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On functionally graded balls and cones

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Abstract. The heat equation, for both steady and unsteady situations, is considered when the material parameters are spherically symmetric functions of position. Explicit separated solutions are derived when the material parameters are exponential functions; the radial part of these solutions is given in terms of confluent hypergeometric functions or Whittaker functions. In the steady case, explicit solutions are found when the conductivity $k(r) = \exp(-\beta r^q)$, where β and q are parameters with $q > 0$. The behaviour near the tip of a spherically-graded cone is also investigated.

Key words: functionally graded materials, spherical grading, heat conduction.

1. Introduction

In recent years, there has been a growing interest in the mechanics of inhomogeneous or 'functionally graded' materials. See, for example, the review of crack problems for such materials by Erdogan [1], or the review by Markworth *et al.* [2]. In many situations, the material is graded in one direction. Thus, if x, y and z are Cartesian coordinates, the material properties are assumed to vary with x, say, but are independent of y and z. Often, specific functional forms for the variation are taken (such as exponentials, polynomials or rational functions), including several adjustable parameters.

We are interested in heat conduction problems, governed by

$$\operatorname{div}(k \operatorname{grad} u) = c\frac{\partial u}{\partial t}. \tag{1}$$

Here, k is the conductivity and $c = \rho C$, where ρ is the density and C is the specific heat of the solid [3, Section 6]. We assume that k and c are smooth functions of position. We are especially interested in the steady form of (1), namely

$$\operatorname{div}(k \operatorname{grad} u) = 0. \tag{2}$$

Again, we assume that k is a given function of position. For example, Gray *et al.* [4] have developed boundary-integral methods for the case $k(x, y, z) = \mathrm{e}^{\beta x}$. Nonlinear problems, in which k also depends on u, have been discussed by Shaw [5]. Anisotropic problems, in which k is replaced by a matrix, have been considered by Clements and Budhi [6].

A known method for tackling (1) or (2) is to change the dependent variable from u to $v = uk^{1/2}$; the resulting equation for v ((8) below) can be reduced to a partial differential equation with constant coefficients if k and c satisfy certain conditions [7, 8]. This will be the case if, for example,

$$\nabla^2\left(k^{1/2}\right) = \lambda k^{1/2} \quad \text{and} \quad c = c_0 k, \tag{3}$$

where λ and c_0 are constants.

In this paper, we consider materials with spherical symmetry, so that k and c are functions of the spherical polar coordinate r (only). A sphere made with such a material could be hard near the surface but tough in its interior, for example. For steel, this can be achieved by 'carburizing' or 'case hardening' (see, for example, [9, Section 6.3] or [10, Chapter 6]), with application to ball bearings [11, Section 1.2.1]. Such heat-treatment problems are, of course, classical.

A new version of these problems was brought to the author's attention by L. J. Gray of the Oak Ridge National Laboratory. He was concerned with a component that currently consists of a two-material composite, comprising a ball of carbon covered by a rhenium shell. When this coated sphere is subjected to thermal loading, the thermal expansion mismatch across the interface between the carbon and the coating can cause the interface to fail. The idea is that this effect may be minimized by grading the material properties, so that the thermal properties change in a continuous manner. The work described herein was motivated by this idea.

For materials with 'spherical grading', the conditions (3) reduce to

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}[k(r)]^{1/2}\right) = \lambda r^2[k(r)]^{1/2} \quad \text{and} \quad c(r) = c_0 k(r).$$

The first of these shows that

$$k(r) = [\kappa(r)/r]^2$$

where $\kappa(r)$ is any solution of $\kappa'' = \lambda\kappa$. In particular, if we want a conductivity that is bounded at $r = 0$, then we obtain

$$k(r) = k_0\left(\frac{\sin\mu_0 r}{r}\right)^2, \tag{4}$$

where k_0 and μ_0 are arbitrary constants.

We are interested in materials with a simple exponential variation in r,

$$k(r) = \mathrm{e}^{-\beta r} \quad \text{and} \quad c(r) = c_0\,\mathrm{e}^{-\beta r}, \tag{5}$$

where β is a constant. For such materials, the first of (3) is *not* satisfied and so the resulting differential equation for v does *not* have constant coefficients. Nevertheless, we are able to find explicit solutions. Specifically, we separate the variables in terms of spherical polar coordinates. It turns out that the radial part of the solution can be expressed in terms of Whittaker functions (or confluent hypergeometric functions). For the steady Equation (2), it is then straightforward to solve boundary-value problems for spherical geometries.

In Section 5, we give a brief discussion of spherically inhomogeneous cones. In particular, we examine the behaviour of the solution near the tip of an exponentially-graded cone.

The paper concludes with a generalization. We consider the steady Equation (2) in which

$$k(r) = \exp(-\beta r^q),$$

where β and q are real parameters, with $q > 0$. Again, we obtain explicit solutions in terms of confluent hypergeometric functions.

Summarising, we have obtained explicit separated solutions of the heat equation (1), for both steady and unsteady situations, in which the material properties, k and c, are exponential functions of r. These solutions can be used in a straightforward way to solve the standard problems for spheres, by separation of variables: one just modifies the radial part of the separated solutions. Such solutions should be useful as benchmarks, and may be useful in their own right.

2. Governing equations

Consider the heat equation (1) where, for the moment, we allow k and c to be smooth functions of position. Subsequently, we shall make choices for k and c.

Introduce a new dependent variable v, defined by

$$u = \ell v,$$

where ℓ will be selected so as to simplify the partial differential equation for v. Substitution gives

$$\operatorname{div}(k \operatorname{grad} u) = k\ell\nabla^2 v + \boldsymbol{a}\cdot\operatorname{grad} v + \alpha v, \tag{6}$$

where

$$\boldsymbol{a} = \operatorname{grad}(k\ell) + k \operatorname{grad} \ell$$

and

$$\alpha = k\nabla^2\ell + (\operatorname{grad} k)\cdot(\operatorname{grad}\ell). \tag{7}$$

Let us eliminate the first derivatives of v in (6). We have

$$\boldsymbol{a} = 2k \operatorname{grad}\ell + \ell \operatorname{grad} k = 2k^{1/2} \operatorname{grad}\left(k^{1/2}\ell\right)$$

and so we obtain $\boldsymbol{a} = \mathbf{0}$ with the choice

$$\ell = k^{-1/2}.$$

Then, we find from (7) that $\alpha = -\nabla^2(k^{1/2})$ and so (1) becomes

$$k^{1/2}\nabla^2 v - v\nabla^2\left(k^{1/2}\right) = ck^{-1/2}\frac{\partial v}{\partial t}. \tag{8}$$

This equation would become a linear second-order partial differential equation with constant coefficients if k and c were chosen to satisfy (3).

3. Spherical grading

Introduce spherical polar coordinates, r, θ and ϕ. Assume that the material of interest is spherically symmetric, with an exponential dependence on r. Thus, we suppose that

$$k(r,\theta,\phi) = \mathrm{e}^{-\beta r} \quad \text{and} \quad c(r,\theta,\phi) = c_0\mathrm{e}^{-\beta r}, \tag{9}$$

where β (the *grading parameter*) and c_0 are given constants.

As $\nabla^2\{f(r)\} = r^{-2}\left[r^2 f'\right]'$, (8) reduces to

$$\nabla^2 v + v\left(\frac{\beta}{r} - \frac{\beta^2}{4}\right) = c_0\frac{\partial v}{\partial t}. \tag{10}$$

Then, solutions of (1) are given by

$$u(r,\theta,\phi,t) = \mathrm{e}^{\beta r/2} v(r,\theta,\phi,t).$$

In this paper, we give some explicit solutions of (10). We seek solutions in the form

$$v(r,\theta,\phi,t) = V_n(r)\, Y_n(\theta,\phi)\, \mathrm{e}^{st}, \tag{11}$$

where s is a constant, n is an integer, Y_n is a spherical harmonic and $V_n(r)$ is to be found by substituting (11) in (10). (A typical spherical harmonic is

$$A_n^m\, P_n^m(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\phi},$$

where P_n^m is an associated Legendre function and A_n^m is a normalisation constant.)

Note that if one wanted to solve an initial-value problem for (10), it would be natural to use a Laplace transform in t. In that case, s would be the transform variable.

We have

$$\nabla^2(V_n Y_n) = V_n \nabla^2 Y_n + 2(\mathrm{grad}\, V_n)\cdot(\mathrm{grad}\, Y_n) + Y_n \nabla^2 V_n. \tag{12}$$

But $(\mathrm{grad}\, V_n)\cdot(\mathrm{grad}\, Y_n) = 0$ because V_n is a function of r and Y_n is a function of θ and ϕ. We also know that $r^n Y_n$ is a separated solution of Laplace's equation, so that

$$0 = \nabla^2\{r^n Y_n\} = r^n \nabla^2 Y_n + Y_n \nabla^2\{r^n\}$$

by (12) and

$$\nabla^2\{r^n\} = r^{-2}\frac{\mathrm{d}}{\mathrm{d}r}\left\{r^2 \frac{\mathrm{d}}{\mathrm{d}r}(r^n)\right\} = n(n+1) r^{n-2}$$

whence $\nabla^2 Y_n = -n(n+1) r^{-2} Y_n$ and then (12) gives

$$\nabla^2(V_n Y_n) = \left\{\nabla^2 V_n - n(n+1) r^{-2} V_n\right\} Y_n.$$

Hence, (10) reduces to

$$V_n'' + \frac{2}{r}V_n' + \left[\frac{\beta}{r} - \left(\frac{1}{4}\beta^2 + c_0 s\right) - \frac{n(n+1)}{r^2}\right] V_n = 0, \tag{13}$$

which is a linear second-order differential equation for $V_n(r)$.

Equation (13) has a regular singularity at $r = 0$, an irregular singularity at $r = \infty$, and no others. Therefore, it can be transformed into the confluent hypergeometric equation. In fact, we transform it into a form of this equation known as *Whittaker's equation*.

Make the substitution

$$V_n(r) = r^{-1} U_n(x) \quad \text{with} \quad x = \delta r$$

in (13). It yields Whittaker's equation for U_n,

$$U_n''(x) + \left[\frac{\kappa}{x} - \frac{1}{4} + \frac{1}{x^2}\left(\frac{1}{4} - \mu^2\right)\right] U_n(x) = 0, \tag{14}$$

wherein $\kappa = \beta/\delta$, $\mu = n + \frac{1}{2}$ and $\delta = \sqrt{\beta^2 + 4c_0 s}$; we assume that δ is real.

The general solution of (14) is given by

$$U_n(x) = A_n\, M_{\kappa,\mu}(x) + B_n\, W_{\kappa,\mu}(x),$$

where A_n and B_n are arbitrary constants and $M_{\kappa,\mu}$ and $W_{\kappa,\mu}$ are Whittaker functions. These functions are discussed in [12, Chapter 16], [13, Section 6.9], [14, Chapter 13], [15], [16, Section 4.9] and [17, Section 4.3]. The computation of confluent hypergeometric functions is discussed in [14, Section 13.8] and in [18].

As n is an integer, 2μ is an odd integer. This is a special case of Whittaker's equation, in that the second solution $W_{\kappa,\mu}(\delta r)$ involves logarithms. Nevertheless, our solutions can be used for various problems involving (1), together with boundary and initial conitions. This can be done by modifying the known method for $\beta = 0$, as described in, for example, [3, Chapter 9] and [19, Chapter 4]. Rather than pursue such transient problems, we prefer to examine the steady problem in more detail.

4. Steady problems for a sphere

If there is no dependence on time, (1) reduces to (2), which we rewrite here for convenience:

$$\operatorname{div}(k \operatorname{grad} u) = 0. \tag{15}$$

For solutions of this equation, with $k = \mathrm{e}^{-\beta r}$, we can put $s = 0$ in (11) (or $c = 0$ in (1)), whence

$$\delta = \beta, \quad \kappa = 1 \quad \text{and} \quad \mu = n + \tfrac{1}{2}.$$

The fact that $\kappa = 1$ as well as $2\mu =$ integer makes the solution of (14) slightly more difficult.

The first solution is straightforward:

$$M_{1,n+1/2}(x) = \mathrm{e}^{-x/2}\, x^{n+1}\, M(n, 2n+2, x) = \mathrm{e}^{-x/2}\, x^{n+1}\, {}_1F_1(n; 2n+2; x),$$

where $M(a, b, z)$ is a *Kummer function* [14, Equation (13.1.2)] and ${}_1F_1(a; b; z)$ is a hypergeometric function. Explicitly, we have

$$M(a, b, z) = \sum_{m=0}^{\infty} \frac{(a)_m}{(b)_m} \frac{z^m}{m!} \tag{16}$$

where Pochhammer's symbol is defined by

$$(a)_m = a(a+1)(a+2)\cdots(a+m-1) \quad \text{with} \quad (a)_0 = 1. \tag{17}$$

Retracing our steps gives one solution of (15) (the exponentials cancel),

$$u(r, \theta, \phi) = M(n, 2n+2, \beta r)\, r^n\, Y_n(\theta, \phi), \quad n = 0, 1, 2, \ldots. \tag{18}$$

This solution is regular at $r = 0$. In particular, as $M(n, 2n+2, 0) = 1$, we obtain the correct result when $\beta = 0$, because (15) reduces to Laplace's equation in this limit. Note also that (18) reduces to a constant when $n = 0$: this is clearly a valid solution of (15).

4.1. A SECOND SOLUTION FOR $n \neq 0$

From [14, Equation (13.1.33)], a second solution of (14) (when $\kappa = 1$) is

$$W_{1,n+1/2}(x) = \mathrm{e}^{-x/2}\, x^{n+1}\, U(n, 2n+2, x),$$

where $U(a, b, z)$ is another Kummer function [14, Equation (13.1.3)]. Standard books, such as [13, 14, 15], do not give explicit formulas for the evaluation of $U(n, 2n+2, x)$ with a non-negative integer n. Therefore, we resort to an integral representation [14, Equation (13.2.5)], namely

$$W_{1,n+1/2}(x) = \frac{\mathrm{e}^{-x/2} x^{n+1}}{(n-1)!} \int_0^\infty \mathrm{e}^{-xt} t^{n-1} (1+t)^{n+1}\, \mathrm{d}t, \tag{19}$$

which is valid for $n = 1, 2, \ldots$; we will consider the case $n = 0$ separately in Section 4.2.

Using the binomial expansion

$$(1+t)^{n+1} = \sum_{j=0}^{n+1} \binom{n+1}{j} t^{n+1-j}$$

in (19) leads to the Laplace integral

$$\int_0^\infty \mathrm{e}^{-xt} t^{2n-j}\, \mathrm{d}t = \frac{(2n-j)!}{x^{2n-j+1}},$$

whence

$$W_{1,n+1/2}(x) = \mathrm{e}^{-x/2}\, \frac{n(n+1)}{x^n} \sum_{j=0}^{n+1} \frac{(2n-j)!}{(n-j+1)!} \frac{x^j}{j!}, \quad n = 1, 2, \ldots. \tag{20}$$

It turns out that the remaining finite series (polynomial) can be written in terms of another Kummer function.

From (17), we have $(-a)_m = (-1)^m a(a-1)(a-2)\cdots(a-m+1)$, whence

$$\frac{(2n-j)!}{(n-j+1)!} = \frac{(2n)!}{(n+1)!} \frac{(-[n+1])_j}{(-2n)_j}.$$

Hence, using (16), we can rewrite (20) as

$$W_{1,n+1/2}(x) = \frac{\mathrm{e}^{-x/2}}{x^n} \frac{(2n)!}{(n-1)!} M(-n-1, -2n, x), \quad n = 1, 2, \ldots. \tag{21}$$

Retracing our steps gives a second independent solution of (15) as

$$u(r, \theta, \phi) = M(-n-1, -2n, \beta r)\, \frac{1}{r^{n+1}}\, Y_n(\theta, \phi), \quad n = 1, 2, \ldots. \tag{22}$$

We emphasise that (unlike in (18)), the Kummer function occurring here is a *polynomial* in βr. Also, (22) has the correct form as $\beta \to 0$ (when (15) reduces to Laplace's equation).

The solution (22) is *not* valid when $n = 0$. We deal with this special case next.

4.2. A SPHERICALLY-SYMMETRIC SOLUTION

The solution for $n = 0$ involves logarithms. In this case, the differential equation (14) reduces to

$$U_0''(x) + \left(\frac{1}{x} - \frac{1}{4}\right) U_0(x) = 0. \tag{23}$$

One solution of this equation is

$$w_1(x) = M_{1,1/2}(x) = x\,\mathrm{e}^{-x/2}.$$

For a second solution, put $U_0(x) = w_1(x)\,f(x)$, whence (23) becomes

$$xf'' = (x-2)\,f',$$

a separable first-order equation for f'; a solution is

$$f(x) = \frac{\mathrm{e}^x}{x} - \int^x \frac{\mathrm{e}^t}{t}\,\mathrm{d}t.$$

Thus, a second solution of (23) is

$$w_2(x) = \mathrm{e}^{x/2} - x\,\mathrm{e}^{-x/2}\,\mathrm{Ei}(x),$$

where Ei is an exponential integral [14, Equation (5.1.2)]. Hence, a second spherically-symmetric solution of (15) is

$$u(r) = \frac{1}{r}\,\mathrm{e}^{\beta r} - \beta\,\mathrm{Ei}(\beta r), \tag{24}$$

the first solution being $u(r) \equiv 1$.

For small βr, we have [14, Equation (5.1.10)]

$$u(r) \sim \frac{1}{r} - \beta \log(\beta r) + \beta(1-\gamma),$$

where $\gamma = 0{\cdot}5772\ldots$ is Euler's constant. This gives the basic spherically-symmetric solution of Laplace's equation when $\beta = 0$, and reveals the logarithmic term for $\beta \neq 0$.

4.3. BOUNDARY-VALUE PROBLEMS

Armed with our two independent solutions of (15), for each n, it is straightforward to solve boundary-value problems involving spherical boundaries. The method to be used is exactly the same as described in textbooks for solving Laplace's equation in spherical polar coordinates. Our second solutions, (22) and (24), are singular at $r = 0$, and so should be excluded if the origin is in the domain in which (15) is to be solved. Similarly, the first solution (18) should be discarded if the domain extends to infinity (exterior problems). Boundary conditions on any surface $r = r_0$, where r_0 is a constant, are easily imposed because the spherical harmonics $\{Y_n(\theta, \phi)\}$ are orthogonal over such surfaces.

For example, suppose that one wants to solve the Dirichlet problem for (15) inside a graded sphere of radius r_0, centred at the origin. For simplicity, suppose that $u(r_0, \theta, \phi) = f(\theta)$, where f is given. This is an axisymmetric problem, so we can write

$$u(r, \theta, \phi) = \sum_{n=0}^{\infty} a_n\, M(n, 2n+2, \beta r)\, r^n\, P_n(\cos\theta)$$

for $r < r_0$, where the coefficients a_n are to be found. As

$$\int_0^\pi P_n(\cos\theta)\, P_\ell(\cos\theta)\, \sin\theta\, d\theta = \frac{2}{2n+1}\,\delta_{n\ell},$$

the boundary condition on $r = r_0$ gives

$$\int_0^\pi f(\theta)\, P_n(\cos\theta)\, \sin\theta\, d\theta = \frac{2}{2n+1}\, a_n\, r_0^n\, M(n, 2n+2, \beta r_0),$$

which gives a_n explicitly. Many other boundary-value problems for steady-state heat conduction with spherical grading and spherical geometries can be solved in a similar manner.

5. Cones

Consider a circular cone, $r > 0$, $0 \le \theta \le \theta_0$, $|\phi| \le \pi$. The method described above will also give separated solutions of (1) and (15) for spherically graded materials. The main change is that n is no longer required to be an integer.

For example, consider axisymmetric solutions (independent of ϕ) of (15) in the form

$$u(r,\theta) = e^{\beta r/2}\, V_\nu(r)\, P_\nu(\cos\theta), \tag{25}$$

where $P_\nu(z)$ is a Legendre function. It follows that V_ν satisfies (13) in which $s = 0$ and $n = \nu$. Solutions for V_ν can be obtained as before; in some sense, they are simpler now because $2\mu = 2\nu + 1$ is no longer an integer, in general. In fact, the allowable values of ν are determined from the boundary condition on the cone $\theta = \theta_0$, and they are exactly the same as for the corresponding boundary-value problem for Lapace's equation. For example, if $u = 0$ on $\theta = \theta_0$, then ν is determined by solving

$$P_\nu(\cos\theta_0) = 0 \qquad \text{for } \nu.$$

Near the tip of the cone at $r = 0$, we have

$$V_\nu(r) = r^\nu \left\{1 - \frac{\beta r}{2(\nu+1)} + O(r^2)\right\}$$

as $r \to 0$; this can be obtained by using the method of Frobenius on (13). It then follows from (25) that

$$u(r,\theta) = r^\nu \left\{1 + \frac{\beta r \nu}{2(\nu+1)} + O(r^2)\right\}$$

as $r \to 0$. Thus, the leading-order behaviour near the cone's tip is exactly as for Laplace's equation. This is to be expected because $k \to 1$ as $r \to 0$; see (9). We see that the grading parameter β appears at the next order.

6. A generalization

The method described above will generalize to other forms of the spherical grading. Thus, if we put $f(r) = k^{1/2}$, we find that (8) can be written as

$$\nabla^2 v - N(r)\, v = M(r)\, \frac{\partial v}{\partial t},$$

where

$$N(r) = \frac{rf'' + 2f'}{rf} \quad \text{and} \quad M(r) = \frac{c(r)}{f^2}.$$

If we then seek solutions in the form (11), we see that $V_n(r)$ must satisfy

$$V_n'' + \frac{2}{r} V_n' - \left[N(r) + sM(r) + \frac{n(n+1)}{r^2} \right] V_n = 0. \tag{26}$$

Hence, explicit solutions of the spherically-graded heat equation can be constructed whenever one can solve (26).

Let us now consider the steady case ($s = 0$), and put $g(r) = -\log f(r)$. Then, (26) becomes

$$V_n'' + \frac{2}{r} V_n' + \left[g'' - (g')^2 + \frac{2}{r} g' - \frac{n(n+1)}{r^2} \right] V_n = 0. \tag{27}$$

Suppose that

$$k(r) = \exp(-\beta r^q), \tag{28}$$

where β and q are real parameters, with $q > 0$. Then $g(r) = \frac{1}{2}\beta r^q$ and (27) becomes

$$V_n'' + \frac{2}{r} V_n' + \left[\frac{1}{2}\beta q(q+1) r^{q-2} - \frac{1}{4}\beta^2 q^2 r^{2q-2} - \frac{n(n+1)}{r^2} \right] V_n = 0. \tag{29}$$

Again, this can be transformed into the confluent hypergeometric equation. Thus, one solution is $r^n \exp(-\frac{1}{2}\beta r^q)\, M(a, b, \beta r^q)$, where $a = n/q$ and $b = (2n + 1 + q)/q$, and another is obtained by replacing M by U. These solutions are obtained by comparing (29) with [14, Equation (13.1.35)]; in the latter, put $A = -n$ and $2f = h = \beta r^q$. These solutions agree with those obtained in Section 4 when $q = 1$.

7. Conclusions

In this paper, we have derived explicit solutions of the steady heat equation, (15), for a two-parameter family of exponentially-graded spherically-symmetric conductivities, $k(r) = \exp(-\beta r^q)$. The special case $q = 1$ was examined in detail. We obtained a complete set of solutions, so that the well-known method of separation of variables can be used to solve a wide variety of boundary-value problems using spherical polar coordinates; simple examples are Dirichlet bounday conditions on the surface of a sphere (interior or exterior problem) or on the surface of a cone. The main value of such solutions is that they are *exact*: they can be used as benchmark solutions to validate numerical methods developed for grading of more general types. The solutions may also have value in their own right. We have also given some solutions for the time-dependent heat equation.

A desirable extension would be to construct a point-source solution for materials with spherical grading, with the source not at the origin. This could then be used as a fundamental solution (Green's function) in the derivation of boundary integral equations for arbitrary geometries. Work in this direction is ongoing.

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