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Electric field and potential calculation for a bioelectric current dipole in an ellipsoid

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Abstract

Computer-based modelling in ellipsoidal geometry can be useful in electroencephalography and gastrography due to the resemblance of the human brain and stomach to an ellipsoid. Both theoretically and computationally, the bioelectric current dipole model is important for the study of electrical activity in these two organs. Computing the electric potential ϕ and electric field \mathbf{E} due to a current dipole located in an ellipsoid requires truncated series expansions involving ellipsoidal harmonics \mathbb{E}_n^m , which are the products of Lamé functions. A theoretical model for this has appeared in the literature only for expansions of order 2 in \mathbb{E}_n^m ; however, this may be insufficient in forward electrogastrography, while an analogous situation is encountered in some geodetic problems where similar expansions are required. In this paper, we propose a generalized model for computing ϕ and \mathbf{E} numerically using harmonic expansions of arbitrary order and degree. The implementation of such a procedure involves finding roots of Lamé polynomials of degree 5 or higher using an optimization technique for solving nonlinear systems of equations. This process can allow one to make a knowledgeable decision concerning the optimal expansion size required for the physical problem under investigation without compromising the overall accuracy of the computation.

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1. Introduction and motivation

The forward problem of bioelectromagnetism plays an important role in the scientific area of biophysical electrodynamics. In human brain studies [20], for example, where the forward problem has been the focus of attention for a considerable period of time, noninvasive recordings of magnetic fields generated in the head have allowed researchers to detect and measure the brain electrical activity directly via electroencephalography (EEG) and

magnetoencephalography (MEG) [1, 35]. In magnetogastrography (MGG), on the other hand, the phenomenon under study is the gastric electrical activity (GEA), generated by the periodic depolarization and repolarization of cells in the stomach [3, 7]. The GEA originates in the corpus of this organ as a wave propagating aborally towards the pylorus through the electric syncytium of the stomach [36]. In the quasistatic approximation, the phenomenon can be modelled as one or several current dipoles. A current dipole \mathbf{Q} is a good approximation for a small source viewed from a distant field point; it is a concentration of some impressed current density \mathbf{J}_i to a single point \mathbf{r}_0 . Anomalies in the characteristics of dipole propagation have been studied [27] and their relevance to the field of medical diagnosis has been the focus of active research [2, 15]. In particular, the use of superconducting quantum interference device (SQUID) magnetometers, pioneered by Cohen *et al* in the 1970s [8–10], has proven to be very suitable for detecting and studying the GEA both in healthy and diseased subjects [2]. An important practical aspect in favour of using SQUIDs for experimental biological data acquisition is the ability to study gastrointestinal electromagnetic phenomena noninvasively, which greatly eases the task of conducting clinical studies. Moreover, the noninvasive GEA studies are encouraging in the light of current efforts to identify effective ways of analysing the phenomenon of abnormal current propagation, which is associated with pathological conditions such as gastroparesis and ischemia [4].

The current dipole approximation has widely been used in the literature to model the biological electrical activity [34]. To study this phenomenon, the body of the stomach has been simulated using cylinders, cones, conoids, ellipsoids and, very recently, using a realistic model of the human body via the finite element and boundary element methods [5]. In 1985 [29, 30], Mirizzi *et al* proposed a mathematical model to simulate the extracellular electrical control activity where an annular band polarized by electric current dipoles moves distally from the mid-corpus to the terminal antrum. In 1995, Mintchev and Bowes constructed a conoidal dipole model of the electrical field produced by the human stomach, where spontaneous depolarization and repolarization due to ionic exchange were simulated [26]. Later, Irimia and Bradshaw constructed a model of the stomach in which an annular band of dipoles advances along a truncated ellipsoid [22], thus simulating the electric potential and electric field recorded by a nasogastric probe.

An important advantage of using the ellipsoidal model in both MGG and EGG is the fact that the problem is approached more realistically than in the case of spherical and conoidal models. Moreover, ellipsoidal geometry offers a suitable ground for the evaluation of inverse problem algorithms in both MEG and MGG. Computing the electric potential ϕ and electric field \mathbf{E} due to an electric current dipole in an ellipsoid requires a truncated expansion of normal ellipsoidal harmonic terms \mathbb{E}_n^m . The general approach to this was first proposed by Kariotou [24] and Dassios [14], who outlined the formalism for this problem but who derived the formulae for ϕ only up to order 2 in \mathbb{E}_n^m . Analogous formulae for the electric field \mathbf{E} have not yet been derived. In our most recent study [23], the electric potential of the stomach was successfully simulated using the low-order ellipsoidal harmonic expansion of Dassios and Kariotou. However, it was found that all ellipsoidal terms included in this expansion (order 1 and 2) contributed substantially to the computed electric potential. This raises the important question as to whether the contributions of higher-order terms may also be significant in electro- and magneto-gastrographic modelling. This issue is significant because the accuracy of the calculation may seriously be affected if an insufficient number of ellipsoidal terms are included in the expansion. The purpose of the present paper is to address this problem by providing a generalized theoretical and computational approach to the calculation of ϕ and \mathbf{E} using an arbitrarily large expansion of ellipsoidal terms. The computer implementation of our proposed formalism would then allow one to investigate the contributions of these terms and to

identify suitable cutoffs to the associated harmonic expansions so that an accurate calculation of the two physical quantities under consideration (ϕ and \mathbf{E}) is made possible.

In the following section, we present the mathematical formalism behind our model. We then continue by deriving formulae for two important quantities in our calculation, namely the gradient ∇ of the normal harmonic functions \mathbb{E}_n^m and the first derivative of the associated Lamé functions E_n^m . Thereafter, generalized expressions for ϕ and \mathbf{E} are found using the mathematical tools developed and computational considerations regarding the overall problem are addressed in the following section. Thus, the material in section 2 is a review of previous work while the remainder of the paper contains novel results. We conclude with a discussion and summary of our model, which we intend to implement numerically with the purpose of answering the important modelling issues raised above.

2. Mathematical formalism

Throughout our derivations, we make use of the standard equation of the ellipsoid

$$\frac{x_1^2}{\alpha_1^2} + \frac{x_2^2}{\alpha_2^2} + \frac{x_3^2}{\alpha_3^2} = 1 \quad (1)$$

where (x_1, x_2, x_3) are the usual Cartesian coordinates (x, y, z) and $0 < \alpha_3 < \alpha_2 < \alpha_1 < +\infty$ are the ellipsoidal semiaxes. As in [21, 24], we also employ the ellipsoidal system, with coordinates ρ, μ and ν and semifocal distances h_1, h_2 and h_3 , defined by

$$h_1^2 = \alpha_2^2 - \alpha_3^2 \quad (2)$$

$$h_2^2 = \alpha_1^2 - \alpha_3^2 \quad (3)$$

$$h_3^2 = \alpha_1^2 - \alpha_2^2. \quad (4)$$

Conversion from ellipsoidal to Cartesian coordinates can be made via the relationships

$$x_1 = \frac{\rho\mu\nu}{h_2h_3} \quad (5)$$

$$x_2 = \frac{\sqrt{\rho^2 - h_3^2}\sqrt{\mu^2 - h_3^2}\sqrt{h_3^2 - \nu^2}}{h_1h_3} \quad (6)$$

$$x_3 = \frac{\sqrt{\rho^2 - h_2^2}\sqrt{h_2^2 - \mu^2}\sqrt{h_2^2 - \nu^2}}{h_1h_2}, \quad (7)$$

where $\rho \in [h_2, +\infty)$, $\mu \in [h_3, h_2]$ and $\nu \in [-h_3, h_3]$. In ellipsoidal coordinates, the Laplace equation has the form

$$(\mu^2 - \nu^2)\frac{\partial^2\phi}{\partial\beta^2} + (\rho^2 - \nu^2)\frac{\partial^2\phi}{\partial\varphi^2} + (\rho^2 - \mu^2)\frac{\partial^2\phi}{\partial\chi^2} = 0, \quad (8)$$

where

$$\beta = \int_{h_2}^{\rho} \frac{d\rho}{\sqrt{\rho^2 - h_3^2}\sqrt{\rho^2 - h_2^2}} \quad (9)$$

$$\varphi = \int_{h_3}^{\mu} \frac{d\mu}{\sqrt{\mu^2 - h_3^2}\sqrt{h_2^2 - \mu^2}} \quad (10)$$

$$\chi = \int_0^v \frac{dv}{\sqrt{h_3^2 - v^2} \sqrt{h_2^2 - v^2}} \quad (11)$$

and ϕ is the electric potential.

To calculate the electric potential ϕ for an ellipsoid, the separation of variables for the Laplace equation in ellipsoidal coordinates leads to the Lamé equation, which assumes the following form for each of the three spatial coordinates $\eta_i = \rho, \mu, \nu$:

$$\begin{aligned} (\eta_i^2 - h_3^2)(\eta_i^2 - h_2^2)E''(\eta_i) + \eta_i(2\eta_i^2 - h_3^2 - h_2^2)E'(\eta_i) \\ + [(h_2^2 + h_3^2)P - n(n+1)\eta_i^2]E(\eta_i) = 0. \end{aligned} \quad (12)$$

Above, P, n are constants, the prime in E' , etc indicates differentiation with respect to the independent variable $\eta_i = \rho, \mu, \nu$, and the quantities E are the so-called Lamé functions that form the normal interior harmonic function

$$\mathbb{E}_n^m(\rho, \mu, \nu) = E_n^m(\rho)E_n^m(\mu)E_n^m(\nu). \quad (13)$$

The corresponding exterior harmonic functions \mathbb{F}_n^m are given by

$$\begin{aligned} \mathbb{F}_n^m(\rho, \mu, \nu) &= (2n+1)\mathbb{E}_n^m(\rho, \mu, \nu)I_n^m(\rho) \\ &= (2n+1)I_n^m(\rho)E_n^m(\rho)E_n^m(\mu)E_n^m(\nu), \end{aligned} \quad (14)$$

where I_n^m are elliptic integrals of the form

$$I_n^m(\rho) = \int_\rho^\infty \frac{dt}{[E_n^m(t)]^2 \sqrt{t^2 - h_2^2} \sqrt{t^2 - h_3^2}} \quad (15)$$

with $n = 0, 1, 2, \dots$, and $m = 1, 2, \dots, 2n+1$. The interior harmonic functions enter the expression for the electric potential only for the space enclosed by the ellipsoid, while the exterior harmonic functions are used to define the potential outside this body. In fact, the internal harmonic terms diverge as $r \rightarrow \infty$, while external terms tend to 0 in the same limit, as expected. Naturally, the surface potential can be computed using either internal or external harmonics since the boundary conditions imposed upon solving the Laplace equation guarantee the absence of any anomalous discontinuities in the potential across the two media.

It was first shown by Lamé that four classes (also called species) of Lamé functions exist, typically denoted by $K(\eta_i), L(\eta_i), M(\eta_i)$ and $N(\eta_i)$, respectively, where η_i is any of the coordinates ρ, μ or ν . These are referred to as Lamé functions of the first (as opposed to second) kind, a label that we omit from this point forward because our theory does not involve Lamé functions of the second kind.

The Lamé functions of the first kind involve polynomials and can be written as

$$K(\eta_i) = \sum_{k=0}^{r+1} a_k \eta_i^{n-2k} \quad (16)$$

$$L(\eta_i) = \sqrt{\eta_i^2 - h_3^2} \sum_{k=0}^{n-r} a_k \eta_i^{n-(k+1)} \quad (17)$$

$$M(\eta_i) = \sqrt{h_2^2 - \eta_i^2} \sum_{k=0}^{n-r} a_k \eta_i^{n-(k+1)} \quad (18)$$

$$N(\eta_i) = \sqrt{(\eta_i^2 - h_3^2)(\eta_i^2 - h_2^2)} \sum_{k=0}^r a_k \eta_i^{n-2(k+1)}, \quad (19)$$

where the coefficients a_k can be obtained by inserting the appropriate Lamé functions into the Laplace equation, according to the approach described by Hobson [21]. The additional restriction must be so placed that the power of each η_i in the expressions for K , L , M and N above must be greater than or equal to zero. The index r in the summations above is given by

$$r = \begin{cases} \frac{n}{2} & \text{for } n \text{ even} \\ \frac{n-1}{2} & \text{for } n \text{ odd,} \end{cases} \quad (20)$$

where n is the degree of the ellipsoidal harmonic \mathbb{E}_n^m . For a harmonic of degree n , there are $2n + 1$ associated Lamé functions; it can be inferred from equation (19) that there are $r + 1$ functions of type K , $n - r$ functions of type L , $n - r$ functions of type M and r functions of type N , for a total of $2n + 1$ Lamé functions. Although not required for our derivations, we give the definition of the Lamé functions of the second kind F_n for completeness. These functions were introduced independently by Liouville and Heine; they involve the Lamé functions of the first kind as well as elliptic integrals. Their general definition is given by

$$F_n(\eta) = (2n + 1)E_n(\eta) \int_{\eta}^{\infty} \frac{d\eta}{\sqrt{\eta^2 - h^2} \sqrt{\eta^2 - k^2}}, \quad (21)$$

where h and k are constants determined by the geometry ([21] discusses this type of functions in more detail).

In the ellipsoidal formalism, the Lamé functions are used to construct ellipsoidal harmonic functions, which are eigenfunctions of the Laplacian operator in ellipsoidal coordinates. Thus, the Lamé functions and the triplet $(E_n^m(\rho), E_n^m(\mu), E_n^m(\nu))$ are analogous to the radial function $R_l^m(r)$ and spherical harmonics $Y_l^m(\theta, \phi)$ —i.e., to the doublet $(R_l^m(r), Y_l^m(\theta, \phi))$ —in spherical harmonic theory.

Products of the form $E_n^m(\mu)E_n^m(\nu)$ are called surface ellipsoidal harmonics because they refer to the ellipsoidal surface $\rho = \rho_0$. We adopt the convention used by Kariotou [24] and label the normalization functions associated with the ellipsoidal harmonics as γ_n^m . These quantities assume the form

$$\gamma_n^m = \oint_{\rho=\rho_0} \frac{[E_n^m(\mu)E_n^m(\nu)]^2}{\sqrt{(\rho_0^2 - \mu^2)(\rho_0^2 - \nu^2)}} dS, \quad (22)$$

where

$$dS = d\mu d\nu (\mu^2 - \nu^2) \sqrt{\frac{(\rho^2 - \mu^2)(\rho^2 - \nu^2)}{(\mu^2 - h_3^2)(h_2^2 - \mu^2)(h_3^2 - \nu^2)(h_2^2 - \nu^2)}} \quad (23)$$

is the ellipsoidal surface element in the same coordinate system [6]. The formulation of ellipsoidal harmonics in Cartesian coordinates is given by

$$\mathbb{E}_n^m(\mathbf{r}) = C_{ij} \prod_{k=1}^m \Theta_k, \quad (24)$$

where $\Theta_k(x, y, z)$ is known as the Niven function [21, 33],

$$\Theta_k = \frac{x^2}{\alpha_1^2 + \theta_k} + \frac{y^2}{\alpha_2^2 + \theta_k} + \frac{z^2}{\alpha_3^2 + \theta_k} - 1, \quad (25)$$

while θ_k is the k th root of the Lamé function E_n^m . C denotes a matrix whose elements are given in Cartesian coordinates and are labelled by subscripts i and j , indicating the corresponding row and column, respectively, of the appropriate entry. C has the form

$$C = \begin{Bmatrix} x & yz \\ 1 & y & zx & xyz \\ z & xy \end{Bmatrix}. \quad (26)$$

Columns in C correspond to each of the function types K , L , M and N , while rows refer to the coordinates in the chosen system, i.e. x , y or z in the Cartesian system. To evaluate \mathbb{E}_n^m using equation (24), one must select appropriate entries in C for each coordinate and multiply the resulting quantity by the product $\prod_{k=1}^m \Theta_k$. Lamé showed that the roots of the functions bearing his name must all be real, distinct and located in the interval $(-\alpha_1^2, \alpha_3^2)$. In ellipsoidal coordinates, the harmonics can be written as

$$\mathbb{E}_n^m(\mathbf{r}) = L_{ij} \prod_{k=1}^m \Psi_k, \quad (27)$$

where L_{ij} denotes the appropriate entry in matrix L given in ellipsoidal coordinates, where

$$L = \begin{Bmatrix} \rho & \sqrt{\rho^2 - h_3^2} & \sqrt{\rho^2 - h_2^2} & \sqrt{(\rho^2 - h_3^2)(\rho^2 - h_2^2)} \\ 1 & \mu & \sqrt{\mu^2 - h_3^2} & \sqrt{(\mu^2 - h_3^2)(h_2^2 - \mu^2)} \\ v & \sqrt{h_3^2 - v^2} & \sqrt{h_2^2 - v^2} & \sqrt{(h_3^2 - v^2)(h_2^2 - v^2)} \end{Bmatrix} \quad (28)$$

and

$$\Psi_k = (\rho^2 - \psi_k^2)(\mu^2 - \psi_k^2)(v^2 - \psi_k^2). \quad (29)$$

In this case, ψ_k are the roots of the corresponding function $\Psi_k(\rho, \mu, v)$ expressed in ellipsoidal coordinates.

3. Derivation of $\nabla \mathbb{E}_n^m$ and $d\mathbb{E}_n^m/d\eta_i$

The two coordinate systems used above (Cartesian and ellipsoidal) are both important throughout our derivations; for this reason, formulae of interest will be given in a form that is independent of the coordinate system chosen. In this section, we derive two particular quantities that are of interest in each of them, namely the gradient of the normal ellipsoidal harmonic function \mathbb{E}_n^m and the derivative of the Lamé polynomial E_n^m .

For any diagonal metric tensor $g_{ij} = g_{ii}\delta_{ij}$ (where δ_{ij} is the usual Kronecker delta function), the scale factors s_i are defined in terms of the parametrizations $x_i = f_i$, where x_i are the Cartesian coordinates and f_i are the functions x_i in terms of some other coordinates η_i . In our case, η_i are the ellipsoidal coordinates ρ, μ and v and the parametrizations f_i are given in equations (5)–(7). For three-dimensional space, the scale factors s_i are defined as

$$s_i = (g_{ii})^{1/2} \quad (30)$$

$$= \left[\sum_{k=1}^3 \left(\frac{\partial f_k}{\partial \eta_i} \right)^2 \right]^{1/2}. \quad (31)$$

In this generalized formalism, the gradient $\nabla w(\eta_i)$ of any function w of three independent variables η_i assumes the form

$$\nabla w = \sum_{i=1}^3 \frac{1}{s_i} \frac{\partial w}{\partial \eta_i} \hat{\mathbf{a}}_i, \quad (32)$$

where $\hat{\mathbf{a}}_i$ are the three unit vectors in the coordinate system η_i . For the Cartesian case, we obtain the familiar expression

$$\nabla = \hat{\mathbf{x}} \frac{\partial}{\partial x} + \hat{\mathbf{y}} \frac{\partial}{\partial y} + \hat{\mathbf{z}} \frac{\partial}{\partial z}. \quad (33)$$

Applying this formalism to the ellipsoidal coordinate case, we obtain

$$\nabla = \frac{1}{s_\rho} \hat{\rho} \frac{\partial}{\partial \rho} + \frac{1}{s_\mu} \hat{\mu} \frac{\partial}{\partial \mu} + \frac{1}{s_v} \hat{v} \frac{\partial}{\partial v}, \quad (34)$$

where inverses of the scale factors [31] are given by

$$\frac{1}{s_\rho} = \sqrt{\frac{(\rho^2 - h_2^2)(\rho^2 - h_3^2)}{(\rho^2 - \mu^2)(\rho^2 - v^2)}} \quad (35)$$

$$\frac{1}{s_\mu} = \sqrt{\frac{(\mu^2 - h_2^2)(\mu^2 - h_3^2)}{(\mu^2 - \rho^2)(\mu^2 - v^2)}} \quad (36)$$

$$\frac{1}{s_v} = \sqrt{\frac{(v^2 - h_2^2)(v^2 - h_3^2)}{(v^2 - \rho^2)(v^2 - \mu^2)}}. \quad (37)$$

Another quantity that will be useful later is the outward unit vector $\hat{\mathbf{n}}$ with respect to the surface of the ellipsoid. In Cartesian coordinates, the ellipsoid can be defined [22] by the implicit equation $F(x, y, z) = 0$, where

$$F(x, y, z) = \frac{x^2}{\alpha_1^2} + \frac{y^2}{\alpha_2^2} + \frac{z^2}{\alpha_3^2} - 1. \quad (38)$$

It follows by a theorem of vector calculus [17] that, in the Cartesian coordinate system, the normal unit vector can be defined as

$$\hat{\mathbf{n}} = \left[\left(\frac{\partial F}{\partial x} \right)^2 + \left(\frac{\partial F}{\partial y} \right)^2 + \left(\frac{\partial F}{\partial z} \right)^2 \right]^{-1/2} \nabla F \quad (39)$$

$$= \left(\frac{x}{\alpha_1^2} \hat{\mathbf{x}} + \frac{y}{\alpha_2^2} \hat{\mathbf{y}} + \frac{z}{\alpha_3^2} \hat{\mathbf{z}} \right) \left(\frac{x^2}{\alpha_1^4} + \frac{y^2}{\alpha_2^4} + \frac{z^2}{\alpha_3^4} \right)^{-1/2}. \quad (40)$$

For ellipsoidal coordinates, the expression for this function is quoted in [13] as being given by

$$\hat{\mathbf{n}} = D_n \hat{\rho}, \quad (41)$$

with

$$D_n = \frac{\alpha_2 \alpha_3}{\sqrt{(\alpha_1^2 - \mu^2)(\alpha_1^2 - v^2)}}. \quad (42)$$

To compute the gradient of the Lamé function, the Cartesian coordinate system is preferable because of the simple form assumed by this operator in terms of x , y and z . Applying the gradient operator to the Cartesian coordinate expression in equation (24) and keeping in mind the product rule of differentiation yields the result

$$\nabla \mathbb{E}_n^m(\mathbf{r}) = \left[\mathbf{G}_{ij} + \left(C_{ij} \sum_{k=1}^m \xi_k \right) \hat{\mathbf{u}} \right] \prod_{l=1}^m \Theta_l, \quad (43)$$

where \mathbf{G} is a vector matrix with entries

$$\mathbf{G} = \begin{Bmatrix} \hat{\mathbf{x}} & y\hat{\mathbf{z}} + z\hat{\mathbf{y}} \\ \mathbf{0} & \hat{\mathbf{y}} & x\hat{\mathbf{z}} + z\hat{\mathbf{x}} & xy\hat{\mathbf{z}} + yz\hat{\mathbf{x}} + xz\hat{\mathbf{y}} \\ \hat{\mathbf{z}} & x\hat{\mathbf{y}} + y\hat{\mathbf{x}} \end{Bmatrix}. \quad (44)$$

The function ξ_k is defined as

$$\begin{aligned} \xi_k(\mathbf{r}) &= \frac{1}{\Theta_k} \nabla \Theta_k \\ &= \frac{2}{\Theta_k} \left(\frac{x}{\alpha_1^2 + \theta_k} + \frac{y}{\alpha_2^2 + \theta_k} + \frac{z}{\alpha_3^2 + \theta_k} \right) \end{aligned} \quad (45)$$

and $\hat{\mathbf{u}} = \hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}$ is composed of the three orthonormal vectors in each of the coordinate directions.

Before we address the problem of computing $\nabla \mathbb{E}_n^m$ in ellipsoidal coordinates, let us compute the first derivative of the Lamé polynomial E_n^m , which has the general form

$$\frac{d}{d\eta_i} E_n^m(\eta_i) = L_{ij} \frac{d}{d\eta_i} B^m + L'_{ij} B^m, \quad (46)$$

the prime in L'_{ij} denoting differentiation of the appropriate entry in matrix L with respect to η_i . The function B^m is defined as

$$B^m = \prod_{k=1}^m (\eta_i^2 - \psi_k^2) \quad (47)$$

$$= \prod_{k=1}^m (\eta_i - \psi_k)(\eta_i + \psi_k). \quad (48)$$

We made use, on the last line above, of the property $\psi_k \in \mathbb{R}$ characteristic of Lamé function roots to factor out the quantity $\eta_i^2 - \psi_k^2$. In other words, since the roots of a Lamé function are always real by definition (see [21]), the quantity $\eta_i^2 - \psi_k^2$ can be written as $(\eta_i - \psi_k)(\eta_i + \psi_k)$. It is also important to note that the symbol η_i is employed to denote the independent variable for E_n^m , where $\eta_i = \rho, \mu$ or ν . This is to emphasize that the B^m function has the same general form for each of all three spatial ellipsoidal coordinates. As expected, the definition of the Lamé polynomials given above is consistent with the separability of the normal ellipsoidal harmonics into functions depending only on one of ρ, μ or ν (see equation (13)); this can be made obvious by noting that the entries in each row of L are the functions of only one variable, whereas only the normal ellipsoidal harmonic function \mathbb{E}_n^m depends on all three spatial coordinates. The entries in the matrix L' can be computed straightforwardly by differentiation. They are

$$L'_{i1} = 0 \quad (49)$$

$$L'_{i2} = 1 \quad (50)$$

$$L'_{i3} = \frac{\rho}{\sqrt{\rho^2 - h_3^2}} \quad (51)$$

$$L'_{i4} = \frac{\rho}{\sqrt{\rho^2 - h_2^2}} \quad (52)$$

$$L'_{15} = \frac{\rho[2\rho^2 - (h_2^2 + h_3^2)]}{\sqrt{(\rho^2 - h_3^2)(\rho^2 - h_2^2)}} \quad (53)$$

$$L'_{23} = \frac{\mu}{\sqrt{\mu^2 - h_3^2}} \quad (54)$$

$$L'_{24} = \frac{-\mu}{\sqrt{h_2^2 - \mu^2}} \quad (55)$$

$$L'_{25} = \frac{\mu[(h_2^2 + h_3^2) - 2\mu^2]}{\sqrt{(\mu^2 - h_3^2)(h_2^2 - \mu^2)}} \quad (56)$$

$$L'_{33} = \frac{-\nu}{\sqrt{h_3^2 - \nu^2}} \quad (57)$$

$$L'_{34} = \frac{-\nu}{\sqrt{h_2^2 - \nu^2}} \quad (58)$$

$$L'_{35} = \frac{\nu[2\nu^2 - (h_2^2 + h_3^2)]}{\sqrt{(h_3^2 - \nu^2)(h_2^2 - \nu^2)}}. \quad (59)$$

Note again that each row i in L' is associated with the Lamé function that depends on the respective variable η_i .

We now turn to the differentiation of B^m . Applying the chain rule of differentiation, we obtain

$$\frac{d}{d\eta_i} B^m = \prod_{k=1}^m (\eta_i - \psi_k) \frac{d}{d\eta_i} \prod_{k=1}^m (\eta_i + \psi_k) + \prod_{k=1}^m (\eta_i + \psi_k) \frac{d}{d\eta_i} \prod_{k=1}^m (\eta_i - \psi_k). \quad (60)$$

Expanding and factoring out the products on the right-hand side, we obtain the following expression:

$$\frac{d}{d\eta_i} B^m = \sum_{d=1}^m \frac{1}{\eta_i + \psi_d} \prod_{k=1}^m (\eta_i - \psi_k)(\eta_i + \psi_k) + \sum_{d=1}^m \frac{1}{\eta_i - \psi_d} \prod_{k=1}^m (\eta_i - \psi_k)(\eta_i + \psi_k). \quad (61)$$

It is useful now to define two functions ζ_{km}^+ and ζ_{km}^- :

$$\zeta_{km}^{\pm} = \sum_{d=1}^m \frac{1}{(\eta_i \pm \psi_d)^k}. \quad (62)$$

Straightforwardly, we can also define a third function ζ_{km} as the sum of the two:

$$\begin{aligned} \zeta_{km} &= \zeta_{km}^+ + \zeta_{km}^- \\ &= \sum_{d=1}^m \left[\frac{1}{(\eta_i + \psi_d)^k} + \frac{1}{(\eta_i - \psi_d)^k} \right]. \end{aligned} \quad (63)$$

It is worthwhile noting that $\zeta_{km} \equiv \zeta_{mk}$, i.e. the permutation of the non-spatial indices k and m does not change the value of $\zeta_{km} B^m$. From this point forward, the subscript m of the ζ 's will be suppressed for simplicity and we will write $\zeta_k \equiv \zeta_{km}$. Using the formalism described

above, one can derive the following result by direct substitution of ζ_k into the expression for the derivative of B^m :

$$\frac{d}{d\eta_i} B^m = B^m \zeta_1. \quad (64)$$

This allows us to write the first derivative of the Lamé function using the simple formula

$$\frac{d}{d\eta_i} E_n^m(\eta_i) = (L_{ij} \zeta_{1m} + L'_{ij}) B^m. \quad (65)$$

We now have the tools required to derive $\nabla \mathbb{E}_n^m(\rho, \mu, \nu)$. The form assumed by the gradient of the normal ellipsoidal harmonic function is far more complicated in the ellipsoidal coordinates than it is in the Cartesian system. Nevertheless, this particular formulation is very important because of the separability property of the normal ellipsoidal harmonics in this coordinate system. Moreover, as will be made obvious in a future section, the simplicity associated with the definition of the ellipsoidal surface in this framework leads to numerous computational advantages, both analytic and numerical. Upon applying the gradient operator in ellipsoidal coordinates, we obtain the formula

$$\nabla \mathbb{E}_m^n = \mathbf{D}_{ij} \prod_{k=1}^m \Psi_k + L_{ij} \nabla \prod_{k=1}^m \Psi_k \quad (66)$$

$$= (\mathbf{D}_{ij} + L_{ij} \nabla) \prod_{k=1}^m \Psi_k, \quad (67)$$

where $\{\mathbf{D}_{ij}\}$ denotes a 3×5 matrix with the following entries:

$$\mathbf{D}_{i1} = \mathbf{0} \quad (68)$$

$$\mathbf{D}_{12} = \frac{1}{s_\rho} \hat{\rho} \quad (69)$$

$$\mathbf{D}_{22} = \frac{1}{s_\mu} \hat{\mu} \quad (70)$$

$$\mathbf{D}_{32} = \frac{1}{s_\nu} \hat{\nu} \quad (71)$$

$$\mathbf{D}_{13} = \frac{1}{s_\rho} \frac{\rho}{\sqrt{\rho^2 - h_3^2}} \hat{\rho} \quad (72)$$

$$\mathbf{D}_{23} = \frac{1}{s_\mu} \frac{\mu}{\sqrt{\mu^2 - h_3^2}} \hat{\mu} \quad (73)$$

$$\mathbf{D}_{33} = \frac{1}{s_\nu} \frac{-\nu}{\sqrt{h_3^2 - \nu^2}} \hat{\nu} \quad (74)$$

$$\mathbf{D}_{14} = \frac{1}{s_\rho} \frac{\rho}{\sqrt{\rho^2 - h_2^2}} \hat{\rho} \quad (75)$$

$$\mathbf{D}_{24} = \frac{1}{s_\mu} \frac{-\mu}{\sqrt{h_2^2 - \mu^2}} \hat{\mu} \quad (76)$$

$$\mathbf{D}_{34} = \frac{1}{s_v} \frac{-v}{\sqrt{h_2^2 - v^2}} \hat{\nu} \quad (77)$$

$$\mathbf{D}_{15} = \frac{[2\rho^2 - (h_3^2 + h_2^2)]\rho}{\sqrt{(\rho^2 - \mu^2)(\rho^2 - v^2)}} \hat{\rho} \quad (78)$$

$$\mathbf{D}_{25} = \frac{[(h_3^2 + h_2^2) - 2\mu^2]\mu}{\sqrt{(\mu^2 - \rho^2)(v^2 - \mu^2)}} \hat{\mu} \quad (79)$$

$$\mathbf{D}_{35} = \frac{[2v^2 - (h_3^2 + h_2^2)]v}{\sqrt{(v^2 - \rho^2)(v^2 - \mu^2)}} \hat{\nu}. \quad (80)$$

Since we have already computed $dB^m/d\eta_i$ using our ζ operator approach, it is now easy to derive $\nabla \prod_{k=1}^m \Psi_k$ because the factorized form of Ψ_k (see equation (29)) allows us to compute the partial derivatives with respect to η_i very easily by holding terms of the form $(\eta_j^2 - \psi_k^2)(\eta_l^2 - \psi_k^2)$ constant, where $j \neq i$ and $l \neq i$. Thus, the same line of reasoning used for finding $dB^m/d\eta_i$ can be employed to compute the partial derivatives of $\prod_{k=1}^m \Psi_k$. The final result is given by

$$\nabla \prod_{k=1}^m \Psi_k = \left[\frac{\zeta_{1m}(\rho)}{s_\rho} \hat{\rho} + \frac{\zeta_{1m}(\mu)}{s_\mu} \hat{\mu} + \frac{\zeta_{1m}(v)}{s_v} \hat{\nu} \right] \prod_{k=1}^m \Psi_k, \quad (81)$$

leading to the following expression for $\nabla \mathbb{E}_n^m$:

$$\nabla \mathbb{E}_n^m = \left\{ \mathbf{D}_{ij} + L_{ij} \left[\frac{\zeta_{1m}(\rho)}{s_\rho} \hat{\rho} + \frac{\zeta_{1m}(\mu)}{s_\mu} \hat{\mu} + \frac{\zeta_{1m}(v)}{s_v} \hat{\nu} \right] \right\} \prod_{k=1}^m \Psi_k. \quad (82)$$

This concludes our derivation of $\nabla \mathbb{E}_n^m$ in the two coordinate systems of our choice.

4. Derivation of the electric potential ϕ and field \mathbf{E}

The mathematical theory of ellipsoidal harmonics is of great interest in a variety of scientific areas, including gravitational astrophysics [40], physical geodesy [16] and numerical analysis, e.g. for obtaining solutions to the ellipsoidal Stokes problem [39]. In biophysics, it is useful for computing the electric potential, electric field and magnetic field due to one or several quasistatic current dipoles located in an organ whose shape is approximately ellipsoidal, such as the human brain or stomach.

Consider a point \mathbf{r}' located inside a body of volume V , where a primary current dipole source with moment \mathbf{Q} is also located. The physics of this problem [19, 41] allows one to model the phenomenon at hand as a concentration of impressed current \mathbf{J}_i to a point \mathbf{r}_0 using the Dirac delta functional $\delta(\mathbf{r} - \mathbf{r}_0)$ via the algebraic expression

$$\mathbf{J}_i(\mathbf{r}) = \mathbf{Q}\delta(\mathbf{r} - \mathbf{r}_0). \quad (83)$$

The electric field \mathbf{E} induced by the impressed current creates an induction current

$$\mathbf{J}_d(\mathbf{r}) = \sigma \mathbf{E}(\mathbf{r}), \quad (84)$$

where σ is the tissue conductivity. Since the anatomical and physiological characteristics of the human body allow for such currents to be considered quasistatic [20, 25, 41, 42], the electric field is irrotational and Poisson's equation can be used to find the electric potential ϕ .

The formulae for ϕ due to the dipoles located inside ellipsoids, spheroids and spheres were derived by Kariotou in [24]. For this reason, we discuss these theoretical results only to the extent that they are necessary for our own derivations. Nevertheless, it is important to take note of the fact that the expressions provided in [24] do not include ellipsoidal harmonic

terms of degree 3 or higher because such terms require numerical evaluations of roots for the Lamé polynomials. In the present study, we provide a generalized numerical and theoretical method for computing the potential using a harmonic expansion of arbitrary degree and order.

In our ellipsoidal coordinate formulation, the general solution to Poisson's equation

$$\Delta\phi^-(\mathbf{r}) = \frac{1}{\sigma}\nabla\cdot\mathbf{J}_i(\mathbf{r}), \quad \mathbf{r} \in V^- \quad (85)$$

is a superposition of an interior harmonic function $\Phi(\mathbf{r})$ and of the function

$$\phi(\mathbf{r}) = \frac{1}{4\pi\sigma}\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\frac{1}{|\mathbf{r}-\mathbf{r}'|}, \quad (86)$$

where the superscripts $(-)$ and $(+)$ denote quantities referring to the interior and exterior, respectively, of the volume for which Poisson's equation is solved. The equation above is cited correctly in [14]. In equations (38) and (40) of [24], however (both [14] and [24] have the same authors), $\nabla_{\mathbf{r}_0}$ is replaced by ∇ ; this is most likely a typographic error because all the other theory in that reference based on this formula is derived correctly using $\nabla_{\mathbf{r}_0}$ instead of ∇ . Upon substitution of the formulae for the interior harmonic function and Laplace operator [32] into equation (85), the interior potential assumes the form

$$\phi^-(\mathbf{r}) = b_0^1 + \sum_{n=0}^{\infty} \sum_{m=1}^{2n+1} \left\{ b_n^m + \frac{1}{\sigma\gamma_n^m} [\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\mathbb{E}_n^m(\mathbf{r}_0)] I_n^m(\rho) \right\} \mathbb{E}_n^m(\mathbf{r}). \quad (87)$$

The symbol b_n^m denotes the coefficient of the normal ellipsoidal harmonic functions \mathbb{E}_n^m , which is given [24] by the formula

$$b_n^m = \frac{1}{\sigma\gamma_n^m} [\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\mathbb{E}_n^m(\mathbf{r}_0)] \left[\frac{1}{\alpha_1\alpha_3 E_n^m(\alpha_1)} \left(\frac{dE_n^m}{d\alpha_1} \right)^{-1} - I_n^m(\alpha_1) \right], \quad (88)$$

where differentiation of $dE_n^m/d\alpha_1$ is with respect to the argument α_1 . As one can see, the interior potential is an infinite summation of terms involving the ellipsoidal harmonics \mathbb{E}_n^m . Substitution of the expression for b_n^m into the equation defining the potential and further manipulations yield the important formula

$$\begin{aligned} \phi^-(\mathbf{r}) = & b_0^1 + \sum_{n=1}^{\infty} \sum_{m=1}^{2n+1} \frac{1}{\sigma\gamma_n^m} [\mathbf{Q}\cdot\nabla_{\mathbf{r}_0}\mathbb{E}_n^m(\mathbf{r}_0)] \mathbb{E}_n^m(\mathbf{r}) \\ & \times \left[I_n^m(\rho) - I_n^m(\alpha_1) + \frac{1}{\alpha_2\alpha_3 E_n^m(\alpha_1)} \left(\frac{dE_n^m}{d\alpha_1} \right)^{-1} \right]. \end{aligned} \quad (89)$$

A similar calculation for ϕ^+ [24] provides the following expression for the exterior potential:

$$\phi^+(\mathbf{r}) = b_0^1 \frac{I_0^1(\rho)}{I_0^1(\alpha_1)} + \sum_{n=1}^{\infty} \sum_{m=1}^{2n+1} \frac{I_n^m(\rho)}{I_n^m(\alpha_1)} \frac{[\mathbf{Q}\cdot\nabla'\mathbb{E}_n^m(\mathbf{r}')] \mathbb{E}_n^m(\mathbf{r})}{\sigma\gamma_n^m\alpha_2\alpha_3 E_n^m(\alpha_1)} \left(\frac{dE_n^m}{d\alpha_1} \right)^{-1}. \quad (90)$$

The value assigned to the real constant b_0^1 is entirely arbitrary and its presence is evocative of the fact that one can add any real constant to a scalar potential without affecting the result obtained when computing the potential difference between two points. In the next section, it will be shown that setting this constant to 0 is computationally advantageous in the calculation of the magnetic field. Although the exterior potential involves the exterior harmonic functions \mathbb{F}_n^m , the potential can also be expressed only in terms of internal harmonics \mathbb{E}_n^m since the former can be defined in terms of the latter. The expressions above were simplified analytically in [24] for ellipsoidal terms of first and second degree. In this section, however, we develop a more general model for obtaining solutions for an arbitrarily large expansion of harmonics.

Using the expressions for ϕ , we can derive the corresponding formulae for the electric field \mathbf{E} that apply both to the interior (\mathbf{E}^-) and to the exterior (\mathbf{E}^+) of the ellipsoid:

$$\mathbf{E}^-(\mathbf{r}) = -\nabla\phi^- \tag{91}$$

$$\begin{aligned} &= -\sum_{n=1}^{\infty} \sum_{m=1}^{2n+1} \frac{1}{\sigma\gamma_n^m} [\mathbf{Q} \cdot \nabla_{\mathbf{r}_0} \mathbb{E}_n^m(\mathbf{r}_0)] \nabla \mathbb{E}_n^m(\mathbf{r}) \\ &\times \left[I_n^m(\rho) - I_n^m(\alpha_1) + \frac{1}{\alpha_2\alpha_3 E_n^m(\alpha_1)} \left(\frac{dE_n^m}{d\alpha_1} \right)^{-1} \right]. \end{aligned} \tag{92}$$

Similarly, we obtain for \mathbf{E}^+

$$\mathbf{E}^+(\mathbf{r}) = -\nabla\phi^+ \tag{93}$$

$$= -\sum_{n=1}^{\infty} \sum_{m=1}^{2n+1} \frac{I_n^m(\rho)}{I_n^m(\alpha_1)} \frac{[\mathbf{Q} \cdot \nabla_{\mathbf{r}_0} \mathbb{E}_n^m(\mathbf{r}_0)] \nabla \mathbb{E}_n^m(\mathbf{r})}{\sigma\gamma_n^m \alpha_2\alpha_3 E_n^m(\alpha_1)} \left(\frac{dE_n^m}{d\alpha_1} \right)^{-1}. \tag{94}$$

This completes our derivation of the electric potential and field.

5. Discussion and computational considerations

We can now summarize our algorithm proposed for the computation of ϕ , \mathbf{B} and \mathbf{E} using an ellipsoidal harmonic expansion of arbitrary order and degree. The generalized formulae for these three quantities are given in equations (89), (90), (92) and (94). The constants γ_n^m can be evaluated numerically using equation (22) as well as the formula for the surface differential dS specified by equation (23). The normal ellipsoidal harmonic functions are given in both Cartesian (equations (24)–(26)) and ellipsoidal (equations (27)–(29)) coordinates. The gradient $\nabla' \mathbb{E}_n^m$ can be computed using equation (82) with inputs for $\{\mathbf{D}_{ij}\}$, $\{L_{ij}\}$ provided in equations (68)–(80) and (28), respectively. Two other required formulas include the elliptic integrals I_n^m (which can be evaluated numerically using equation (15)) and the first derivative of the Lamé function (provided by equation (65)). Finally, the function D_n is specified by equation (41).

A number of computational issues should be addressed with reference to the problem at hand. As explained in [24], ellipsoidal harmonics can be expressed analytically in terms of the α_i only for $n \leq 3$ because higher-degree harmonic parameters lead to irreducible polynomial equations of cubic or higher degree. In this work, we choose to work only with the general formula for the ellipsoidal harmonics of arbitrary order and degree. According to a result by Stieltjes [37, 38], the Lamé function $E_n^m(\rho)$ has at most m real zeros ψ_1, \dots, ψ_m , $m \leq 2n + 1$, none of which are repeated. Because identifying all roots is algebraically impossible for polynomials of order 5 and higher, better approximations to the electric potential can be obtained only by implementing a numerical algorithm. To find the characteristic equations associated with Lamé polynomials, one must substitute the general expressions for \mathbb{E}_n^m into the Laplace equation and write down the relations that must hold in order for this equation to be satisfied; the details of this process are demonstrated in detail by Hobson, whose work on ellipsoidal harmonics [21] is an excellent reference. After tedious manipulations, it can be shown that the set of characteristic equations is given by

$$\sum_{d=1}^3 \frac{z_d}{\alpha_d^2 + \theta_p} + \sum_{q=1, q \neq p}^m \frac{1}{\theta_p - \theta_q} = 0, \tag{95}$$

Table 1. Values of the coefficients z_d , $d = 1, \dots, 3$ in the characteristic equations of the Lamé polynomials.

Function type	Value		
	z_1	z_2	z_3
K	1/4	1/4	1/4
L	3/4	1/4	1/4
M	1/4	3/4	3/4
N	3/4	3/4	3/4

where $\theta_1, \dots, \theta_m$ are the m roots sought and the constants z_d have the values shown in table 1. The left-hand side in this set of equations is the logarithmic differential coefficient with respect to θ_p of the product

$$E_n^m = \prod_{p=1}^m (\alpha_1^2 + \theta_p)^{z_1} (\alpha_2^2 + \theta_p)^{z_2} (\alpha_3^2 + \theta_p)^{z_3} \prod_{q \neq p}^m |\theta_p - \theta_q|, \quad (96)$$

which is known as Stieltjes' formulation of the Lamé function. The system of equations defined above can be manipulated using an efficient method for solving nonlinear equations; for example, a subspace trust region method based on the interior-reflective Newton method [11, 12] was found by the author to exhibit excellent convergence behaviour. In this approach, each iteration involves the approximate solution of a large linear system using the method of preconditioned conjugate gradients [12].

Numerical integration must be used to compute elliptic integrals of the form shown in equation (15), as well as the constants γ_n^m . In the case of the I_n^m , a simple analysis of the physical problem demonstrates that contributions to the integral are minute for the values of the integration variable t greater than some constant multiple of α_1 , i.e. for $t > c\alpha_1$, where c is of $\mathcal{O}(1)$ and $c > 1$. Hence, the upper integration limit can appropriately be fixed in this case to a suitable value.

The results presented in this paper show that the calculation of higher-order contributors to the electric potential and field in ellipsoidal geometry is a tedious and computationally-demanding task. This raises the question as to whether simpler techniques—such as the finite or boundary element methods—may be superior. This may indeed be the case for the forward problem of MEG or MGG; nevertheless, a certain important advantage associated with our method is not available in the BEM or FEM formalisms. This advantage refers to the fact that neither of the latter methods can clarify the issue as to how many higher-order contributors are necessary for accurate calculations of ϕ and \mathbf{E} in the ellipsoidal formalism. Because of this, the issue of accuracy associated with the localization of sources from inverse procedures applied to MGG or foetal EEG data (see [18] and the discussion in [23]) cannot be settled only from an application of FEM or BEM. More research is therefore required to determine how appropriate the ellipsoidal model is in comparison with the realistic models.

6. Conclusion and future research

In this paper, we have presented a generalized theoretical and numerical method for computing the electric potential, electric field and magnetic field due to a quasistatic bioelectric current dipole located inside an ellipsoid. The electric potential field can be expressed as a truncated infinite series of terms involving the normal ellipsoidal harmonic functions \mathbb{E}_n^m and their gradients. On the other hand, the magnetic field is given by a double infinite summation of ellipsoidal terms, which potentially makes its computation more intensive by two orders of

magnitude. Our computational technique requires one to find the roots of Lamé functions, a task that has already been successfully approached using a standard nonlinear optimization algorithm. In our future endeavour, we intend to implement the algorithm described here numerically and to investigate the quantitative importance of high-order terms in the calculation of ϕ , \mathbf{E} and \mathbf{B} for the electro- and magneto-gastrographic forward problem.

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