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Approximate Eigensolutions of

$$(d^2\phi/dx^2) + [a + b(e^{-x}/x)]\phi = 0$$

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THE equation in question has been studied by various authors, (1)–(8)† inspired mainly by its connection with the deuteron problem. The present work, which forms a sequel to earlier papers ((4)–(6)) by one of the authors, was started because it was desirable to extend the previous calculations for the sake of certain applications, e.g., the photo-disintegration of the deuteron and the capture of neutrons by protons (9). In the course of the work, however, we took an interest in the mathematical aspect of the problem and accordingly studied it more closely than was strictly necessary from the point of view of the physical applications. We hope that the results may also be of interest to other than theoretical physicists occupied with the deuteron problem.

I. VARIATIONAL METHOD APPLIED TO GROUND STATE

Consider the differential equation

$$(d^2\phi/dx^2) + a\phi + bv(x)\phi = 0 \quad (1)$$

with the boundary conditions

$$\phi(0) = \phi(\infty) = 0, \quad (2)$$

the potential function $v(x)$ being continuous, at least sectionally, and bounded in the whole domain, except at $x=0$, where we assume

$$\lim_{x \rightarrow 0} x^2 v(x) \rightarrow \Psi, \quad \Psi \leq 0. \quad (3)$$

Further, we take

$$v(x) \rightarrow 0, \quad x \rightarrow \infty. \quad (4)$$

Now it is well known that Eq. (1) can be regarded as the Euler equation of a variational problem, e.g., the

following: Search for extremum of the integral

$$J = \int_0^\infty (\phi'^2 - a\phi^2) dx \quad (5)$$

with the accessory condition

$$N = \int_0^\infty v(x)\phi^2 dx = \text{const} \neq 0 \quad (\text{e.g.} = 1), \quad (6)$$

where ϕ is a continuous function with continuous ϕ' , satisfying conditions (2). Introducing a lagrange multiplier λ , we obtain

$$\delta J - \lambda \delta N = 0, \quad (7)$$

which is equivalent to Eq. (1), with λ for b . For a ϕ satisfying Eq. (1) we have, multiplying (1) by ϕ and integrating,

$$b = J_{\text{extremal}}/N. \quad (8)$$

An alternative formulation of the variational problem (see, for example, work by Zeilon; reference 10) is to drop the condition (6) and seek extremum of J/N . This gives

$$\delta(J/N) = (1/N)[\delta J - (J/N)\delta N] = 0, \quad (9)$$

which again leads to Eq. (1), provided

$$b = (J/N)_{\text{extremal}}. \quad (10)$$

The reason why we choose a as the known parameter and b as the eigenvalue—we might as well have done the reverse—is a purely practical one. In the application to problems of the nuclear force type, $v(x)$ is a function which decreases rather rapidly with increasing x . In such cases the eigenfunction of a bound state ($a < 0$) tends asymptotically to $\exp[-(-a)^{1/2}x]$ which is a natural starting point for choosing the trial function in

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† Numbered references are at end of article.

TABLE I.

$(-a)^{\frac{1}{2}}$	b_1	$(\alpha = 2(-a)^{\frac{1}{2}} + 1)$	h_1/h_0	h_2/h_0	h_3/h_0	$(\sigma_0 - 1) \cdot 10^8$	$(\sigma_\infty - 1) \cdot 10^8$
0	1.679933	0.679933	0.53567	—	—	-4.14	-10.05
0	1.679853	0.679853	0.57807	-0.05161	—	+4.40	-5.45
0	1.679819 ₆	0.679819 ₆	0.62081 ₆	-0.17699	0.09816	-2.28	-2.81
0.05	1.792570	0.692570	0.54323	—	—	-3.15	-10.28
0.05	1.792510	0.692510	0.58169	-0.04520	—	+3.93	-5.85
0.05	1.792481	0.692481	0.62420	-0.16555	0.09249	-2.01	-3.03
0.10	1.904045	0.704045	0.55025	—	—	-2.31	-10.44
0.10	1.904001	0.704001	0.58479	-0.03930	—	+3.52	-6.24
0.10	1.903977	0.703977	0.62718	-0.15532	0.08760	-1.77	-3.24
0.15	2.014534	0.714534	0.55679	—	—	-1.59	-10.51
0.15	2.014502	0.714502	0.58746	-0.03383	—	+3.17	-6.60
0.15	2.014480	0.714480	0.62979	-0.14611	0.08336	-1.58	-3.44
0.20	2.124173	0.724173	0.56293	—	—	-0.97	-10.53
0.20	2.124150 ₆	0.724150 ₆	0.58975	-0.02871	—	+2.87	-6.95
0.20	2.124131 ₆	0.724131 ₆	0.63166	-0.13661	0.07883	-1.38	-3.66
0.25	2.233074	0.733074	0.56877	—	—	-0.45	-10.47
0.25	2.233059 ₇	0.733059 ₇	0.59175	-0.02393	—	+2.60	-7.28
0.25	2.233043 ₀	0.733043 ₀	0.63352	-0.12843	0.07514	-1.23	-3.85
0.30	2.341331	0.741331	0.57430	—	—	0.00	-10.37
0.30	2.341320 ₉	0.741320 ₉	0.59356	-0.01953	—	+2.37	-7.60
0.30	2.341306 ₂	0.741306 ₂	0.63514	-0.12084	0.07181	-1.10	-4.04
0.35	2.449016	0.749016	0.57959	—	—	+0.37	-10.21
0.35	2.449010 ₂	0.749010 ₂	0.59514	-0.01537	—	+2.17	-7.91
0.35	2.448997 ₃	0.748997 ₃	0.63657	-0.11379	0.06877	-0.99	-4.22
0.40	2.556194 ₆	0.756194 ₆	0.58467	—	—	+0.72	-10.02
0.40	2.556191 ₄	0.756191 ₄	0.59654	-0.01146	—	+1.99	-8.20
0.40	2.556179 ₉	0.756179 ₉	0.63784	-0.10721	0.06600	-0.89	-4.39
0.45	2.662919 ₈	0.762919 ₈	0.58955	—	—	+1.01	-9.78
0.45	2.662918 ₅	0.762918 ₅	0.59779	-0.00778	—	+1.83	-8.49
0.45	2.662908 ₂	0.762908 ₂	0.63898	-0.10108	0.06347	-0.80	-4.56

a Rayleigh–Ritz procedure (11). Now this is a simple requirement if a is a known quantity, but if a is the eigenvalue it is not very convenient to work with a trial function containing a . Of course, it is perfectly possible to replace $\exp[-(-a)^{\frac{1}{2}}x]$ by $\exp(-\mu x)$, taking μ as an indeterminate parameter, but this would not be appropriate either. According to general experience it is in most cases advisable to use a trial function, which is linear in the indeterminate parameters.

Suppose ϕ is expanded in terms of a complete function system f_ν , thus

$$\phi(x) = \sum_1^{\infty} c_\nu f_\nu(x). \quad (11)$$

Retaining a finite number of terms, say, the n first ones, we have a possible trial function. Inserting in (5) and minimizing with (6) as accessory condition, we obtain

$$(\partial J / \partial c_\nu) - \lambda(\partial N / \partial c_\nu) = 0, \quad \nu = 1, \dots, n, \quad (12)$$

which is a linear and homogeneous system of equations for the parameters c_ν . The smallest value λ which makes the determinant of the system (12) vanish then gives the minimum value of J/N , i.e., an approximation for b .

Now it is well known that the solution of a determinant equation often requires an unwieldy precision in the numerical work, if the roots are wanted with some accuracy, and the case treated below is no exception. Therefore, we proceeded as follows. Suppose the equation system (12) has been solved, by using n parameters $c_1 \cdots c_n$, and the smallest root of the determinant equation is $\lambda^{(n)}$, which is then an approximation to the lowest eigenvalue b_1 of (1) and (2). This value $\lambda^{(n)}$ is inserted into (12), with $\nu = 2, 3, \dots, n+1$, which gives a set of values $c_1', c_2', \dots, c_{n+1}'$ (or rather the ratios $c_2'/c_1', c_3'/c_1', \dots, c_{n+1}'/c_1'$). We then calculate

$$\lambda^{(n)'} = J(c_1', c_2', \dots, c_{n+1}') / N(c_1', c_2', \dots, c_{n+1}'), \quad (13)$$

which is, in general, closer to the eigenvalue b_1 than was $\lambda^{(n)}$. After inserting $\lambda^{(n)'}$ into (12), we get a new set of quantities c_1'', \dots, c_{n+1}'' , and $\lambda^{(n)''}$ is obtained from (13). In the cases treated below this procedure turns out to converge rapidly, giving at the end $\lambda^{(n+1)}$ —the smallest root of (12) with $(n+1)$ parameters—and the corresponding set c_1, \dots, c_{n+1} . Thus, (12) can be solved for any number of parameters without resorting to the determinant equation, except for $n=2$. (The

TABLE I.—Continued.

$(-a)^{\frac{1}{2}}$	b_1	$\frac{b_1 - \alpha}{(\alpha = 2(-a)^{\frac{1}{2}} + 1)}$	h_1/h_0	h_2/h_0	h_3/h_0	$(\sigma_0 - 1) \cdot 10^8$	$(\sigma_\infty - 1) \cdot 10^8$
0.50	2.769237	0.769237	0.59424	—	—	+1.25	-9.52
0.50	2.769237	0.769237	0.59891	-0.00431	—	+1.69	-8.76
0.50	2.769227 ₉	0.769227 ₉	0.63998	-0.09531	0.06113	-0.72	-4.73
0.75	3.295925 ₄	0.795925 ₄	0.61561	—	—	+2.04	-7.77
0.75	3.295923 ₂	0.795923 ₂	0.60305	0.01053	—	+1.17	-10.01
0.75	3.295917 ₉	0.795917 ₉	0.64377	-0.07135	0.05198	-0.46	-5.47
1.0	3.816632 ₂	0.816632 ₂	0.63424	—	—	+2.38	-5.58
1.0	3.816624 ₀	0.816624 ₀	0.60558	0.02222	—	+0.85	-11.08
1.0	3.816620 ₇	0.816620 ₇	0.64617	-0.05319	0.04564	-0.30	-6.11
1.5	4.846964 ₆	0.846964 ₆	0.66583	—	—	+2.48	-0.59
1.5	4.846945 ₇	0.846945 ₇	0.60808	0.03965	—	+0.50	-12.86
1.5	4.846944 ₃	0.846944 ₃	0.64893	-0.02748	0.03766	-0.15	-7.16
2.0	5.868308 ₅	0.868308 ₅	0.69199	—	—	+2.31	+4.56
2.0	5.868284 ₄	0.868284 ₄	0.60884	0.05219	—	+0.32	-14.30
2.0	5.868283 ₆	0.868283 ₆	0.65045	-0.01027	0.03308	-0.08	-7.97
2.5	6.884243 ₆	0.884243 ₆	0.71421	—	—	+2.07	+9.53
2.5	6.884217 ₆	0.884217 ₉	0.60874	0.06176	—	+0.23	-15.52
2.5	6.884217 ₅	0.884217 ₅	0.65133	0.00216	0.03018	-0.05	-8.62
3.0	7.896638 ₉	0.896638 ₉	0.73337	—	—	+1.83	+14.18
3.0	7.896614 ₀	0.896614 ₀	0.60819	0.06935	—	+0.16	-16.58
3.0	7.896613 ₈	0.896613 ₈	0.6519 ₅	0.0114 ₄	0.0282 ₇	-0.03	-9.15
3.5	8.90657 ₆	0.90657 ₆	0.7501 ₈	—	—	+1.61	+18.46
3.5	8.906555 ₃	0.906555 ₃	0.6074 ₅	0.0755 ₃	—	+0.13	-17.49
3.5	8.906554 ₉	0.906554 ₉	0.6518	0.0194	0.0266	-0.02 ₅	-9.69
4.0	9.91473 ₉	0.91473 ₉	0.7647 ₇	—	—	+1.44	+22.41
4.0	9.914717	0.914717	0.6065 ₄	0.0807 ₁	—	+0.10	-18.31
4.0	9.914716 ₆	0.914716 ₆	0.6489	0.0289	0.0240	-0.02	-10.60
9.0	19.95423 ₅	0.95423 ₅	0.8519 ₂	—	—	+0.54	+108.6
9.0	19.954228	0.954228	0.5979	0.1071	—	+0.02	-23.42
9.0	19.954227 ₈	0.954227 ₈	0.644	0.061	0.019	-0.01	-13.75

number of effectively varied parameters is only $n-1$, because one parameter, say, c_1 , is needed for the normalization of ϕ .)

The equation to be solved here is

$$(d^2\phi/dx^2) + [a + b(e^{-x}/x)]\phi = 0, \quad (14)$$

with the boundary conditions

$$\phi(0) = 0, \quad \phi(\infty) = 0. \quad (15)$$

In one of the previous papers (4) it was pointed out that the solution can be written as follows (see also Sec. III below):

$$\phi(x) = \exp[-(-a)^{\frac{1}{2}}x] \sum_1^\infty \omega_\nu (1 - e^{-x})^\nu. \quad (16)$$

Thus, it would be justified to use (16) with a finite number of terms as a trial function. However, any such finite sum can be written in the following way

$$\phi(x) = (1 - e^{-x}) \exp[-(-a)^{\frac{1}{2}}x] \sum_{\nu=0}^n h_\nu e^{-\nu x}. \quad (17)$$

This form of the trial function has already been used in reference 6 because it simplifies the calculations, and we

choose it here for the same reason. Inserting (17) into (5) and (6) we obtain

$$J = \sum_{\mu=0}^n \sum_{\nu=0}^n h_\mu h_\nu \times \left[\frac{\mu\nu}{\alpha + \mu + \nu - 1} - \frac{2(\mu+1)\nu}{\alpha + \mu + \nu} + \frac{(\mu+1)(\nu+1)}{\alpha + \mu + \nu + 1} \right], \quad (18)$$

$\alpha = 2(-a)^{\frac{1}{2}} + 1,$

and

$$N = b \sum_{\mu=0}^n \sum_{\nu=0}^n h_\mu h_\nu I(\alpha + \mu + \nu, 2) \quad (19)$$

with (see reference 4)

$$I(\beta, m) = \int_0^\infty \frac{(1 - e^{-x})^m}{x} e^{-\beta x} dx \quad (20)$$

$$= \sum_{\mu=0}^m (-1)^{\mu+1} \binom{m}{\mu} \ln(\beta + \mu) \quad (m \text{ integer } \geq 1).$$

The Eqs. (12) are then easily written down. The results

obtained for the lowest eigenvalue b_1 with one, two and three effective parameters are given in Table I. Some of the results have been published earlier (6).

A certain check on the accuracy of the eigenfunctions is furnished by the quantities σ_0 and σ_∞ which are defined in the following way (6)

$$\begin{aligned}\sigma_0 &= b \int_0^\infty \exp[-(-a)^{\frac{1}{2}}x] \cdot \frac{e^{-x}}{x} \cdot \phi(x) dx / \phi'(0) \\ &= b \sum_{\nu=0}^n h_\nu \ln \frac{\alpha+\nu+1}{\alpha+\nu} / \sum_{\nu=0}^n h_\nu, \quad (21)\end{aligned}$$

$$\begin{aligned}\sigma_\infty &= b \int_0^\infty \sinh((-a)^{\frac{1}{2}}x) \cdot \frac{e^{-x}}{x} \cdot \phi(x) dx / (-a)^{\frac{1}{2}} \\ &= \frac{b}{2(-a)^{\frac{1}{2}}} \sum_{\nu=0}^n h_\nu \left(\ln \frac{2+\nu}{1+\nu} - \ln \frac{\alpha+\nu+1}{\alpha+\nu} \right). \quad (22)\end{aligned}$$

As shown in a previous paper (6), these ratios would equal 1 if the solutions $\phi(x)$ were exact. The deviation from 1 gives an idea of the accuracy of the eigenfunction, or, more precisely: errors in the region of small x will preferably affect σ_0 , whereas σ_∞ substantially reflects the shortcomings of the approximate $\phi(x)$ at relatively large x .

For small values of $(-a)^{\frac{1}{2}}$, the eigenvalue b_1 and the corresponding parameters can be developed in power series. Using the variational method we obtain with one effective parameter,

$$\begin{aligned}b_1 &= 1.679933 + 2.265775\epsilon - 0.276306\epsilon^2 + \dots, \\ h_1/h_0 &= 0.53567 + 0.15765\epsilon - 0.13782\epsilon^2 + \dots, \\ \epsilon &= (-a)^{\frac{1}{2}} = (\alpha-1)/2;\end{aligned} \quad (23)$$

with two parameters,

$$\begin{aligned}b_1 &= 1.679853 + 2.266217\epsilon - 0.277277\epsilon^2 + \dots, \\ h_1/h_0 &= 0.57807 + 0.07857\epsilon - 0.13320\epsilon^2 + \dots, \\ h_2/h_0 &= -0.05160 + 0.13343\epsilon - 0.11099\epsilon^2 + \dots;\end{aligned} \quad (24)$$

and with three parameters,†

$$\begin{aligned}b_1 &= 1.6798195 + 2.266313_8\epsilon - 0.277437_9\epsilon^2 \\ &\quad + 0.332012_5\epsilon^3 - 0.518899\epsilon^4 + \dots, \\ h_1/h_0 &= 0.62082 + 0.07377\epsilon - 0.23822\epsilon^2 + \dots, \\ h_2/h_0 &= -0.17699 + 0.23938\epsilon - 0.18131\epsilon^2 + \dots, \\ h_3/h_0 &= 0.09816 - 0.12007\epsilon + 0.26354\epsilon^2 + \dots.\end{aligned} \quad (25)$$

For very large values of $(-a)^{\frac{1}{2}}$ it proves convenient to express the eigenvalue and parameters as power series in terms of

$$\tau = 1/(\alpha+1) = 1/[2(-a)^{\frac{1}{2}}+2]. \quad (26)$$

With one effective parameter, the variation procedure

† We are indebted to Mr. V. Grinvalds for making these calculations and checking some of the earlier ones.

then gives

$$\begin{cases} b_1 = (1/\tau) - \tau + 2\tau^2 - (22/3)\tau^3 + \dots, \\ h_1/h_0 = 1 - 4\tau + 28\tau^2 + \dots. \end{cases} \quad (27)$$

We shall return to the question of the asymptotic expansions in Sec. III but already wish to point out here that the b_1 value in (27) is exact as far as the first three terms are concerned (the fourth one is wrong by a factor 44/45—it ought to be $-(15/2)\tau^3$).

II. THE VARIATIONAL METHOD APPLIED TO HIGHER EIGENVALUES

Returning to Eq. (1) with boundary conditions (2), we assume that the lowest eigenvalue is b_1 and the corresponding eigenfunction ϕ_1 . To obtain the next eigenvalue b_2 with its eigenfunction ϕ_2 , one may then proceed as follows. Take an arbitrary function ϕ which satisfies the boundary conditions (2), and calculate J according to (5). J is then minimized with the accessory conditions (6) and

$$M = \int_0^\infty \phi(x)v(x)\phi_1(x)dx = 0, \quad (28)$$

which expresses the orthogonality of ϕ and ϕ_1 .

Introducing lagrange multipliers λ and μ , we write the necessary condition for minimum of J

$$\delta J - \lambda \delta N - \mu \delta M = 0, \quad (29)$$

or after partial integrations

$$\int_0^\infty \delta\phi \left\{ \left[\frac{d^2}{dx^2} + a + \lambda v(x) \right] \phi + \frac{\mu}{2} v(x) \phi_1 \right\} dx = 0. \quad (30)$$

This is valid for all $\delta\phi$ only if

$$\left[\frac{d^2}{dx^2} + a + \lambda v(x) \right] \phi + \frac{\mu}{2} v(x) \phi_1 = 0. \quad (31)$$

A comparison with (1) suggests that $\mu=0$, which can be confirmed in the following way.‡ Multiplying (31) by ϕ , we have after partial integrations, making use of (2),

$$\begin{aligned} \int_0^\infty \phi \left(\frac{d^2\phi_1}{dx^2} + a\phi_1 \right) dx + \lambda \int_0^\infty \phi_1 v(x) \phi dx \\ + \frac{\mu}{2} \int_0^\infty v(x) \phi_1^2 dx = 0, \end{aligned}$$

or, since b_1 is the eigenvalue connected with the eigenfunction ϕ_1 ,

$$\frac{\mu}{2} \int_0^\infty v(x) \phi_1^2 dx + (\lambda - b_1) \int_0^\infty \phi_1 v(x) \phi dx = 0,$$

‡ See, for example, reference 12, p. 258.

TABLE II.

$(-a)^{\frac{1}{2}}$	b_2	$b_2 - 2\alpha$	h_1/h_0	h_2/h_0	h_3/h_0	$(\sigma_0 - 1) \cdot 10^3$	$(\sigma_\infty - 1) \cdot 10^3$
0	6.44849 ₀	4.44849 ₀	-0.33674	-3.47154	—	+15.15	-3.18
0	6.44771 ₅	4.44771 ₅	-0.47238	-2.99632	-0.36459	+5.24	-11.26
0.25	7.63588	4.63588	-0.03277	-3.14148	—	+17.41	+5.07
0.25	7.63399 ₆	4.63399 ₆	-0.27719	-2.39865	-0.50719	+3.75	-14.21
0.5	8.77351 ₉	4.77351 ₉	+0.1707 ₆	-2.9760 ₂	—	+18.12	+15.33
0.5	8.77057 ₅	4.77057 ₅	-0.1828 ₁	-2.0106 ₉	-0.5978 ₇	+2.72	-17.90
4	23.442 ₀	5.442 ₀	+1.770	-3.52 ₁	—	+8.5	+260
4	23.439 ₆	5.439 ₆	-0.029	-0.66 ₆	-0.846	-0.5	-50.5
9	43.675 ₈	5.675 ₃	-3.74	-5.30	—	+1050	-5780
9	43.674 ₄	5.674 ₄	-0.10	-0.26	-0.91	-8	-76

which gives, considering (6) and (28):

$$\mu = 0. \quad (32)$$

Equation (31) then becomes identical with (1). Multiplying (31) by ϕ and integrating we obtain

$$\lambda = J_{\text{extremal}}/N. \quad (33)$$

Equation (32) means that the orthogonality condition need not enter into the practical calculations. Thus, the problem of the higher eigenvalues and eigenfunctions can be treated by the formalism already developed in Sec. I, the lowest eigenvalue but one being approximated by the second root λ_2 of the equation system (12).^{||} The approximate eigenfunctions ϕ_2 and ϕ_1 are then automatically orthogonal, as may be directly proved in the following way.

Let ϕ be linear in the parameters c_ν . J and N are then homogeneous quadratic functions of the parameters:

$$\begin{cases} J = \sum_{\mu} \sum_{\nu} j_{\mu\nu} c_{\mu} c_{\nu} \\ N = \sum_{\mu} \sum_{\nu} n_{\mu\nu} c_{\mu} c_{\nu} \end{cases} \quad (34)$$

with symmetrical coefficients $j_{\mu\nu}$ and $n_{\mu\nu}$. The expression for M is

$$M = \sum_{\mu} \sum_{\nu} n_{\mu\nu} c_{\mu}^{(2)} c_{\nu}^{(1)}, \quad (35)$$

where $n_{\mu\nu}$ are the same quantities as in (34), and the coefficients $c_{\nu}^{(1)}$, $c_{\mu}^{(2)}$ characterize the functions ϕ_1 and ϕ_2 , respectively. If each of the two sets of coefficients makes J stationary, with N constant, then according to

(12) the following equations are satisfied:

$$\sum_{\nu} j_{\mu\nu} c_{\nu}^{(1)} - \lambda_1 \sum_{\nu} n_{\mu\nu} c_{\nu}^{(1)} = 0,$$

$$\sum_{\nu} j_{\mu\nu} c_{\nu}^{(2)} - \lambda_2 \sum_{\nu} n_{\mu\nu} c_{\nu}^{(2)} = 0.$$

Multiplying the first equation by $c_{\mu}^{(2)}$, the second by $c_{\mu}^{(1)}$, summing μ from 1 to n and subtracting, we obtain

$$(\lambda_2 - \lambda_1) \sum_{\mu} \sum_{\nu} n_{\mu\nu} c_{\mu}^{(1)} c_{\nu}^{(2)} = 0;$$

thus, either $\lambda_2 = \lambda_1$, or $M = 0$.

This implies that one of the parameters $c_{\nu}^{(2)}$ is used up in making ϕ_2 orthogonal to ϕ_1 , whence the number of effective parameters available for approximating b_2 and ϕ_2 is only $n-2$, against $n-1$ for b_1 and ϕ_1 . If the same number of parameters is used, b_2 and ϕ_2 are always less accurate than b_1 and ϕ_1 . This is illustrated by a comparison between Tables I and II.

It should also be pointed out that the convergence region is much smaller in the case of higher eigenvalues, therefore the eigenvalue must already be known with fair accuracy before the procedure is started.

III. THE ASYMPTOTIC EXPANSIONS FOR LARGE EIGENVALUES

With the variational method we obtained an approximate asymptotic expansion (27) for the eigenvalue b_1 in terms of the parameter τ , defined in (26). The simplicity of the expression for b_1 suggests that τ is an appropriate parameter, whence we use this parameter τ in the following discussion, which is otherwise quite independent of the variational method.

TABLE III.

$(-a)^{\frac{1}{2}}$	b_3	$b_3 - 3\alpha$	h_1/h_0	h_2/h_0	h_3/h_0	$(\sigma_0 - 1) \cdot 10^3$	$(\sigma_\infty - 1) \cdot 10^3$
0	14.37 ₃	11.37 ₃	-1.20 ₄	-13.04 ₃	+17.17 ₉	+42	+20
0.25	16.221 ₅	11.721 ₅	-0.422	-11.988	+14.006	+42	+38
0.5	17.99	11.99	+0.16	-11.73	+12.49	+42	+67

^{||} In treating the case $v(x) = e^{-x}/x$ [Eq. (14)] a first approximation for b_2 and b_3 was obtained from earlier results,⁴ including a comparison with the exact solutions in the case $v(x) = e^{-x}/(1 - e^{-x})$. Alternatively, the asymptotic expansion of b_2 could be used, especially for large a (see Sec. III).

First, we transform Eq. (14) by introducing

$$\begin{cases} \phi(x) = \exp[-(-a)^{\frac{1}{2}}x]\omega(\xi) \\ \xi = 1 - e^{-x} \end{cases} \quad (36)$$

and obtain the following equation

$$(1-\xi)\frac{d^2\omega}{d\xi^2} - \alpha\frac{d\omega}{d\xi} - b\frac{1}{\ln(1-\xi)}\omega = 0, \quad (37)$$

$$\alpha = 1 + 2(-a)^{\frac{1}{2}} \geq 1$$

with the boundary conditions

$$\omega(0) = 0, \quad (1-\xi)^{(-\alpha)^{\frac{1}{2}}}\omega(\xi) \rightarrow 0, \quad \text{as } \xi \rightarrow 1. \quad \P (38)$$

We start by studying the extreme limiting case $\alpha = \infty$ or $\tau = 0$. Putting

$$\lim_{\alpha \rightarrow \infty} (b/\alpha) = \lim_{\tau \rightarrow 0} b\tau = m, \quad (39)$$

we write (37) as follows:

$$(d\omega/d\xi) + [m/\ln(1-\xi)]\omega = 0. \quad (40)$$

The general solution of (40) is

$$\begin{aligned} \omega = \Omega(\xi) &= C \exp\left\{-m \int [d\xi/\ln(1-\xi)]\right\} \\ &= C \exp[m \operatorname{li}(1-\xi)]. \end{aligned} \quad (41)$$

If the eigenfunctions and eigenvalues of (37) depend analytically on τ , every such eigenfunction must pass into a function (41), when $\tau \rightarrow 0$. Thus, we see that m must be a finite number $\neq 0$; otherwise, (40) would only have the trivial solution $\omega(\xi) \equiv 0$. Furthermore, the eigenvalue b can be expressed as a power series in τ , say,

$$b = (\beta_{-1}/\tau) + \beta_0 + \beta_1\tau + \beta_2\tau^2 \cdots, \quad \beta_{-1} = m. \quad (42)$$

The point $\xi = 0$ is a regular singularity of Eq. (37), and in the neighborhood of $\xi = 0$ we have a regular integral of the following type

$$\omega(\xi) = \sum_{\nu=\nu_0, \nu_0+1, \dots}^{\infty} \omega_{\nu} \xi^{\nu} \quad (43)$$

(ν_0 a priori not necessarily an integer). Inserting this in Eq. (37), we get the recurrence formula

$$\nu(\nu+1)\omega_{\nu+1} = (\nu(\nu+\alpha-1)-b)\omega_{\nu} - b \sum_{\mu=\nu_0}^{\nu-1} L_{\nu-\mu}\omega_{\mu}, \quad (44)$$

\P It seems that the last condition can be replaced by $\omega(1)$ finite, without changing the results (see reference 4, p. 3, footnote).

where the coefficients L_{λ} are defined by

$$\begin{cases} L(x) = -\frac{x}{\ln(1-x)} = \sum_{\lambda=0}^{\infty} L_{\lambda}x^{\lambda}; \\ L_0 = 1, \\ L_{\lambda} = -\left(\frac{1}{2}L_{\lambda-1} + \frac{1}{3}L_{\lambda-2} + \cdots + 1/(\lambda+1)L_0\right).^{**} \end{cases} \quad (45)$$

From (44) we obtain, choosing $\nu = \nu_0 - 1$, the indicial equation $(\nu_0 - 1)\nu_0 = 0$. However, putting $\nu = \nu_0 = 0$ in (44), we have: $\omega_{\nu_0} = 0$. Thus, the only possibility is

$$\omega(\xi) = \sum_{\nu=1}^{\infty} \omega_{\nu} \xi^{\nu}. \quad (46)$$

This solution satisfies the first of the boundary conditions (38). Inversely, all solutions of (37) vanishing at $\xi = 0$ can be expressed in the form of (46). $\dagger\dagger$

The second boundary condition (38) is too complicated to be directly used for determining the eigenvalues. However, we know that the solution in the limiting case $\tau = 0$ is given by (41). Using

$$\operatorname{li}(1-\xi) = \ln\xi + \sum_{\mu=1}^{\infty} \frac{L_{\mu}}{\mu} \xi^{\mu} - \sum_{\mu=1}^{\infty} \frac{L_{\mu}}{\mu}, \quad (47)$$

which follows from (45), we can rewrite (41):

$$\Omega(\xi) = C \xi^m \exp\left(m \sum_{\mu=1}^{\infty} \frac{L_{\mu}}{\mu} \xi^{\mu}\right). \quad (48)$$

When τ tends to zero, every eigenfunction must pass into this form. As all eigenfunctions can be represented by (46), this is only possible if m (defined in (39)) is a positive integer. Furthermore, when $\tau \rightarrow 0$, the quantities ω_{ν} must have finite limits, viz., the coefficients in the Maclaurin expansion of (48). This puts a very heavy restriction on the ω_{ν} 's. Indeed, assuming that they depend analytically on τ , we can express ω_{ν} as a power series without negative powers of τ :

$$\omega_{\nu} = \sum_{\lambda=0}^{\infty} \omega_{\nu, \lambda} \tau^{\lambda}. \quad (49)$$

Inserting this in (44) and using (42), we obtain the

** The first L_{μ} 's are:

$$\begin{array}{ll} L_0 = 1, & L_6 = -3/160, \\ L_1 = -\frac{1}{2}, & L_7 = -863/2^5 \cdot 3^3 \cdot 7 \cdot 10, \\ L_2 = -1/12, & L_8 = -275/2^7 \cdot 3^3 \cdot 7, \\ L_3 = -1/24, & L_9 = -33953/2^6 \cdot 3^4 \cdot 700, \\ L_4 = -19/720, & L_{10} = -8183/2^7 \cdot 3^4 \cdot 100. \end{array}$$

$\dagger\dagger$ The other regular integral of (37) can be written as

$$\chi(\xi) = \omega(\xi) \ln\xi + \sum_{\mu=0}^{\infty} \chi_{\mu} \xi^{\mu}, \quad \chi_0 \neq 0,$$

where $\omega(\xi)$ is given by (46).

following recurrence formula:

$$n(n+1)\omega_{n+1,\mu} = n(n-2)\omega_{n,\mu} + n\omega_{n,\mu+1} - \sum_{\nu=1}^n L_{n-\nu} \sum_{\kappa=1}^{\mu} \beta_{\kappa}\omega_{\nu,\mu-\kappa} \quad (50)$$

$(n=1, 2, 3, \dots; \mu=0, 1, 2, \dots)$.

This makes it possible to calculate all quantities β_{μ} and

$\omega_{\nu,\lambda}$ in terms of the first non-vanishing coefficient in ω_1 , say, $\omega_{1,m-1}$. Here it is, of course, essential to use the condition that no negative powers are allowed to appear in (49). In this way we obtain the m 'th eigenvalue b_m and its appending eigenfunction.

A more practical way to calculate the solutions is as follows. The coefficients $\omega_{\nu,0}$ can be directly taken from the Maclaurin expansion of (41) ($m=1, 2, 3, \dots$). Putting C in (48) = 1, we have:

$$\left. \begin{aligned} \omega_{1,0} &= \omega_{2,0} = \dots = \omega_{m-1,0} = 0 \\ \omega_{m,0} &= 1 \\ \omega_{m+1,0} &= -\frac{m}{2} \\ \omega_{m+2,0} &= \frac{m(3m-1)}{24} \\ \omega_{m+3,0} &= -\frac{m(3m^2-3m+2)}{16 \cdot 9} \\ \omega_{m+4,0} &= \frac{m(15m^3-30m^2+45m-38)}{2^6 \cdot 3^2 \cdot 10} \\ \omega_{m+5,0} &= -\frac{m(90m^4-300m^3+750m^2-1340m+1296)}{2^7 \cdot 3^3 \cdot 100} \\ \omega_{m+6,0} &= \frac{m(630m^5-3150m^4+11550m^3-32690m^2+65212m-69040)}{2^9 \cdot 3^4 \cdot 7 \cdot 100} \\ \omega_{m+7,0} &= -m \cdot \frac{7m(45m^5-315m^4+1575m^3-6265m^2+19348m-41716)+330000}{2^9 \cdot 3^4 \cdot 49 \cdot 100} \\ &\text{etc.} \end{aligned} \right\} \quad (51)$$

It is easy to prove that

$$\omega_{\nu,\lambda} = 0, \quad \text{if } \nu + \lambda < m. \quad (52)$$

Furthermore, ω_1 in (46) includes an indefinite normalizing factor, and here it is convenient to choose $\omega_1 = \tau^{m-1}$, that is,

$$\omega_{1,\nu} = \begin{cases} 1, & \nu = m-1, \\ 0, & \nu \neq m-1. \end{cases} \quad (53)$$

Putting $n=1$ in (50) we thus obtain:

$$2\omega_{2,\mu} = -\omega_{1,\mu} + \omega_{1,\mu+1} - \beta_{\mu-m+1}, \quad (54)$$

which gives, combined with (42) and (53):

$$\beta_{\nu} = \begin{cases} 0, & \nu < -1, \\ 1 - 2\omega_{2,m-2}, & \nu = -1, \\ -1 - 2\omega_{2,m-1}, & \nu = 0, \\ -2\omega_{2,\nu+m-1}, & \nu > 0. \end{cases} \quad (55)$$

$\omega_{\nu,\lambda}$ and β_{μ} can now be successively calculated from (50), starting with those which have $\nu + \lambda = m$, then $\nu + \lambda = m + 1$, etc. In determining the quantities β_{μ} , i.e., $\omega_{2,m-2}$, $\omega_{2,m-1}$, \dots , it is important to observe that $\omega_{n,\mu+1}$ cancels out of (50), if we take $n=m$.

Among those results which are generally valid we mention

$$\omega_{\nu,m-\nu} = \frac{(-1)^{\nu-1}}{\nu!} \binom{m-1}{\nu-1}. \quad (56)$$

Specially for $\nu=m$:

$$\omega_{m,0} = \frac{(-1)^{m-1}}{m!}. \quad (57)$$

The condition (53), thus, implies that Ψ must be chosen $= (-1)^{m-1}/m!$ in (48), whence the quantities in (51) should be multiplied by the same factor.

For $m=1, 2$, and 3 , the following results are obtained.

Lowest eigenvalue.

$$b_1 = \frac{1}{\tau} - \tau + 2\tau^2 - \frac{15}{2}\tau^3 + 33\tau^4 - \frac{1001}{6}\tau^5 + \frac{2783}{3}\tau^6 \dots \quad (58)$$

$$\omega_1 = 1$$

$$\omega_2 = -\frac{1}{2} + \frac{1}{2}\tau - \tau^2 + \frac{15}{4}\tau^3 - \frac{33}{2}\tau^4 + \frac{1001}{12}\tau^5 - \frac{2783}{6}\tau^6 \dots$$

$$\omega_3 = \frac{1}{12} - \frac{1}{3}\tau + \frac{25}{24}\tau^2 - \frac{13}{3}\tau^3 + \frac{1511}{72}\tau^4 - \frac{1018}{9}\tau^5 \dots$$

$$\omega_4 = -\frac{1}{72} + \frac{5}{72}\tau - \frac{19}{48}\tau^2 + \frac{911}{16 \cdot 27}\tau^3 - \frac{5165}{16 \cdot 27}\tau^4 \dots$$

$$\omega_5 = -\frac{1}{720} + \frac{1}{80}\tau - \frac{29}{360}\tau^2 + \frac{311}{540}\tau^3 \dots$$

$$\omega_6 = -\frac{31}{8 \cdot 27 \cdot 100} + \frac{1}{1200}\tau - \frac{49}{5400}\tau^2 \dots$$

$$\omega_7 = -\frac{859}{16 \cdot 81 \cdot 7 \cdot 100} + \frac{1073}{16 \cdot 81 \cdot 7 \cdot 100}\tau \dots$$

$$\omega_8 = -\frac{8669}{32 \cdot 81 \cdot 49 \cdot 100} \dots$$

Second eigenvalue.

$$b_2 = \frac{2}{\tau} + 4 - 8\tau + 40\tau^2 - 290\tau^3 + 2484\tau^4 - \frac{71428}{3}\tau^5 \dots \quad (59)$$

$$\omega_1 = \tau$$

$$\omega_2 = -\frac{1}{2} + \frac{5}{2}\tau + 4\tau^2 - 20\tau^3 + 145\tau^4 - 1242\tau^5 + \frac{35714}{3}\tau^6 \dots$$

$$\omega_3 = \frac{1}{2} - \frac{4}{3}\tau + \frac{10}{3}\tau^2 - \frac{29}{2}\tau^3 - 88\tau^4 + \frac{5453}{9}\tau^5 \dots$$

$$\omega_4 = -\frac{5}{24} + \frac{1}{18}\tau - \frac{25}{72}\tau^2 + \frac{58}{9}\tau^3 - \frac{8881}{4 \cdot 27}\tau^4 \dots$$

$$\omega_5 = \frac{1}{18} - \frac{161}{720}\tau + \frac{137}{90}\tau^2 - \frac{14869}{4 \cdot 27 \cdot 10}\tau^3 \dots$$

$$\omega_6 = -\frac{13}{1440} + \frac{2083}{16 \cdot 27 \cdot 10}\tau - \frac{9481}{4 \cdot 27 \cdot 100}\tau^2 \dots$$

$$\omega_7 = \frac{287}{8 \cdot 27 \cdot 7 \cdot 100} - \frac{8609}{8 \cdot 81 \cdot 7 \cdot 100}\tau \dots$$

$$\omega_8 = \frac{451}{32 \cdot 81 \cdot 7 \cdot 100} \dots$$

Third eigenvalue.

$$b_3 = \frac{3}{\tau} + 12 - 27\tau + 222\tau^2 - \frac{4929}{2}\tau^3 + 31887\tau^4 \dots \quad (60)$$

$$\omega_1 = \tau^2$$

$$\omega_2 = -\tau - \frac{13}{2}\tau^2 + \frac{27}{2}\tau^3 - 111\tau^4 + \frac{4929}{4}\tau^5 - \frac{31887}{2}\tau^6 \dots$$

$$\omega_3 = \frac{1}{6} - \frac{10}{3}\tau + \frac{29}{4}\tau^2 - 3\tau^3 - \frac{595}{8}\tau^4 + 1633\tau^5 \dots$$

$$\omega_4 = -\frac{1}{4} + \frac{41}{12}\tau - \frac{11}{8}\tau^2 - \frac{145}{8}\tau^3 + \frac{4545}{16}\tau^4 \dots$$

$$\omega_5 = \frac{1}{6} - \frac{19}{12}\tau + \frac{149}{80}\tau^2 - \frac{1519}{80}\tau^3 \dots$$

$$\omega_6 = \frac{5}{72} - \frac{27}{80}\tau + \frac{1843}{2400}\tau^2 \dots$$

$$\omega_7 = \frac{29}{1440} - \frac{43}{2400}\tau \dots$$

$$\omega_8 = \frac{67}{14400} \dots$$

We have not been able to prove that these expansions converge; they are most likely to be semiconvergent. At any rate, the eigenvalues obtained in this way agree, for reasonably small values of τ , with those calculated by the variational method, as may be clear from Table IV.

An alternative method to bring out the asymptotic expansions by successive approximations should also be indicated. Introducing τ according to (26) in Eq. (37), we have

$$\tau(1-\xi) \frac{d^2\omega}{d\xi^2} - (1-\tau) \frac{d\omega}{d\xi} - \frac{b\tau}{\ln(1-\xi)} \omega = 0. \quad (61)$$

TABLE IV.

τ	Variational method 3 param.	b_1		Variational method 3 param.	b_2	
		Asymptotic expansion Eq. (58)	Last term omitted		Asymptotic expansion Eq. (59)	Last term omitted
0.2	4.847	4.879	4.819			
0.125	7.8966	7.8981	7.8946			
0.1	9.9147	9.9151	9.9141	23.44	23.32	23.56
0.05	19.954227 ₈	19.954231	19.954217	43.674 ₄	43.671	43.679

We now take

$$\omega(\xi) = \sum_{\nu=0}^{\infty} f_{\nu}(\xi) \cdot \tau^{\nu}, \quad (62)$$

and insert this in (61), replacing b by (42). Arranging according to powers of τ and annihilating the coefficient of τ^n , we get the following equation for $f_n(\xi)$ ($n=0, 1, 2, \dots$):

$$f_n' + m/[\ln(1-\xi)] \cdot f_n = F_n, \quad (63)$$

with

$$F_n = (1-\xi)f_{n-1}'' + f_{n-1}' - \frac{1}{\ln(1-\xi)} \sum_{\mu=1}^n \beta_{\mu-1} f_{n-\mu}, \quad (64)$$

which contains f_0, f_1, \dots, f_{n-1} and $\beta_0, \dots, \beta_{n-1}$. For $n=0$, (63) reduces to (40), with the solution (41) (or (48)). The general solution of (63) is

$$f_n(\xi) = f_0(\xi) \left\{ C_n + \int [F_n(\xi)/f_0(\xi)] d\xi \right\}, \quad (65)$$

where C_n can be put $=0$, because its only effect is to change the constant factor of f_0 . Thus, the eigenfunctions can be obtained asymptotically for small τ by successive approximations in terms of the coefficients β_{μ} . These quantities can then be determined from the boundary condition (38), which implies that all $f_n(\xi)$ must vanish at $\xi=0$. However, this way of determining the eigenvalues turns out to be more complicated than the procedure used above. On the other hand, once the coefficients β_{-1}, β_0 , etc., are known, the expression (65) gives more information about the eigenfunctions than do the expansions (58a)–(60a).

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BIBLIOGRAPHY

- (1) N. Kemmer, Proc. Cambridge Phil. Soc. **34**, 364 (1938). (Calculations by Miss Littleton.)
- (2) A. H. Wilson, Proc. Cambridge Phil. Soc. **34**, 365–374 (1938).
- (3) R. Sachs and M. Goepfert-Mayer, Phys. Rev. **53**, 991–993 (1938).
- (4) L. Hulthén, Arkiv Mat., Astron. Fysik **23A**, No. 5, 1–12 (1942).
- (5) E. A. Hylleraas and V. Risberg, Avhandl. Norsk Videnskaps-Akad. Oslo I, No. 3 (1941).
- (6) L. Hulthén, K. Fysiograf. Sällsk. Lund. Förhandlingar **15**, Nr 22, 6–8 (Printed by Håkan Ohlsson, Lund, 1945).
- (7) E. A. Hylleraas, Fra Fysikkens Verden **7** (Printed by Grøndahl & Son, Oslo, 1945), 175–179.
- (8) L. Rosenfeld, *Nuclear Forces* (North-Holland Publishing Company, Amsterdam, 1948), chapter V.
- (9) I. F. E. Hansson and L. Hulthén, Phys. Rev. **76**, 1163–1165 (1950); L. Hulthén, Phys. Rev. **79**, 166–167 (1950); I. F. E. Hansson, Phys. Rev. **79**, 909–910 (1950).
- (10) N. Zeilon, Lunds Universitets årskrift, New Series, Sec. 2, Vol. 43, Nr 10, (C. W. K. Gleerup, Lund, 1947), and unpublished manuscript. One of the authors (L.H.) is indebted to Prof. Zeilon for discussions on the Rayleigh-Ritz method.
- (11) R. Courant und D. Hilbert, *Methoden der Mathematischen Physik I* (Berlin, Julius Springer, 1931), second edition, chapter 6.
- (12) H. Margenau and G. M. Murphy, *The Mathematics of Physics and Chemistry* (D. Van Nostrand Company, Inc., New York, 1943), pp. 256ff.