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Note

On the Limitations of Spherical Harmonics for the Solution of Laplace's Equation

INTRODUCTION

This note is concerned with the use of the series sum of spherical harmonics to solve Laplace's equation for situations in which either (a) convergence cannot be guaranteed, or (b) boundary conditions exist for which there is no corresponding set of coefficients that would satisfy them. It is shown, through simple examples, that the boundary conditions do not have to be extreme, or particularly unusual, for the spherical harmonic sum to fail. It appears that problems arise when the boundary surface is aspherical and the likelihood of the spherical harmonic sum failing as a solution of Laplace's equation increases with deviation of the boundary surface from spherical shape. For example, it is demonstrated that the spherical harmonic series for the solution of a conducting prolate spheroid in an electric field fails when the ratio of major to minor axes exceeds $\sqrt{2}$.

I am motivated to write this note because from time to time spherical harmonic sums are used as solutions to Laplace's equation outside their limit of applicability. To the author's knowledge there are three papers [1–3] on just a single subject, namely the deformed drop in an electric field, where spherical harmonics have been used in good faith, but I believe beyond their limit of applicability, to develop solutions for an electrostatic field. I would be surprised if there were not more such examples in the literature.

BACKGROUND

In spherical polar co-ordinates (r, θ, ϕ), the separated solutions of Laplace's equation may be written:

$$\psi = \sum_{m,n} (a_{mn} \cos(m\phi) + b_{mn} \sin(m\phi)) P_n^m(\cos\theta) \left(\frac{r}{a}\right)^n \tag{1}$$

for the solution bounded at $r = 0$, and

$$\psi = \sum_{m,n} (a_{mn} \cos(m\phi) + b_{mn} \sin(m\phi)) P_n^m(\cos\theta) \left(\frac{a}{r}\right)^{n+1} \tag{2}$$

for the solution bounded at $r = \infty$.

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In Eqs. (1) and (2), a is a suitable scaling for the radial co-ordinate. These equations will be found in any of the standard works on mathematical physics (see [4, 5], for example). However, these works do not stress the limitations of (1) and (2). Indeed casual reference to them would tend to leave one with the view that (1) and (2) were perfectly general.

For simplicity, we consider the exterior Dirichlet problem (where the potential is defined over a boundary surface enclosing the origin and is bounded for $r \to \infty$) and impose cylindrical symmetry. For cylindrical symmetry, the appropriate form of Eq. (2) is:

$$\psi = \sum_{n=0}^{\infty} a_n P_n(\cos\theta) \left(\frac{a}{r}\right)^{n+1} \tag{3}$$

It is, I believe, the compelling simplicity of (3) that often leads researchers to infer a generality it does not possess. We shall now demonstrate through a simple example that Eq. (3) cannot be used to solve all cylindrically symmetric potential problems (and by implication the same conclusion follows for the more general Eqs. (1) and (2)).

The Problem

Figure (1) depicts a cylindrically symmetric but aspherical body. Exterior to the body we specify that a scalar potential field exists and has a boundary value on the surface of the body derived from an interior point source on the axis of symmetry. Clearly the solution is $1/R$ everywhere, R being the distance from source. Normally, for such a trivial case, one would not seek solution by considering the boundary value of ψ at the intersection of the surface of some arbitrarily shaped body with the Green's function, $1/R$. However, in our case this example serves a useful purpose, because $1/R$ may be expressed in terms of a spherical harmonic sum about a point different from the source, thus

$$\frac{1}{R} = \frac{1}{(r^2 + a^2 - 2ra\cos\theta)^{1/2}} = \frac{1}{a} \sum_{n=0}^{\infty} \left(\frac{a}{r}\right)^{n+1} P_n(\cos\theta) \tag{4}$$

(cf. Morse and Feshbach [5]).

In Eq. (4), a is the separation of source and origin of the spherical harmonic sum and θ is the polar angle in the spherical coordinate system.

Now the series (4) is uniformly convergent for $r > a$ and convergent for $r = a$ (see [5], for example; i.e., exterior to that sphere centred on the origin, and in whose surface the source is embedded). However, the series (4) is clearly *divergent*

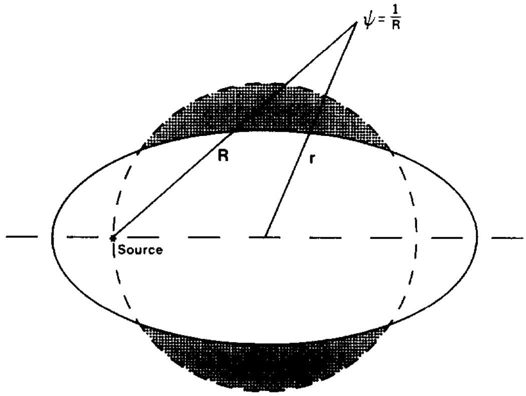

FIG. 1. A boundary surface configuration (solid line) for which the spherical harmonic sum solution of Laplace's equation may fail. For an external field equivalent to a single source as shown, divergence occurs in the strippled region.

anywhere inside the sphere. So returning to Fig. 1 we see that there is a region *outside* the body, yet *inside* the sphere where the correct spherical harmonic sum is now known to diverge. Note that the boundary value on the surface of the body is everywhere smooth, so an "extreme" example has not been chosen by any means.

Consider now what may happen to the unwary investigator who seeks to develop a solution as a spherical harmonic sum to a problem, such as described above. Two possibilities may arise:

(i) The coefficients of the sum are deduced in some approximate manner such that the series (2) converges everywhere outside the body. But these coefficients have to be wrong because we know that the correct coefficients do not give a convergent solution everywhere. Thus the field computed from such coefficients will not be correct *anywhere.*

(ii) The coefficients of the sum are deduced correctly but there exist regions exterior to the boundary where the solution blows up.

Further, it follows that, if volume integrals of the potential are required (e.g., to calculate a potential energy of a field), these integrals will be wrong in the case of (i) and not exist in the case of (ii).

Neither of the possibilities above is very attractive to the computational physicist and what is needed is a method of solution that does not depend upon specific geometries (spherical harmonics require a spherical geometry to ensure their success).

We should note that the interior Dirichlet problem suffers from the same problem as may be illustrated by rewriting the series (3) as:

$$\frac{1}{R} = a \sum_{n=0}^{\infty} \left(\frac{r}{a}\right)^n P_n(\cos\theta) \tag{5}$$

This time, divergence occurs for $r > a$ and similar reasoning as with the exterior problem shows that non-spherical boundary surfaces may have interior regions in which the series solution of Eq. (1) blows up.

A Case Study—The Electrified Drop

Although it was shown that the spherical harmonic sum may fail for aspherical boundary surfaces it is not sufficient to assume that it did fail in [1–3] without further study of their particular problem. In this section, we demonstrate that, for one of the central results of [2, 3], namely the critical electric field for the instability of a conducting drop, the spherical harmonic sum does fail.

It has been established theoretically [6–8], experimentally [9], and using a numerical model [10] that a conducting drop of radius, R_0, and surface tension, T, situated in an electric field, E, (in e.s. units) becomes unstable when $E\sqrt{(R_0/T)}$ exceeds 1.6. At the instability point, the drop is very nearly spheriodal and has a distortion ratio, a/b (the ratio of major to minor axes), of 1.85 ± 0.05. This result is at variance with those of [2], for which values of $E\sqrt{(R_0/T)} = 1.9$ and $a/b = 2.75$ are predicted, and [3], for which a value of 1.745 is given for $E\sqrt{(R_0/T)}$. Unfortunately no explicit value for a/b is given in [3], but we can infer that it is similar to that of [2] from their Figs. 1 and 2. If we are to believe the results of [2] or [3], and discount the results derived from the spheroidal approximation (implicitly done so in [2] and, explicitly, in [3]), then their model for the electric field (the spherical harmonic expansion) must have a domain of applicibility that encompasses the prolate spheroid of distortion ratio 1.9. We now prove that their model does not have such a domain.

Figure 2 shows that geometry of a conducting polate spheroid of major axis, a, and minor axis, b, as referred to in cylindrical coordinate system (r, z), and situated in a uniform field, E, parallel to the major axis. Suppose now that the perturbation to the external field be represented by the field due to a line charge of variable density, $\sigma(Z)$, distributed along the major axis of the spheriod. Then application of elementary potential theory (potential = charge/distance) yields the result that the spheriod surface is at zero potential if the Fredholm equation

$$Ez = \int_{-a}^{a} \frac{\sigma(z')\,dz'}{\sqrt{(b^2(1 - z^2/a^2) + (z - z')^2)}} \tag{6}$$

is satisfied. The coefficients, a_n, of Eq. (3) follow by application of Eq. (4):

$$a_n = \int_{-a}^{a} z'^n \sigma(z')\,dz' \tag{7}$$

and, referred to a *spherical* coordinate system (R, θ), the potential outside the spheriod may be written thus:

$$V(R, \theta) = -ER\cos\theta + \sum_{n=0}^{\infty} \left\{ \int_{-a}^{a} \left(\frac{z'}{R}\right)^n \sigma(z')\,dz' \right\} \frac{1}{R} P_n(\cos\theta). \tag{8}$$

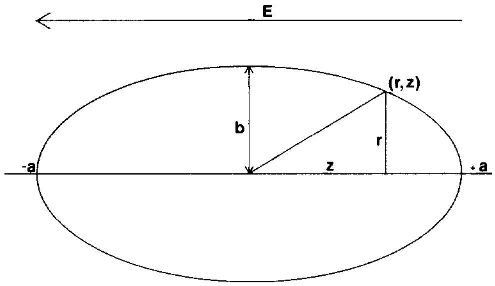

FIG. 2. The geometry of a prolate spheriod in an electric field and referred to a cylindrical co-ordinate system.

Clearly a divergent region exists exterior to the spheriod, rendering Eq. (8) inadmissable as a solution for the electric potential, if $\sigma(z')$ is non-zero for $|z'| > b$.

Now, the analytical solution of a conducting prolate spheriod in a field is well known [5] and easily yields the solution to Eq. (6) as

$$\begin{aligned} \sigma(z) &= \frac{Ez}{\ln((1+e)/(1-e)) - 2e} \qquad \text{for} \quad -\sqrt{(a^2-b^2)} < z < \sqrt{(a^2-b^2)} \\ &= 0 \qquad \text{otherwise} \end{aligned} \tag{9}$$

where $e = \sqrt{(1 - b^2/a^2)}$; i.e., $\sigma(z)$ is non-zero only between the spheriod foci, varying linearly from a positive value at one focus to an equally negative value at the other. The details of derivation of $\sigma(z)$ have been omitted, because of the ease of verification of the result by substitution of Eq. (9) into Eq. (6).

The condition that the spherical harmonic sum fails occurs when some of the internal charge, σ, falls outside the largest incribed sphere (see Eqs. (4) and (8)), namely

$$\sqrt{(a^2 - b^2)} > b$$

or

$$\frac{a}{b} > \sqrt{2}. \tag{10}$$

Thus, we have a precise and perhaps surprising result that spherical harmonic sum for the field about the prolate spheroid is convergent everywhere outside the spheriod only if the distortion ratio does not exceed 1.414. So we are only justified in using the spherical harmonic sum for prolate spheriods of distortion ratios less than 1.414. Because a drop has a much larger distortion at its critical point for stability, it is now clear why the results of [2, 3] for the critical value of $E\sqrt{(R_0/T)}$ should differ so markedly from the accepted value.

One might conjecture that, although the spherical harmonic sum fails for the prolate spheriod, perhaps it did not fail for the *particular* drop shapes at instability, as calculated in [2, 3]. However, the fact that it fails for even the *simplest* deformation from spherical shape is very serious and means that such a conjecture cannot be sustained.

Conclusions

We must conclude that, although the spherical harmonic sum may be used for the solution of either the Dirichlet or the Neumann problems, where the boundary surfaces are aspherical, the question of convergence must be addressed with each application. For the examples cited here [1–3] we have demonstrated that the correct coefficients of the spherical harmonic sum led to a divergent solution for that situation central to one of their principal conclusions.

However, the computational physicist can avoid all of these difficulties as fairly robust schemes exist for the solution of the Laplace's equation (see [11] for a comprehensive review). A method I have used successfully in a number of applications [10] distributes sources just under the boundary surface for the exterior problem or just outside for the interior problem and their strengths are calculated so as to satisfy the boundary conditions. I believed at the time that the method was original, but am comforted to find that there is (at least) one earlier example of its use [12].

I hope that this note serves to warn future researchers as to the insidiously attractive appearance of the spherical harmonic sum for general solution of problems in potential theory and that the spherical harmonic sum may fail for aspherical boundary surfaces.

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