THE NUMERICAL DETERMINATION OF CHARACTERISTIC NUMBERS

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Abstract

A method is developed for the numerical calculation of characteristic energy levels in cases where the wave equation contains, or can be reduced so as to contain, a single space variable. The procedure consists in the numerical integration of an auxiliary differential equation for several chosen values of the energy, after which the characteristic values are obtained by interpolation. The method is one of considerable generality so far as the form of the differential equation is concerned, and is capable of giving any preassigned degree of accuracy.

1. The entrance of wave mechanics into modern physics gives new interest to boundary value problems associated with linear differential equations, especially those problems treated by Weyl[1] and others which have to do with the Sturm-Liouville equation

$$\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right] - q(x)y + \lambda\rho(x)y = 0 \tag{1}$$

in the intervals $0<x<\infty$ or $-\infty<x<\infty$. A problem of particular physical interest is the determination of those characteristic values of λ (eigenwerte) for which (1) possesses solutions that are finite at both ends of the interval.[2] In several important special cases the complete analytical solution of this problem is known,[3] but in other instances it is necessary to resort to approximate methods.

The object of this note is to describe a numerical procedure for obtaining the characteristic values of λ belonging to the equation

$$\frac{d^2u}{dx^2}+G(x,\lambda)u=0. \tag{2}$$

Equation (1) can be reduced to this form by the substitution $y=up^{-1/2}$, provided p has first and second derivatives and does not vanish in the interval.

[1] Weyl, Mathematische Annalen **68,** 220 (1910), and Göttinger Nachrichten, (1910), p. 442. Hilb, Mathematische Annalen **76,** 333 (1915). Milne, Trans. Amer. Math. Soc. **30,** 797 (1928).

[2] Schrödinger, Ann. d. Physik **79,** 361 (1926). See p. 363. Kemble, Phys. Rev. Supplement **1,** 157 (1929), see p. 177.

[3] Cf. e.g. Kemble, reference 2, pp. 183–186. Condon and Morse, Quantum Mechanics, (McGraw-Hill, 1929) Chapter II.

Equation (2) contains as a special case the wave equations of the type

$$\frac{d^2u}{dx^2}+\frac{8\pi^2\mu}{h^2}[W-V(x)]u=0, \tag{3}$$

as is seen by setting

$$\lambda=\frac{8\pi^2\mu W}{h^2}$$

and

$$G(x,\lambda)=\lambda-\frac{8\pi^2\mu}{h^2}V(x).$$

Equation (2), however, is considerably more general than (3).

With regard to $G(x,\lambda)$ we assume that $\partial G/\partial\lambda$ exists and is positive, that $G(x,\lambda)$ is continuous in x, that when $|x|$ is sufficiently large $G(x,\lambda)$ is negative for the values of λ under consideration, and (if the interval is $0<x<\infty$) $\lim_{x=0} G(x, \lambda)=-\infty$.

2. For simplicity we consider only the case in which the interval is $-\infty<x<\infty$. Let x_0 be a value of x in the interval, and let $u_1(x)$ and $u_2(x)$ be two solutions of Eq. (2) satisfying the conditions

$$\begin{aligned} u_1(x_0)&=1, & u_2(x_0)&=0,\\ u_1'(x_0)&=0, & u_2'(x_0)&=a\neq 0. \end{aligned} \tag{4}$$

The constant a is arbitrary and in any particular case is to be determined so as to make the numerical work as simple as possible. These solutions satisfy the well-known identity

$$u_1(x)u_2'(x)-u_2(x)u_1'(x)\equiv a. \tag{5}$$

Let a function $w(x)$ be defined by the equation

$$w(x)=[u_1^2(x)+u_2^2(x)]^{1/2} \tag{6}$$

By differentiating this equation twice, eliminating $u_1''(x)$ and $u_2''(x)$ by means of (2), and simplifying with the aid of (5) we find that the function $w(x)$ satisfies the simple differentiation equation

$$\frac{d^2w}{dx^2}+G(x,\lambda)w-\frac{a^2}{w^3}=0. \tag{7}$$

Now the general solution of (2) can be expressed in the form

$$u(x)=Cw(x)\sin\left\{a\int_{x_0}^{x} w^{-2}dx-\alpha\right\}, \tag{8}$$

in which C and α are arbitrary constants. Since with the given hypotheses $w(x)$ does not approach zero at either end of the interval, it is clear that a solution satisfying the desired conditions at both ends of the interval can be found if and only if

$$\frac{a}{\pi}\int_{-\infty}^{\infty} w^{-2}dx = n \tag{9}$$

in which n is a positive integer.

3. Now the integral

$$N = \frac{a}{\pi}\int_{-\infty}^{\infty} w^{-2}dx \tag{10}$$

is an increasing function of λ, so that if we select k values of λ for which this integral is finite (values of λ for which N is infinite belong to the continuous spectrum and do not interest us here), say $\lambda^1 < \lambda^2 \cdots < \lambda^k$, we obtain k values of N, say $N_1 < N_2 \cdots < N_k$. If an integer n lies in the interval $N_1 < n < N_k$, we may use the method of interpolation to obtain approximately the corresponding value of λ, $\lambda = \lambda_n$, which will be precisely the n-th characteristic value of λ counted in order of magnitude.

To put this plan into execution we proceed as follows:

First, we solve Eq. (7) with the initial conditions $w(x_0) = 1$, $w'(x_0) = 0$ for each of the k values of λ, $\lambda,^1 \lambda^2 \cdots \lambda^k$. For this purpose we may use any one of several well-known methods for the numerical integration of differential equations.

Second, using in turn each of the solutions now obtained, we evaluate by numerical quadrature the integral (10) and get the k values of N, N_1, $N_2, \cdots, N_k$.

Lastly, we obtain by interpolation the values of λ corresponding to each integer in the interval N_1 to N_k.

When the characteristic value of λ has been found it is then possible to integrate (7) using this value of λ and then obtain the corresponding wave function itself by means of (8). As a matter of fact, however, it will generally be easier to obtain $w(x)$ and $\int_0^x w^{-2}\,dx$ by interpolation from the computations already performed.

Naturally the speed and accuracy of the method depend largely on good judgment in the selection of the trial values $\lambda^1, \lambda^2 \cdots \lambda^k$. This is perhaps best illustrated by means of an example.

4. We take as an illustrative example the differential equation

$$\frac{d^2u}{dz^2} + \frac{8\pi^2\mu}{h^2}[W - kz^4]u = 0,$$

which upon the substitutions

$$z = \frac{h^{1/3}}{(8\pi^2\mu k)^{1/6}}x,$$

$$\lambda = \left[\frac{64\pi^4\mu^2}{h^4 k}\right]^{1/3} W,$$

reduces to

$$\frac{d^2u}{dx^2}+(\lambda-x^4)u=0.$$

For simplicity we choose $x_0=0$, $a=\lambda^{1/2}$, so that equation (7) becomes

$$\frac{d^2w}{dx^2}+(\lambda-x^4)w-\lambda w^{-3}=0, \tag{11}$$

with the initial conditions $w=1$, $w'=w''=w^{(3)}=w^{(4)}=w^{(5)}=0$ at $x=0$. The desired solution is even, so that we need to compute it for positive values of x only.

The critical values of λ are evidently positive, and when n is large their order of magnitude can be obtained from the formula[4]

$$\pi n=\lambda_n{}^{3/4}\int_0^1 s^{1/4}(1-s)^{-1/2}ds+R_n,$$

in which R_n is bounded. This gives

$$\lambda_n=n^{4/3}[2.184+E/_n]$$

where E is bounded. It appears, therefore, that λ_1 will probably lie somewhere between 1 and 4, so we choose the four trial values $\lambda^1=1$, $\lambda^2=2$, $\lambda^3=3$, $\lambda^4=4$, and calculate the solution of (11) for each of these values. The method actually used was that described by the author elsewhere.[5] With the aid of a calculating machine and Barlow's Tables the integration can be done rapidly. The values of $1/w^2$ and $1/w^3$ are read directly in the columns headed "square" and "cube" respectively. We retained only enough significant figures in w to give $1/w^2$ to four places of decimals. The first one of the four computations is shown below to illustrate the general method. The integrals

$$I(\lambda)=\int_{-\infty}^{\infty}w^{-2}dx=2\int_0^{\infty}w^{-2}dx$$

were found with the calculating machine, using Weddle's rule and were checked with Simpson's rule. They proved to be as follows:

λ	$I(\lambda)$	ΔI	$\Delta^2 I$	$\Delta^3 I$
1	3.0469			
		621		
2	3.1090		8	
		629		6
3	3.1719		14	
		643		
4	3.2362			

[4] Milne, Trans. Amer. Math. Soc. **31**, 907–918 (1929), see formula (25) p. 914.

[5] Milne, Numerical Integration of Ordinary Differential Equations, Amer. Math. Monthly **33**, 455 (1926).

From (8), since $a=\lambda^{1/2}$, we get

$$\lambda_n=\left[\pi n/I(\lambda)\right]^2$$

and by a few trials find from this that the values of the first two characteristic numbers are

$$\lambda_1=1.0605$$

$$\lambda_2=3.7998.$$

COMPUTATION I. $\lambda=1$.

x	w	w'	w''	$[x^4-1]$	$1/w^3$	$1/w^2$
0	1.0000	.0000	.0000	−1.0000	1.0000	1.0000
.1	1.0000	.0000	.0001	−.9999	1.0000	1.0000
.2	1.0000	.0001	.0016	−.9984	1.0000	1.0000
.3	1.0000	.0005	.0081	−.9919	1.0000	1.0000
.4	1.0001	.0021	.0252	−.9744	.9997	.9998
.5	1.0005	.0061	.0605	−.9375	.9985	.9990
.6	1.0015	.0151	.1238	−.8704	.9955	.9970
.7	1.0038	.0322	.2258	−.7599	.9886	.9924
.8	1.0084	.0620	.3798	−.5904	.9752	.9833
.9	1.0168	.1104	.6016	−.3439	.9513	.9673
1.0	1.0314	.1853	.9114	.0000	.9114	.9400
1.1	1.0551	.2966	1.341	.4641	.8514	.8983
1.2	1.0924	.4590	1.940	1.0736	.7671	.8380
1.3	1.1493	.6930	2.792	1.8561	.6587	.7570
1.4	1.2344	1.031	4.039	2.8416	.5316	.6563
1.5	1.3606	1.522	5.924	4.0625	.3971	.5402
1.6	1.5467	2.251	8.859	5.5536	.2703	.4181
1.7	1.8232	3.353	13.57	7.3521	.1650	.3008
1.8	2.2377	5.067	21.34	9.4976	.0893	.1997
1.9	2.8706	7.803	34.58	12.0321	.0423	.1213
2.0	3.856	12.32	57.83	15.0000	.0175	.0673
2.1	5.440	20.01	100.4	18.4481	.0062	.0338
2.2	8.058	33.66	180.7	22.425	.0019	.0154
2.3	12.60	58.74	338.6	26.98	.0005	.0063
2.4	20.57	106.9	661.6	32.18		.0024
2.5	36.5	230.0	1387.	38.06		.0007
2.6	60.	410.0				.0003

$\int_{-\infty}^{\infty} w^{-2}dx=3.0469$ by Weddle.
3.04688 by Simpson.