TOWARDS A METHOD FOR THE ACCURATE SOLUTION OF THE SCHRÖDINGER WAVE EQUATION IN MANY VARIABLES

II. A SIMPLE NUMERICAL ILLUSTRATION

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Summary

The method described in Part I is here applied to an eigenvalue problem in two variables

$$\mathscr{H}\psi(x,y)=\lambda\psi(x,y).$$

The results show that an accurate estimate of the fundamental eigenvalue (to seven significant figures) and eigenfunction can be obtained for this problem with only four terms in the series expression for ψ,

$$\psi=\sum_k a_k(x)b_k(y).$$

An application of the Rayleigh-Ritz method to the same problem gives a four-term solution of much lower accuracy (Table 5). The example shows that the individual functions a_k and b_k are not uniquely determined. It shows that a calculation based on a coarse interval can provide good initial estimates of the $a_k(x)$ and $b_k(y)$ and, moreover, predict the accuracy of the corresponding solution obtainable without numerical approximation.

I. NUMERICAL ILLUSTRATION

The method† described in Part I‡ has been applied to the equation

$$(-\partial^2/\partial x^2-\partial^2/\partial y^2+9xy)v(x,y)=\lambda v(x,y),$$

where the eigenfunction $v(x,y)$ is defined within and vanishes on the boundary of the square $0\leqslant x\leqslant 1$, $0\leqslant y\leqslant 1$. Three values of h were used, $\frac{1}{8}$, $\frac{1}{16}$, and $\frac{1}{32}$.

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† In the second formulation, given in Section III, Part I, in which it is formulated as a method of solving a numerical form of the eigenfunction problem.

‡ BASSETT, I. M. (1959).—*Aust. J. Phys.* **12** : 430.

For $h=\frac{1}{8}$, the matrix H is the 49×49 matrix:

$$
\begin{matrix}
\frac{-4}{h^2}+\frac{3}{8}\cdot\frac{3}{8} & & & & & & & 1/h^2 & & \\
& \frac{-4}{h^2}+\frac{3}{8}\cdot\frac{6}{8} & & & & & & & 1/h^2 & \\
& & \frac{-4}{h^2}+\frac{3}{8}\cdot\frac{9}{8} & & & & & & & \\
& & & \frac{-4}{h^2}+\frac{3}{8}\cdot\frac{12}{8} & & & & & & \cdots \\
& & & & \frac{-4}{h^2}+\frac{3}{8}\cdot\frac{15}{8} & & & & & \\
& & & & & \frac{-4}{h^2}+\frac{3}{8}\cdot\frac{18}{8} & & & & \\
& & & & & & \frac{-4}{h^2}+\frac{3}{8}\cdot\frac{21}{8} & & & \\
1/h^2 & & & & & & & \frac{-4}{h^2}+\frac{6}{8}\cdot\frac{3}{8} & & \\
& 1/h^2 & & & & & & & \frac{-4}{h^2}+\frac{6}{8}\cdot\frac{6}{8} & \\
& & & & & & & & & \cdots \\
& & \cdots & & & & & & &
\end{matrix}
$$

in which the zeros have been omitted.

The equation to be solved for f, namely,

$$\sum_y gHgf-\Lambda\sum_y g^2f+\sum_y gHu-\Lambda\sum_y gu=0,$$

becomes

$$-f''\sum_y g^2+f(-\sum_y g''g+9x\sum_y g^2y-\Lambda\sum_y g^2)$$
$$+\sum_k\{-a_k\sum_y gb_k''-a_k''\sum_y gb_k+9a_kx\sum_y gb_ky-\Lambda a_k\sum_y gb_k\}=0,$$

where $u(x,y)=\sum_k a_k(x)b_k(y)$ and f'' stands for the vector whose jth element is

$$(1/h^2)[f\{(j-1)h\}-2f(jh)+f\{(j+1)h\}].$$

If the last equation is rewritten in the form

$$f''+p(x)f(x)+q(x)=0,$$

after dividing through by $-\sum_y g^2$, then the elements of f are the solution of

$$
\begin{aligned}
-2f(h)+f(2h)+h^2p(h)f(h)+h^2q(h)&=0,\\
f(h)-2f(2h)+f(3h)+h^2p(2h)f(2h)+h^2q(2h)&=0,\\
f(2h)-2f(3h)+f(4h)+h^2p(3h)f(3h)+h^2q(3h)&=0,\\
\cdots\quad&\\
-2f(rh)+f\{(r-1)h\}+h^2p(rh)f(rh)+h^2q(rh)&=0.
\end{aligned}
$$

Results of the calculations are shown in Tables 1–5.

TABLE 1

$h=\frac{1}{8}$

	$a_0=b_0$	Term 1			Term 2			Term 3		
		$\bar{a}_1$	$\bar{b}_1$	g_0	$\bar{a}_2$	$\bar{b}_2$	g_0	$\bar{a}_3$	$\bar{b}_3$	g_0
	0·3827	0·125	0·125	0·64775962	—0·125	0·125	0·01	0·125	0·125	0·01
	0·7071	0·2272427654	0·2272948014	1·14374253	—0·164159598	0·166741626	0·01	0·15647423	0·17322713	0·01
	0·9239	0·2903877106	0·2905471896	1·40105055	—0·105516293	0·113146656	0·01	0·13417524	0·16026166	0·01
	1·0000	0·3065020806	0·3067841048	1·40476502	0·010737892	0·002453142	0·01	0·12259124	0·14493200	0·01
	0·9239	0·2760799732	0·2764400832	1·19617773	0·121094932	—0·104475358	0·01	0·14270564	0·15765280	0·01
	0·7071	0·2065678800	0·2069098306	0·84767007	0·167524435	—0·151795674	0·01	0·15328570	0·16994080	0·01
	0·3827	0·1099309538	0·1101422600	0·43193433	0·121350239	—0·111596213	0·01	0·10631966	0·12476700	0·01
Modulus of first element		1·31561279	0·75260925		0·17604305	0·12488933		0·05871633	0·00588043	
Q	5·43443226	263·37321470			263·36285907			263·41846382		
N	0·250010228	12·14228421			12·14271222			12·14527603		
Q/N	21·7368397	21·69058227			21·68896489			21·68896475		
Number of cycles ..		10			$3\frac{1}{2}$			5		
Mean square residual	1·408	0·09045			0·00001574			0·000001207		
Root mean square residual	1·187	0·3007			0·003967			0·001099		

TABLE 2

$h=\frac{1}{32}$

$a_0=b_0$	Term 1			Term 2			Term 3		
	$\bar{a}_1$	$\bar{b}_1$	g_0	$\bar{a}_2$	$\bar{b}_2$	g_0	$\bar{a}_3$	$\bar{b}_3$	g_0
0·0980	0·03125	0·03125	0·071574	−0·03125	0·03125	0·036241	0·03125	0·03125	0·00174273
0·1951	0·0621216443	0·0621248084	0·141453	−0·0607994448	0·0609203250	0·069125	0·061077129	0·060915748	0·00331087
0·2902	0·0922642635	0·0922737323	0·210395	−0·0873194620	0·0877365696	0·099687	0·079362905	0·087632960	0·00475409
0·3827	0·1213152603	0·1213401183	0·276127	−0·1096142003	0·1106376143	0·124819	0·100155996	0·110364443	0·00592337
0·4714	0·1489737318	0·1490202186	0·339297	−0·1269819229	0·1289021393	0·144981	0·108404481	0·128376227	0·00682318
0·5555	0·1749409837	0·1750168388	0·397962	−0·1388694202	0·1420137271	0·158795	0·107220891	0·141451815	0·00744015
0·6344	0·1989363265	0·1990524081	0·452619	−0·1449252516	0·1496710412	0·166197	0·107698016	0·149630178	0·00773929
0·7071	0·2207376205	0·2209014152	0·501779	−0·1451838148	0·1518447289	0·167380	0·099677205	0·153412671	0·00782561
0·7730	0·2401328703	0·2403525962	0·545790	−0·1397785321	0·1486600345	0·161872	0·089440800	0·153461643	0·00764220
0·8315	0·2569470834	0·2572303943	0·583606	−0·1290546694	0·1404252755	0·151091	0·080175949	0·150741236	0·00735981
0·8819	0·2710496613	0·2714009997	0·615422	−0·1135799193	0·1276219969	0·134264	0·066745610	0·146253338	0·00691877
0·9239	0·2823233882	0·2827479612	0·640657	−0·0939527258	0·1108202615	0·113709	0·059271230	0·141043304	0·00649813
0·9569	0·2907087287	0·2912071703	0·659351	−0·0710114323	0·0907408213	0·088466	0·049317375	0·136095476	0·00605303
0·9808	0·2961529187	0·2967266055	0·671381	−0·0455405185	0·0681324615	0·061413	0·047918138	0·132260950	0·00571808
0·9952	0·2986596875	0·2993054439	0·676650	−0·0185123656	0·0438460719	0·031524	0·047216460	0·130200443	0·00547472
1·0000	0·2982501533	0·2989629765	0·675446	+0·0091396180	0·0187367925	0·001877	0·049011910	0·130316140	0·00537865
0·9952	0·2949738891	0·2957470624	0·667550	+0·0364796896	−0·0063348919	−0·028513	0·055189196	0·132789238	0·00544302
0·9808	0·2889133484	0·2897373038	0·653621	+0·0625610820	−0·0305136239	−0·056687	0·062862604	0·137454864	0·00562836
0·9569	0·2801753820	0·2810379566	0·633341	0·0864836739	−0·0529831778	−0·083487	0·069321477	0·143886959	0·00597631
0·9239	0·2688761953	0·2697656294	0·607666	0·1074839441	−0·0730117453	−0·106388	0·081709045	0·151443987	0·00636195
0·8819	0·2551766424	0·2560767015	0·576199	0·1247559865	−0·0898973721	−0·126004	0·088556873	0·159199149	0·00684469
0·8315	0·2392289389	0·2401247555	0·540129	0·1377397817	−0·1030845260	−0·140492	0·098203070	0·166114233	0·00724633

TABLE 2 (*Continued*)

	$a_0=b_0$	Term 1			Term 2			Term 3		
		$\bar{a}_1$	$\bar{b}_1$	g_0	$\bar{a}_2$	$\bar{b}_2$	g_0	$\bar{a}_3$	$\bar{b}_3$	g_0
	0·7730	0·2212243197	0·2220977013	0·499011	0·1458723800	—0·1120821827	—0·150161	0·100863513	0·171063081	0·00762817
	0·7071	0·2013458858	0·2021800389	0·454184	0·1488400165	—0·1165653912	—0·154085	0·102371152	0·172853833	0·00780633
	0·6344	0·1797972054	0·1805749120	0·405178	0·1464272821	—0·1163277042	—0·152206	0·100627142	0·170405425	0·00782438
	0·5555	0·1567930324	0·1574962466	0·353403	0·1385657697	—0·1113064413	—0·144702	0·090641957	0·162827583	0·00755159
	0·4714	0·1325311018	0·1331459924	0·298374	0·1254823944	—0·1016438153	—0·131114	0·084106310	0·149395111	0·00699514
	0·3827	0·1072397948	0·1077512310	0·241550	0·1074451315	—0·0875996927	—0·112820	0·071396304	0·129794790	0·00613349
	0·2902	0·0811374706	0·0815315836	0·182467	0·0849766464	—0·0696362033	—0·088895	0·050644888	0·104160069	0·00492102
	0·1951	0·0544171921	0·0546866907	0·122514	0·0589339328	—0·0484529881	—0·062116	0·037541913	0·073100040	0·00349462
	0·0980	0·0273073794	0·0274436751	0·061692	0·0301869423	—0·0248751081	—0·032485	0·017805372	0·037763715	0·00185428
Modulus of first element		0·61244964	0·10705947		0·04671489	0·03742186		0·01782422	0·00153148	
Q ..	5·49321185	268·34276156			268·33665109			268·37386641		
N ..	0·24999404	12·23648429			12·23706945			12·23876670		
Q/N ..	21·973371	21·92972713			21·92817914			21·92817895		
Mean sq. residual	1·45	0·0915			0·0000428			0·00000449		
Root mean sq. res.	1·20	0·303			0·00654			0·00212		
Number of cycles ..		2			2			1		

TABLE 3

$h=\frac{1}{8}$ AND $h=\frac{1}{16}$

	$h=\frac{1}{8}$			$h=\frac{1}{16}$		
	$\bar{a}_1$	$\bar{b}_1$	g_0	$\bar{a}_1$	$\bar{b}_1$	g_0
	0·125	—0·125	0·2	0·0625	—0·0625	0·0625
	0·2567267570	—0·25671942	0·2	0·1268290283	—0·1268266729	0·1303710
	0·3805350478	—0·38051271	0·2	0·1930585893	—0·1930501860	0·2056846
	0·4656209639	—0·46558162	0·2	0·2607784330	—0·2607594424	0·2893524
	0·4789506184	—0·47890051	0·2	0·3268765612	—0·3268430642	0·3772544
	0·3990173670	—0·39896985	0·2	0·3876155807	—0·3875648942	0·4638023
	0·2287914444	—0·22876210	0·2	0·4387724283	—0·4387036028	0·5421943
				0·4756925444	—0·4756067925	0·6045265
				0·4941653416	—0·4940660623	0·6432952
				0·4905300346	—0·4904227652	0·6516494
				0·4625313841	—0·4624232590	0·6249084
				0·4093291761	—0·4092284337	0·5606269
				0·3321804714	—0·3320954907	0·4598159
				0·2348250951	—0·2347632457	0·3277130
				0·1216740439	—0·1216414385	0·1706619
Modulus of first element ..	0·091266394	0·125000000		0·06527578	0·03949496	
Q	3·854003014			3·96983820		
N	0·177694173			0·18143552		
Q/N	21·688967			21·880160		
No. of cycles ..	$4\frac{1}{2}$			10		
Mean square residual	0·000261					
R.M.S. residual ..	0·0162					

TABLE 4

VALUES OF Λ AND DECREMENTS, CORRESPONDING TO SUCCESSIVE TERMS

	Term 0	Term 1	Term 2	Term 3
First solution (Tables 1 and 2)				
$h=\frac{1}{8}$	21·7368398	21·69058227 0·0463	21·68896489 0·00162	21·68896475 $1{\cdot}4\times10^{-7}$
$h=\frac{1}{16}$	21·9258745	21·8817581 0·0441	21·8801570 0·00160	21·8801570 0×10^{-7}
$h=\frac{1}{32}$	21·973371	21·92972713 0·0436	21·92817914 0·00155	21·92817895 $1{\cdot}9\times10^{-7}$
Second solution (Table 3)				
$h=\frac{1}{8}$	21·7368398	21·688967 0·0479		
$h=\frac{1}{16}$	21·9258745	21·880160 0·0457		

TABLE 5

COMPARISON OF MEAN SQUARE RESIDUALS OBTAINED BY THE RAYLEIGH-RITZ METHOD AND THE PRESENT METHOD

	Term 0	Term 1	Term 2	Term 3
Rayleigh-Ritz method ..	1·4	0·73	0·073	0·011
Present method ($h=\frac{1}{32}$) ..	1·4	0·092	0·000043	0·0000045

The approximate solution which is first guessed (the zeroth term) is written $a_0(x)b_0(y)$. a_0 and b_0 are equal, and are the values of sin πx, sin πy at the lattice points. This choice was made since sin πx sin πy is the exact solution of the original problem with the term $9xy$ omitted. The notation $\bar{a}_1$ means $a_1 h/|\, a_1(h)\,|$ that is, the vector obtained from a_1 by dividing by the modulus of the first element, and then multiplying by h. The moduli of the first elements are given and the vectors themselves can be calculated from these. The "number of cycles" is one if, from the initially assumed g_0, one f has been determined, and from that a new g; a cycle is a determination of an f *and* a g. The "mean square residual" is

$$\sum_{xy} (Hv-\Lambda v)^2 / \sum_{xy} v^2,$$

and the square root of this is the "root mean square residual". For $h=\frac{1}{8}$ the mean square residual was calculated from the residuals—the 7^2 individual values of $Hv-\Lambda v$. For $h=\frac{1}{32}$ the mean square residual was calculated from integrals, using the identity

$$\sum_{xy} (Hv-\Lambda v)^2 = \sum_{xy} (Hv)^2 - \Lambda Q.$$

Calculation by this method, as the mean square residual is small and Q is large, provided a sensitive check on arithmetic errors in the calculation of Λ.

The character of the solution is essentially independent of h. The shapes of the functions a_k, the sizes of the mean square residuals, the rapidity of convergence of the iterative process for determining the products $a_k(x)b_k(y)$, and the decrements of Λ (Table 4) all point to this conclusion.

These same properties would certainly persist no matter how small h were taken, so that an expression of the form

$$\sum_0^3 a_k(x)b_k(y)$$

would provide a solution of the original problem of similar accuracy. This illustrates, too, that calculations based on a coarse interval can provide good initial estimates of the eigenfunction for a refined calculation, and can be used to predict the accuracy of that refined calculation, the truncation error associated with the coarseness of the interval being irrelevant to that prediction.*

* The further refinement of the solution was not undertaken, as lack of computing facilities made the labour seem not worth while, in view of the strong indications already obtained that the accuracy and other characteristics of the solution are independent of h.

Two different solutions to the problem were obtained from different g_0's used in the calculation of the first term $a_1(x)b_1(y)$. One solution is shown in Tables 1 and 2 and the other in Table 3. Note that the existence of two solutions does not contradict theorem 3 (Part I).

The cyclic improvement of f and g was stopped when it seemed that no essential further changes would take place. While the vectors $a_1(x)$, $b_1(y)$ at which $\Lambda(a_0b_0+a_1b_1)$ is stationary with respect to a_1 and b_1 evidently satisfy $a_1(t)=\pm b_1(t)$, $a_1(x)$ and $b_1(y)$ were left in the slightly unsymmetrical form in which they were got.

A rough idea of the degree of accuracy of the eigenvector can be got from the magnitude of the root mean square residual. Since Λ is approximately 20, if the absolute values of the errors in v cluster around 10^{-4}, the root mean square residual must be about 2×10^{-3}. Since this is the approximate size of the root mean square residual to the third term for $h=\frac{1}{8}$ and $h=\frac{1}{32}$, the eigenvector to the third term must be right to about one part in 10,000 (the table of residuals for $h=\frac{1}{8}$ and samples of the residuals for $h=\frac{1}{32}$ showed the error to be fairly uniformly spread over the eigenvector). An approximate upper limit on the absolute error in the eigenvalue estimate can also be set in the following way: for $h=\frac{1}{8}$ and $h=\frac{1}{32}$ the third term reduces the mean square residuals by a factor of about 10, and probably reduces the error in the eigenvalue estimate by a similar factor. Those figures in the eigenvalue estimates which are unchanged by the third terms, namely, 21·688965 and 21·928179, are therefore probably correct; both are almost certainly correct to seven significant figures; this is supported by the coincidence to seven significant figures in the case of $h=\frac{1}{8}$ of the eigenvalue estimate belonging to the other solution (Table 3).

The mean square residuals obtained in a Rayleigh-Ritz calculation are shown in Table 5. For the zeroth term, $\sin \pi x \sin \pi y$ was used, and the subsequent terms were multiples of $\sin \pi x \sin 2\pi y$, $\sin 2\pi x \sin \pi y$, and $\sin 2\pi x \sin 2\pi y$ respectively; the solution to term 3 is the best linear combination of these four functions.

The accuracy obtained by the present method, and the comparison with the Rayleigh-Ritz method, are both satisfactory, but the evidence is of course not weighty. The main function of this example is to show that the equations developed are formally correct and that the method can work in a simple case.

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