ON THE COULOMB AND HULTHÉN POTENTIALS

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Summary

This paper contains the results of two investigations. (i) The Hulthén potential is considered as a modification of the Coulomb potential. The transition from the former to the latter is investigated. (ii) The zeros of the Fredholm determinant for the Hulthén potential are calculated from the first two terms of its power-series expansion. These approximate results are compared with the exact values.

I. INTRODUCTION

It is well known that the general theory of scattering is not immediately applicable to the case of the Coulomb potential because it decreases too slowly as the distance increases (Mott and Massey 1949). In order to apply the general theory to the scattering by the Coulomb field, modifications of the Coulomb potential have been considered in the literature. A procedure introduced by Gordon (1928) consists in cutting off the field at a large distance R and making R go to infinity in the final result. Another procedure consists in replacing the Coulomb potential by the Yukawa potential, and subsequently making the exponential factor approach unity. Gordon's treatment leads to closed asymptotic expressions for large values of R. Treatment along the other line has been carried out by the method of Born approximations.

An object of the present paper is to investigate the use of the Hulthén potential (Hulthén 1942, Rosenfeld 1948) as a modified form of the Coulomb potential. Since the wave equation for the S-states can be solved exactly in the case of the Hulthén potential, we are able to trace the transition from the modified to the true Coulomb potential without making approximations.

A second issue that concerns us in this paper is the determination of discrete bound states from the zeros of the Fredholm determinant for a scattering problem. This has recently been done in work on field theories (Fubini 1953 ; Green 1954). In field theories it is often the case that the Fredholm determinant can be evaluated only in the form of a power series, and the first few terms of the series alone can be computed without excessive calculations. It is therefore of interest to see whether reasonably good results can be obtained for bound states by considering just the first few terms of the Fredholm determinant.

As a test, we consider the case of the Hulthén potential. We shall calculate the zeros of the Fredholm determinant from the first two terms of its expansion, and compare them with the zeros of its exact form. It will be seen that the

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approximate calculation, rough as it is, gives reasonably well the general trend of the zeros for coupling not too strong, although the numerical agreement is not good for the binding energies of the bound states.

II. Transition from the Hulthén to the Coulomb Potential

We write the wave equation for the S-states in the form

$$\left[\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2+k^2\right]u(r)=U(r)u(r), \quad \ldots\ldots\ldots\ldots \quad (1)$$

where k^2 is the total energy E divided by $\hbar^2/8\pi^2m$ and $U(r)$ is the potential energy $V(r)$ divided by the same factor. In the case of the Hulthén potential, $U(r)$ may be written in the form

$$U(r)=-\frac{\lambda\mu \mathrm{e}^{-\mu r}}{1-\mathrm{e}^{-\mu r}} \quad (\mu>0). \quad \ldots\ldots\ldots\ldots \quad (2)$$

For positive-energy continuum states, k is a positive real number. The solution of (1) that has the asymptotic form $\mathrm{e}^{-\mathrm{i}kr}$ is (Jost 1947)

$$f(k, r)=\mathrm{e}^{-\mathrm{i}kr}F(a, b, c, z), \quad \ldots\ldots\ldots\ldots \quad (3)$$

where F is the hypergeometric function (Magnus and Oberhettinger 1949) with

$$a=\left(\frac{\mathrm{i}k}{\mu}\right)\left[1-\left(1-\frac{\lambda\mu}{k^2}\right)^{\frac{1}{2}}\right], \quad \ldots\ldots\ldots\ldots \quad (4)$$

$$b=\left(\frac{\mathrm{i}k}{\mu}\right)\left[1+\left(1-\frac{\lambda\mu}{k^2}\right)^{\frac{1}{2}}\right], \quad \ldots\ldots\ldots\ldots \quad (5)$$

$$c=1+2\frac{\mathrm{i}k}{\mu}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (6)$$

and

$$z=\mathrm{e}^{-\mu r}. \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (7)$$

The value of $f(k, r)$ at $r=0$ is

$$f(k,0)=F(a, b, c, 1), \quad \ldots\ldots\ldots\ldots \quad (8)$$

or

$$f(k,0)=\frac{\Gamma(c)}{\Gamma(1+a)\Gamma(1+b)}, \quad \ldots\ldots\ldots\ldots \quad (9)$$

or

$$f(k,0)=\prod_{n=1}^{\infty}\frac{k+\mathrm{i}\gamma_n}{k-\mathrm{i}n\mu/2}, \quad \ldots\ldots\ldots\ldots \quad (10)$$

with

$$\gamma_n=\tfrac{1}{2}\left(\frac{\lambda}{n}-n\mu\right). \quad (n=1, 2, \ldots) \quad \ldots\ldots \quad (11)$$

The matrix element $S(k)$ of the S-matrix for an S-state, which is connected with the phase $\delta(k)$ by the relation

$$S(k)=\mathrm{e}^{2\mathrm{i}\delta(k)}, \quad \ldots\ldots\ldots\ldots\ldots \quad (12)$$

is given by

$$S(k)=\frac{f(k)}{f(-k)}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (13)$$

or, on account of (9),

$$S(k)=\frac{\Gamma(1+a^*)\Gamma(1+b^*)\Gamma(c)}{\Gamma(1+a)\Gamma(1+b)\Gamma(c^*)}. \quad \ldots\ldots\ldots \quad (14)$$

For each positive real γ_n there is a bound state with the eigenvalue

$$E_n=-\frac{h^2\gamma_n^2}{8\pi^2 m}. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (15)$$

The corresponding wave function is given by (3) with $k=-i\gamma_n$,

$$a=-n, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (16)$$

$$b=\frac{\lambda}{n\mu}. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (17)$$

The first two normalized wave functions are

$$u_1(r)=\left(\frac{1}{\mu}\right)\left[\lambda\left(\frac{\lambda^2-\mu^2}{2}\right)\right]^{\frac{1}{2}}(1-z)e^{-\gamma_1 r}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (18)$$

$$u_2(r)=\left(\frac{1}{16\mu}\right)[\lambda(\lambda^2-16\mu^2)]^{\frac{1}{2}}(1-z)\left[4-\left(2+\frac{\lambda}{\mu}\right)(1-z)\right]e^{-\gamma_2 r}. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (19)$$

We pass from the Hulthén potential energy to the Coulomb potential energy

$$V(r)=-\frac{Ze^2}{r} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (20)$$

by putting

$$\lambda=\frac{8\pi^2 mZe^2}{h^2}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (21)$$

and making μ approach zero. For small μ we have

$$\frac{\Gamma(1+a^*)}{\Gamma(1+a)}=S'(k)+0(\mu), \quad \ldots\ldots\ldots\ldots \quad (22)$$

where

$$S'(k)=\frac{\Gamma\left(1-\frac{i\lambda}{2k}\right)}{\Gamma\left(1+\frac{i\lambda}{2k}\right)} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (23)$$

is a familiar expression in the theory of Coulomb scattering, and $0(\mu)$ means a term that vanishes as μ tends to zero. Also,

$$\frac{\Gamma(1+b^*)\Gamma(c)}{\Gamma(1+b)\Gamma(c^*)}=e^{i\omega(k)}, \quad \ldots\ldots\ldots\ldots\ldots \quad (24)$$

with (Jahnke and Emde 1945)

$$\omega(k)=\left(\frac{\lambda}{k}\right)\ln\left(\frac{2k}{\mu}\right)+0(\mu). \quad \ldots\ldots\ldots\ldots (25)$$

Thus

$$S(k)=S'(k)e^{i\omega(k)}, \quad \ldots\ldots\ldots\ldots\ldots (26)$$

with $\omega(k)$ given by (25). This result is similar to the previous result of Gordon (Gordon 1928 ; Møller 1946), which is given by (23), (25), and (26), with $1/R$ instead of μ.

Equations (25) and (26), which are valid for small μ, may also be useful if one uses the Hulthén potential to represent a screened Coulomb potential.

In the limit $\mu=0$ we see from (11) that γ_n becomes simply $\lambda/2n$. There are then an infinite number of bound states having the energy spectrum $E_n=-h^2\lambda^2/32\pi^2mn^2$ of an electron in the Coulomb field. It is easy to verify that the normalized wave functions (16) and (17) pass over to the normalized Coulomb wave functions of the $1s$ and $2s$ states respectively.

III. Application of the Fredholm Theory to the Hulthén Potential

According to the Fredholm theory of integral equations (Whittaker and Watson 1946), the integral equation

$$X(s)=Y(s)+\lambda\int_A^B K(s,t)X(t)\mathrm{d}t, \quad \ldots\ldots\ldots\ldots (27)$$

under certain general conditions on the kernel K, has the solution

$$X(s)=Y(s)+D^{-1}\int_A^B D(s,t)Y(t)\mathrm{d}t, \quad \ldots\ldots\ldots (28)$$

if the Fredholm determinant D does not vanish. If the kernel K is such that D vanishes, there exists a solution of the homogeneous equation

$$X(s)=\lambda\int_A^B K(s,t)X(t)\mathrm{d}t. \quad \ldots\ldots\ldots\ldots\ldots (29)$$

The solution of (1) that describes a state of positive energy $h^2k^2/8\pi^2m$ in the scattering problem satisfies an integral equation of the form (27). The kernel $K(r, r')$ satisfies the differential equation

$$\lambda\left[\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^2+k^2\right]K(r,r')=U(r)\delta(r-r'), \quad \ldots\ldots\ldots (30)$$

and the integral term $\lambda\int_0^\infty K(r,r')u(r')\mathrm{d}r'$ varies as $\exp(ikr)$ for large r. The Fredholm determinant D is a function of λ and k. Since we are concerned with the dependence of D on k rather than on λ, we shall denote it by $D(k)$ from now on. Corresponding to any k such that

$$D(k)=0, \quad \ldots\ldots\ldots\ldots\ldots (31)$$

there is a wave function $u(r)$ satisfying the homogeneous integral equation

$$u(r)=\lambda\int_0^\infty K(r, r')u(r')\mathrm{d}r'. \quad \ldots\ldots\ldots\ldots\ldots (32)$$

There is no real k that satisfies (**31**). If k is an imaginary number, $\mathrm{i}\gamma$, the wave function $u(r)$ varies as $\mathrm{e}^{-\gamma r}$ for large r and thus describes a bound state of energy $-h^2\gamma^2/8\pi^2 m$ when $\gamma>0$. There may also be complex zeros of $D(k)$ which correspond to complex energies of radioactive states.

According to the idea of analytic continuation adopted by Heisenberg in the theory of S-matrix (Heisenberg 1946 ; Møller 1946 ; Jost 1947), bound and radioactive states are connected with imaginary and complex values of k satisfying the equation

$$f(k)=0. \quad \ldots\ldots\ldots\ldots\ldots (33)$$

That equations (**31**) and (**33**) give the same results for the problems under consideration here can be seen from the identity

$$D(k)=f(-k) \quad \ldots\ldots\ldots\ldots\ldots (34)$$

proved by Jost and Pais (1951).

In the case of the Hulthén potential, the Fredholm determinant is known in closed form on account of (**34**). The zeros of $f(k)$ or $D(k)$ are all purely imaginary. There are no complex zeros that correspond to complex energies.* The power-series expansion of $D(k)$ may be obtained by expanding $f(k)$ in powers of λ or from the general formula of the Fredholm theory. As already explained in Section I, it is our intention to compare the zeros of the first two terms of $D(k)$ with the exact zeros.

Expanding in powers of λ and retaining only the first two terms, we obtain from (**4**) and (**5**)

$$\Gamma(1+a)=1-\frac{\mathrm{i}\lambda C}{2k}, \quad \ldots\ldots\ldots\ldots\ldots (35)$$

$$\Gamma(1+b)=\Gamma\left(1+\frac{2\mathrm{i}k}{\mu}\right)\left[1-\frac{\mathrm{i}\lambda}{2k}\Psi\left(\frac{2\mathrm{i}k}{\mu}\right)\right], \quad \ldots\ldots\ldots (36)$$

where C is Euler's constant and Ψ is the logarithmic derivative of the factorial function (Jahnke and Emde 1945). Substituting in (**9**) and using (**6**), we obtain, up to the term linear in λ,

$$f(k)=1+\frac{\mathrm{i}\lambda}{2k}\left[\Psi\left(\frac{2\mathrm{i}k}{\mu}\right)+C\right]. \quad \ldots\ldots\ldots\ldots (37)$$

* In this respect the Hulthén potential is different from the square-well potential or the following potential :

$$V(r)=V_0 \quad (r_1<r<r_2) \quad (V_0>0),$$
$$=0 \quad (r<r_1 \text{ or } >r_2).$$

The complex energies for the last potential are known from the Gamow-Condon-Gurney theory (Møller 1946). According to Blatt and Weisskopf (1952), there exist complex energies for the square-well potential.

Let $-i\gamma_n'$ $(n=1, 2, \ldots)$ denote the zeros of the right hand side of (37). Let

$$x_n=\frac{2\gamma_n}{\mu}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (38)$$

with γ_n given by (11), and let x_n' be similarly defined in terms of γ_n'. We have then

$$x_n=\frac{\lambda}{n\mu}-n, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (39)$$

$$1-\frac{\lambda}{\mu}\frac{\Psi(x_n')+C}{x_n'}=0. \quad \ldots\ldots\ldots\ldots \quad (40)$$

Each positive x_n corresponds to a bound state.

We give below some numerical results for the first three zeros of the Fredholm determinant calculated from (39) and (40).

(i) $\lambda=-\mu$:

$x_1=-2$, $x_2=-5/2$, $x_3=-10/3$;
$x_1'=-1\cdot4$, $x_2'=-2\cdot4$, $x_3'=-3\cdot3$.

(ii) $\lambda=\frac{1}{2}\mu$:

$x_1=-1/2$, $x_2=-7/4$, $x_3=-17/6$;
$x_1'=-0\cdot24$, $x_2'=-1\cdot8$, $x_3'=-2\cdot8$.

(iii) $\lambda=\mu$:

$x_1=0$, $x_2=-3/2$, $x_3=-8/3$;
$x_1'=1$, $x_2'=-1\cdot7$, $x_3'=-2\cdot8$.

(iv) $\lambda=2\mu$:

$x_1=1$, $x_2=-1$, $x_3=-7/3$;
$x_1'=4\cdot3$, $x_2=-1\cdot7$ $x_3'=-2\cdot7$.

We have confined our attention to real solutions of (40). Since the exact form of $f(k)$ has no complex zeros, it is probable that its approximate form has no complex zeros either.

The general trend of the above approximate results seems to be as good as can be expected, although the numerical values for the binding energies of bound states are not accurate. The agreement becomes very bad, of course, in the case of strong coupling. For a very large value of λ/μ, (39) gives many bound states, but (40) only one.

IV. Acknowledgments

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V. References

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Note Added in Proof

A. The above results calculated from (**40**) are encouraging, and suggest that one might attain quite good accuracy by using the expansion of $f(-i\gamma)$ up to the quadratic term, namely

$$f(-i\gamma)=1+\frac{\lambda}{\mu}f_1(-i\gamma)+\left(\frac{\lambda}{\mu}\right)^2 f_2(-i\gamma). \quad \ldots\ldots\ldots\ldots \quad (41)$$

As may be easily verified,

$$f_1(-i\gamma)=-\left[\frac{\Psi(x)+C}{x}\right], \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (42)$$

$$f_2(-i\gamma)=\left[\frac{\Psi(x)+C}{x^3}\right]+\left[\frac{\Psi(x)+C}{2x^2}\right]^2-\left[\frac{\Psi'(x)+\pi^2/6}{2x^2}\right], \quad \ldots \quad (43)$$

where $x=2\gamma/\mu$ and the function Ψ' is that of Jahnke and Emde (1945). There is, however, a simpler method which has been used in Adelaide for improving the accuracy, as Professor H. S. Green kindly informed the writer. Applied to the problem considered here, the simplified method amounts to dealing with a modified form of $f(k)$, namely,

$$f_A(k)=f(k)e^{\sigma\lambda/\mu}, \quad \ldots\ldots\ldots\ldots\ldots \quad (44)$$

where σ is chosen such that the quadratic term in the expansion of $f_A(-i\gamma)$ vanishes, so that, to this degree of accuracy,

$$f_A(-i\gamma)=\frac{1-\lambda}{\mu}(f_1^2-2f_2)^{\frac{1}{2}}. \quad \ldots\ldots\ldots\ldots \quad (45)$$

Let $-i\gamma_n''$ denote the zeros of f_A and $x_n''=2\gamma_n''/\mu$. One then gets, using (42) and (43), the equation

$$1-\frac{\lambda}{\mu}\left\{\left[\frac{\Psi'(x_n'')+\pi^2/6}{x_n''^2}\right]-2\left[\frac{\Psi(x_n'')+C}{x_n''^3}\right]\right\}^{\frac{1}{2}}=0. \quad \ldots\ldots\ldots \quad (46)$$

Dr. I. E. McCarthy of the University of Adelaide has obtained numerical values for the first zero x_1'' of (46). For our cases (iii) and (iv), his results are $x_1''=-0\cdot1$ and $x_1''=1\cdot15$ respectively, which are much better than the results x_1' obtained from (40).

B. Application of the Fredholm theory to scattering problems has recently been investigated in several papers. In particular, Dr. P. Swan of the University of Melbourne has called the writer's attention to his recent work on the reduction of the Schrödinger and the second order linear integro-differential equation to Fredholm's equation. Our present paper differs from these papers in that we are mainly concerned with a bound-state problem.