhood. For we have then, on account of Eqs. (40) and (35),

$$S(k) = (i\gamma + k)/(i\gamma - k), \quad (53)$$

and

$$\cot[\delta(k)] = -\gamma/k. \quad (54)$$

The quantity γ here takes the place of the quantity α of Sec. IIA. As before, the scattering cross section is approximately given by

$$\sigma(k) = 4\pi/(k^2 + \gamma^2). \quad (55)$$

If $\gamma > 0$ there is a bound state having the energy $E_\gamma = -\gamma^2$ and we can express $\sigma(k)$ in the form

$$\sigma(k) = 4\pi/(E_k + |E_\gamma|). \quad (56)$$

If $\gamma < 0$ there is no bound state, but one can retain Eq. (56) by introducing a virtual state whose energy is numerically equal to γ^2 .

This situation is the same as in Sec. IIA. However, our discussion suggests the following *exact* definition of the virtual state. A real number γ satisfying Eq. (47) corresponds to a bound or virtual state according as γ is positive or negative. If the magnitude of the potential energy is varied so that γ decreases from a positive value to a negative value, a bound state disappears and is replaced by a virtual state. Interpretation of the virtual state along this line has been proposed by several authors. The definition of virtual state expressed by Eq. (12) and that mentioned in Sec. IIC are consistent with this interpretation.

It should be noted that the validity of the preceding considerations depends on the assumption expressed by Eq. (52). This is true of the special problems in which the question of virtual state has arisen.

Besides zeros and poles on the imaginary axis, there are complex zeros and poles that are of physical interest. They are related to what are usually called the decaying or radioactive states.^{4,6,26} Without entering into a detailed discussion, we shall merely mention the

²⁶ W. Heitler and N. Hu, *Nature* **159**, 776 (1947).

analogous of Eqs. (47), (48), and (49) for the decaying states, namely

$$f(-k_c) = 0, \quad (57)$$

$$S(-k_c) = 0, \quad (58)$$

$$S(k_c) = \infty, \quad (59)$$

$$f(k_c^*) = 0, \quad (57)^*$$

$$S(k_c^*) = 0, \quad (58)^*$$

$$S(-k_c^*) = \infty. \quad (59)^*$$

In these equations k_c stands for a complex number. The complex energies $E_c = k_c^2$ have played an important part in the theory of α decay²⁷ and the theory of resonance scattering and reactions.²⁸

C. Examples

The following potentials provide simple illustrations for the bound states and their passage into virtual states according to the discussion of the preceding section.

(i) The square-well potential: In this case

$$f(k, r) = \exp(-ikr) \quad (r \geq a) \quad (60)$$

and

$$f(k, r) = \{ (k' - k) \exp[ik'(r - a)] + (k' + k) \times \exp[-ik'(r - a)] \} \exp(-ika)/2k' \quad (r \leq a) \quad (61)$$

with $k' = (V_0 + k^2)^{1/2}$. Hence

$$f(k) = [\cos(k'a) + ik \sin(k'a)/k'] \exp(-ika), \quad (62)$$

so that the general conditions expressed by Eqs. (47) and (57) reduce to Eqs. (12) and (26), respectively.

(ii) The attractive exponential potential

$$V(r) = -V_0 \exp(-r/a) \quad (V_0 > 0): \quad (63)$$

In this case

$$f(k) = (z/2)^{-\nu} \Gamma(1 + \nu) J_\nu(z), \quad (64)$$

with $\nu = 2iak$, and $z = 2aV_0^{1/2}$. The function $f(k)$ is singular at $\nu = -n$ ($n = 1, 2, \dots$) or $k = in/2a$. For $\nu \neq -n$, Eq. (64) may be written as²⁹

$$f(k) = \prod_{n=1}^{\infty} [1 - (z/j_{\nu, n})^2], \quad (65)$$

where the $j_{\nu, n}$ are zeros of $z^{-\nu} J_\nu(z)$. For $z \geq 0$, ν real, the equation¹

$$J_\nu(z) = 0 \quad (66)$$

gives an infinite number of curves starting from the points $\nu = -n$ on the ν axis with z increasing mono-

²⁷ G. Gamow and C. L. Critchfield, *Theory of Atomic Nucleus and Nuclear Energy Sources* (Oxford University Press, Oxford, 1949).

²⁸ J. Humblet, *Mem. soc. roy. scien. Liège* **12**, No. 4 (1952); N. G. Van Kampen, *Phys. Rev.* **89**, 1072 (1953). See also the previous papers mentioned in these publications.

²⁹ W. Magnus and F. Oberhettinger, *Special Functions of Math. Physics* (Chelsea Publishing Company, New York, 1949), p. 25.

tonically with ν . These curves cross the z axis at the points $z_1=2,40$, $z_2=5.52$, etc. A bound state disappears at every critical point $V_0=(z_n/2a)^2$.

(iii) Hulthén's potential^{22,30}

$$V(r) = -V_0 \exp(-r/a) / [1 - \exp(-r/a)] \quad (-\infty < V_0 < \infty): \quad (67)$$

Here

$$f(k) = \prod_{n=1}^{\infty} (k + i\gamma_n) / (k - i\gamma_n'), \quad (68)$$

with

$$\left. \begin{aligned} \gamma_n &= (V_0 a^2 - n^2) / 2an, \\ \gamma_n' &= n/2a. \end{aligned} \right\} \quad (69)$$

A bound state disappears at every critical point $V_0=(n/a)^2$.

(iv) An Eckart potential^{22,23}

$$V(r) = -V_0 \exp(-r/a) / [1 + (V_0 a^2 / 2) \exp(-r/a)]^2 \quad (V_0 a^2 > -2): \quad (70)$$

Here

$$f(k) = (k + i\gamma_1) / (k - i\gamma_1'), \quad (71)$$

with

$$\left. \begin{aligned} \gamma_1 &= (1/2a)(V_0 a^2 - 2) / (V_0 a^2 + 2), \\ \gamma_1' &= 1/2a. \end{aligned} \right\} \quad (72)$$

There is a bound state when $V_0 a^2 > 2$.

In examples (iii) and (iv) the function $f(k)$ is of the form

$$f(k) = \prod_{n=1}^N (k + i\gamma_n) / (k - i\gamma_n'), \quad (73)$$

where N may be finite or infinite. Hence

$$S(k) = \prod_{n=1}^N \sigma_n \sigma_n', \quad (74)$$

where

$$\sigma_n = (k + i\gamma_n) / (k - i\gamma_n), \quad (75)$$

and σ_n' is given by Eq. (75) with γ_n' instead of γ_n . The zero $-i\gamma_n$ of the factor σ_n corresponds to a bound or virtual state according as $\gamma_n >$ or < 0 . The zero $-i\gamma_n'$ of σ_n' is a redundant zero and γ_n' is always positive. If we take the argument of each factor σ_n or σ_n' to be zero when $k \rightarrow +\infty$, then, as $k \rightarrow +0$, the argument of σ_n becomes $\pm\pi$ or 0 according as $\gamma_n \geq$ or $= 0$, and the argument of σ_n' becomes π . Thus the validity of Levinson's theorem expressed by Eq. (46) is obvious for the class of problem specified by Eqs. (73)-(75). Special examples of this general theorem can also be found in the books of Bethe¹ and Mott and Massey.⁹

³⁰ L. Hulthén, Ark. Mat. Astron. Fysik. **28A**, No. 5 (1942).

D. The Effective-Range Theory in Factorized Form

To see the connection of the bound and virtual states of Sec. IIC with the function $S(k)$, we write

$$k \cot[\delta(k)] \pm ik = (r_0/2)(k \pm i\gamma)(k \pm i\gamma'). \quad (76)$$

Comparison of Eqs. (27) and (76) gives

$$\gamma + \gamma' = 2/r_0, \quad (77)$$

$$\gamma\gamma' = 2\alpha/r_0. \quad (78)$$

It follows from these equations that γ and γ' both satisfy the quadratic equation (29). The numerically smaller root is given by Eq. (30). The other root is

$$\gamma' = [1 + (1 - 2\alpha r_0)^{1/2}] / r_0. \quad (79)$$

Substituting Eq. (76) into Eq. (34) we obtain

$$S(k) = (k + i\gamma)(k + i\gamma') / (k - i\gamma)(k - i\gamma'), \quad (80)$$

showing that $S(k)$ has two pairs of zeros and poles $\pm i\gamma$, $\pm i\gamma'$.

The connection between $\pm i\gamma$ and the bound and virtual states of Sec. IIC is consistent with the general definition suggested by the theory of the S matrix. As has been mentioned in Sec. IIIB, there may be zeros and poles of $S(k)$ that have no connection with any bound or virtual state. This is the case with $\pm i\gamma'$. Jost and Kohn have shown the function $f(k)$ for the deuteron is of the form

$$f(k) = (k + i\gamma) / (k - i\gamma'), \quad (81)$$

which shows that $-i\gamma'$ is a zero of $S(k)$ but not a zero of $f(k)$.

Using Eq. (76) or Eq. (80) we obtain the factorized form

$$\sigma(k) = 4\pi(\gamma + \gamma')^2 / (k^2 + \gamma^2)(k^2 + \gamma'^2) \quad (82)$$

for the scattering cross section. This formula is identical with Eq. (32), though it looks somewhat simpler. Factorization of $S(k)$ and $\sigma(k)$ is possible also for the higher approximation in the expansion of $k \cot[\delta(k)]$,

$$k \cot[\delta(k)] = -\alpha + \frac{1}{2}r_0 k^2 - T k^4. \quad (83)$$

The equation

$$k \cot[\delta(k)] \pm ik = -T \prod_{n=1}^4 (k \pm i\gamma^{(n)}) \quad (84)$$

determines four numbers $\gamma^{(n)}$. The functions S and σ can be factorized as follows:

$$S(k) = \prod_{n=1}^4 (k + i\gamma^{(n)}) / (k - i\gamma^{(n)}), \quad (85)$$

$$\sigma(k) = (4\pi/T^2) \prod_{n=1}^4 (k^2 + \gamma^{(n)2})^{-1}. \quad (86)$$

IV. THE VIRTUAL LEVEL ACCORDING TO THE THEORY OF RESONANCE LEVELS

 A. The Functions R and Q

The R matrix of Wigner and Eisenbud reduces in the present problem to the derivative function $R(E)$.³¹ For real nonnegative E , the function $R(E)$ is defined by

$$R(E) = [u_k(r)/(d/dr)u_k(r)]_{r=a}, \quad (87)$$

where $E = E_k = k^2$ and a is the range of the short-range interaction. The variable E is, in general, a complex number. The function R is the reciprocal of the logarithmic derivative of $u_k(r)$ at $r=a$, which we shall denote by $L(E)$. The connection of the latter with the resonance levels has been investigated by Feshbach, Peaslee, and Weisskopf.^{6,32}

We shall confine our attention to the function R for those problems in which $V(r)$ vanishes for $r > a$ but is arbitrary otherwise. We have then

$$R(E) = (1/k) \tan[ka + \delta(k)], \quad (88)$$

and so

$$\cot[\delta(k)] = [kR(E) \sin(ka) + \cos(ka)] / [kR(E) \cos(ka) - \sin(ka)], \quad (89)$$

$$\sin^2[\delta(k)] = [kR(E) \cos(ka) - \sin(ka)]^2 / [k^2 R(E)^2 + 1]. \quad (90)$$

It follows from Eqs. (33) and (88) that the functions R and S are connected by the following formulas:

$$R(E) = (1/ik) [S(k) \exp(2ika) - 1] / [S(k) \exp(2ika) + 1], \quad (91)$$

$$S(k) = \exp(-2ika) [1 + ikR(E)] / [1 - ikR(E)]. \quad (92)$$

The function $R(E)$ admits of an expansion of the form

$$R(E) = \sum_{\lambda} \omega_{\lambda} / (E_{\lambda} - E), \quad (93)$$

where ω_{λ} and E_{λ} are real numbers, $\omega_{\lambda} > 0$. This is a special case of a general result of references 5, 31. It shows that R is a meromorphic function of E whose poles E_{λ} are all on the real axis. When $E_k = E_{\lambda}$, the derivative of $u_k(r)$ vanishes at $r=a$. The energies E_{λ} are often referred to as the resonance energies because of their relation to observed resonance levels. The condition for such resonance energies may be put in the form^{32a}

$$R(E_{\lambda}) = \infty. \quad (94)$$

³¹ E. P. Wigner, Ann. Math. **53**, 36 (1951); Proc. Camb. Phil. Soc. **47**, 790 (1951); Revista Mexicana de Fisica **1**, 91 (1952); Am. Math. Mon. **59**, 669 (1952); W. Schützer and J. Tiomno, Phys. Rev. **83**, 249 (1951).

³² Feshbach, Peaslee, and Weisskopf, Phys. Rev. **71**, 145 (1947).
^{32a} For positive values $E_{\lambda} = \lambda^2$, Eq. (94) is equivalent to Eq. (24). There may also be negative values E_{λ} and E_{ρ} that satisfy Eq. (94) and Eq. (98) below.

Wigner and Teichmann have considered a Q matrix³³ that shows resonance features like the R matrix. The Q matrix is connected with the S matrix by the general relation

$$S = (1+iQ)/(1-iQ). \quad (95)$$

The function

$$Q(E) = \tan[\delta(k)] \quad (96)$$

is related to the Q matrix in the same way as the functions $R(E)$ and $S(k)$ are related to the R and S matrices. It follows from Eqs. (5) and (96) that

$$\sigma(k) = 4\pi/k^2 \{1 + [1/Q(k)]^2\}. \quad (97)$$

The condition for resonance expressed by Eq. (25) may be written in the form^{33a}

$$Q(E_{\rho}) = \infty. \quad (98)$$

B. One-Level Formulas

It is the object of this section to discuss representation of the low-energy scattering cross section by means of a low-energy resonance level E_{λ} or E_{ρ} .

Equation (27) of the effective-range theory may be rewritten as

$$Q(E) = (2k/r_0)/(E - E_{\rho}), \quad (99)$$

where

$$E_{\rho} = 2\alpha/r_0 \quad (100)$$

is a resonance energy according to Eq. (98). Equation (100) shows that E_{ρ} is positive for 3S and negative for 1S . Substituting Eq. (99) into Eq. (97) we find

$$\sigma(k) = 4\pi/[E + (E - E_{\rho})^2 r_0^2 / 4]. \quad (101)$$

This is just Eq. (31) written in a slightly different form.

In the neighborhood of a resonance level E_{λ} , $R(E)$ is approximately given by

$$R(E) = \omega_{\lambda} / (E_{\lambda} - E). \quad (102)$$

Using this one-level formula, we see that, for small E and E_{λ} , Eq. (89) may be approximately written in the form of Eq. (27) with

$$\alpha = -E_{\lambda} / \omega_{\lambda}, \quad (103)$$

$$r_0 = 2(\omega_{\lambda} a - 1) / \omega_{\lambda}. \quad (104)$$

Conversely, given Eq. (27) we obtain Eq. (102) by using Eq. (88). Owing to the approximations we have made, the values of α and r_0 given by Eqs. (103) and (104) are only nearly the same as the values of these constants in the effective-range theory. The correspondence between the resonance levels E_{λ} and E_{ρ} is given by the relation

$$E_{\rho} = E_{\lambda} / (1 - \omega_{\lambda} a). \quad (105)$$

³³ As mentioned by these authors, the Q matrix is equal to Heitler's K matrix multiplied by a numerical factor.

^{33a} As has been mentioned in Sec. IIIB, a further condition for resonance levels expressed in terms of the function S exists in the literature.

We have seen in Sec. IIID that Eqs. (27) and (80) are equivalent. There is therefore a simple connection between E_λ and the energy E_γ of the S matrix theory.^{33b} Using Eq. (103) we obtain approximately

$$|E_\gamma| = |E_\alpha| = (E_\lambda/\omega_\lambda)^2. \quad (106)$$

The scattering cross section can be given in terms of E_λ as follows. From Eqs. (4) and (90) we obtain, expanding in powers of E and E_λ and retaining only the first two terms in the numerator and denominator,

$$\sigma(k) = 4\pi \{1 - (a/\omega_\lambda)[E(a\omega_\lambda - 2) + 2E_\lambda]\} / [E + (E - E_\lambda)^2/\omega_\lambda^2]. \quad (107)$$

Similarly, from Eqs. (5) and (89),

$$\sigma(k) = 4\pi / \{E + [E_\lambda + (\omega_\lambda a - 1)E]^2/\omega_\lambda^2\}. \quad (108)$$

These formulas are generalizations of Eqs. (19) and (20), respectively. Eq. (108) is identical with Eq. (101). For $E \ll |E_\lambda|$, $|E_\rho|$ the denominators of Eqs. (101) and (108) are approximately equal to $E + (E_\rho r_0/2)^2$ and $E + (E_\lambda/\omega_\lambda)^2$, respectively. These are the same as the denominator $E + |E_\alpha|$ in Eq. (9).

In the case of the square-well potential the function

^{33b} Eqs. (103)–(106) are valid for small E_λ . For $E_\lambda \gg \omega_\lambda^2/4$ we find from Eqs. (92) and (102) that $S(k)$ has zeros near $k = \pm E_\lambda^{1/2} + i\omega_\lambda/2$ and poles near $k = \pm E_\lambda^{1/2} - i\omega_\lambda/2$.

$R(E)$ is given by

$$R(E) = \tan[(V_0 + E)^{1/2}a] / (V_0 + E)^{1/2}. \quad (109)$$

It can therefore be expanded in the form³⁴

$$R(E) = (2/a) \sum_{n=0}^{\infty} [(n + \frac{1}{2})^2(\pi/a)^2 - V_0 - E]^{-1}. \quad (110)$$

Hence

$$\omega_\lambda = 2/a, \quad (111)$$

and

$$E_\lambda = (\pi/2a)^2 - V_0 \quad (112)$$

for the lowest E_λ . From Eq. (112) it follows that E_λ is positive for 1S and negative for 3S . By Eq. (105),

$$E_\rho = -E_\lambda, \quad (113)$$

showing that E_λ and E_ρ are opposite in sign.

The condition for the bound states and the various definitions for the virtual level can also be stated simply in terms of the logarithmic derivative $L(E)$. The Eqs. (12), (15), and (18) for the square-well potential determine the zeros of the functions $L(-x^2) + x$, $L(x^2) - x$, and $L(x^2)$, respectively. Given any suitable function of $L(\pm x^2)$, there is a one-level representation for a low-energy scattering formula.

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³⁴ E. C. Titchmarsh, *Theory of Functions* (Oxford University Press, Oxford, 1939), p. 113.