NUCLEAR SCIENCE AND ENGINEERING: **13,** 197–200 (1962)

Letters to the Editors

Eigenvalues for the Wilkins Equation

In the study of thermalization problems based on the heavy gas scattering kernel for a $1/v$ absorber one is often faced with the task of solving for the eigenvalues, α^2, of the following equation

$$\epsilon\phi'' + \epsilon\phi' + [1 + \alpha^2 - \Delta/(4\sqrt{\epsilon})]\phi = 0 \qquad (1)$$

where ϵ is the energy in units of kT and Δ is the usual absorption parameter, i.e., $\Delta = 4\sigma_a(kT)/(\xi\sigma_0)$. The general problem has been considered by many investigators (*1–5*). In particular Michael considered the numerical solutions of the secular equation resulting from Eq. (1) by assuming solutions of the form $\phi = \sum_m A_m\, \epsilon \exp(-\epsilon) L_m^{(1)}(\epsilon)$ where $L_m^{(1)}(\epsilon)$ are the associated Laguerre polynomials. It can be shown that this is equivalent to a variational solution and hence the calculated fundamental eigenvalue is necessarily an upper bound to the true eigenvalue. More recently de Sobrino and Clark (*6*) published an extensive study dealing with the solutions of Eq. (1). Included in their paper is an expression for the eigenvalues of Eq. (1) in the form

$$\alpha_n^2 = n + a_n\Delta + b_n\Delta^2 \qquad (2)$$

with analytical expressions for the coefficients a_n and b_n. In this note we develop a similar expansion for the eigenvalues including the coefficient of the cubic term in Δ. Numerical values for the coefficients in Eq. (2) are given. The fundamental eigenvalue is given to the cubic term in Δ. In addition, a formulation of the eigenvalue in terms of the WKBJ method is also included. In his paper, Michael (*3*) points out that calculations of this type have been previously carried out by Corngold.

To solve Eq. (1), the flux, $\phi(\epsilon)$, and α^2 are expanded in powers of Δ, i.e., $\phi(\epsilon) = \sum \Delta^n\phi_n(\epsilon)$ and $\alpha^2 = \sum \Delta^n a_n$. Substituting the above in Eq. (1) and equating like powers of Δ gives

$$\begin{aligned}\epsilon\phi_n'' + \epsilon\phi_n' + (1 + a_0)\phi_n \\ = [1/(4\sqrt{\epsilon}) - a_1]\phi_{n-1} - a_2\phi_{n-2} - \cdots - a_n\phi_0\end{aligned} \qquad (3)$$

where the right hand side vanishes for $n = 0$. These equations are solved recursively using the conditions of vanishing flux at $\epsilon = 0$ and ∞. If $a_0 = k$ where $k = 0, 1, 2, \cdots$, then ϕ_0 is given by $A_k\, \epsilon \exp(-\epsilon) L_k^{(1)}(\epsilon)$ where the A_k are arbitrary. This solution satisfies the homogeneous boundary conditions. For the solution correct to the first order in Δ, consider Eq. (3) with $n = 1$; that is,

$$\begin{aligned}\epsilon\phi_1'' + \epsilon\phi_1' + (1 + k)\phi_1 \\ = A_k[1/(4\sqrt{\epsilon}) - a_1]\, \epsilon\, e^{-\epsilon} L_k^{(1)}(\epsilon).\end{aligned} \qquad (4)$$

The complimentary integral is given by

$$B_k\, \epsilon\, e^{-\epsilon} L_k^{(1)}(\epsilon) \qquad (5)$$

and for the particular integral assume a solution of the form

$$\phi_1 = \sum_n b_n\, \epsilon\, e^{-\epsilon} L_n^{(1)}(\epsilon) \qquad (6)$$

where the B_k are arbitrary and the b_n are to be determined. Substituting Eq. (6) into (4), multiplying by $L_j^{(1)}(\epsilon)\, d\epsilon$ and using the orthogonality relation,

$$\int_0^\infty \epsilon e^{-\epsilon} L_k^{(1)}(\epsilon) L_j^{(1)}(\epsilon)\, d\epsilon = (1 + k)\delta_{kj},$$

gives

$$(k - j)(1 + j)b_j = A_k[(1/4)v_{jk}^{-1} - a_1(1 + k)\delta_{kj}]. \qquad (7)$$

Solving Eq. (7) gives for

$$k \neq j \qquad b_j = A_k v_{jk}^{-1}/[4(k - j)(1 + j)] \qquad (8)$$

$$\left.\begin{aligned} k = j \qquad & b_k = \text{arbitrary} \\ \text{and} \qquad & a_1 = v_{kk}^{-1}/[4(1 + k)]\end{aligned}\right. \qquad (9)$$

where

$$v_{jk}^{-1} = \int_0^\infty x e^{-x} L_j^{(1)}(x)(1/\sqrt{x}) L_k^{(1)}(x)\, dx. \qquad (10)$$

Therefore, summarizing our results, the kth eigenvalue to the first order in Δ is given by

$$\alpha_k^2 = k + \Delta v_{kk}^{-1}/[4(1 + k)] \qquad (11)$$

and similarly the kth eigenfunction is given by

$$\phi_k(\epsilon) = \sum_j b_{jk}\, \epsilon\, e^{-\epsilon} L_j^{(1)}(\epsilon) \qquad (12)$$

where

$$\begin{aligned} b_{jk} &= \Delta v_{jk}^{-1}/[4(k - j)(1 + j)], \qquad k \neq j \\ &= 1, \qquad k = j. \end{aligned} \qquad (13)$$

The arbitrary constant in Eq. (12) was determined by normalization. Carrying out calculations similar to the above, the kth eigenvalue to the third order in Δ is given by

$$\begin{aligned}\alpha_k^2 = k + \frac{\Delta v_{kk}^{-1}}{4(1 + k)} + \frac{\Delta^2}{16(1 + k)} \sum_j{}' \frac{(v_{jk}^{-1})^2}{(k - j)(1 + j)} \\ + \frac{\Delta^3}{64(1 + k)} \left\{ \sum_{j,n}{}' \frac{(v_{jk}^{-1})(v_{nj}^{-1})(v_{kn}^{-1})}{(k - j)(1 + j)(k - n)(1 + n)} \right. \\ \left. - \frac{(v_{kk}^{-1})}{(1 + k)} \sum_j{}' \frac{(v_{jk}^{-1})^2}{(k - j)^2(1 + j)} \right\} + O(\Delta^4)\end{aligned} \qquad (14)$$

TABLE I

EIGENVALUES

$\alpha_k^2 = k + a_1\Delta + a_2\Delta^2 + a_3\Delta^3 + \cdots$

Order, k	a_1	a_2[a]	a_3[a]
0	0.221557	−0.0081912 ± 4	0.00049 ± 2
1	0.193862	−0.00408 ± 1	
2	0.176553	−0.00253 ± 2	
3	0.164220	−0.00175 ± 2	
4	0.154768	−0.00130 ± 3	
5	0.147176	−0.00101 ± 3	
6	0.140878	−0.00081 ± 4	
7	0.135525	−0.00067 ± 5	
8	0.130892	−0.00057 ± 6	
9	0.126821	−0.00049 ± 7	
10	0.123202	−0.00042 ± 8	
11	0.119953	−0.00037 ± 9	
12	0.117012	−0.0003 ± 1	
13	0.114330	−0.0003 ± 1	

[a] Note the uncertainty applies to the last significant digit reported.

TABLE II

FUNDAMENTAL EIGENFUNCTION

$$\phi_0 = \sum_j d_{j0}\, \epsilon e^{\epsilon} L_j^{(1)}(\epsilon)$$

$$d_{j0} = a_1\Delta(1 + a_2\Delta), \qquad j \neq 0$$

$$d_{00} = 1 + a_2\Delta^2$$

j	a_1	a_2[a]
0	—	−0.003468
1	0.0553892	−0.0164 ± 1
2	0.0138477	−0.1582 ± 1
3	0.0057697	−0.2070 ± 3
4	0.0030290	−0.2317 ± 4
5	0.0018174	−0.2467 ± 5
6	0.0011900	−0.2567 ± 7

[a] Note the uncertainty applies to the last significant digit reported.

where the primes on the summations indicate $j, n \neq k$. The eigenfunction to second order in Δ is given by

$$\phi_k(\epsilon) = \sum_j d_{jk}\, \epsilon\, e^{-\epsilon} L_j^{(1)}(\epsilon)$$

where

$$d_{kk} = 1 - \frac{\Delta^2}{32(1+k)} \sum_j{}' \frac{(v_{jk}^{-1})^2}{(k-j)^2(1+j)} \qquad (15)$$

and for $k \neq j$

$$d_{jk} = \frac{\Delta v_{jk}^{-1}}{4(k-j)(1+j)} + \frac{\Delta^2}{16(k-j)(1+j)} \sum_n{}' \cdot \frac{v_{nk}^{-1} v_{nj}^{-1}}{(k-n)(1+n)} - \frac{\Delta^2 v_{kk}\, v_{jk}}{16(k-j)^2(1+k)(1+j)}.$$

Before proceeding with the numerical evaluation of the above some comments on the matrix elements v_{jk}^{-1} are necessary. Using the series definition for the Laguerre polynomials

$$L_j^{(1)}(x) = \sum_{n=0}^{j} \binom{j+1}{j-n} (-x)^n/n!$$

Eq. (10) becomes

$$v_{jk}^{-1} = \sum_{n=0}^{j} \binom{j+1}{j-n} [(-1)^n/(n!)] \int_0^\infty x^{n+1/2} e^{-x} L_k^{(1)}(x)\, dx. \qquad (16)$$

The integral in Eq. (16) is of the standard form and is given by Bateman (7), substituting for the integral, Eq. (16) becomes

$$v_{jk}^{-1} = \sum_{n=0}^{j} \binom{j+1}{j-n} \frac{(-1)^n\, \Gamma(k-n+\frac{1}{2})\Gamma(n+3/2)}{n!\, k!\, \Gamma(\frac{1}{2}-n)}. \qquad (17)$$

By the use of the generating function for the Laguerre polynomials, Häfele and Dresner (5) have previously derived an equivalent expression for the v_{jk}^{-1}'s. Using the definition for the gamma functions and noting that for $k \geq n$

$$\frac{\Gamma(k-n+\frac{1}{2})}{\Gamma(\frac{1}{2}-n)} = \frac{(-1)^n(2k-2n)!\,(2n)!}{\{2^{2k}(k-n)!\,n!\}}. \qquad (18)$$

The restriction that $k \geq n$ introduces no particular difficulty since v_{jk}^{-1} is symmetrical. Therefore, the final expres-

TABLE III

COMPARISON OF EIGENVALUES

Δ	α_0^2		α_1^2		α_2^2	
	M	G	M	G	M	G
0.25	0.0549	0.05488	1.0483	1.0482	2.0441	2.0440
0.5	0.1089	0.1088	1.0961	1.0959	2.0880	2.0876
1	0.2140	0.2138	1.1904	1.1898	2.1754	2.1740
2	0.4144	0.4142	1.3736	1.3714	2.3471	2.3430
3	0.6031	0.604	1.5492	1.5449	2.5135	2.5069
4	0.7819	0.786	1.7178	1.7102	2.6740	2.6657
5	0.9523	0.964	1.8799	1.867	2.8286	2.820
10	1.7124	1.88	2.6156	2.531	3.5359	3.513

Note: The values designated by M were calculated by Michael, for the most part they were obtained from the diagonalization of a 5 × 5 matrix. G indicates the values obtained by this work.

sion for v_{jk}^{-1} is given by

$$v_{kj}^{-1} = \frac{(j+1)\Gamma(\frac{1}{2})}{2^{2k}\,k!} \sum_{n=0}^{j} \cdot \frac{(2n+1)!(2k-2n)!(2n)!}{(j-n)!(n+1)(n!)^4(k-n)!2^{2n+1}}, \qquad k \geqq j \qquad (19)$$

where $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. Examination of Eq. (19) shows that

$$v_{kk}^{-1} \to \sqrt{k} \ln k \text{ as } k \to \infty. \qquad (20)$$

Using Stirling's approximation to the factorials similarly it can be shown that

$$v_{k0}^{-1} = 1/\sqrt{4k}, \qquad k \gg 1. \qquad (21)$$

The following relation involving the v_{jk}^{-1}'s is of interest in numerical calculations. By orthogonality it can be shown that

$$\frac{L_j^{(1)}(x)}{\sqrt{x}} = \sum_{n=0}^{\infty} \frac{v_{jn}^{-1}\, L_n^{(1)}(x)}{(1+n)}. \qquad (22)$$

Squaring the above and multiplying by $x \exp(-x)$ and integrating gives

$$j + 1 = \sum_{k=0}^{\infty} \frac{(v_{jk}^{-1})^2}{(1+k)}. \qquad (23)$$

Equation (23) is useful in obtaining crude estimates of the convergence of sums involving the matrix elements v_{jk}^{-1}.

With a tabulation of the v_{ij}^{-1}'s it is a simple matter to calculate the sums as given in Eqs. (14) and (15). For the fundamental eigenvalue, $k = 0$, the expression for a_2 is readily evaluated by summing the first several terms exactly and then summing the remaining terms by the use of Euler's summation formula using Eq. (21). The expression for a_3 for $k = 0$ is evaluated in a similar fashion and also by recognizing that v_{jk}^{-1} is a decreasing function for increasing j for $j > k$. The higher order eigenvalues were evaluated only to the second order in Δ. The expression for a_2 was evaluated by summing the first 40 terms exactly and then using Euler's summation formula to get an upper estimate of the remainder. The coefficients for the eigenvalues are summarized in Table I. It should be noted that, as the order of the eigenvalue increases, the coefficient of Δ^2 decreases quite rapidly and that for moderate values of Δ the first order coefficient a_1 is sufficient. Using

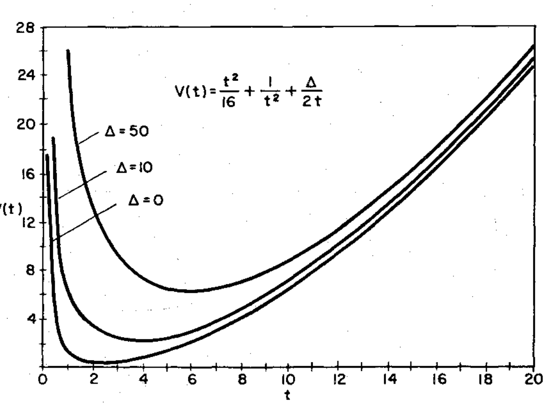

FIG. 1. "Potential function" for the Wilkins equation

TABLE IV

COMPARISON OF EIGENVALUES

Δ	α_0^2	
	WKBJ	Michael
0.1^a	0.0242	0.02208
10	1.720	1.7124
50	5.88	
500	30.2	

[a] Equation (14) gives a value of 0.022068.

the asymptotic form for v_{kk}^{-1}, Eq. (20), and applying l'Hospital's rule it should be noted that $a_1 \to 0$ for $k \to \infty$ and hence the eigenvalues approach integers.

The second order correction term for the eigenvectors was evaluated in a similar manner to the method used for the eigenvalues. The expressions for the eigenvectors are given in Table II.

A comparison between the eigenvalues calculated in this work and those calculated by Michael is given in Table III. For the most part the values given by Michael were computed by the diagonalization of a 5×5 matrix. The eigenvalues for $\Delta = 10$ were obtained from the diagonalization of a 20×20 matrix. It should be noted for values of Δ up to about 5, the perturbation technique gives eigenvalues which are in agreement to better than 1%.

For large values of Δ, the perturbation technique is of limited value and other techniques must be used. The eigenvalues can be approximated by the WKBJ method as developed for the solution of the eigenvalues of the one-dimensional Schrödinger wave equation for bound particles. The procedure followed here is that used by Morse and Feshbach (*8*) as developed for radial wave equations. The eigenvalues for Eq. (1), $\alpha_n^2 = k^2 - 1$, are given by the solution of

$$\int_{t_1}^{t_2} \left\{ k^2 - \left[\frac{t^2}{16} + \frac{1}{t^2} + \frac{\Delta}{(2t)} \right] \right\}^{1/2} dt = (n + \tfrac{1}{2})\pi \qquad (24)$$

where t_2 and t_1 are value of t for which the integrand of Eq. (24) vanishes. A plot of the "potential function"

$$V(t) = \frac{t^2}{16} + \frac{1}{t^2} + \frac{\Delta}{(2t)}$$

as given in Eq. (24) is shown in Fig. 1. For zero absorption the above integral can be integrated in closed form, giving the condition that $k^2 = n + 1$ or $\alpha_n^2 = n$. The exact eigenvalue for the case of zero absorption. For $\Delta \neq 0$, Eq. (24) can be expressed in terms of elliptic integrals of the third kind, an intractable form for numerical calculations. The integral was evaluated numerically using Simpson's rule for several values Δ and the results are given in Table IV.

The plot of the potential function, $V(t)$, as given in Fig. 1 is convenient for estimating the turning points, t_1 and t_2, and the initial value of the eigenvalue. For $\Delta = 10$, the agreement with the value as calculated by Michael is better than 1%. Examination of Eq. (24) shows that for large values of k^2, the term $(\Delta/2t)$ in the integrand can be neglected in comparison to the other terms and, hence, the integral is equivalent to the case of zero absorption for large values of n. It can, therefore, be concluded that the eigenvalues approach integers; i.e., $\alpha_n{}^2 \to n$ for $n \to \infty$.

REFERENCES

1. H. HURWITZ, JR. AND M. S. NELKIN, *Nuclear Sci. and Eng.* **3,** 1 (1958).
2. M. S. NELKIN, *J. Nuclear Energy* **8,** 48 (1958).
3. P. MICHAEL, *Nuclear Sci. and Eng.* **8,** 426 (1960).
4. N. CORNGOLD AND L. ZAMICK, *Trans. Am. Nuclear Soc.* **3,** 504 (1960).
5. W. HÄFELE AND L. DRESNER, *Nuclear Sci. and Eng.* **7,** 304 (1959).
6. L. DE SOBRINO AND M. CLARK, JR., *Nuclear Sci. and Eng.* **10,** 388 (1961).
7. H. BATEMAN, "Tables of Integral Transforms," Vol. II, p. 292. Compiled by the Staff of the Bateman Project, A. Erdelyi, Editor. McGraw Hill, New York, 1953.
8. P. M. MORSE AND H. FESHBACH, "Methods of Theoretical Physics," Part II. McGraw Hill, New York, 1953.

E. GARELIS

Vallecitos Atomic Laboratory
General Electric Company
Received November 28, 1961
Revised January 31, 1962

Effective Diffusion Coefficient in Void Regions

The multigroup diffusion theory for a virtually critical medium, with homogeneous regions, gives rise to the following system of differential equations (*1, 2*).

$$D_i^l \nabla^2 \phi_i^l - \left(\Sigma_{ia}^l + \sum_{j=i+1}^{g} \Sigma_{i\to j}^l\right)\phi_i^l + \sum_{j=1}^{i-1} \Sigma_{j\to i}^l \phi_i^l + \frac{1}{K}\sum_{j=1}^{g} f_i^l (\nu\Sigma_j)_j^l \phi_j^l = 0 \tag{1}$$

$i = 1, 2, \cdots, g$ (number of groups); $l = 1, 2, \cdots r$ (number of regions), with the boundary conditions of continuity of fluxes and currents at the interfaces.

This system, when applied in one dimensional cylindrical geometry to a void region, $l = v$, with $\Sigma_{xi}^v = 0$, $x = a$, $i \to j, f$, and $D_i^v \to \infty$ (it is assumed to be arbitrarily large in the codes WANDA, AIM-5, $\cdots$), results in

$$D_i^v \nabla^2\phi_i^v = D_i^v \frac{1}{r}\frac{d}{dr}\left(r\frac{d\phi_i^v}{dr}\right) = 0 \tag{2}$$

then

$$\phi_i^v(r) = a_i^v \ln r + b_i^v \tag{3}$$

with the boundary conditions, at the inner interface of radius $r_{v-1} \neq 0, \infty$

$$D_i^{v-1} \nabla\phi_i^{v-1}(r_{v-1}) = D_i^v \nabla\phi_i^v(r_{v-1}) = D_i^v a_i^v r_{v-1}^{-1} \tag{4}$$

$$\phi_i^{v-1}(r_{v-1}) = \phi_i^v(r_{v-1}) = a_i^v \ln r_{v-1} + b_i^v \tag{5}$$

This system of equations determines a_i^v, b_i^v. When $D_i^v \to \infty$, $a_i^v \to 0$, a flux $\phi_i^v \to b_i^v$ = constant is obtained.

Depending on whether the net current flow through the gap is inwards or outwards, this theory overestimates or underestimates the fraction of neutrons entering the void from the outer interface which reaches the inner interface. Actually, current flow through the gap produces a discrete jump in the value of the flux which has been calculated by Newmarch (*3*) to be

$$\phi_i^v(r_v) - \phi_i^v(r_{v-1}) = 2\alpha D_i^{v-1}\nabla\phi_i^{v-1}(r_{v-1}) \tag{6}$$

with

$$r_v D_i^v \nabla\phi_i^v(r_v) - r_{v-1} D_i^v \nabla\phi_i^v(r_{v-1}) = 0 \tag{7}$$

and

$$\alpha = 1 - \frac{2}{\pi}\arc\sin\frac{r_{v-1}}{r_v} - \frac{2}{\pi}\frac{r_{v-1}}{r_v}\left(1 - \frac{r_{v-1}^2}{r_v^2}\right)^{1/2} \tag{8}$$

For this correction to be applied more easily, an effective diffusion coefficient in the void can be considered, which must satisfy Eqs. (4) and (6). Equation (5) can be used to determine b_i^v, and Eq. (7) is always satisfied along with Eq. (3).

Substitution of Eq. (3) into (6), gives

$$a_i^v = \frac{2\alpha D_i^{v-1}\nabla\phi_i^{v-1}(r_{v-1})}{\ln(r_v/r_{v-1})} \tag{9}$$

which substituted into Eq. (4), gives in turn

$$D_{\text{eff}}^v = \frac{r_{v-1}\ln(r_v/r_{v-1})}{2\alpha} = r_{v-1} f(r_{v-1}/r_v) \tag{10}$$

with

$$D_{\text{eff}}^v \to \infty, \quad \text{if } r_{v-1} \to r_v; \quad D_{\text{eff}}^v = (1 \pm 0.2) r_{v-1}, \quad \text{if } 0,15 \leqq r_{v-1}/r_v \leqq 0,85 \tag{11}$$

Therefore, in one-dimensional cylindrical multigroup diffusion equations, void may be represented by purely diffusive media, with cross sections equal to zero, and effective diffusion coefficient given by Eq. (10). In this way the Newmarch correction is taken into account.

REFERENCES

1. O. J. MARLOWE, WAPD-TM-28 (1956).
2. H. P. FLATT, D. C. BALLER, AND E. R. COHEN, NAA-SR-4694 (1960).
3. D. A. NEWMARCH, *J. Nuclear Energy* **2,** 52–58 (1955).

G. VELARDE

Div. Reactores
Junta de Energía Nuclear
Madrid, 3, Spain
Received November 28, 1961