A STUDY OF THE WAVE EQUATION
FOR THE DIPOLE

by

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A STUDY OF THE WAVE EQUATION

FOR THE DIPOLE

In 1923 Louis de Broglie suggested that waves and particles may be intimately bound together in the phenomena of radiant energy. Soon after, Erwin Schroedinger published a mathematical approach to the determination of the energy states of a radiating atom. His method of treatment has come to be known as "wave mechanics" and involves the equation

$$(1) \quad \frac{\partial^2\psi}{\partial\xi^2} + \frac{\partial^2\psi}{\partial\eta^2} + \frac{\partial^2\psi}{\partial\zeta^2} + \frac{8\pi m}{h^2}(E - \bar{V}_{(\xi,\eta,\zeta)})\psi = 0,$$

called the Schroedinger wave equation.

This wave equation follows from the idea that there is some sort of a de Broglie wave associated with the motion of a particle whose total energy is E and whose potential energy is $\bar{V}_{(\xi,\eta,\zeta)}$ the potential energy being a function of the Cartesian coordinates ξ, η, ζ of the particle. The assumption is made that the allowable energy levels are those values of E that determine finite and single valued solutions of the wave equations through-out space.

This assumption becomes the working rule of wave mechanics and permits the calculation of allowed energy levels of an electron moving in a field of potential energy $\tilde{V}(\xi, \eta, \zeta)$.

Since no attempt will be made to check our findings against experimental results they need not be expressed in terms of the usual physical quantities. Therefore, our work will be greatly simplified by the introduction of new independent variables x, y and z such that

$$\frac{1}{8\pi m/h^2}\left(\frac{\partial^2\psi}{\partial\xi^2} + \frac{\partial^2\psi}{\partial\eta^2} + \frac{\partial^2\psi}{\partial\zeta^2}\right) = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}.$$

We can now write (1) as

$$(1)' \quad \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + (E - V_{(x,y,z)})\psi = 0,$$

where $V_{(x,y,z)} = \tilde{V}_{(\xi,\eta,\zeta)}$,

and use this form as the basis of our investigation.

PARTICULAR PROBLEM

The problem treated in this paper is that of setting up the wave equation in the case of an electron found in the neighborhood of an electric dipole and of finding the least values of the parameters involved for which solutions of this equation are possible.

It is to be stated at the outset that there is no intention of reading into the results any physical significance other than that of the most general nature. The problem was undertaken with the idea of gaining some insight into the methods and technics of wave mechanics.

EXPLANATION OF DIAGRAM

The position of the electron in three dimensional space is given in terms of the spherical coordinates r, θ, ϕ, where

$$x = r\cos\phi \cdot \sin\theta,$$

$$y = r\sin\phi \cdot \sin\theta,$$

$$z = r\cos\theta.$$

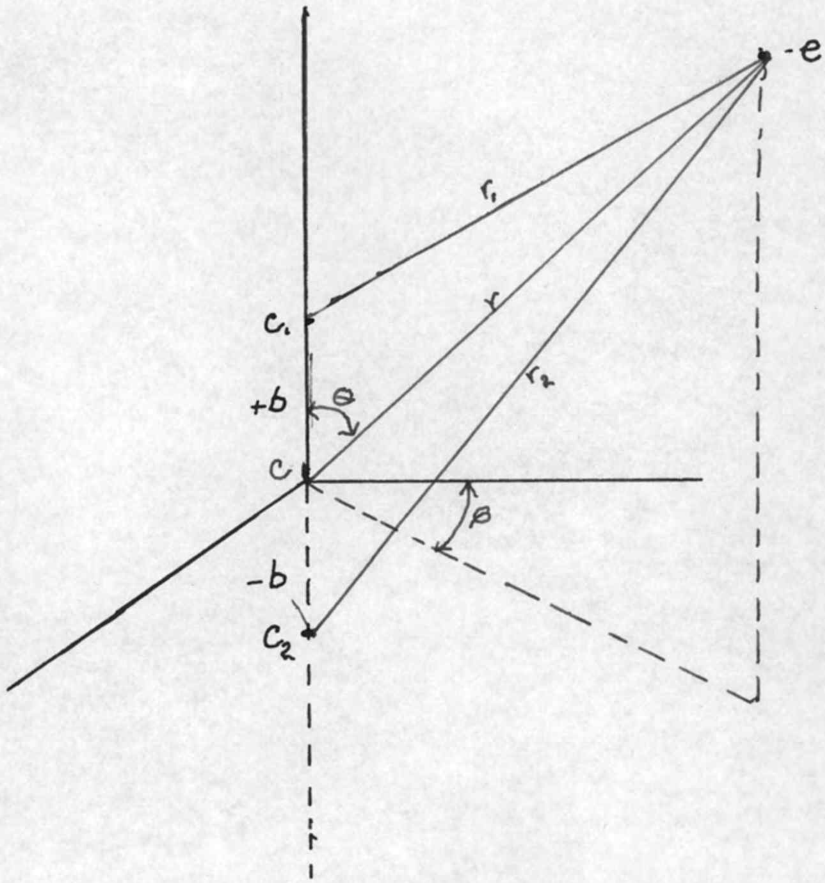

Figure 1 (a). Space diagram for the dipole problem.

If C is used to denote the midpoint of the line joining the charges C_1 and C_2 of the dipole then C may be thought of as the limiting position of the two charges as the distance 2b between them is made very small.

SETTING UP THE WAVE EQUATION

The wave equation for finding the allowed energy levels of a free electron moving in a potential field contains an expression for the total energy as well as one for the potential. The total energy is hereafter denoted by E and the determination of its lowest permissible values is the plan of this paper. The allowed values of E are those for which the wave function satisfies the condition that the integral

$$\int |\psi|^2 dv$$

is finite throughout all space.

The electrostatic potential due to the nucleus, as considered in this paper, is to be thought of as the limiting case of the potential due to two single charges, one positive and the other negative, as the distance between them approaches zero. We will denote by V the potential energy of the electron in the field of the nucleus.

For the purposes of this paper let C_1 be the charge at (o, o, b), C_2 that at (o, o, -b) and, furthermore, let these charges be defined by the following expressions

$$C_1 = -\frac{e}{2} + \frac{k}{2b} \quad ,$$

$$C_2 = -\frac{e}{2} - \frac{k}{2b} \quad .$$

The expression for the potential energy V may now be written as the sum of the potentials energies due to each of the individual charges C_1 and C_2 and, consequently, is given by

$$\frac{V}{e} = \frac{-\frac{e}{2} + \frac{k}{2b}}{r_1} + \frac{-\frac{e}{2} - \frac{k}{2b}}{r_2} \quad .$$

On combining the terms in the right hand expression we have

$$\frac{V}{e} = - \frac{e/2\,(r_1 + r_2) + k/2b\,(r_1 - r_2)}{r_1 r_2} \quad .$$

Turning back to the diagram on page 4 it is seen that, by use of the law of cosines, r_1 and r_2 may be expressed in terms of r, b and the angle θ so that

$$r_1^2 = r^2\left(1 + \frac{b^2}{r^2} - \frac{2b}{r}\cos\theta\right) \quad ,$$

$$r_2^2 = r^2\left(1 + \frac{b^2}{r^2} + \frac{2b}{r}\cos\theta\right) \quad .$$

Expanding r_1 and r_2 in powers of b/r we have

$$r_1 \; = r\left[1 - \frac{b}{r}\cos\theta + \frac{b^2}{r^2}\frac{(1-\cos^2\theta)}{2} + \text{higher powers}\right],$$

and

$$r_2 \; = r\left[1 + \frac{b}{r}\cos\theta + \frac{b^2}{r^2}\frac{(1-\cos^2\theta)}{2} + \text{higher powers}\right].$$

Hence

$$r_1 + r_2 = r\left[2 + 0 + \text{2nd and higher powers}\right],$$

$$r_1 - r_2 = r\left[-\frac{2b\cos\theta}{r} + \text{3rd and higher powers}\right].$$

On substituting these last two results in the expression for the potential we get

$$\frac{V}{e} = -\frac{\frac{er}{2}\left(2 + \begin{smallmatrix}\text{2nd and higher}\\ \text{powers}\end{smallmatrix}\right) - \frac{kr}{2b}\left(\frac{2b}{r}\cos\theta + \begin{smallmatrix}\text{3rd and}\\ \text{higher powers}\end{smallmatrix}\right)}{r^2\left(1 - \frac{b}{r}\cos\theta + \cdots\right)\left(1 + \frac{b}{r}\cos\theta + \cdots\right)}.$$

As b is allowed to approach zero the above equation becomes:

$$\frac{V}{e} = \frac{-er + k\cos\theta}{r^2},$$

$$V = -\frac{e^2}{r} + \frac{ke}{r^2}\cos\theta \; .$$

The wave equation may now be written as

(2)

$$\nabla^2\psi + \left[E + \frac{e^2}{r} - \frac{ke}{r^2}\cos\theta\right]\psi = 0 \; .$$

On writing the explicit expression for $\nabla^2\psi$ in spherical coordinates the above equation becomes

$$\frac{1}{r^2}\,\frac{\partial\left(r^2\frac{\partial\psi}{\partial r}\right)}{\partial r}+\frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2\psi}{\partial\phi^2}+\frac{1}{r^2\sin\theta}\cdot\frac{\partial\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)}{\partial\theta}+$$

$$\left[E+\frac{e^2}{r}-\frac{ke\cos\theta}{r^2}\right]\psi=0 \quad .$$

SEPARATION OF THE VARIABLES

In order to treat the foregoing wave equation effectively we will separate the variables in the manner commonly employed when dealing with central force problems expressed in spherical coordinates. On letting

$$\psi = \Phi(\phi) \cdot \Theta(\theta) \cdot R(r)$$

equation (3) may be separated into the following three differential equations of the second order,*

(4) $$\Phi''(\phi) + C_1 \Phi(\phi) = 0,$$

(5) $$\frac{1}{\sin\theta} \frac{\partial\left[\sin\theta \frac{\partial\Theta}{\partial\theta}\right]}{\partial\theta} + \left[k e \cos\theta + \lambda - \frac{C_1}{\sin^2\theta}\right]\Theta = 0,$$

(6) $$r^2 \frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + r^2\left[E + \frac{e^2}{r} - \frac{\lambda}{r^2}\right] R = 0.$$

The determination of the characteristic values of the parameters C_1, λ and E, appearing in the above e equations, is the object of this thesis. These values must be such that there will exist non zero, single valued solutions of the differential equations for which the space integral $\int \psi^2 dv$ expressed in spherical coordinates as

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} R^2 \Phi^2 \Theta^2 r^2 \sin\theta \, d\phi \, d\theta \, dr$$

is finite.

* The symbol C_1 does not denote the same quantity as C_1 previously used.

The above integral may be expressed in the following form:

$$\left[\int_0^\infty R^2 \cdot r^2 dr\right]\cdot\left[\int_0^\pi \Theta^2 \sin\theta\, d\theta\right]\cdot\left[\int_0^{2\pi} \Phi^2 d\phi\right] = 1,$$

from which it is evident that, in order for the triple integral to be finite, it is necessary for each of the single integrals to remain finite in the indicated intervals.

It is seen that for all values of C_1 the angular equation in Φ will possess solutions making

$$\left[\int_0^{2\pi} \Phi^2 d\phi\right]$$

finite. However, the necessary condition of single valueness for solutions of the differential equation

$$\Phi''(\phi) + C_1 \Phi(\phi) = 0$$

restricts the selection of values for the parameter C_1. Therefore, the only values of C_1 that are acceptable are those for which the solutions of the differential equation are both single valued and finite, and for which the single integral previously mentioned is finite.

Before a similar inquiry is made into the angular equation in Θ certain substitutions will be made. These substitutions are those that were found necessary to bring the differential equation

(5) $$\left[\frac{1}{\sin\Theta}\,\frac{\partial\left(\sin\Theta\,\frac{\partial\oplus}{\partial\Theta}\right)}{\partial\Theta}\right] + \left[ke\cos\Theta + \lambda - \frac{C_1}{\sin^2\Theta}\right]\oplus = 0$$

into a form permitting the numerical calculation of λ .

In order to simplify the work we will set ke=1, and let C =0 the least of its allowed values.*

If we now introduce the new independent variables

$$\cos\Theta = x \quad , \quad \oplus = y \, ,$$

and note that

$$\frac{d\oplus}{d\Theta} = \frac{dy}{dx}\cdot\frac{dx}{d\Theta} = -\frac{dy\,\sin\Theta}{dx}$$

equation (5) takes the form

(6) $$\frac{d\left[(1-x^2)\frac{dy}{dx}\right]}{dx} + \left[x+\lambda\right]y = 0$$

or

$$(1-x^2)\,y'' - 2xy + \left[x+\lambda\right]y = 0 \, .$$

This equation in its present form has simple singular points at +1 and -1, and since the behavior as **x** varies from -1 to +1 is desired, a substitution is made to increase the range of investigation so as to include the end values. This may be done by multiplying equation (6) through by $(1-x^2)$ and making the substitutions

$$\frac{(1-x^2)}{dx} = \frac{1}{dz} \quad , \quad z = \tanh^{-1}x \quad , \quad x = \tanh z$$

* A complete treatment of this problem would involve determining the effect of giving k a value such that ke $\neq$ 1.

giving

$$(7) \quad (1-x^2)\frac{d\left[(1-x^2)\dfrac{dy}{dz(1-x^2)}\right]}{dz\ (1-x^2)} +$$

$$\left[(\tanh z+\lambda)(1-\tanh^2 z)\right]y = 0 .$$

On simplifying (7) becomes

$$(8) \quad \frac{d^2y}{dz^2} + \left[\operatorname{sech}^2 z\ (\tanh z+\lambda)\right]y = 0 .$$

We note that on making the substitution

$$-\sin\Theta\, d\Theta = \operatorname{sech}^2 z\, dz$$

the single integral

$$\int_0^{\pi} \Theta^2 \sin\Theta\, d\Theta$$

becomes

$$(9) \quad -\int_{+\infty}^{-\infty} \Theta^2 \operatorname{sech}^2 z\, dz = \int_{-\infty}^{\infty} \Theta^2 \operatorname{sech}^2 z\, dz$$

Thus we see that the allowed values of λ are those for which the solutions of (8) are finite and single valued throughout the specified range, and (9) is finite.

It now follows that for any determined value of λ the allowed values of the energy parameter are precisely those for which

$$\int_0^{\infty} R^2 r^2 dr$$

is finite in the given interval and R is a non-zero, single valued solution of

$$r^2 \frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + r^2\left(E + \frac{e^2}{r} - \frac{\lambda}{r^2}\right) R = 0$$

THE ANGULAR EQUATION FOR ϕ.

If the arbitrary constant C_1 is set equal to N^2 the angular equation in becomes

$$\Phi''(\phi) + N^2\Phi(\phi) = 0.$$

In order that this solution be single valued throughout the region investigated it is apparent that certain values of N must be barred.

Only positive values of N need be considered since negative values of N do not give new solutions. Non-integral values of N make the solution multiple valued thus barring them.

This leaves positive whole integer values of N as the allowable characteristic values of the parameter N appearing in the angular equation for ϕ.

NUMERICAL DETERMINATION OF THE CHARACTERISTIC VALUES OF λ.

An equation that has been studied a great deal in connection with wave mechanics is the well known Sturm-Liouville[1] equation

(10)
$$\frac{d\left[P(z)\frac{dy}{dz}\right]}{dz} - q(z)y + \lambda p(z)y = 0$$

in the intervals $0<z<\infty$ or $-\infty<z<\infty$. By the substitution $y = Up^{-\frac{1}{2}}$ this equation becomes

(11)
$$\frac{d^2U}{dz^2} + G(z,\lambda)U = 0$$

provided p does not vanish in the interval and its first and second derivative exist.

It[2] has been shown that (11) contains wave equations of the type of equation (80) if it is noted that

$$G(z,\lambda) = \operatorname{sech}^2 z\,(\tanh z + \lambda)$$

1. Milne, W.E., Physical Review, 35, 863 (1930).
2. Ibid.

It is assumed that $G(z,\lambda)$ is continuous in z and when z is large

$$G\ (z,\lambda) \rightarrow 0$$

for all values of λ discussed.

Now the necessary and sufficient condition that a given set of solutions $U_1(z)$ and $U_2(z)$ of a second order differential equation be linearly independent is that

$$\begin{vmatrix} U_1 & U_2 \\ U_1' & U_2' \end{vmatrix} \neq 0 .$$

Let two such solutions of (11) satisfy

$$U_1(z_0) = 1 , \quad U_2(z_0) = 0 ,$$

$$U_1'(z_0) = 0 , \quad U_2'(z_0) \neq 0 ,$$

where z_0 is a value of z in the interval $-\infty < z < +\infty$.

These solutions satisfy the identity

(12) $$U_1(z)\cdot U_2(z) - U_2(z)\cdot U_2'(z) \equiv \alpha$$

where a is arbitrary. It has been shown by Milne[1] that a new function $W(z)$ may be defined in terms of these two solutions as

(13) $$W\ (z) = \left[U_1^2(z) + U_2^2(z) \right]^{\frac{1}{2}}$$

1. Milne, W.E., Physical Review, 35, 863 (1930).

whose first and second derivatives are

$$W' = \frac{1}{2}\,(U_1^2\ U_2^2)\,(2\,U_1U_1' + 2\,U_2U_2')$$

and

$$W'' = -\,\frac{4}{4}\,(U_1^2 + U_2^2)^{-\frac{3}{2}}\,(U_1U_1' + U_2U_2')^2 +$$

$$\frac{2}{2}\,(U_1^2 + U_2^2)^{-\frac{1}{2}}\,(U_1U_1'' + U_1'^2 + U_2U_2'' + U_2'^2)\ .$$

Using the relationships;

$$W'' = -\,G\,(\lambda, z)\,W \quad ,$$

$$W = (U_1^2\ U_2^2)^{\frac{1}{2}} \quad , \qquad U_1U_2' - U_2U_1' \equiv a \quad ,$$

we may now write

(14) $$W'' + G\,(\lambda\,,\,z)\,W - \frac{a^2}{W^3} = 0$$

of which (13) is a solution. The general solution of (11) is not known[1] but can be expressed in the form of

(15) $$U(z) = C\,W(z)\,\sin\left\{a\int_{z_0}^{z} W^{-2}\,dz - \alpha\right\} ,$$

in which C and α are arbitrary constants. Since with the given boundary conditions $W(z)$ remains finite at

1. Milne, W.E., Physical Review, 35, 863 (1930).

either end of the interval, it is apparent that (15) will satisfy these conditions if, and only if,

(16)
$$\frac{a}{\pi}\int_{-\infty}^{\infty} W^{-2}\,dz = n \quad ,$$

where n is a positive integer.

The integral

(17)
$$N = \frac{a}{\pi}\int_{-\infty}^{\infty} W^{-2}\,dz$$

is an increasing function of λ so that if the integral is evaluated for several values of the parameter λ there will be obtained an equal number of different values for the integral N,

$$N_1,\ N_2,\ N_3,\ ---\ N_K \quad .$$

If the integer n is found between N_1 and N_K , then the corresponding value of λ may be found by interpolation, which will be precisely the n-th characteristic value of λ counted in order of magnitude.

The procedure for determining the characteristic values of λ for the equation

$$\frac{d^2W}{dz^2} + \operatorname{sech}^2 z\ (\tanh z + \lambda) = 0$$

will now be outlined.

NUMERICAL DETERMINATION OF CHARACTERISTIC

VALUES OF λ FOR THE EQUATION

$$W'' + \operatorname{sech}^2 z\,(\tanh z + \lambda)\,W = 0 .$$

If, as previously shown, a function $W(z)$ be defined in terms of two solutions U_1 and U_2 of (8) as

$$W^2(z) = U_1^2(z) + U_2^2(z) ,$$

where

$$U_1(z_0) = 1 , \qquad U_2(z_0) = 0 ,$$

$$U_1'(z_0) = 0 , \qquad U_2'(z_0) = a \neq 0 ,$$

then W(z) satisfies the equation

(18)
$$W'' + \operatorname{sech}^2 z\,(\tanh z + \lambda)\,W - \frac{a^2}{W^3} = 0 .$$

Since $\underline{a}$ is an arbitrary constant it may be set equal to $\lambda^{\frac{1}{2}}$ so that (18) becomes:

(19) $$W'' + \operatorname{sech}^2 z\,(\tanh z + \lambda)\,W - \frac{\lambda}{W^3} = 0 .$$

This equation will now be integrated numerically for the following values of λ:

-1, 0, +0.001, 0.0625, 1.0 and 2.0.

The initial conditions are

$$W(z_0) = 1, \qquad W'(z_0) = 0.$$

In order to start the numerical integration of (19) it will be necessary to have three values of W besides the initial value. These may be obtained from a Taylor's series for W, the first four terms of which are found as follows:

$$W_{(z_0)} = 1 ,$$

$$W'_{(z_0)} = 1 ,$$

$$W''_{(z_0)} = \frac{\lambda}{W^3} - \operatorname{sech}^2 z_0 (\tanh z_0 + \lambda) = 0$$

$$\begin{aligned} W'''_{(z_0)} = {} & -3\lambda W^{-4} W' - (\operatorname{sech}^4 z_0 - 2\operatorname{sech}^2 z_0 \tanh^2 z_0 \\ & -2\lambda \operatorname{sech}^2 z_0 \tanh z_0) W \\ & -(\operatorname{sech}^2 z_0 \tanh z_0 + \lambda \operatorname{sech}^2 z_0) W = 1 , \end{aligned}$$

$$\begin{aligned} W''_{(z_0)} = {} & 12\lambda W^{-5} W' - 3\lambda W^{-4} W'' - (-4\operatorname{sech}^4 z_0 \tanh z_0 \\ & + 4\operatorname{sech}^2 z_0 \tanh^3 z_0 + 4\operatorname{sech}^4 z_0 \tanh z_0 \\ & - 4\lambda \operatorname{sech} z_0 \tanh^2 z_0 - \lambda \operatorname{sech}^4 z_0) W \\ & + (\text{terms in } \operatorname{sech} z \text{ \& } \tanh z) W \\ & - (\quad " \quad " \quad " \quad " \quad " \quad) W'' = 2\lambda . \end{aligned}$$

$$W^{v} = -60W^{-6} + 12W^{-5}W'' - 3W^{-4}W'''$$

$$-(+16\operatorname{sech}^2 z \tanh^2 z - 4\operatorname{sech}^6 z + 12\operatorname{sech}^4 z \tanh^2 z$$

$$+4\operatorname{sech}^6 z - 8\operatorname{sech}^2 z \tan^4 z + 4\lambda \operatorname{sech} z \tanh^3 z$$

$$-4\operatorname{sech}^4 z \tanh^2 z - 8\lambda \operatorname{sech}^3 z \tanh z$$

$$+8\lambda \operatorname{sech}^4 z \tanh z)W$$

$$-(-4\operatorname{sech}^4 z \tanh z + 4\operatorname{sech}^2 z \tanh^3 z$$

$$+4\operatorname{sech}^4 z \tanh z - 4\operatorname{sech} z \tanh^2 z$$

$$-2\lambda \operatorname{sech}^4 z)W' + \left(\begin{array}{c}\text{terms in sech}\, z\\ \text{and tanh}\, z.\end{array}\right)W'$$

$$+\left(\begin{array}{c}\text{terms in sech}\, z\\ \text{and tanh}\, z.\end{array}\right)W'' - (\operatorname{sech}^2 z \tanh z$$

$$+\lambda \operatorname{sech}^2 z)W''' = 3\lambda\ .$$

The Taylor series, for the first four terms may now be written

$$w = 1 - \frac{z^3}{3!} + \frac{2\lambda z^4}{4!} + \frac{3\lambda z^5}{5!} + - \cdot\cdot - ,$$

from which the starting values of w may be obtained for use in the numerical method of integration[1].

1. Milne, W.E., Amer. Math. Monthly, XL, 322, (1933).

An attempt to carry the numerical calculations forward for negative values of λ will give extremely large values for the integral

$$\int_{-\infty}^{+\infty} W\,dz \,.$$

For all such values it is apparent that for positive values of z the right hand member of

$$W'' = -\operatorname{sech}^2 z\,(\tanh z + \lambda)\,W - \frac{\lambda}{W^2}$$

will be negative. It then follows that the W's in the predictor and corrector formulas :

$$W_{n+1} = W_n + W_{n-2} - W_{n-3} + \frac{h^2}{4}\,(5W_n'' + 2W_{n-1}'' + 5W_{n-3}'')\,,$$

$$W_n = 2W_{n-1} - W_{n-2} + \frac{h^2}{12}\,(W_n'' + 10\,W_{n-1}'' + W_{n-2}'')\,,$$

actually used in the numerical work will be negative for all positive values of z thus causing W to diminish through zero. For increasingly small W's the integral of $1/W^2$ will become increasingly large over the specified range.

For $\lambda = 0$ the same reasoning holds causing us to rule out zero and all negative numbers as possible values of λ.

For $\lambda = 0.001$, since $N = \frac{\lambda^{\frac{1}{2}}}{\pi}\int_{-\infty}^{+\infty} \frac{1}{W^2}\,dz$, our calculations show $N < 1.0$. For $\lambda = 1$ the value is over 1.0. This is an encouraging start as it indicates that the N's are an increasing function of λ.

The following tables show the values of $G(\lambda, z)$ and the initial numerical steps used in determining the first two characteristic values of λ. The actual interval used, however, was 0.1 and the computations were carried out with this interval over the range indicated at the head of each table. The interval was then doubled and the work proceeded until W became a linear function of z.

At this point the linear relationship is expressed by

$$W = az + b$$

and the value of

$$\int_{x_1}^{\infty} \frac{1}{az + b}$$

is found. Since $G(\lambda, z)$ is not even in z it is necessary to calculate both ways from zero. The complete evaluation of N, therefore, consists of four applications of Simpson's rule and the determination of two definite integrals.

It is to be noted that, in this method of determining characteristic values of the parameter being investigated, the integral

$$\int_{-\infty}^{\infty} W^{-2}\,dz$$

must be finite. Therefore, it is essential that W increase steadily as z increases in either the positive or negative direction. The following pages show this condition to be satisfied and on page 36 appear the least values of λ as obtained by the Milne method[1].

1. Milne, W.E., Physical Review, 35, 863 (1930).

TABLE I (a).

Computation of $G(\lambda, z)$ for $\lambda = 0.001$.

z	$G(\lambda,-z)$	$G(\lambda,+z)$
0.0	0.001	0.001
0.2	0.191	0.191
0.4	0.324	0.326
0.6	0.381	0.383
0.8	0.371	0.372
1.0	0.319	0.320
1.2	0.254	0.254
1.4	0.191	0.191
1.6	0.138	0.138
1.8	0.098	0.098
2.0	0.067	0.068
2.2	0.047	0.047
2.4	0.032	0.032
2.6	0.027	0.027
2.8	0.015	0.015
3.0	0.008	0.008

TABLE I (b)

Numerical integration of $W'' + \operatorname{sech}^2 z\,(\tanh z + \lambda)W - \frac{\lambda}{W^3} = 0$

z	W	W''	1/1000W³	1/W²
+0.2	0.999	0.189	0.001	1.0020
0.0	1.000	0.000	0.001	1.0000
-0.2	1.001	0.190	0.001	0.9980
-0.4	1.010	0.330	0.001	0.9807
-0.6	1.032	0.396	0.001	0.9388
-0.8	1.070	0.399	0.001	0.8733
-1.0	1.118	0.352	0.001	0.7999
-1.2	1.180	0.302	0.001	0.7181
-1.4	1.254	0.240	0.001	0.6360
-1.6	1.338	0.185	0.000	0.5586
-1.8	1.429	0.140		0.4897
-2.0	1.526	0.104		0.4295
-2.2	1.627	0.077		0.3777
-2.3	1.731	0.052		0.3337
-2.6	1.837	0.047		0.2964
-2.8	1.945	0.027		0.2643
-3.0	2.054	0.014		0.2371
-3.2	2.165	0.008		0.2133
-3.4	2.276	0.003		0.1930
-3.6	2.387	0.001		0.1754

TABLE I (c).

Numerical integration of $W'' + \operatorname{sech}^2 z(\tanh z + \lambda)W - \frac{\lambda}{W^3} = 0$.

z	W	W''	1/1000W^3	1/W^2
-0.2	1.001	0.000	0.001	
0.0	1.001	0.000	0.001	1.0000
0.2	0.999	-0.189	0.001	1.0020
0.4	0.991	-0.322	0.001	1.0181
0.6	0.970	-0.371	0.001	1.0629
0.8	0.934	-0.346	0.001	1.1449
1.0	0.884	-0.282	0.001	1.2791
1.2	0.823	-0.207	0.002	1.4762
1.4	0.754	-0.142	0.002	1.7582
1.6	0.679	-0.091	0.003	2.1697
1.8	0.600	-0.054	0.005	2.7688
2.0	0.519	-0.028	0.007	3.7133
2.2	0.437	0.006	0.012	5.2349
2.4	0.355	0.011	0.022	7.9298
2.6	0.273	0.043	0.049	13.4175
2.8	0.193	0.136	0.139	26.8427
3.0	0.120	0.578	0.579	69.4388
3.2	0.075	2.368	2.369	177.6889
3.4	0.113	0.693	0.693	78.3048
3.6	0.183	0.162	0.133	29.8552

3.8	0.261	0.055	0.056	14.6765
4.0	0.341	0.024	0.025	8.5966
4.2	0.422	0.013	0.013	5.6169
4.4	0.504	0.007	0.007	3.9362
4.6	0.586	0.005	0.005	2.9104
4.8	0.668	0.003	0.003	2.2410
5.0	0.750	0.002	0.002	1.7768
5.2	0.832	0.001	0.001	1.7366
5.4	0.914	0.000	0.001	1.1968
5.6	0.996		0.001	1.0080
5.8	1.078		0.001	0.8611
6.0	1.160		0.001	0.7430

$$\int_{-3.6}^{-\infty} \frac{1}{(0.41z - 0.130)^2}\,dz + \int_{-3.6}^{6.0} \frac{1}{W^2}\,dz + \int_{6.0}^{+\infty} \frac{1}{(0.553z + 0.389)^2}\,dz$$

$$= 94.492 .$$

TABLE II (a).

Computation of $G(\lambda,x)$ for $\lambda = 1/16$.

z	G(1/16,-z)	G(1/16,+z)
0.0	0.062	0.062
0.2	0.129	0.249
0.4	0.271	0.378
0.6	0.337	0.426
0.8	0.336	0.406
1.0	0.293	0.346
1.2	0.235	0.273
1.4	0.177	0.204
1.6	0.129	0.147
1.8	0.091	0.104
2.0	0.063	0.071
2.2	0.043	0.049
2.4	0.029	0.032
2.6	0.020	0.022
2.8	0.013	0.013
3.0	0.007	0.008
3.2	0.006	0.005
3.4	0.004	0.003
3.6	0.002	0.002
3.8	0.001	0.001
4.0	0.000	0.001

TABLE II (b).

Numerical integration of

$$W'' + \operatorname{sech}^2 z\,(\tan z + \lambda)W - \frac{\lambda}{W^3} = 0. \qquad \lambda = \frac{1}{16}.$$

z	W	W″	1/16W³	1.W²
+0.2	0.998	-0.186	0.062	1.0040
0.0	1.000	0.000	0.062	1.0000
-0.2	1.001	0.191	0.062	0.9980
-0.4	1.009	0.335	0.060	0.9820
-0.6	1.030	0.394	0.057	0.9424
-0.8	1.006	0.409	0.051	0.8798
-1.0	1.118	0.372	0.044	0.7999
-1.2	1.185	0.314	0.037	0.7121
-1.4	1.264	0.253	0.030	0.6250
-1.6	1.353	0.201	0.025	0.5461
-1.8	1.450	0.141	0.020	0.4755
-2.0	1.552	0.114	0.016	0.4151
-2.2	1.659	0.084	0.013	0.3633
-2.4	1.769	0.062	0.011	0.3192
-2.6	1.881	0.046	0.009	0.2825
-2.8	1.995	0.033	0.007	0.2512
-3.0	2.110	0.021	0.006	0.2245
-3.2	2.226	0.018	0.005	0.2017
-3.4	2.342	0.014	0.004	0.1822
-3.6	2.458	0.008	0.004	0.1654

-3.8	2.574	0.005	0.003	0.1509
-4.0	2.690	0.004	0.003	0.1381
-4.2	2.806	0.002	0.002	0.1269
-4.4	2.922	0.002	0.002	0.1171
-4.6	3.038	0.002	0.002	0.1083
-4.8	3.154	0.001	0.001	0.1004
-5.0	3.270	0.001	0.001	0.0935

$$\int_{0}^{-5} \frac{1}{W^2} dz + \int_{-5}^{-\infty} \frac{1}{(0.5802z + 0.37)^2} dz = 2.5540.$$

TABLE II (c).

Numerical integration of

$$W'' + \operatorname{sech}^2 z\,(\tan z + \lambda)\,W - \frac{\lambda}{W^3} = 0. \qquad \lambda = \frac{1}{16}.$$

z	W	W''	$1/16W^3$	$1/W^2$
-0.2	1.001	0.191	0.062	0.9980
0.0	1.000	0.000	0.062	1.0000
0.2	0.998	-0.186	0.062	1.0040
0.4	0.990	-0.298	0.065	1.0201
0.6	0.970	-0.345	0.068	1.0629
0.8	0.936	-0.305	0.075	1.1406
1.0	0.890	-0.219	0.082	1.2611
1.2	0.836	-0.122	0.106	1.4304
1.4	0.777	-0.025	0.133	1.6563
1.6	0.717	0.061	0.168	1.9432
1.8	0.659	0.149	0.217	2.3012
2.0	0.607	0.236	0.279	2.7126
2.2	0.564	0.321	0.348	3.1435
2.4	0.534	0.389	0.406	3.5043
2.6	0.519	0.448	0.459	3.7094
2.8	0.522	0.432	0.438	3.6672
3.0	0.542	0.387	0.392	3.4040
3.2	0.577	0.322	0.325	3.0032
3.4	0.624	0.254	0.256	2.5664
3.6	0.681	0.197	0.198	2.1550

3.8	0.746	0.149	0.150	1.7956
4.0	0.817	0.113	0.114	1.4981
4.2	0.892	0.088	0.088	1.2566
4.4	0.971	0.068	0.068	1.0588
4.6	0.053	0.053	0.053	0.9017
4.8	1.137	0.042	0.042	0.7735
5.0	1.222	0.034	0.034	0.6695
5.2	1.309	0.027	0.207	0.5844
5.4	1.398	0.021	0.021	0.5116
5.6	1.488	0.017	0.017	0.4515
5.8	1.578	0.015	0.015	0.4015
6.0	1.668	0.013	0.013	0.3594

$$\int_0^6 \frac{1}{W^2}dz + \int_6^\infty \frac{1}{(0.45z-1.032)^2}dz = 11.5870.$$

TABLE III (a).

Computation of G(λ z) for λ = 1 .

z	G(λ,-z)	G(λ,+z)
0.0	1.000	1.000
0.2	0.771	1.150
0.4	0.530	1.179
0.6	0.329	1.093
0.8	0.187	0.930
1.0	0.100	0.739
1.2	0.050	0.559
1.4	0.024	0.407
1.6	0.011	0.289
1.8	0.005	0.201
2.0	0.002	0.138
2.2	0.001	0.092
2.4	0.000	0.064
2.6	-----	0.043
2.8	-----	0.029
3.0	-----	0.019
3.2	---	0.007
3.4	---	0.004
3.6	---	0.002
3.8	-	0.001
4.0	-	0.000

TABLE III (b).

Numerical integration of $W'' + \operatorname{sech}^2 z\,(\tanh z + \lambda)\,W - \frac{\lambda}{W^3} = 0$.

z	W	W''	$1/W^3$	$1/W^2$
+0.2	0.998	−0.146	1.003	1.0020
0.0	1.000	0.000	1.000	1.0000
-0.2	1.001	0.227	0.997	0.9980
-0.4	1.011	0.432	0.967	0.9783
-0.6	1.038	0.552	0.893	0.9279
-0.8	1.086	0.584	0.780	0.8478
-1.0	1.157	0.530	0.645	0.7470
-1.2	1.249	0.451	0.513	0.6409
-1.4	1.359	0.342	0.398	0.5414
-1.6	1.482	0.291	0.307	0.4552
-1.8	1.616	0.228	0.236	0.3829
-2.0	1.759	0.180	0.183	0.3231
-2.2	1.909	0.142	0.143	0.2743
-2.4	2.065	0.113	0.113	0.2344
-2.6	2.225	0.090	0.090	0.2019
-2.8	2.388	0.073	0.073	0.1753
-3.0	2.554	0.060	0.060	0.1532
-3.2	2.722	0.049	0.049	0.1349
-3.4	2.891	0.041	0.041	0.1196
-3.6	3.061	0.034	0.034	0.1066

-3.8	3.232	0.029	0.029	0.0957
-4.0	3.404	0.025	0.025	0.0862
-4.2	3.577	0.021	0.021	0.0781
-4.4	3.751	0.018	0.018	0.0710
-4.6	3.925	0.016	0.016	0.0649
-4.8	4.099	0.014	0.014	0.0595
-5.0	4.273	0.012	0.012	0.0547

$$\int_0^{-5} \frac{1}{W^2}\,dz + \int_{-5}^{-\infty} \frac{1}{(1.37z-2.517)^2}\,dz = 2.0802.$$

TABLE III (c).

Numerical integration of $W'' + \operatorname{sech}^2 z\,(\tanh z + \lambda)W - \dfrac{\lambda}{W^3} = 0$,

z	W	W″	$1/W^3$	$1/W^2$
-0.2	1.001	0.227	0.997	0.9980
0.0	1.000	0.000	1.000	1.0000
0.2	0.998	-0.146	1.003	1.0020
0.4	0.992	- 0.147	1.023	1.0150
0.6	0.980	- 0.014	1.058	1.0383
0.8	0.968	0.122	1.099	1.0650
1.0	0.962	0.410	1.121	1.0795
1.2	0.972	0.545	1.088	1.0580
1.4	1.002	0.582	0.991	0.9942
1.6	1.056	0.544	0.849	0.8966
1.8	1.132	0.460	0.689	0.7803
2.0	1.225	0.373	0.543	0.6656
2.2	1.334	0.296	0.420	0.5616
2.4	1.454	0.230	0.324	0.4722
2.6	1.584	0.182	0.251	0.3981
2.8	1.721	0.146	0.197	0.3388
3.0	1.864	0.117	0.154	0.1575
3.2	2.011	0.107	0.122	0.2471
3.4	2.162	0.097	0.098	0.2133
3.6	2.3175	0.075	0.082	0.1826

3.8	2.475	0.064	0.065	0.1634
4.0	2.635	0.052	0.052	0.1440
4.2	2.797	0.045	0.045	0.1278
4.4	2.961	0.038	0.038	0.1140
4.6	3.127	0.032	0.032	0.1022
4.8	3.295	0.027	0.027	0.0920
5.0	3.462	0.024	0.024	0.0834
5.2	3.630	0.020	0.020	0.0759
5.4	3.799	0.018	0.018	0.0692
5.6	3.968	0.016	0.016	0.0635
5.8	4.137	0.014	0.014	0.0586
6.0	4.306	0.012	0.012	0.0539

$$\int_0^6 \frac{1}{W^2}\,dz + \int_6^\infty \frac{1}{(0.845z+0.764)^2}\,dz = 3.1643.$$

TABLE IV (a).

Computation of G(λ, z) for $\lambda = 2$.

z	G(λ,-z)	G(λ,-z)
0.0	2.000	2.000
0.2	1.732	2.111
0.4	1.386	2.036
0.6	1.041	1.805
0.8	0.746	1.489
1.0	0.520	1.159
1.2	0.353	0.864
1.4	0.240	0.623
1.6	0.162	0.439
1.8	0.109	0.305
2.0	0.073	0.209
2.2	0.049	0.142
2.4	0.033	0.096
2.6	0.022	0.065
2.8	0.014	0.044
3.0	0.010	0.029
3.2	0.006	0.0019
3.4	0.004	0.013
3.6	0.003	0.008
3.8	0.002	0.005
4.0	0.001	0.003

TABLE IV (b).

Numerical integration of $W'' + \operatorname{sech}^2 z\,(\tanh z + \lambda)W - \frac{\lambda}{W^3} = 0$.

z	W	W'	$1/W^3$	$1/W^2$
+0.2	0.999	0.105	2.006	1.0020
-0.0	1.000	0.000	2.000	1.0000
-0.2	1.001	0.262	1.994	0.9980
-0.4	1.012	0.521	1.929	0.9763
-0.6	1.044	0.671	1.757	0.9173
-0.8	1.102	0.672	1.494	0.8233
-1.0	1.186	0.582	1.198	0.7108
-1.2	1.293	0.468	0.924	0.5979
-1.4	1.419	0.350	0.699	0.4966
-1.6	1.559	0.274	0.527	0.4113
-1.8	1.710	0.213	0.399	0.3418
-2.0	1.869	0.170	0.306	0.2862
-2.2	2.035	0.137	0.236	0.2414
-2.4	2.206	0.114	0.186	0.2054
-2.6	2.381	0.096	0.148	0.1763
-2.8	2.559	0.083	0.119	0.1526
-3.0	2.740	0.070	0.097	0.1331
-3.2	2.924	0.062	0.079	0.1168
-3.4	3.108	0.054	0.066	0.1034
-3.6	3.294	0.046	0.055	0.0921

-3.8	3.481	0.041	0.047	0.0824
-4.0	3.669	0.036	0.040	0.0742
-4.2	3.858	0.034	0.034	0.0671
-4.4	4.048	0.030	0.030	0.0610
-4.6	4.239	0.026	0.026	0.0556
-4.8	4.431	0.022	0.022	0.0509
-5.0	4.624	0.020	0.020	0.0467
-5.2	4.818	0.017	0.017	0.0430
-5.4	5.012	0.015	0.015	0.0398
-5.6	5.206	0.014	0.014	0.0369
-5.8	5.400	0.012	0.012	0.0342
-6.0	5.594	0.011	0.011	0.0319

$$\int_0^{-6} \frac{1}{W^2}\,dz + \int_{-6}^{-\infty} \frac{1}{(0.970z - 0.0226)^2}\,dz = 1.9751.$$

TABLE IV (c).

Numerical integration of $W'' + \operatorname{sech}^2 z\,(\tanh z + \lambda)\,W - \frac{\lambda}{W^3} = 0.$

z	W	W''	$2/W^3$	$1/W^2$
-0.2	1.001	0.266	1.998	0.9980
0.0	1.000	0.000	2.000	1.0000
0.2	0.999	0.105	2.006	1.0020
0.4	0.995	0.005	2.030	1.0100
0.6	0.991	0.266	2.054	1.0180
0.8	0.997	0.534	2.018	1.0060
1.0	1.024	0.676	1.862	0.9535
1.2	1.074	0.685	1.612	0.8658
1.4	1.151	0.593	1.310	0.7548
1.6	1.251	0.471	1.021	0.6388
1.8	1.369	0.362	0.779	0.5334
2.0	1.501	0.277	0.591	0.4193
2.2	1.644	0.219	0.450	0.3699
2.4	1.796	0.183	0.345	0.3099
2.6	1.955	0.140	0.267	0.2616
2.8	2.119	0.117	0.210	0.2226
3.0	2.288	0.099	0.166	0.1909
3.2	2.461	0.087	0.134	0.1650
3.4	2.637	0.075	0.109	0.1437
3.6	2.816	0.065	0.089	0.1260

+3.8	2.997	0.060	0.074	0.1112
+4.0	3.180	0.053	0.062	0.0988
+4.2	3.365	0.046	0.052	0.0822
+4.4	3.551	0.040	0.044	0.0792
+4.6	3.738	0.035	0.038	0.0715
+4.8	3.926	0.031	0.033	0.0648
+5.0	4.115	0.027	0.028	0.0590
+5.2	4.304	0.024	0.025	0.0539
+5.4	4.494	0.022	0.022	0.0495
+5.6	4.685	0.019	0.019	0.0455
+5.8	4.876	0.017	0.017	0.0420
+6.0	5.067	0.015	0.015	0.0389

$$\int_0^{+6} \frac{1}{W^2}\,dz + \int_6^{\infty} \frac{1}{(0.955z-0.663)^2}\,dz = 2.4667.$$

The calculations shown on the preceding pages together with the extended evaluations of

$$\int_0^{z_1} \frac{1}{W^2}\, dz$$

and

$$\int_{z_1}^{\pm\infty} \frac{1}{(az+b)^2}\, dz$$

give the following values of the N's for the respective values of the λ's investigated;

λ	N
0.001	$3.000/\pi$
0.0625	$3.5352/\pi$
1.000	$5.2445/\pi$
2.000	$6.2833/\pi$

From these values, and a trial calculation for $\lambda = 0.002$ giving $N = 3.142$, the first two characteristic values of λ are found to be 0.002 and 2.000. These values will now be used in the determination of the least values of the energy parameter.

THE EQUATION IN R.

$$r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + r^2(E + \frac{e}{r} - \frac{\lambda}{r^2})R = 0 .$$

The above equation, on setting

$$R = \frac{S}{r}$$

becomes

(20) $$S'' + (E + \frac{e^2}{r} - \frac{\lambda}{r^2})S = 0$$

This may be put into a neater form if a new parameter η and a new variable x (not to be confused with previous x) are introduced according to the equations

$$E = \pm\frac{e^4}{4n^2} \quad , r = \frac{nx}{e^2} \quad ,$$

so that (20) becomes

(21) $$S'' + (\pm\frac{1}{4} + \frac{n}{x} - \frac{\lambda}{x^2})S = 0 \quad .$$

Striking out the terms that approach zero in value as $x \longrightarrow \infty$, we may write (21) as

$$S'' \pm \frac{1}{4}S = 0 \quad .$$

Considering the negative sign, one of the two solutions

1. Condon and Morse, Quantum Mechanics, Chapt. II, McGraw and Hill, 1929.

$e^{-\frac{x}{2}}$ and $e^{+\frac{x}{2}}$ remain finite as $x \longrightarrow \infty$. Since only negative values of E are being considered , the following substitution is made;

$$S = yx^{\int+1} e^{-\frac{x}{2}} \quad ,$$

so that the differential equation (21) becomes

(22)

$$xy'' + [2(\int+1) - x]y' + (n - \int - 1)y = 0$$

for whose power series solution the relation between successive coefficients is found as follows. Let

$$y = a + a_1x + a_2x^2 + \text{---------} a_nx^n$$

Taking the first and second derivatives and substituting in (22) the following array is arrived at:

$$4\int a + 2\int a_2x + 3\int a_3x^2 + 4\int a_4x^3 + \text{-----}$$

$$+2a_1 + 4a_2x + 6a_3x^2 + 4a_4x^3 + \text{------}$$

$$-a_1x - 2a_2x^2 - 3a_3x^3 + \text{---------}$$

$$+ na_0 + na_1x + na_2x^2 + na_3x^3 + \text{----------}$$

$$-\int a_0 - \int a_1x - \int a_2x^2 - \int a_3x^3 + \text{----------}$$

$$-a_0 - ax - a_1x - a_2x^2 - a_3x^3 - \text{---------}$$

$$+4\int a_nx^{n-1} + 4a_nx^{n-1} + na_{n-1}x^{n-1}$$

$$-\int ax^{n-1} - a_{n-1}x^{n-1} = 0 \quad .$$

The relationship between successive coefficients of like powers of x is now found to be

$$a_{j+1}\,(j+1)(j+2l+2) = a_j\,(j+l+1-n),$$

$$j = 0, +1, +2, +3, \ldots .$$

It is apparent that the series will break off and give a polynomial solution if n is set equal to

$$j + l + 1$$

where l is related to λ by the equation

$$l(l+1) = \lambda .$$

Since 0.002 is the least value of λ it follows that there are two corresponding values of n, that is;

$$n = j + \frac{-1 \pm \sqrt{1+4\lambda}}{2} + 1 = \begin{cases} -0.0019 \\ +1.0019, \end{cases}$$

of which the smaller and negative value is, of course, the least value of n that is being sought for.

These allowed values of n give us, in turn, the allowed values of E for negative energies. Recalling our previous substitution

$$E = \pm \frac{e^4}{4 n^2} ,$$

we may write

$$E = - \frac{e^4}{1.444} \cdot 10^5 ,$$

$$E = - \frac{e^4}{4} ,$$

as allowed values of E for which λ as determined by ($1'$) is finite and single-valued throughout space.

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