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Angular Singularities of Elliptic Problems

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1. INTRODUCTION

Criticality calculations for nuclear reactors are commonly based [8, 12, 13[on 5-point difference approximations to the multigroup diffusion equations in plane sections, which have a low order of accuracy: $O(h^2)$ if the mesh is uniform, and only $O(h)$ if the mesh is nonuniform. The results reported here concern the possibility of developing "finite element" variational methods having higher-order accuracy which could advantageously replace them.[1]

For elliptic problems whose solution is sufficiently smooth (e.g., of class $C^{(2m)}$), variational methods using Hermite interpolation or spline subspaces of piecewise polynomial functions are known[2] to give sets of algebraic equations whose solution yields a function approximating the exact solution with order of accuracy $O(h^{2m})$. However, plane sections of nuclear reactors are typically *piecewise homogeneous media* separated by *interfaces with corners*, where the "flux" becomes *nonanalytic* and has what may be called an *angular singularity*. Analogous "angular singularities" occur in elliptic problems arising in many other branches of physics, such as electromagnetic theory.

To develop "finite elements", some linear combination of which will approximate to a high order of accuracy the exact solution of the multigroup diffusion equations in such reactors, one must know the analytical nature of the angular singularities of the exact solution (flux) near such corners. When difference methods are used, one typically "subtracts out" the leading

[1] The research reported here was supported by the Atomic Energy Commission under Contract AT(30-1)-3971. The author wishes to thank George Fix, Bruce Kellogg, and Robert E. Lynch for valuable comments.

[2] See [2, Lectures 7–8] for references to the original proofs by Varga, Schultz, and the author.

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terms of the singularity [7, pp. 302–3] and [14]; to obtain an analytic (or smooth) remainder, one must know their coefficients. Fortunately, with the Rayleigh–Ritz–Galerkin method, it is enough to know the *form* of the singularity; the coefficients can be determined to the specified order of accuracy from the variational conditions. Thus one need only guess the right *singular basis functions*; these, combined with piecewise bicubic polynomial functions, are known [5; 3, p. 137], and [2, Lecture 8] to give the Rayleigh–Ritz method a high order of accuracy.

Unfortunately, the nature of angular singularities seems to be unknown even in the simplest two-region cases.

The simplest case at all typical for nuclear reactor theory is that of the *one-group diffusion equation*. This is an elliptic partial differential equation of the particular form

$$\nabla \cdot (p\nabla u) + (\lambda\rho - q)u = s(x, y); \tag{1}$$

I shall assume that the coefficient functions $p(x)$, $\rho(x)$, $q(x)$, $s(x)$ are regionwise constant, and in general (for simplicity) that most of them vanish.

My ultimate objective is *algorithmic*: To find the simplest possible singular basis functions which will achieve a given order of accuracy. To quote Rayleigh, I shall "neither seek nor avoid mathematical difficulties." And I shall be concerned only indirectly with general theorems about the existence, uniqueness, and most general function space membership of solutions, questions which have been considered by Ladyzhenskaya [9], Kellogg,[3] and others.

By a *simple angular singularity* of the *DE* (1), I mean a point near which, in suitable polar coordinates, the coefficient functions p, ρ, q, s are piecewise constant in prescribed angular sectors (α_{i-1}, α_i) for $i = 1,..., s$, so that

$$\left.\begin{matrix} p(r, \theta) = p_i\,, & \rho(r, \theta) = \rho_i \\ q(r, \theta) = q_i\,, & s(r, \theta) = s_i \end{matrix}\right\} \quad \text{for } \theta \in (\alpha_{i-1}, \alpha_i). \tag{1'}$$

This paper will be concerned with the explicit solution of one-group diffusion equations of the form (1) near simple angular singularities of the form (1′). I shall assume the *interface condition* that u and $p\partial u/\partial n$ are continuous across interfaces, so that (for $r > 0$), $u(r, \alpha_i^-) = u(r, \alpha_i^+)$ and

$$p_i(\partial u/\partial\theta)(r, \alpha_i^-) = p_{i+1}(\partial u/\partial\theta)(r, \alpha_i^+); \tag{2}$$

this is appropriate for reactor theory [8, p. 102].

[3] See R. Bruce Kellogg, "On the Poisson equation with intersecting interfaces," Tech. Note BN-643, Feb., 1970.

Condition (2) is "natural," in the sense that it is automatically fulfilled by functions which make stationary the variational expression appropriate to the one-group diffusion problem. When $\rho = 0$ (the true source problem), this is

$$J[u] = \iint \{p\nabla u \cdot \nabla u + qu^2 - 2s\,u\}\,dx\,dy. \tag{3}$$

In the *source-free* (homogeneous) case $s = 0$, the *DE* (1) reduces in each region to $p\nabla^2 u + \alpha u = 0$, or $\nabla^2 u + k^2 u = 0$ for $k^2 = (\alpha/p)$, and so it is reasonable to refer to (1) as a *piecewise Helmholtz equation.* When $s = 0$ (the eigenfunction problem), the appropriate variational expression is the Rayleigh quotient

$$R[u] = \iint \{p\nabla u \cdot \nabla u + qu^2\}\,dx\,dy \Big/ \iint \rho u^2\,dx\,dy. \tag{3'}$$

For the fact that (2) is natural, we refer the reader to [6, section 19.4; 11].

2. Source in Quadrant

I shall treat first the simplified case of a *Poisson equation* [(1) with $p = 1$ and $q = \rho = 0$], whose source term has an angular singularity. The case of a uniform source in one quadrant is typical. Symmetrizing, we have

$$\nabla^2 u = \begin{cases} 1 & \text{if } \ |\theta| < \pi/4, \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

This problem can be solved in the plane by using Fourier series. Expanding the source term in (4), we get

$$s = s(\theta) = \frac{1}{4} + \frac{1}{\pi}\left\{\sum_{n=1}^{\infty} \alpha_n \cos n\theta\right\}, \tag{5}$$

where

$$\alpha_n = \left\{\begin{matrix} 0 & \text{if } \ n \equiv 0 \text{ or } 4 \\ \pm 2/n & \text{if } \ n \equiv \pm 2 \\ \pm\sqrt{2}/n & \text{if } \ n \equiv \pm 1 \text{ or } \pm 3 \end{matrix}\right\} \quad (\text{mod } 8). \tag{5'}$$

Since $\nabla^2(r^2 \cos n\theta) = (4 - n^2)\cos n\theta$ and

$$\nabla^2(r^2 \ln r \cos 2\theta) = 4\cos 2\theta,$$

we can solve (5) term by term, getting the particular solution

$$u = r^2 \left\{ -\frac{1}{16} + \frac{1}{\pi} \left[-\sqrt{2} \cos \theta + \frac{\ln r}{4} \cos 2\theta + \sum_{n=3}^{\infty} \frac{\alpha_n}{n^2 - 4} \cos n\theta \right] \right\}. \quad (6)$$

We can also solve (4) in the disc $|r| \leqslant a$ for the boundary condition $u(a, \theta) = 0$, by subtracting from it the harmonic function

$$h(r, \theta) = a^2 \left\{ -\frac{1}{16} + \frac{1}{\pi} \left[-\sqrt{2} \frac{r}{a} \cos \theta + \frac{r^2 \ln a}{4a^2} \cos 2\theta + \sum_{n=3}^{\infty} \frac{\alpha_n^2}{n^2 - 4} \frac{r^n}{a^n} \cos n\theta \right] \right\} \quad (7)$$

which assumes the same values on $r = a$ as u in (6).

To solve (4) analytically in a *square* is more complicated; a typical problem might concern a uniform source in the first quadrant of a square as in Fig. 1.

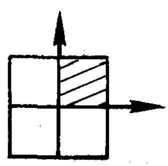

FIGURE 1

Fortunately, the *nature* of the ("simple") angular singularity near the center is presumably independent of the shape of the boundary. If we can describe it as a linear combination of a small number of "singular basis functions," we can hope to apply successfully the variational methods used in [5] (and reviewed in [3, p. 137; 1, Lecture 8]).

The terms of (6) are all $O(r^2)$ or $O(r^2 \ln r)$; individually, they would give an infinite sequence of singular basis functions which, when rotated through 45° to conform to Fig. 1, are

$$(x + y)r, \qquad xy \ln r, \qquad (x^3 - 3x^2y - 3xy^2 + y^3)/r, \qquad \text{etc.}$$

To omit any one would give an error which was $O(r^2)$.

However, all the terms except $xy \ln r$ are of the form $r^2 h_k(\theta)$. Hence we can use as singular basis functions $xy \ln r$ and a *single* solution $r^2 G(\theta)$ of $\nabla^2 u = \sigma(\theta)$, where $\sigma(\theta)$ is the part of $s(\theta)$ in (5) orthogonal to $\cos 2\theta$, where $\theta = 0$ bisects the first quadrant.

To determine $G(\theta)$, we solve

$$G''(\theta) + 4G(\theta) = G(\theta), \qquad G(\theta + 2\pi) = G(\theta), \tag{8}$$

where G is given and (scaling for numerical convenience and letting the x and y axes be $\theta = \pm\pi/4$ for analytical convenience) by

$$G(\theta) = \begin{cases} \pi - \theta \sin 2\theta & \text{if } \quad |\,\theta\,| < \pi/4, \\ (\pi - \theta) \sin 2\theta & \text{if } \quad \pi/4 < |\,\theta\,| < \pi. \end{cases} \tag{9}$$

One easily verifies that this $G(\theta)$ satisfies (8) and $G'(\pm\pi) = 0$, $G(\pi/4) = 3\pi/4$, and $G'(\pi/4) = 1$, whence $G \in C^1$ is the desired function.

To apply the method of [5] and [3], one wants singular basis functions whose *support is confined to a few mesh rectangles*, but whose behavior near $r = 0$ matches that of the two singular basis functions just obtained.[4] One should therefore replace the functions $xy \ln r$ and $r^2 G(\theta)$ by something like $xy\, B(x)\, B(y) \ln r$ and $B(x)\, B(y)\, r^2 G(\theta)$, where $B(x) = 16h^3 - 6hx^2 + |\,x\,|^3$ satisfies $B(\pm 2h) = B'(\pm 2h) = 0$.

Remark. The singular basis functions derived above for the Poisson Eq. (4) are adequate much more generally. Thus, suppose we wish to match the angular singularity of the solution $u(r, \theta)$ of the source problem

$$\nabla^2 u - k^2 u = s(\theta), \tag{10}$$

where $s(\theta)$ is given by (5)–(5′). Then, comparing with the derivation of (6) and (9), we see that the exact solution $v = [r^2 \ln r \cos 2\theta]/4 + r^2 G(\theta)$ of (4) satisfies $\nabla^2 v - k^2 v = s(\theta) + O(r^2 \ln r)$. Hence the solution of Eq. (10) is $v(r, \theta) + w(r, \theta)$, where $\nabla^2 w - k^2 w = O(r^2 \ln r)$ and so (presumably) $w = O(r^4 \ln r)$. The angular singularity of the actual solution is thus presumably acceptably approximated by the singular basis functions $xy\, B(x)B(y) \ln r$ and $B(x)B(y)r^2\, G(\theta)$.

3. Piecewise Laplace Equation

Since the angular singularity at the origin $r = 0$ of the system (1)–(1′) is dominated by the first term of (1) in the sense that this term of the operator multiplies functions by a factor $O(r^{-2})$ in general, it is appropriate to consider first the special case $\rho = q = 0$ of the *piecewise Laplace* equation $\nabla \cdot (p\nabla u) = 0$ [subject to the interface condition (2)]. Angular singularities of this equation have been of interest since the time of Poisson, in connection

[4] Specifically, the *general* solution of the quadrant source problem is just the sum of the particular solution (6) and a harmonic function (which is analytic).

with electrostatics. For a straight interface (the two-sector case of (1′), with $\alpha_i = \pm\pi/2$), see [8a, sections 135–8 and 224–5]; the general case $s = 2$ is discussed in [4, Vol. 1, p. 55].

For the piecewise Laplace equation, a general class of solutions can be found by separating variables. Thus, trying $u = r^\nu g(\theta)$, we find that (1) is equivalent to

$$\nabla \cdot (p\nabla u) = r^{\nu-2}\, p[\nu^2 g(\theta) + g''(\theta)] = 0;$$

hence for $r > 0$ to

$$g'' + \nu^2 g(\theta) = 0 \qquad \text{in each sector } (\alpha_{i-1}, \alpha_i). \tag{11}$$

Note that the function $p(\theta)$ intervenes only through the interface conditions (2), or

$$p_i g'(\alpha_i^-) = p_{i+1}\, g'(\alpha_i^+). \tag{11′}$$

Indicial periodic Sturm-Liouville system.

I shall call the system (11)–(11′), together with the condition that $g(\theta)$ be periodic of period 2π, the *indicial periodic Sturm–Liouville system* associated with the simple angular singularity of (1)–(1′)–(2). It determines an infinite sequence of *eigenfunctions* $g_m(\theta)$, each with one or two *characteristic exponents* $\nu = \nu(m)$, in much the same way that the regular singular point of $f''(r) + r^{-1}f'(r) = \nu^2 f(r)$ determines the characteristic exponents $\nu = 0, 1, 1, 2, 2,...$ in the case of the Laplace equation

$$\nabla^2 u = 0, \quad g_{2k}(\theta) = \cos k\theta, \quad g_{2k-1}(\theta) = \sin k\theta.$$

The preceding analysis shows that the piecewise Laplace DE $\nabla \cdot (p\nabla u) = 0$, with $p(\theta) = p_i$ in (α_{i-1}, α_i), has solutions of the special form $r^\nu g(\theta)$, where $\nu = \nu(m)$ and $g(\theta)$ are, respectively, an eigenvalue and eigenfunction of the indicial periodic Sturm–Liouville system (11)–(11′) associated with $\nabla \cdot (p\nabla u) = 0$. Because (11) is a second-order system, one can use the Prüfer substitution to compute an infinite sequence of (at most double) eigenvalues. The numbers $\nu = \nu(m)$ will be called *characteristic exponents*. The particular function $g_0(\theta) \equiv 1$ is always a trivial eigenfunction, with eigenvalue $\nu(0) = 0$. For large ν, since the total change in the Prüfer phase-angle $\arctan(u/u')$ differs from $2\pi\nu^2$ by at most $s\pi/2$, the number $N(\nu)$ of characteristic exponents $\nu(m) \leqslant \nu$ satisfies $N(\nu) = 2\nu + O(1)$.

The preceding theoretical statements are special cases of results of Lynch [11] on Surm–Liouville problems with piecewise analytic coefficient functions. In particular, the g_m are the eigenfunctions of the piecewise smooth Sturm–Liouville system

$$(pg')' + pg = 0, \tag{12}$$

orthogonal with respect to the weight function $p(\theta)$, or *p orthogonal.* Since $p(\theta)$ is bounded away from 0 and ∞, square integrability is equivalent to the condition $\oint |u(\theta)|^2 \, d\theta < +\infty$, and the $g_m(\theta)$ are a (complete) *p-orthogonal basis* for periodic square-integrable functions (on the unit circle).

This follows perhaps most generally from the theory of integral equations. For any $\lambda < 0$ we can construct a symmetric, continuous, positive periodic *Green's function* $G(\theta_0, \theta)$ whose first derivative makes a unit jump at $\theta = \theta_0$. This is a *compact* operator, of Hilbert–Schmidt type in the Hilbert space with norm $[\oint p(\theta)u^2(\theta)d\theta]^{1/2}$.

Orthonormalizing the $g_m(\theta)$, and integrating with respect to $pg_m(\theta)d\theta$, we can therefore expand any solution of (1) and (2) into a *mean-square convergent* series of the form

$$u(r, \theta) = \sum f_m(r) \, g_m(\theta), \qquad f_m(r) = \oint pug_m \, d\theta. \tag{13}$$

To prove the *termwise differentiability* of the resulting series requires other considerations, which I shall present now.

Dirichlet problems.

The functions $r^{\nu(m)}g_m(\theta)$ are appropriate "singular functions" for any piecewise Laplace *DE* $\nabla \cdot (p\nabla u) = 0$ for which $p = p(\theta)$ is given by (1′), i.e., is piecewise constant in angular sectors. For the Dirichlet problem in any disc D: $r \leqslant a$, with $u(a, \theta) = U(\theta)$ given on the boundary, the solution of

$$\nabla \cdot [p(\theta)\nabla u] = 0 \tag{14}$$

can be written down by inspection. It is

$$u(r, \theta) = \sum c_m r^{\nu(m)} g_m(\theta), \tag{15}$$

where the c_m are chosen to satisfy the boundary conditions on $r = a$. That is, we make

$$\sum c_m a^{\nu(m)} g_m(\theta) = U(\theta).$$

The condition for this equation to hold is (by the "p-orthogonality" of the $g_m(\theta)$ with respect to the weight function $p(\theta)$):

$$c_m = a^{-\nu(m)} \oint p(\theta)U(\theta)g_m(\theta)d\theta. \tag{15′}$$

For any square-integrable $U(\theta)$, we have $\sum c_m{}^2 a^{2\nu(m)} < +\infty$; therefore for $r < a$, the series (15) and *all its partial derivatives* with respect to r and θ are uniformly convergent on any disc $r < a < \epsilon$ $(\epsilon > 0)$. On each ray $\theta = \alpha_i$, for $r < a$, the normal derivative $\partial u/r\partial\theta$ therefore has a jump which satisfies (2).

It follows that, for the approximating subspace spanned by piecewise bicubic polynomial functions of class C^1 and singular basis functions $B(x)B(y)r^{\nu(m)}g_m(\theta)$ with $0 < \nu(m) < 4$, the Rayleigh–Ritz method should give approximate solutions differing from the exact solutions by $O(h^4)$.

4. Two-Region Case

The nature of angular singularities of the piecewise Laplace equation[5] is well illustrated by the case of *two* regions (sectors). The formulas become simpler if we take advantage of the symmetry, and locate the two interfaces along the rays $\theta = \pm\alpha$, separating two homogeneous angular sectors $R_0 : |\theta| \leqslant \alpha$ and $R_1 : \alpha \leqslant |\theta| \leqq \pi$ (Fig. 2); the case $\alpha = \pi/4$ of a quadrant

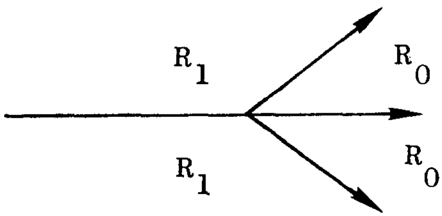

Figure 2

is typical. Then $g_0(\theta) = 1$ is a degenerate eigenfunction $c_0(\theta)$; the other even eigenfunctions of $\nabla \cdot (p\nabla u) = 0$ have the form

$$g_{2n}(\theta) = c_n(\theta) = \begin{cases} A_0 \cos \nu\pi & \text{in } R_0 : |\theta| \leqslant \alpha, \\ A_1 \cos \nu(\pi - \theta) & \text{in } R_1 : \alpha \leqslant |\theta| \leqslant \pi, \end{cases} \tag{15a}$$

while the odd eigenfunctions have the form

$$g_{2n-1}(\theta) = s_n(\theta) = \begin{cases} B_0 \sin \nu\theta & \text{in } R_0, \\ B_1 \sin \nu(\pi - \theta) & \text{in } R_1. \end{cases} \tag{15b}$$

The interface conditions for such solutions have, respectively, the forms

$$p_0 \tan \nu\alpha = -p_1 \tan \nu(\pi - \alpha) \tag{16a}$$

and

$$p_1 \tan \nu\alpha = -p_0 \tan \nu(\pi - \alpha). \tag{16b}$$

For fixed α, the left sides of (16a)–(16b) are increasing functions, while the

[5] The formulas of this section are taken from a report on "Angular singularities of polyharmonic functions" written by me in January, 1969.

right sides are decreasing functions. Hence the number of eigenvalues (characteristic exponents) in the range $0 < \nu < N$ satisfies

$$n(N) = (N\pi/\alpha) + [N\pi/(\pi - \alpha)] + O(1), \tag{17}$$

which is the number of times that $\tan \nu\alpha$ and $\tan \nu(\pi - \alpha)$ pass through ∞ in the range $0 < \nu < N$. Note that, normally, the roots of (16a) and (16b) are different. Hence, in contrast to the one-region problem whose eigenvalues have multiplicity 2, the two-region problem normally has simple eigenvalues.

For instance, suppose $\alpha = \pi/4$, and let β denote $\pi\nu/4$. Then, in (16a), $(\pi - \alpha) = 3\pi\nu/4 = 3\beta$, and one can compute the n-th characteristic exponent $\nu(n)$ for even eigenfunctions by trigonometric algebra. This gives

$$\tan 3\beta = (3 \tan \beta - \tan^3\beta)/(1 - 3 \tan^2\beta). \tag{18}$$

Therefore, when $\alpha = \pi/4$, (16a) is equivalent to

$$\frac{3 \tan \beta - \tan^3 \beta}{1 - 3 \tan^2 \beta} = -P \tan \beta, \qquad P = p_0/p_1 . \tag{19}$$

The equation has a common factor $\tan \beta = 0$, which gives the solution $E_0(\theta) = 1$ with $\nu = 0$, and also the integral characteristic exponents $\nu = 4$, 8, 12,..., which correspond to *analytic* solutions (no singularity) of (1) and (2). These describe the angular variation of the even harmonic functions satisfying (2):

$$1, \quad r^4 \cos 4\theta, \quad r^8 \cos 8\theta, \ldots ;$$

see Remark 4 below.

Factoring out $\tan \beta$, we get from (19) also

$$(3 + P) = (3P + 1) \tan^2 \beta, \qquad \text{or } \tan \beta = \left| \frac{3 + P}{3P + 1} \right|^{1/2} \tag{20}$$

This has roots $\pm \beta_0$, where

$$\beta_0 = \arctan [(3 + P)/(3P + 1)]^{1/2} \tag{20a}$$

lies in the interval $(\arctan 1/\sqrt{3}, \arctan \sqrt{3}) = (\pi/6, \pi/3)$. By the periodicity of $\tan \theta$, this gives characteristic exponents

$$\nu_\pm(n) = \frac{4}{\pi} [\pm\beta_0 + n\pi] = \pm(4\beta_0/\pi) + 4n \tag{21a}$$

associated with *even* eigenfunctions (with (15a) and (16a)).

Similarly, we can compute from (16b) the characteristic exponents of *odd* eigenfunctions (15b). These correspond to the odd harmonic functions which satisfy (2), namely:

$$r^2 \sin 2\theta, \quad r^6 \sin 6\theta, \quad r^{10} \sin 10\theta, \ldots .$$

The other odd eigenfunctions can be derived from an analog of (18), but replacing the number P by $1/P$. This replaces β_0 by β_1 in (20b) $\beta_1 = \arctan [(3P + 1)/(3 + P)]^{1/2} = \operatorname{arccot}(\tan \beta_0) = \pi/2 - \beta_0$, and hence (21a) by

$$\tilde{\nu}_{\pm}(n) = \mp(4\beta_0)/\pi) + 4n + 2. \tag{21b}$$

Remark 1. The reader should be cautioned that formulas (18)–(21b) are only valid in the special case $\alpha = \pi/4$. The case $\alpha = \pi/2$ (of the Schwarz Reflection Principle) is presumably easier; the one-region analog has been studied in depth by H. Lewy and others. The special solutions

$$u = \begin{cases} Pax + by, & |\, \theta \,| \leqslant \pi \\ \ ax + by, & |\, \theta - \pi \,| \equiv \pi \end{cases}$$

are noteworthy; the "angle of refraction" of the lines of flow satisfies $(\tan i)/(\tan r) = P$, instead of Snell's Law. The extension of other polynomials across the interface is equally easy (but not unique; see Remark 4).

Remark 2. For any α (in the two-region case $s = 2$ of (1′)), the even eigenfunctions $g_{2k}(\theta) = c_k(\theta)$ and the odd eigenfunctions $g_{2k-1}(\theta) = s_k(\theta)$ are analogs of the cosine and sine functions, respectively. When restricted to the interval $[0, \pi]$, each of these sets of eigenfunctions is the set of all eigenfunctions of an essentially *regular* Sturm–Liouville system, with piecewise constant coefficients. Thus all eigenvalues are *simple*.

Remark 3. Consider the eigenfunction problem for a *disc* of radius a divided into two sectors $R_i (i = 0,1)$ as above, for the *DE*

$$\nabla \cdot [p(\theta)\nabla u] + k^2 \rho u = 0, \tag{22}$$

where

$$p(\theta) = p_i, \qquad \rho(\theta) = \rho_i \text{ in } R_i \qquad [i = 1, 2], \tag{22′}$$

and $\rho_0/p_0 = \rho_1/p_1$. The eigenfunctions are the products $J_{\nu(m)}(kr)c_m(\theta)$ and $J_{\nu'(m)}(kr)s_m(\theta)$. For $\alpha = \pi/4$, the $\nu(m)$ are given by (22a) and (22b).

Hence for $s = 2$, $\alpha = \pi/4$, a suitable set of singular basis functions, augmenting piecewise bicubic polynomials of class $\tilde{C}^1$ (the modified "bicubic Hermite" approximating subspace), is provided (with the x- and y-axis located on the lines $\theta = \pm\, \pi/4$), by the functions $B(x)B(y)r^{\nu(m)}c_m(\theta)$ with $m = 1, 2, 3$ (for *even* eigenfunction calculations).

Remark 4. In two-region problems, it is nontrivial to determine the appropriate subspaces of *Hermite approximations* by piecewise polynomial functions; the interface condition (2) prevents *linear* polynomials defined on R_1 from being continued to analytic functions on R_0 (which we take to be the first quadrant for simplicity). To be sure, the functions 1 and x^n, y^n for $n > 1$ satisfy (2) trivially, and so does any function

$$u_F(x, y) = \begin{cases} xy\, F(x, y) \text{ on } R_1 \\ Pxy\, F(x, y) \text{ on } R_0 , \end{cases}$$

for example, for $F(x, y)$ any polynomial. Hence one can extend any polynomial with missing linear terms from R_1 to one of the same degree on R_0, so as to satisfy the interface conditions (2). However, it is not clear how one should extend the even (in θ) linear function $x + y = \sqrt{2}\, r \cos(\theta - \pi/4)$ or the odd linear function from R_1 to R_0. For $\tan(\pi\mu/4) = 1/P$, one can extend the latter to $r \sin \mu(\theta - \pi/4)$, but the odd "singular" function $r^{\bar{\nu}(1)} s_1(\theta - \pi/4)$ described earlier in this section is probably preferable (and $r^{\nu(1)} c_1(\theta - \pi/4)$ probably preferable to any even extension of $x + y$).

Note that the continuation of higher-degree polynomials across the interface is not *unique*. Thus any piecewise polynomial function of the form

$$u(x, y) = \begin{cases} x^2y^2\, G_0(x, y) \text{ on } R_0 \\ x^2y^2\, G_1(x, y) \text{ on } R_1 \end{cases}$$

satisfies (2).

5. Source Problems with $q = 0$

We next apply the formal expansion of Section 3, (13), to *source problems* with $q = 0$, that is, to the generalized Poisson equation[6]

$$\nabla \cdot (p \nabla u) = s(r, \theta) = \sum s_k(r)\, g_k(\theta). \tag{23}$$

Here the $g_k(\theta)$ are the orthonormalized eigenfunctions of the indicial periodic Sturm–Liouville system (10)–(10′), so that

$$s_k(r) = \oint p(\theta)\, g_k(\theta)\, s(r, \theta)\, d\theta.$$

Assuming termwise differentiability, we are led heuristically to expect that the series (13) will satisfy (23) if and only if

$$f''_m(r) + \frac{1}{r} f'_m(r) - \frac{\nu(m)^2}{r^2} f_m = s_m(r). \tag{24}$$

[6] This expansion has been used by R. Bruce Kellogg, op. cit. supra, but with other aims in view.

This is evidently an inhomogeneous linear ordinary *DE* with a regular singular point at $r = 0$, and the following remarks refer to this general situation; cf. [1, p. 17].

First, we simplify our notation by suppressing the subscript m and we set $f_m(r) = f(r) = r^\nu \psi(r)$, where (in our general notation) $\nu = \nu(m)$. Since r^ν is a solution of the reduced equation

$$L[f] = f''(r) + \frac{1}{r} f'(r) - \frac{\nu^2}{r^2} f(r) = 0, \tag{25}$$

the function $h(r) = \psi'(r)$ satisfies

$$r^{2\nu+1}\, h'(r) + (2\nu + 1) r^{2\nu}\, h(r) = r^{\nu+1}\, s(r),$$

or

$$\frac{d}{dr}\, [r^{2\nu+1} h(r)] = \frac{d}{dr}\, [r^{2\nu+1} \psi'(r)] = r^{\nu+1} s(r).$$

Integrating, we get

$$\psi'(r) = h(r) = \frac{1}{r^{2\nu+1}} \left[A + \int_0^r r^{\nu+1} s(r)\, dr \right]. \tag{26}$$

For $s(r) = O(r^\beta)$, therefore, $\psi'(r) = Ar^{-2\nu-1} + O(r^{\beta+1-\nu})$, whence

$$\psi(r) = ar^{-2\nu} + b + O(r^{\beta+2-\nu}), \tag{27}$$

for suitable constants a and b.

This shows that $f_m(r) = r^\nu \psi(r)$ is bounded and satisfies (24) with $s_m(r) = O(r^\beta)$ if and only if

$$f_m(r) = br^\nu + O(r^{\beta+2}). \tag{28}$$

For simplicity, I have ignored above the possibility of a logarithmic factor. This will arise in (26) if $\beta = -2 - \nu$ and in integrating (26) to get (27) if $\beta = \nu - 2$. Hence it arises if $\beta = \pm (\nu - 2)$. This is to be expected from dimensional considerations, since this is the case that the operator L in (25), applied to $a(r) = r^{\pm\nu}$ would give zero; it arose in the example of Section 2.

The inhomogeneous linear *DE* (24) can also be attacked in two other ways. If

$$s(r) = s_0 r^\beta + s_1 r^{\beta+2} + s_2 r^{\beta+4} + \cdots = \sum_{k=0}^{\infty} s_k r^{\beta+2k} \tag{29}$$

is the product of r^β times an *analytic* function, then we can apply the method of undetermined coefficients to the formal power series

$$f(r) = f_1 r^{\beta+2} + f_2 r^{\beta+4} + f_3 r^{\beta+6} + \cdots = \sum_{k=1}^{\infty} f_k r^{\beta+2k} \tag{29'}$$

Differentiating the series (29′) termwise, substituting in (24):

$$f'' + r^{-1}f' - \nu^2 r^{-2} f = s(r),$$

and equating coefficients of r^{β}, $r^{\beta+2}$, we get the infinite sequence of algebraic equations

$$[(\beta + 2)^2 - \nu^2]f_1 = s_0\,, \qquad [(\beta + 4)^2 - \nu^2]f_2 = s_1\,,\ldots, \tag{30}$$

which can be uniquely solved unless $\nu - \beta$ is an even positive integer. Moreover, the series (29′) obtained from (29) by (30) has the same radius of convergence as (29).

Green's function approach.

A second, more general approach to solving (24) consists in constructing the Green's function of the *DE* (25), for the condition that the solution f of (24) be bounded at the origin and satisfy $f(R) = 0$ for some specified $R > 0$.[7] To construct this Green's function, we set as usual (to satisfy the boundary conditions):

$$G(r, \rho) = \begin{cases} Ar^{\nu} & \text{for } \; r \in [0, \rho], \\ B[(r/R)^{\nu} - (R/r)^{\nu}] & \text{for } \; r \in [\rho, R]. \end{cases} \tag{31}$$

The continuity condition that $G(\rho^-, \rho) = G(\rho^+, \rho)$ gives

$$A\rho^{\nu} = B[(\rho/R)^{\nu} - (R/\rho)^{\nu}]. \tag{31′}$$

The condition that $\partial G/\partial r$ have a jump of one[8] across $r = \rho$ is equivalent to

$$A\rho^{\nu} + \mu = B[(\rho/R)^{\nu} + (R/\rho)^{\nu}], \qquad \mu = \rho/\nu. \tag{31″}$$

Subtracting (31′) from (31″), $B = \mu(\rho/R)^{\nu}/2$; back-substituting into (31′), $A = (\mu/2R^{\nu})[(\rho/R)^{\nu} - (R/\rho)^{\nu}]$. Now substituting into (31), we get

$$G(r, \rho) = \begin{cases} \dfrac{\mu}{2}\,[R^{-2\nu}(\rho r)^{\nu} - (r/\rho)^{\nu}] & r \in [0, \rho], \\[2ex] \dfrac{\mu}{2}\,[R^{-2\nu}(\rho r)^{\nu} - (\rho/r)^{\nu}] & r \in [\rho, R]. \end{cases} \tag{32}$$

This is evidently bounded for any fixed ρ.

Consequently, for any nonnegative integer m, the operator $\mathscr{G}_m[s]$ defined for each $\nu = \nu(m)$ by the Green's function $G = G_m$ of formula (32) is *bounded* on $C[0, R]$.

[7] The *general* solution $f(r)$ of (24) which is bounded on $[0, R]$ will then be the sum of the particular solution constructed as $\int_0^{\infty} G(x, \rho)s(\rho)\,d\rho$ and an arbitrary multiple of r^{ν}.

[8] See Birkhoff-Rota, "Ordinary Differential Equations," 2nd ed., p. 309. In (24) above, clearly $p_0(r) = 1$.

6. One-Group Diffusion Equation

A similar algorithm yields for *any specified* λ a formal solution of the one-group diffusion equation

$$\nabla \cdot [p(\theta)\nabla u] = Q(\theta)u, \qquad Q = q(\theta) - \lambda\rho(\theta), \tag{33}$$

in ascending powers of r. We look for a series solution of the form

$$u(r, \theta) = \sum_{k=0}^{\infty} r^{\nu+2k} G_{2k}(\theta) = r^{\nu} \sum_{k=0}^{\infty} r^{2k} G_{2k}(\theta). \tag{34}$$

We start the series by a term $r^{\nu}G_0(\theta)$ where, as in Section 3, the choices $\nu = \nu(m)$ and $G_0(\theta) = g_m(\theta)$ give a solution of the *DE* $\nabla \cdot (p\nabla u) = 0$. We then compute $G_{2k}(\theta)$ recursively from $G_{2k-2}(\theta)$, for $k = 1, 2, 3,\ldots$, by substituting from (34) into (33) and setting the coefficient of $r^{\nu+2k-2}$ equal to zero. The result is the inhomogeneous linear *DE*

$$[pG'_{2k}(\theta)]' + (\nu + 2k)^2\, G_{2k}(\theta) = Q(\theta)\, G_{2k-2}(\theta); \tag{35}$$

$G_{2k-2}(\theta)$ is a *known* periodic function; we seek for the *unknown* periodic function $G_{2k}(\theta)$ which satisfies (35) and (2). It is computable from the Green's function of the operator $d(pd/d\theta)/d\theta + (\nu + 2k)^2$ and the periodicity condition; this Green's function is always *positive* if $Q(\theta)$ is.

In the simplest case $p \equiv 1$, $Q(\theta) = \kappa^2$, the above algorithm gives the solution $I_m(\kappa r)\left\{\begin{smallmatrix}\cos\\ \sin\end{smallmatrix}\right\}m\theta$, where I_m is the modified Bessel function and $\nu(m) = m^2$.

The example just given is atypical, not only because no singularity is involved, but more essentially because $q(\theta) = ap(\theta)$ and $\rho = bp(\theta)$ for *constants* $a = 0$ and $b = 1$. The coefficient functions p, q, ρ are all proportional; as a result, the functions $G_{2k}(\theta)$ are independent of λ. Indeed, they are all proportional to $\cos m\theta$ or $\sin m\theta$, regardless of λ or k.

Although the method used above could be generalized to singularities of this special type, I prefer to go directly to the general case. I do this especially because, in the eigenfunction problem, $Q(\theta)$ is not positive, but negative or of mixed sign.

Eigenfunction problem.

To handle the general eigenfunction problem with λ as an unknown parameter, (33) should be rewritten as

$$L[u] = -\nabla \cdot [p(\theta)\nabla u] + q(\theta)u = \lambda\rho(\theta)u. \tag{36}$$

Note that $L = -\nabla \cdot [p\nabla] + q$ has a *positive Green's function* $G(x, y; \xi, \eta)$, which expresses the conditional probability that a neutron "born" at (x, y) will produce a "fission" at (ξ, η). Our objective is to construct a small set of (*local*) singular basis functions which will be independent of the unknown λ. This is essentially because λ is determined by *global* considerations.)

Physically, ρ can be thought of as the fission cross section, q as the absorption cross section, and p as the neutron diffusivity. If we consider the u on the right side of (36) as a "source" density (of neutron population or flux), then the u on the left represents the density of "fission" neutrons of the next generation.

Two-region problems.

It would be misleading to suggest that I "know" the nature of the resulting singularity in any rigorous sense. However, the preceding considerations suggest that the local behavior can be matched pretty well, for *two*-region problems, by linear combinations of functions of the form $r^{\nu(m)+2k} g_m(\theta)$, where the $g_m(\theta)$ are the functions described in Section 4. One or two terms of the form $r^{\nu(m)} \ln g_m(\theta)$ may also be needed (e.g., for $\nu(m) = 2$; see Section 3)

For the somewhat more general source problem:

$$L[u] = -\nabla \cdot [p(\theta)\nabla u] + q(\theta)u = \lambda\rho(\theta)u + s(x, y), \tag{37}$$

we can expand in a power series in λ in the "subcritical" case. Properly normalizing $s(x, y)$ with respect to the "subcriticality" $\lambda_c - \lambda$, we can then achieve the "critical" u as a *limit* of solutions of $L[u^{(n+1)}] = u^{(n)}$, i.e., of "n-th" generation" neutrons. By the formulas of Sections 3 and 4, these can also be obtained by setting $u_0(x, y) = s(x, y)$ and, recursively,

$$-\nabla \cdot [p(\theta)\nabla u] = Q(\theta)u, \qquad Q(\theta) = \lambda\rho(\theta) - q(\theta). \tag{38}$$

This would seem to yield only terms of the kind described above.

Added in proof: Many of the results here have been generalized by R. B. Kellogg, "Singularities in interface problems," in *SYNSPADE 1970* (Bert Hubbard, Ed.), Academic Press, 1971, pp. 351–400.

Prof. R. E. Lynch has pointed out that, although the source problem (4) is "well-set" in the Sobolev space $W_1{}^2$ of functions whose Laplacian is square-integrable, it is even better set (pointwise well-set) if one defines $s(\theta) = \frac{1}{2}$ for $\theta = \pm\pi/4$, $r > 0$, and $s = \frac{1}{4}$ for $r = 0$. In this case, the sum of the series (6) has a Laplacian which can be computed term-by-term in polar coordinates, by a pointwise convergent series.

He has also pointed out that one can solve (4) analytically in the square $[-\pi/2, \pi/2] \times$

$[-\pi/2, \pi/2]$ of Fig. 1, for the boundary conditions $u(x, y) = 0$ for $x = \pm\pi/2$ or $y = \pm\pi/2$, by using double Fourier series. The solution is

$$\begin{aligned} u(x, y) = &-\frac{1}{\pi^2} \sum_{\text{odd } j,k} \sum \frac{1}{jk} \frac{1}{j^2 + k^2} \sin 2jx \sin 2ky \\ &- \frac{1}{4\pi} \sum_{\text{odd } m} \frac{1}{m^3} [\sin 2mx + \sin 2my] \\ &- \frac{4}{\pi^2} \sum_{\text{odd } j,k} \sum \frac{(-1)^{(j+k-2)/2}}{jk(k^2 + j^2)} \cos jx \cos ky \\ &+ \frac{1}{4\pi} \sum_{\text{odd } m} \frac{1}{m^3} \frac{1}{\sinh 2\pi m} [\sin 2mx S_m(y) + \sin 2my S_m(x)], \end{aligned}$$

where $S_m(t) = \sinh(2mt + m\pi) - \sinh(2mt - m\pi)$.]

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