Potential and Field of a Homogeneous Magnetic Spheroid of Arbitrary Direction in a Homogeneous Magnetic Field in Cartesian Coordinates.

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1 Introduction

We derive expressions for the potential and the magnetic field of prolate and oblate spheroids with permeability $\mu_2$ inserted into a static homogeneous magnetic field in a medium with permeability $\mu_1$. Both directions, that of the primary field and that of the symmetry axis, are completely arbitrary. The potential and the field components as well as the arguments of these functions are expressed in Cartesian coordinates. Though the centre of the spheroid is at the origin, it is easy to change all the formulas for another position of the spheroidal centre. This grants more freedom, flexibility and ease for building complex structures composed of arbitrarily arranged spheroids.

Our derivations start from previous work (Kuchel and Bulliman, 1989) where the two problems have been solved for spheroids in prolate or oblate spheroidal coordinates with the z-axis as the symmetry axis and a homogeneous static external field of arbitrary direction. The potentials and the fields have also been expressed in Cartesian coordinates except for three functions in $\cosh \eta$ (in the prolate case) or in $\sinh \eta$ (in the oblate case), where $\eta$ is the quasi-radial variable. We succeeded in replacing these hyperbolic functions by square root expressions involving Cartesian coordinates. These square roots depend on the square of the radius, a rotation invariant, and on $z^2$, which is invariant under rotations around the symmetry axis. All other terms of the potentials depend on similar invariants. These dependences permit one to go from the $z$-axis to an arbitrary vector as the symmetry axis. The gradients of the potentials are needed to determine the field expressions. For this purpose the gradients of

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the three functions occurring in the potentials are computed and simplified. All these expressions are derived in the third and fourth section.

When deriving these potentials and fields we had in mind magnetic resonance imaging (MRI) and magnetic resonance spectroscopy (MRS). These make use of the Larmor resonance signals emitted by protons precessing in the local magnetic induction, which is excited by an external static magnetic field. In general, the MR signal is highly sensitive to the magnetic properties of the matter surrounding the nuclei. Theoretical studies of the resonance signal behaviour in situations of varying magnetic susceptibilities and dynamic physiological processes as for instance diffusion utilize the analytical magnetostatic solutions of specific geometrical bodies. Models of structures like cells or blood vessels can be built up from arrays of simple magnetic bodies. In particular prolate and oblate spheroids are used as such building blocks to analyse the local magnetic field distribution in the vicinity of blood cells in MRS of cells (Kuchel and Bulliman, 1989). The magnetic susceptibilities of biological matter are small. Hence the total field a proton experiences consists of the primary field and of the perturbation fields of all the spheroids used to model the structure under investigation. Since the magnetic susceptibilities of the biological materials are small the interaction between the various spheroids may be neglected. So the proposed approach described below gives a good approximation.

In this way a toolbox for MRI and MRS resonance signal analyses with flexible instruments is provided capable of modelling several biological tissues of interest such as trabecular bone, microvascular network and general interfaces of adjacent tissues. We give only a short survey of such applications in the fifth section. More detailed accounts of such investigations will be submitted to pertinent journals of medical physics.

Conclusions regarding the results obtained and listing of motivation and other applications are contained in the sixth section.

2 Primary and Total Field

The primary field is a homogeneous static magnetic field. In the general case this is written as

\[
\mathbf{H}_0 = (H_{0x}, H_{0y}, H_{0z}) = H_0 (\sin \beta \cos \alpha, \sin \beta \sin \alpha, \cos \beta)
\]

with the corresponding potential

\[
\Phi_0(x, y, z) = -(H_{0x} x + H_{0y} y + H_{0z} z)
\]

A spheroid with magnetic permeability \(\mu_2 = \mu_0(1 + \chi_2)\) is surrounded by an infinite medium with magnetic permeability \(\mu_1 = \mu_0(1 + \chi_1)\). The total external field \(\mathbf{H}_1\) and the corresponding potential \(\Phi_1\) must assume the asymptotic values

\[
\lim_{|r| \to \infty} \mathbf{H}_1 = \mathbf{H}_0, \quad \lim_{|r| \to \infty} \Phi_1 = \Phi_0.
\]

The presence of the spheroid induces perturbation fields in the exterior and the interior, with potentials \(\Phi_{1r}\) and \(\Phi_{2r}\). The corresponding total fields, \(\Phi_1 = \)
\( \Phi_1 + \Phi_0 \) and \( \Phi_2 = \Phi_2 + \Phi_0 \) must fulfil the following two continuity conditions at the surface of the spheroid:

\[
r = r_s : \quad \Phi_1 = \Phi_2, \quad \mu_1 \left( s \cdot \nabla \Phi_1 \right) \bigg|_{r=r_s} = \mu_2 \left( s \cdot \nabla \Phi_2 \right) \bigg|_{r=r_s}. \tag{4}
\]

\( s \) is the normal to the surface of the spheroid. All these conditions define a unique solution to be found in the next chapters for prolate and oblate spheroids.

### 3 A Prolate Spheroid in a Homogeneous Magnetic Field

For a prolate spheroid (semi-axes \( a_p, a_p, c_p; c_p > a_p \)) with magnetic permeability \( \mu_2 \) in a medium with magnetic permeability \( \mu_1 \) and in an external homogeneous field (1) the boundary value problem has been solved in prolate spheroidal coordinates (Kuchel and Bulliman, 1989). The symmetry axis is the z-axis. The direction of the primary field is arbitrary (cf. eq.(1)). We repeat just the essential equations of this reference. Then we use these expressions to go over to Cartesian coordinates. Finally these expressions are generalized to the case where both the symmetry axis and that of the primary field are completely arbitrary.

#### 3.1 The reaction field in prolate spheroidal coordinates

At first the boundary value problem is solved in prolate spheroidal coordinates (s., for example, (Moon and Spencer, 1988), Fig.1.06).

\[
x = e_p \sinh \eta \sin \theta \cos \psi, \tag{5}
\]
\[
y = e_p \sinh \eta \sin \theta \sin \psi, \tag{6}
\]
\[
z = e_p \cosh \eta \cos \theta; \tag{7}
\]
\[
e_p = \sqrt{c_p^2 - a_p^2} \tag{8}
\]

for a spheroid, whose symmetry axis coincides with the z-axis. The potential equation can be solved by separation.

\[
\Phi(\eta, \theta, \psi) = H(\eta) \Theta(\theta) \Psi(\psi). \tag{9}
\]

The particular solutions of the resulting ordinary differential equation for the quasi-radial functions \( H(\eta) \) are Legendre polynomials or functions in \( \cosh \eta \). The solutions \( \Theta(\theta) \) must be Legendre polynomials in \( \cos \theta \); Legendre functions in \( \cos \theta \) are singular at \( \theta = 0, \pi \); so they must be excluded. In each term the order \( n \) of the quasi-radial functions must agree with that of the Legendre polynomial \( P_n^m(\cos \theta) \). \( \Psi(\psi) \) are the trigonometric functions \( \cos(m\psi) \) or \( \sin(m\psi) \).

The interface separating the two domains is the spheroid:

\[
\frac{x^2}{a_p^2} + \frac{y^2}{a_p^2} + \frac{z^2}{c_p^2} = 1 \iff \eta = \eta_p = \text{Arcoth}(c_p/a_p). \tag{10}
\]

One starts inserting the spheroidal coordinates into the primary potential (2). Thereafter these are replaced by the corresponding particular solutions of
the potential equation using

\[ P_0^0(\cos \theta) = \cos \theta, \quad P_1^1(\cos \theta) = \sin \theta; \quad P_0^0(\cosh \eta) = \cosh \eta, \quad P_1^1(\cosh \eta) = \sinh \eta \]

(11)
to give:

\[ \Phi_0 = -e_\rho P_1^1(\cosh \eta) P_1^1(\cos \theta) (H_{0x} \cos \psi + H_{0y} \sin \psi) \\
- e_\rho P_0^0(\cosh \eta) P_0^1(\cos \theta) H_{0z}. \quad (12) \]

The perturbation field in the exterior must vanish at infinity. This is ensured by the Legendre functions of the quasi-radial variable in the following series expansions:

\[ \eta \geq \eta_p : \]

\[ \Phi_{1r} = \sum_{m=0}^{\infty} A_m P_m(\cosh \eta) P_m(\cos \theta) \cos(m\psi) + \]
\[ + B_m P_m(\cosh \eta) P_m(\cos \theta) \sin(m\psi). \quad (13) \]

In the interior the total field must be finite at the origin. This excludes the Legendre functions for the quasi-radial variable.

\[ \eta \leq \eta_p : \]

\[ \Phi_2 = \sum_{m=0}^{\infty} A_m P_m(\cosh \eta) P_m(\cos \theta) \cos(m\psi) + \]
\[ + B_m P_m(\cosh \eta) P_m(\cos \theta) \sin(m\psi). \quad (14) \]

These sums are inserted into the two continuity conditions (4). The normal derivative \( s \cdot \nabla \) becomes just the derivation \( \partial / \partial \eta \) up to a metric coefficient, which cancels on both sides of the equation. In view of the orthogonality of the Legendre polynomials \( P_m^n(\cos \theta) \) and of the trigonometric functions these two conditions involving sums are decomposed into three system of two linear equations for the expansion coefficients. Each system comprises just a single pair of the parameters \( n \) and \( m \). Solving these systems gives the expansion coefficients listed below.

One may start with a more general expansion comprising infinite sums in \( n \) and \( m \). One inserts these infinite sums into the two continuity conditions (4). The aforementioned orthogonality leads to an infinite system of pairs of linear equations. But for \( n \neq 1 \) and \( m \neq 0 \) nor \( \neq 1 \) these systems are linear homogeneous equations for the unknown coefficients \( 2A_m, 2B_m, 1A_m \) and \( 1B_m \) giving zero solutions. So the simple approach as well as the more complicated
one give the same solutions:

\[ 1A_1^0 = e_p H_{0x} (\mu_2 - \mu_1) P_0 \frac{P_0' Q_1}{P_1 Q_1'} = e_p H_{0z} L_0, \]

\[ 2A_1^0 = e_p H_{0z} \mu_1 \left( \frac{P_0' Q_0 - P_0 Q_0'}{\mu_1 P_0 Q_0'} \right) = e_p H_{0z} M_0; \quad (15) \]

\[ 1A_1^1 = e_p H_{0x} (\mu_2 - \mu_1) \frac{P_1' Q_1}{P_1 Q_1'} = e_p H_{0x} L_1, \]

\[ 1B_1^1 = e_p H_{0y} L_1, \quad (16) \]

\[ 2A_1^1 = e_p H_{0x} \mu_1 \left( \frac{P_1' Q_1 - P_1 Q_1'}{\mu_1 P_1 Q_1'} \right) = e_p H_{0x} M_1, \]

\[ 2B_1^1 = e_p H_{0y} M_1. \quad (17) \]

The argument of all the Legendre polynomials and functions in the above equations is \( \cosh \eta_p \). The solutions have been obtained with the help of Mathematica. The corresponding notebook named ProlateCoefficients.nb can be found at a website (Kraiger and Schnizer, 2011). The solutions agree with those of (Kuchel and Bulliman, 1989). In the same reference it has been shown that the Legendre functions and polynomials may be replaced with elementary functions

\[ Q_0'(cosh \eta) = \cosh \eta \text{Arcoth} (cosh \eta) - 1, \]

\[ Q_1'(cosh \eta) = \sinh \eta \text{Arcoth} (cosh \eta) - \coth \eta. \quad (21) \]

The above results are inserted into eq.(14); the total interior potential comes out as that of a homogeneous field:

\[ \eta \leq \eta_p : \quad \Phi_2 = e_p M_1 (H_{0x} \cos \psi + H_{0y} \sin \psi) \sin \eta \sin \theta \]

\[ + e_p M_0 H_{0z} \cosh \eta \cos \theta, \]

\[ \Phi_2(x, y, z) = M_1 (H_{0x} x + H_{0y} y) + M_0 H_{0z} z. \quad (22) \]

Similarly one gets for the exterior reaction field:

\[ \eta \geq \eta_p : \quad \Phi_{r1} = e_p (H_{0x} \cos \psi + H_{0y} \sin \psi) \times \]

\[ \times L_1 (\sin \eta \text{Arcoth} (cosh \eta) - \coth \eta) \sin \theta \]

\[ + e_p H_{0z} L_0 (\cosh \eta \text{Arcoth} (cosh \eta) - 1) \cos \theta, \]

\[ = L_1 (H_{0x} x + H_{0y} y) (f_1(\eta) - f_2(\eta)) + L_0 H_{0z} z (f_1(\eta) - f_3(\eta)), \quad (23) \]
with
\[
\begin{align*}
    f_1(\eta) &= \text{Arcoth}(\cosh \eta), \quad (24) \\
    f_2(\eta) &= \frac{\cosh \eta}{\sinh^2 \eta}, \quad (25) \\
    f_3(\eta) &= \frac{1}{\cosh \eta}. \quad (26)
\end{align*}
\]

The functions \(f_1(\eta), f_2(\eta), f_3(\eta)\) above depend solely on the quasi-radial variable \(\cosh \eta\). In the exterior of the spheroid is \(\eta \geq \eta_p > 1\); so the three functions just introduced are well-defined, real, finite and non-zero in the exterior of the spheroid.

Inserting the substitutions (11), (21) and their derivatives into the definitions of the constants \(L_0, L_1, M_0, M_1\) above and going over to the susceptibilities the expressions for these constants become after some algebra:

\[
\begin{align*}
    L_0 &= \frac{(\chi_1 - \chi_2) \cosh \eta_p}{1 + \chi_2 - (1 + \chi_1) \coth^2 \eta_p + (\chi_1 - \chi_2) \cosh(\eta_p) \text{Arcoth}(\cosh \eta_p)}, \quad (27) \\
    L_1 &= \frac{\chi_1 - \chi_2}{(2 + \chi_1 + \chi_2) \csch^2 \eta_p \sech \eta_p + (\chi_1 - \chi_2) (\text{Arcoth}(\cosh \eta_p) - \sech \eta_p)}, \quad (28) \\
    M_0 &= -\frac{1 + \chi_1}{1 + \chi_1 + (\chi_1 - \chi_2) \sinh^2 \eta_p (1 - \cosh \eta_p) \text{Arcoth}(\cosh \eta_p)}, \quad (29) \\
    M_1 &= -\frac{2 (1 + \chi_1)}{(2 + \chi_1 + \chi_2) - (\chi_1 - \chi_2) \sinh^2 \eta_p (1 - \cosh \eta_p) \text{Arcoth}(\cosh \eta_p)}. \quad (30)
\end{align*}
\]

If both media are the same the above coefficients become:

\[
\begin{align*}
    \chi_2 &\rightarrow \chi_1: \quad L_0 \rightarrow 0, \quad L_1 \rightarrow 0, \quad M_0 \rightarrow -1, \quad M_1 \rightarrow -1. \quad (31)
\end{align*}
\]

The exterior reaction potential, eq.(23), then assumes the value zero. The total interior potential, eq.(22), becomes equal to the primary potential, eq.(2). So the interior reaction potential is:

\[
\Phi_2(x, y, z) = \Phi_2(x, y, z) = \\
= (H_{0x} x + H_{0y} y) (M_1 + 1) + H_{0z} z (M_0 + 1). \quad (32)
\]

3.2 The reaction field in Cartesian coordinates

We want expressions for the potential which depend on \(x, y, z\) only. So \(\cosh \eta\) must be replaced with a corresponding expression in Cartesian coordinates. From eqs.(5) to (7) one finds:

\[
\cosh^2 \eta = \frac{1}{2} \left(1 + \frac{r^2}{e^2} \pm \sqrt{\left(1 + \frac{r^2}{e^2}\right)^2 - 4 \frac{z^2}{e^2}} \right) .
\]
Intense numerical studies show that only the plus sign applies. So we have:

\[
\cosh \eta = \frac{1}{\sqrt{2}} \sqrt{1 + \frac{r^2}{e_p^2} + w_p(r, e_z)} := \frac{u_p(r, e_z)}{\sqrt{2}},
\]

\[
w_p(r, e_z) = \sqrt{\left(1 + \frac{r^2}{e_p^2}\right)^2 - 4 \frac{\mathbf{e}_z \cdot \mathbf{r}^2}{e_p^2}} = \sqrt{\left(1 + \frac{r^2}{e_p^2}\right)^2 - 4 \left(\mathbf{e}_z \cdot \mathbf{r}\right)^2},
\]

\[
r^2 = x^2 + y^2 + z^2.
\]

Inserting this expression for \(\cosh \eta\) into eqs.(24) to (26)

\[
f_1(r, e_z) = \text{Arcoth}(u_p(r, e_z)/\sqrt{2}),
\]

\[
f_2(r, e_z) = \frac{\sqrt{2} u_p(r, e_z)}{u_p(r, e_z)^2 - 2},
\]

\[
f_3(r, e_z) = \frac{\sqrt{2}}{u_p(r, e_z)}.
\]

and inserting the resulting expressions for \(f_1, f_2, f_3\) into eq.(23) we get the final expression for the exterior potential as a pure function of the Cartesian coordinates \(x, y, z\):

\[
\Phi_{r1}(x, y, z) = L_1 \left(H_{0z} x + H_{0y} y\right) \left(f_1(r, e_z) - f_2(r, e_z)\right) + L_0 H_{0z} z \left(f_1(r, e_z) - f_3(r, e_z)\right).
\]

As stated after eqs.(26) these functions encounter no problems in the exterior of the spheroid. The interior potential, eq.(32), is already a simple function of the Cartesian coordinates.

### 3.3 Potential and field for an arbitrary direction of the spheroidal symmetry axis

For applications it is necessary to consider spheroids whose symmetry axis has an arbitrary direction. The corresponding expressions for the potential will be derived from those given in eqs.(39) and (32). These are rewritten in a way suggesting a general form:

\[
\Phi_{r1}(x, y, z) = \left(H_{0z} \cdot \mathbf{r}_{\perp}\right) L_1 \left(f_1(r, e_z) - f_2(r, e_z)\right) + \left(H_{0z} \cdot \mathbf{r}\right) L_0 \left(f_1(r, e_z) - f_3(r, e_z)\right),
\]

\[
\Phi_{r2}(x, y, z) = \left(H_{0z} \cdot \mathbf{r}_{\perp}\right) (M_1 + 1) + \left(H_{0z} \cdot \mathbf{r}\right) (M_0 + 1).
\]

The vectors \(\mathbf{H}_{0z}, \mathbf{r}\) give the projections of the corresponding vector parallel to the symmetry axis, i.e. the \(z\)-axis. Similarly, the vectors \(\mathbf{H}_{0z} = (H_{0x}, H_{0y}, 0)\), \(\mathbf{r}_{\perp} = (x, y, 0)\) give the vector corresponding to the projection onto the \(x, y\)-plane, which is perpendicular to the symmetry axis.

Now it is easy to accomplish the substitutions for an arbitrary direction of the symmetry axis given by the unit vector \(\mathbf{n}\). Any vector \(\mathbf{s}\) may be decomposed into a component parallel to \(\mathbf{n}\) and one perpendicular to that vector:

\[
\mathbf{s} = \mathbf{s}_{\parallel} + \mathbf{s}_{\perp} = \mathbf{n}(\mathbf{s} \cdot \mathbf{n}) + (\mathbf{s} - \mathbf{n}(\mathbf{s} \cdot \mathbf{n})).
\]
In \( w_p(r, e_z) \), eq.(34), only the variable \( z = (e_z \cdot r) \), the component of the position vector along \( e_z \), must be replaced by \( (n \cdot r) \) giving:

\[
\cosh \eta = \frac{1}{\sqrt{2}} \sqrt{1 + \frac{r^2}{e_p^2} + w_p(r, n) := u_p(r, n)/\sqrt{2},}
\]

\[
w_p(r, n) = \sqrt{\left(1 + \frac{r^2}{e_p^2}\right)^2 - 4 \frac{(n \cdot r)^2}{e_p^2}}.
\]

The functions \( f_i \), eqs.(36) to (38), remain the same except that \( u_p(r, e_z) \) and \( w_p(r, e_z) \) must be replaced with \( u_p(r, n) \) and \( w_p(r, n) \) giving the new functions \( f_i(r, n) \):

\[
f_1(r, n) = \text{Arcoth}(u_p(r, n)/\sqrt{2}),
\]

\[
f_2(r, n) = \frac{\sqrt{2} u_p(r, n)}{(u_p(r, n))^2 - 2},
\]

\[
f_3(r, n) = \frac{\sqrt{2}}{u_p(r, n)},
\]

Inserting all these new functions into eqs.(40) gives the potential for a prolate spheroid whose symmetry axis is given by the arbitrary unit vector \( n \):

\[
\Phi_{v1}(x, y, z) = L_1 (H_0 \cdot r) \left( f_1(r, n) - f_2(r, n) \right) + \nonumber
\]

\[
+ (H_0 \cdot n)(n \cdot r) \left[ L_0 \left( f_1(r, n) - f_2(r, n) \right) - L_1 \left( f_1(r, n) - f_2(r, n) \right) \right],
\]

\[
\Phi_{v2}(x, y, z) = \left( H_0 \cdot r \right) (M_1 + 1) + (H_0 \cdot n)(n \cdot r) \left[ M_0 - M_1 \right].
\]

The evaluation of the magnetic field requires the gradients of the functions \( f_i(r, n) \). These are done by symbolic computation. Since the resulting expressions consist again of polynomials and the square roots already occurring in the potential it is possible to find simpler expressions. These are again checked against the original gradients by symbolic computation. All gradients are proportional to the vector \( r_p \):

\[
r_p := \frac{\sqrt{2}}{e_p^2} \left( r - 2n \frac{(n \cdot r)}{[u_p(r, n)]^2} \right).
\]

\[
\nabla f_1(r, n) - \nabla f_2(r, n) = \frac{u_p(r, n)}{w_p(r, n)} \frac{4}{[(u_p(r, n))^2 - 2]^2} r_p,
\]

\[
\nabla f_1(r, n) - \nabla f_3(r, n) = \frac{2}{[2 - (u_p(r, n))^2]} \frac{u_p(r, n) w_p(r, n)}{w_p(r, n)} r_p.
\]

The corresponding checks are contained in the notebook ProlatePotDeriva-
tives.nb (Kraiger and Schnizer, 2011).

The vector \( r_p \) and all the gradients listed above are well-defined and real in the exterior of the spheroid, including the interface, where \( \eta \geq \eta_p \), which
is equivalent with the condition (55) in Cartesian coordinates. In fact, a more detailed analysis shows that on the interface:

\[ u_p(r, n) = \sqrt{2} \cosh \eta_p, \tag{52} \]

\[ w_p(r, n) = \sqrt{z^4/(\eta_p \cosh(\eta_p))^4 - 2z^2/\eta_p^2 + \cosh^4 \eta_p} \tag{53} \]

\[ \sinh^2 \eta_p \leq w_p(r, n) \leq \cosh^2 \eta_p. \tag{54} \]

For example, for \( a = 1, c = 2, (e_p = \sqrt{3}) \) one finds \( \sqrt{2} \cosh \eta_p = 2\sqrt{2/3} = 1.63... > \sqrt{2}; 1/3 \leq w_p(r, n) \leq 4/3. \)

### 3.4 Final formulas for the field

So the final formulas for the reaction field excited in an arbitrary homogeneous primary field \( H_0 \) by a prolate spheroid with arbitrary symmetry axis given by a unit vector \( n \) is in the exterior:

\[ \frac{r^2 - (n \cdot r)^2}{a_p^2} + \frac{(n \cdot r)^2}{c_p^2} \geq 1 : \quad H_{r1}(x, y, z) = -H_0 \quad L_1 \quad \left(f_1(r, n) - f_2(r, n)\right) - n(H_0 \cdot n)\left[L_0 \quad \left(f_1(r, n) - f_3(r, n)\right) - L_1 \quad \left(f_1(r, n) - f_2(r, n)\right)\right] \]

\[ -r_p \quad (H_0 \cdot r) \quad L_1 \quad \frac{u_p(r, n)}{w_p(r, n)} \quad \frac{4}{\left[(u_p(r, n))^2 - 2\right]^2} \]

\[ -r_p \quad (H_0 \cdot n)(r \cdot n) \quad L_0 \quad \frac{2}{\left[(u_p(r, n))^2 - 2\right]}; \tag{56} \]

and in the interior:

\[ \frac{r^2 - (n \cdot r)^2}{a_p^2} + \frac{(n \cdot r)^2}{c_p^2} \leq 1 : \quad H_{r2}(x, y, z) = -H_0 \quad (M_1 + 1) - n \quad (H_0 \cdot n) \quad [M_0 - M_1]. \tag{57} \]

### 3.5 Concluding remarks for the field of the prolate spheroid

A prolate spheroid is inserted into an external homogeneous magnetic field \( H_0 \) of arbitrary direction. Its permeability is \( \mu_2 = \mu_0 (1 + \chi_2) \); while that of the surrounding medium is \( \mu_1 = \mu_0 (1 + \chi_1) \). The spheroid has semi-axes \( a_p, a_p, c_p, c_p > a_p \); these determine the excentricy \( e_p \) and the quasi-radial parameter \( \eta_p \), eqs.(8) and (10). These in turn determine the coefficients \( L_0, L_1, M_0, M_1 \), eqs.(27) to (30). The spheroid’s symmetry axis is the arbitrary unit vector \( n \). The reaction field due to the presence of the spheroid in the external field is given in Cartesian coordinates, \( r = (x, y, z) \), by eq.(56) in the exterior, by eq.(57) in the interior. The functions \( f_1(r, n), \quad f_2(r, n), \quad f_3(r, n), \) eqs.(44) to (46), depend on the variables \( u_p(r, n) \) and \( w_p(r, n) \), eqs.(42) and (43). The needed gradients of the \( f_i(r, n) \) are given in eqs.(50) and (51). Eqs.(56) and eq.(57) are for a spheroid, whose centre is at the origin. If the centre is at the point \( r_0 = (x_0, y_0, z_0) \) then the vector \( r \) must replaced simply with \( r - r_0 \).
4 A Single Oblate Spheroid in a Homogeneous Magnetic Field

An oblate spheroid (semi-axes $a_o, b_o, c_o$; $c_o < a_o$) with magnetic permeability $\mu_2 = \mu_0(1 + \chi_2)$ is in a medium with magnetic permeability $\mu_1 = \mu_0(1 + \chi_1)$ and in an external field (1). The solution of this boundary value problem has been sketched in (Kuchel and Bulliman, 1989). We use a notation for the coefficients which differs somewhat from that employed in this reference. The derivations are quite analogous to those performed in the previous chapter. The main difference is the different analytical form of the quasi-radial particular solutions.

4.1 The reaction field in oblate spheroidal coordinates

The spheroid induces a reaction field represented by the potentials $\Phi_\text{r1}(x, y, z)$ in the exterior, by $\Phi_\text{r2}(x, y, z)$ in the interior. This problem has been solved in (Kuchel and Bulliman, 1989) in oblate spheroidal coordinates (s., for example, (Moon and Spencer, 1988), Fig.1.07).

\begin{align*}
x &= e_o \cosh \eta \sin \theta \cos \psi, \tag{58} \\
y &= e_o \cosh \eta \sin \theta \sin \psi, \tag{59} \\
z &= e_o \sinh \eta \cos \theta; \tag{60} \\
e_o &= \sqrt{a_o^2 - c_o^2} \tag{61}
\end{align*}

for a spheroid, whose symmetry axis coincides with the z-axis. $\Phi_0$, $\Phi_1 = \Phi_0 + \Phi_{r1}$, $\Phi_2 = \Phi_0 + \Phi_{r2}$ must be solutions of the potential equation in oblate coordinates. This partial differential equation can be solved by separation. The particular solutions of the separated equations suitable for the problem under investigation are Legendre polynomials or functions in $i \sinh \eta$; Legendre polynomials in $\cos \theta$; trigonometric functions in $\psi$.

The interface separating the two domains is the spheroid:

\begin{equation}
\frac{x^2}{a_o^2} + \frac{y^2}{b_o^2} + \frac{z^2}{c_o^2} = 1 \iff \eta = \eta_o = \text{Artanh}(c_o/a_o). \tag{62}
\end{equation}

The potential and the normal component of the magnetic induction must be continuous across this interface. So conditions (4) apply again.

One starts with expansion in the particular solutions fulfilling the boundary conditions. We already know from the previous chapter that only the parameter values $n = 1$, $m = 0$ and 1 are needed. We want to get real expansion coefficients. According to (Kuchel and Bulliman, 1989), eqs.(A64), the $P_m^n(i \sinh \eta)$ are purely imaginary, the $Q_m^n(i \sinh \eta)$ are real:

\begin{align*}
P_0^0(i \sinh \eta) &= i \sinh \eta, \\
P_1^0(i \sinh \eta) &= i \cosh \eta; \tag{63} \\
Q_1^0(i \sinh \eta) &= \sinh \eta \text{arccot}(\sinh \eta) - 1, \\
Q_1^1(i \sinh \eta) &= \cosh \eta \text{arccot}(\sinh \eta) - \tanh \eta. \tag{64}
\end{align*}

These reality properties are taken into account below by inserting imaginary units in the expansions for the potentials. The primary potential is expressed
as:
\[
\Phi_0 = i e_o H_{0z} P_1^0(i \sinh \eta) P_1^0(\cos \theta) - i e_o (H_{0x} \cos \psi + H_{0y} \sin \psi) P_1^1(i \sinh \eta) P_1^1(\cos \theta) \tag{65}
\]
by eqs. (58) to (60) and (63). The total potentials are assumed as:

\( \eta \geq \eta_o : \)
\[
\Phi_1 = \Phi_0 + \sum_{m=0}^{1} i A_1^m Q_1^m(i \sinh \eta) P_1^m(\cos \theta) \cos(m \psi) + 1 B_1^1 Q_1^1(i \sinh \eta) P_1^1(\cos \theta) \sin \psi ; \tag{66}
\]

\( \eta \leq \eta_o : \)
\[
\Phi_2 = \sum_{m=0}^{1} i 2 A_1^m P_1^m(i \sinh \eta) P_1^m(\cos \theta) \cos(m \psi) + i 2 B_1^1 P_1^1(i \sinh \eta) P_1^1(\cos \theta) \sin \psi . \tag{67}
\]

The sums are inserted into the continuity conditions (4). In view of the orthogonality of the Legendre polynomials \( P_n^m(\cos \theta) \) and of the trigonometric functions these two conditions involving sums are decomposed into three independent systems with the solutions:

\[
1 A_1^0 = i e_o H_{0z} \mu_2 (\mu_2 - \mu_1) P_1^0 \frac{P_1^0 P_1^0}{P_1^0 Q_1^0 - \mu_1 P_1^0 Q_1^0} \]
\[
:= e_o H_{0z} \bar{L}_0 , \tag{68}
\]

\[
2 A_1^0 = e_o H_{0z} \mu_1 \left( \frac{P_1^0 Q_1^0 - P_1^0 Q_1^0}{P_1^0 Q_1^0 - \mu_1 P_1^0 Q_1^0} \right) \]
\[
:= e_o H_{0z} \bar{M}_0 ; \tag{69}
\]

\[
1 A_1^1 = i e_o H_{0x} (\mu_1 - \mu_2) P_1^1 \frac{P_1^1 P_1^1}{P_1^1 Q_1^1 - \mu_1 P_1^1 Q_1^1} \]
\[
:= e_o H_{0x} \bar{L}_1 , \tag{70}
\]

\[
1 B_1^1 = e_o H_{0y} \bar{L}_1 , \tag{71}
\]

\[
2 A_1^1 = e_o H_{0z} \mu_1 \left( \frac{P_1^1 Q_1^1 - P_1^1 Q_1^1}{P_1^1 Q_1^1 - \mu_1 P_1^1 Q_1^1} \right) \]
\[
:= e_o H_{0z} \bar{M}_1 , \tag{72}
\]

\[
2 B_1^1 = e_o H_{0y} \bar{M}_1 . \tag{73}
\]

The solutions are given in the notebook OblateCoefficients.nb (Kraiger and Schnizer, 2011). The argument of all the Legendre polynomials and functions in all of the above equations is \( i \sinh \eta_o \). Inserting these solutions and thereafter the elementary functions (63) and (64) we get the total interior potential as that of a homogeneous field:

\( \eta \leq \eta_o : \)
\[
\Phi_2 = - e_o \bar{M}_1 (H_{0z} \cos \psi + H_{0y} \sin \psi) \cosh \eta \sin \theta - e_o \bar{M}_0 H_{0z} \sinh \eta \cos \theta , \]
\[
\Phi_2(x, y, z) = - \bar{M}_1 (H_{0x} x + H_{0y} y) - H_{0z} z . \tag{74}
\]
Similarly we get for the external reaction field:

\[ \eta \geq \eta_0 : \]

\[ \Phi_{r1} = e_o (H_{0x} \cos \psi + H_{0y} \sin \psi) \times \]

\[ L_1 \left( \cosh \eta \arccot(\sinh \eta) - \tanh \eta \sin \theta \right) + e_o H_{0z} L_0 \left( \sinh \eta \arccot(\sinh \eta) - 1 \right) \cos \theta , \]

\[ = - L_1 \left( H_{0x} x + H_{0y} y (g_1(\eta) - g_2(\eta)) - L_0 H_{0z} z (g_1(\eta) - g_3(\eta)) \right). \]  

(75)

The functions \( g_1, g_2, g_3 \) depend solely on the function \( \sinh \eta \):

\[ g_1(\eta) = \arccot(\sinh \eta), \quad (76) \]

\[ g_2(\eta) = \frac{\sinh \eta}{\cosh^2 \eta} = \frac{\sinh \eta}{1 + \sinh^2 \eta}, \quad (77) \]

\[ g_3(\eta) = \frac{1}{\sinh \eta}. \quad (78) \]

Substituting eqs.(63) and (64) and their derivatives into the definitions of the constants \( \bar{L}_0, \bar{L}_1, \bar{M}_0, \bar{M}_1 \) and going over to the susceptibilities the expressions for the constants become after some algebra:

\[ \bar{L}_0 = \frac{(\chi_1 - \chi_2) \sinh \eta_0}{(1 + \chi_2) - (1 + \chi_1) \tanh^2 \eta_0 + (\chi_1 - \chi_2) \sinh \eta_0 \arccot(\sinh \eta_0)}, \quad (79) \]

\[ \bar{L}_1 = - \frac{(\chi_1 - \chi_2) \cosh^2 \eta_0 \sinh \eta_0}{2 + \chi_1 + \chi_2 + (\chi_1 - \chi_2) \cosh^2 \eta_0 \left( 1 - \sinh \eta_0 \arccot(\sinh \eta_0) \right)}, \quad (80) \]

\[ \bar{M}_0 = \frac{(1 + \chi_1) \sech^2 \eta_0}{(1 + \chi_2) - (1 + \chi_1) \tanh^2 \eta_0 + (\chi_1 - \chi_2) \sinh \eta_0 \arccot(\sinh \eta_0)}, \quad (81) \]

\[ \bar{M}_1 = \frac{2(1 + \chi_1)}{2 + \chi_1 + \chi_2 + (\chi_1 - \chi_2) \cosh^2 \eta_0 \left( 1 - \sinh \eta_0 \arccot(\sinh \eta_0) \right)}. \quad (82) \]

The corresponding transformations are also given in the notebook OblateCoefficients.nb (Kraiger and Schnizer, 2011).

If both media are the same the external reaction potential must be zero. The internal potential must become the primary potential. Indeed, the limits of the four coefficients

\[ \chi_2 \rightarrow \chi_1 : \quad \bar{L}_0 \rightarrow 0, \quad \bar{L}_1 \rightarrow 0, \quad \bar{M}_0 \rightarrow 1, \quad \bar{M}_1 \rightarrow 1 \quad (83) \]

ensure this. In view of these results the reaction potentials, \( \Phi_{r1} \) and \( \Phi_{r2} \), may be rewritten as:

\[ \Phi_{1r} = (H_{0x} x + H_{0y} y) \bar{L}_1 (g_1 - g_2) + H_{0z} z \bar{L}_0 (g_1 - g_3), \quad (84) \]

\[ \Phi_{2r}(x, y, z) = (H_{0x} x + H_{0y} y) (1 - \bar{M}_1) + H_{0z} z (1 - \bar{M}_0). \quad (85) \]
4.2 The reaction field in Cartesian coordinates

We want expressions for the potential which depend on \(x, y, z\) only. So \(\sinh \eta\) must be replaced with a corresponding expression in Cartesian coordinates. From eqs.(58) to (60) one finds:

\[
\sinh^2 \eta = \frac{1}{2} \left( -1 + \frac{r^2}{e_0^2} \pm \sqrt{\left( -1 + \frac{r^2}{e_0^2} \right)^2 + 4 \frac{z^2}{e_0^2}} \right).
\]

Since the square root is larger than the preceding polynomial it is obvious that only the plus sign applies. This is also confirmed by intense numerical studies. So we have:

\[
\sinh \eta = \frac{1}{\sqrt{2}} \sqrt{\left( -1 + \frac{r^2}{e_0^2} \right)^2 + 4 \frac{z^2}{e_0^2}},
\]

(86)

\[
w_\ell(r, e_z) = \sqrt{\left( -1 + \frac{r^2}{e_0^2} \right)^2 + 4 \frac{z^2}{e_0^2},}
\]

(87)

\[
r^2 = x^2 + y^2 + z^2.
\]

(88)

Inserting this expression for \(\sinh \eta\) into eqs.(76) to (78) and inserting the resulting expressions for \(g_1, g_2, g_3\)

\[
g_1 = \text{acoth}(u_\ell(r, e_z)/\sqrt{2}),
\]

(89)

\[
g_2 = \frac{\sqrt{2}}{u_\ell(r, e_z)} \frac{1}{\sqrt{w_\ell(r, e_z)^2 + 2}},
\]

(90)

\[
g_3 = \frac{\sqrt{2}}{u_\ell(r, e_z)}.
\]

(91)

into eq.(84) we get the final expression for the exterior potential as pure function of the Cartesian coordinates \(x, y, z\):

\[
\Phi_{r1}(x, y, z) = (H_{0x} x + H_{0y} y) \hat{L}_1 (g_1 - g_2) + H_{0z} z \hat{L}_0 (g_1 - g_3),
\]

(92)

The interior potential, eq.(85), is already a pure function of the Cartesian coordinates.

4.3 Potential and field for an arbitrary direction of the spheroidal symmetry axis

For applications it is necessary to consider spheroids whose symmetry axis has an arbitrary direction. The corresponding expressions for the potential will be derived from those given in eqs.(92) and (85). These are rewritten in a way suggesting a general form:

\[
\Phi_{r1}(x, y, z) = (H_{0\perp} \mathbf{r}_\perp) \hat{L}_1 (g_1 - g_2) + (H_{0\parallel} \mathbf{r}_\parallel) \hat{L}_0 (g_1 - g_3),
\]

\[
\Phi_{r2}(x, y, z) = (H_{0\perp} \mathbf{r}_\perp) (1 - \hat{M}_1) (H_{0\parallel} \mathbf{r}_\parallel)(1 - \hat{M}_0).
\]

(93)

The meaning of the subscripts \(\perp\) and \(\parallel\) has already been explained above before and in eq.(41). \(n\) is a unit vector giving the symmetry axis of the spheroid.
In \( w_o \), eq.(87), only the variable \( z \), the component of the position vector along the z-axis, i.e. the symmetry axis, must be replaced by \((n \cdot r)\) giving:

\[
\sinh \eta = \frac{1}{\sqrt{2}} \sqrt{1 + \frac{r^2}{e_o^2} + \bar{w}_o(r, n)} := \bar{u}_o(r, n)/\sqrt{2}, \tag{94}
\]

\[
\bar{w}_o(r, n) = \sqrt{1 + \frac{r^2}{e_o^2} + \frac{(n \cdot r)^2}{e_o^2}}, \tag{95}
\]

The functions \( g_i \), eqs.(89) to (91), remain the same except that \( u_o(r, e_z) \) and \( w_o(r, e_z) \) must be replaced with \( \bar{u}_o(r, n) \) and \( \bar{w}_o(r, n) \) giving the new functions \( \bar{g}_i \):

\[
\bar{g}_1 = \text{acoth}(\bar{u}_o(r, n)/\sqrt{2}), \tag{96}
\]
\[
\bar{g}_2 = \frac{\sqrt{2}}{[\bar{u}_o(r, n)]^2 + 2}, \tag{97}
\]
\[
\bar{g}_3 = \frac{\sqrt{2}}{\bar{u}_o(r, n)}. \tag{98}
\]

Inserting all these new functions into eqs.(93) gives the potential for an oblate spheroid whose symmetry axis is given by the arbitrary unit vector \( n \):

\[
\Phi_{r1}(x, y, z) = (H_0 \cdot r) \bar{L}_1 (\bar{g}_1 - \bar{g}_2) + (H_0 \cdot n)(n \cdot r) [\bar{L}_0 (\bar{g}_1 - \bar{g}_3) - \bar{L}_1 (\bar{g}_1 - \bar{g}_2)], \tag{99}
\]

\[
\Phi_{r2}(x, y, z) = (H_0 \cdot r) (1 - M_1) + (H_0 \cdot n)(n \cdot r) [M_1 - M_0]. \tag{100}
\]

The evaluation of the magnetic field requires the gradients of the functions \( \bar{g}_i \). These are obtained in symbolic computation. Since the resulting expressions consist again of polynomials and the square roots already occurring in the potential it is possible to find simpler expressions. These are again checked against the original gradients by symbolic computation. All these derivatives are proportional to the vector \( r_o \)

\[
r_o := \frac{\sqrt{2}}{e_o^2} \left( r + 2n \frac{(n \cdot r)}{[\bar{u}_o(r, n)]^2} \right). \tag{101}
\]

\[
\nabla \bar{g}_1 - \nabla \bar{g}_2 = -\frac{\bar{u}_o(r, n)}{\bar{w}_o(r, n)} \frac{4}{[(\bar{u}_o(r, n))^2 + 2]^2} r_o, \tag{102}
\]

\[
\nabla \bar{g}_1 - \nabla \bar{g}_3 = \frac{2}{[2 + (\bar{u}_o(r, n))^2]} \frac{\bar{u}_o(r, n)}{\bar{w}_o(r, n)} \bar{w}_o(r, n) r_o. \tag{103}
\]

The corresponding checks are contained in the notebook OblatePotDerivatives.nb (Kraiger and Schnizer, 2011).

The vector \( r_o \) and all the gradients listed above are well-defined and real in the exterior of the oblate spheroid, where \( \eta > \eta_o \); which is equivalent with the condition (107) in Cartesian coordinates. In fact, a more detailed analysis shows that on the interface:

\[
\bar{u}_o(r, n) = \sqrt{2} \sinh \eta_o, \tag{104}
\]

\[
\bar{w}_o(r, n) = \sqrt{\frac{z^4}{(e_o \sinh(\eta_o))^2} + 2z^2/e_o^2} \sinh^4 \eta_o \tag{105}
\]

\[
\sinh^2 \eta_o \leq \bar{w}_o(r, n) \leq \cosh^2 \eta_o. \tag{106}
\]
In the exterior of the spheroid $\bar{u}_o(r, \mathbf{n})$, $\bar{w}_o(r, \mathbf{n})$ respectively are always larger than $\sqrt{2} \sinh \eta_o \sinh^2 \eta_o$ respectively. For $a = 1$, $c = 2$, $(e_o = \sqrt{3})$ one finds $\sqrt{2} \sinh \eta_o = \sqrt{2/3} = 0.816...$ ; $1/3 \leq \bar{w}_o(r, \mathbf{n}) \leq 4/3$.

4.4 Final formulas for the field

So the final formulas for the reaction field excited in an arbitrary homogeneous primary field $\mathbf{H}_0$ by an oblate spheroid with arbitrary symmetry axis given by a unit vector $\mathbf{n}$ is in the exterior:

$$\frac{r^2 - (\mathbf{n} \cdot \mathbf{r})^2}{a_o^2} + \frac{(\mathbf{n} \cdot \mathbf{r})^2}{c_o^2} \geq 1 :$$

$$\mathbf{H}_r(x, y, z) = - \mathbf{H}_0 L_1 (\hat{g}_1 - \hat{g}_2) - \mathbf{n}(\mathbf{H}_0 \cdot \mathbf{n})[L_0 (\hat{g}_1 - \hat{g}_3) - L_1 (\hat{g}_1 - \hat{g}_2)] + \frac{4}{\bar{w}_o(r, \mathbf{n})} \frac{2}{[2 + (\bar{u}_o(r, \mathbf{n}))^2]^2} \bar{u}_o(r, \mathbf{n}) \bar{w}_o(r, \mathbf{n})$$

$$- \frac{r_o (\mathbf{H}_0 \cdot \mathbf{r}) L_1}{\bar{w}_o(r, \mathbf{n})} \frac{4}{[2 + (\bar{u}_o(r, \mathbf{n}))^2]^2} \bar{u}_o(r, \mathbf{n}) \bar{w}_o(r, \mathbf{n})$$

$$- \frac{r_o (\mathbf{H}_0 \cdot \mathbf{r}) (\mathbf{r} \cdot \mathbf{n}) L_1}{\bar{w}_o(r, \mathbf{n})} \frac{4}{[2 + (\bar{u}_o(r, \mathbf{n}))^2]^2} \bar{u}_o(r, \mathbf{n}) \bar{w}_o(r, \mathbf{n})$$

and in the interior:

$$\frac{r^2 - (\mathbf{n} \cdot \mathbf{r})^2}{a_o^2} + \frac{(\mathbf{n} \cdot \mathbf{r})^2}{c_o^2} \leq 1 :$$

$$\mathbf{H}_r(x, y, z) = \mathbf{H}_0 (1 - M_1) + \mathbf{n} \mathbf{H}_0 \cdot \mathbf{n} [M_1 - M_0].$$

4.5 Concluding remarks for the field of an oblate spheroid

An oblate spheroid is inserted into an external homogeneous magnetic field $\mathbf{H}_0$ of arbitrary direction. Its permeability is $\mu_2 = \mu_0(1 + \chi_2)$; while that of the surrounding medium is $\mu_1 = \mu_0(1 + \chi_1)$. The spheroid has semi-axes $a_o, a_o, c_o, c_o < a_o$; these determine the excentricy $e_o$ and the quasi-radial parameter $\eta_o$, eqs.(61) and (62). These in turn determine the coefficients $L_0, L_1, M_0, M_1$, eqs.(79) to (82). The spheroid’s symmetry axis is the arbitrary unit vector $\mathbf{n}$. The reaction field due to the presence of the spheroid in the external field is given in Cartesian coordinates, $\mathbf{r} = (x, y, z)$, by eq.(108) in the exterior, by eq.(109) in the interior. The functions $g_1, g_2, g_3$, eqs.(96) to (98), depend on the functions $\bar{u}_o(r, \mathbf{n})$ and $\bar{w}_o(r, \mathbf{n})$, eqs.(94) and (95). The needed gradients of the $g_i$ are given in eqs.(102) and (103). Eqs.(108) and eq.(109) are for a spheroid, whose centre is at the origin. If the centre is at the point $\mathbf{r}_0 = (x_0, y_0, z_0)$ then the vector $\mathbf{r}$ must replaced simply with $\mathbf{r} - \mathbf{r}_0$. 
5 Application: modelling trabecular bone

5.1 Introduction

Generally, in magnetic resonance experiments disturbances of the homogeneous main magnetic field have an essential impact on the formation of the resonance signal. In principle magnetic inhomogeneities can be classified with respect to their origin and strength, and their influence on the formation of the signal decay (Yablonksy and Haacke, 1994). Especially in MR-Osteodensitometry insights on the microarchitectural status of cancellous bone can be gained (Majumdar and Genant, 1992; Wehrli et al., 2006). In the space of spongy bone the relaxation properties of bone marrow are changed due to the susceptibility effects induced by the discontinuities of the magnetic susceptibility across the surface of the network of branching bone spicules (Davis et al., 1986). In several studies direct relations between the effective transversal relaxation time $T^*_2$, a measure sensitive to field disturbances, and bone mineral density (BMD) (Grampp et al., 1995; Link et al., 1996; Arokoski et al., 2002) and as well mechanical competence of trabecular bone (Chung et al., 1993; Brismar et al., 1997; Beuf et al., 2001) were reported.

The resonance signal decay in a gradient echo MR experiment obeys, in case of these inhomogeneities being of Lorentzian characteristics, the following empirical expression:

$$S(T_E) \propto e^{-R^*_2 T_E} \text{ with } R^*_2 = 1/T_2 + R'_2,$$

with $T_2$ giving the intrinsic transversal relaxation time and $T_E$ the echo time. The quantity $R'_2$ accounts for the additional contribution, originating from the local field inhomogeneities, to the effective transversal relaxation rate $R^*_2 = 1/T_2$. Further, $R'_2 \approx \gamma \Delta B$ with $\Delta B$ representing the field variation and $\gamma$ the gyromagnetic ratio.

Computer simulations modelling the magnetic field distortion make it possible to gain insight into the interrelationship between the temporal characteristics of the resonance signal and the histomorphometrical parameters of the bone lattice. Hence interactions of morphometric quantities such as inter trabecular distance, trabecular thickness, bone volume fraction and the induced line broadening of the resonance spectra can be studied, as has been shown in (Kraiger, 2012) for situations of trabecular microcracks in a simplified model of vertebrae.

5.2 Simulation

A two-compartment model, consisting of bone marrow and the mineralized bone, was applied evaluating the magnetic field distribution. For the simulation of architectures made up by plate-like trabeculae, as they can be found in the epiphysis of long bones like the femur, oblate spheroids were used. Hence, in a three-dimensional unit cell representing the volume of interest (VOI) ellipsoids were arranged appropriately to model the known trabecular microstructure (Hildebrand et al., 1999).

Following the approach described by (Bakker et al., 1992), the reaction fields induced by the susceptibility difference between the ellipsoids (trabeculae) and the background (bone marrow) were computed at first. Subsequently the time
course of the resonance signal was computed applying a Fourier Transformation of the spatial magnetic field distribution with respect to time (Ford et al., 1993).

In a homogeneous magnetic field the precession frequency of spins is determined through the magnetic induction $B$. Now introducing a sample with a different susceptibility - in the current experiment trabecular bone ($\chi_2$) is surrounded by bone marrow ($\chi_1$) - the resulting magnetic induction $B_z$ can be generally written as:

$$B_z = \mu (H_{0z} + M_z (r)) = \mu_0 (1 + \chi) (H_{0z} + M_z (r)),$$  \hspace{1cm} (111)

with $M_z$ characterising the induced reaction field. Herein the units are given in the MKS-system, and susceptibility units are per unit volume.

Since the transversal magnetization decay of mineralized bone is several magnitudes faster comparing to bone marrow, the received resonance signal in MR-Osteodensitometry is governed by the magnetization arising within the marrow. Hence $M_z$ corresponds to the computed reaction field $\Delta H_{r1, z}$ caused by the difference in magnetic property between bone and marrow.

Within the unit cell the distribution of the reaction field originating from the $n$ ellipsoids was determined as the sum of all individual contributions $H_{r1, z}$:

$$\Delta H_{r1, z} (r) = \sum_{i=1}^{n} H_{r1, i} (r).$$  \hspace{1cm} (112)

Interactions between the trabeculae have been neglected. This assumption is valid, since such interactions include susceptibility effects of the second order, which will give rise to field contributions of $H_0 (\Delta \chi)^2$, or $\approx H_0 \cdot 10^{-12}$.

In a simple MR experiment, RF excitation followed by an acquisition period, the signal of the free induction decay (FID) can be written as:

$$S(t) = \text{const} \int \text{VOI} d^3 r e^{-i\omega(r)t} e^{-t/T_2};$$  \hspace{1cm} (113)

with $\omega(r) = \gamma B_z (r)$ it follows:

$$S(t) = \text{const} \int \text{VOI} d^3 r e^{-i\gamma B_z (r)t} e^{-t/T_2}.$$  \hspace{1cm} (114)

Applying (111) again, the following expression in $H_z$ can be found:

$$S(t) = \text{const} \int \text{VOI} d^3 r e^{-i\gamma t \mu_0 (1+\chi_1) (H_{0z} + \Delta H_{r1, z}(r))} e^{-t/T_2}.$$  \hspace{1cm} (115)

This integral must be extended over the entire unit cell enclosing all ellipsoids.

In order to compare the simulation results with commonly acquired MR magnitude images $S(t)$ has to be further processed. From eq.(115) it is clear, that except for the dissipative relaxation phenomenon $e^{-t/T_2}$ the expressions are purely oscillatory in $H_{0z}$. Hence, the essential decay for the analysis of the signal course can be expressed as:

$$|S(t)| = \text{const} \int \text{VOI} d^3 r e^{-i\gamma t \mu_0 (1+\chi_1) \Delta H_{r1, z}(r)}.$$  \hspace{1cm} (116)
\( \Delta H_{1,z}(r) \) can be computed according to (112) as the sum over all the reaction fields of the individual ellipsoids, where \( \mu(1 + \chi) \) describes the magnetic permeability at the location \( r \).

### 5.2.1 Algorithm

Utilizing the expression developed for the reaction field of an oblate ellipsoid eq.(108) the simulations were implemented in Mathematica (Wolfram Research, Inc.). As input parameters the spacing of the trabeculae in x-, y- and z-direction, the dimensions of the ellipsoids and the position of the symmetry axis with respect to the z-axis of the coordinate system had to be defined. Further, the susceptibilities of the bones, the background and the orientation of the applied homogenous main magnetic field had to be set. The program computed the field distribution of the z-component of the reaction fields in the sense of a histogram and generated the MR signal curve according to (116). The obtained signal was subsequently processed within a fitting-procedure yielding the relaxation constant \( R'_2 \).

![Diagram](image)

**Figure 1:** a.) Schematic depiction of six oblate ellipsoids forming the three-dimensional plate-like microstructure of Model I; b.) Detailed view of the applied unit cell; dimensions are given in mm. The centres of the ellipsoids are indicated by crosses, the subscripts \( v, h \) denote the horizontal and vertical flat ellipses representing the trabeculae in the array; \( C \) indicates the origin.

### 5.2.2 \( T'_2 \) Data fitting

From the simulated signal curves the relaxation time was estimated assuming a Gaussian signal model (Selby et al., 1996; Fransson et al., 1998). The signal intensities computed at the echo times ranging from 0 to 50 ms (eq.(116)), 2.5 ms increment, were used to generate a single \( T'_2 \) value by means of a non linear least-squares-approximation to a three parameter fit function:

\[
S(t) = A + B \ e^{-t^2/(2T'_2)}.
\]  

(117)
The fitting model is equivalent to a bi-Gaussian function with one term having a decay constant greater than the maximum $T_E$ (50 ms). A high value of the ratio $A/B$ corresponds to a decay that deviates significantly from a single Gaussian (Newitt et al., 1996; Fransson et al., 1998).

### 5.2.3 Model: plate-like trabecular structure

The effect of the loss of bone mass within a three-dimensional plate-like trabecular model was analysed using oblate ellipsoids. Hence, stepwise decreasing of the bone volume fraction $\varsigma = BV/TV$, bone volume ($BV$)/total volume ($TV$), was performed. In accordance with the findings of (Hildebrand et al., 1999), $\varsigma$ values ranging from 0.530–0.406 were investigated. The bone remodelling was simulated as a simultaneous decrease of the thickness of the horizontal and vertical ellipsoids by 12.5 $\mu$m.

The configuration of the 3D unit cell and the parameter settings are shown in Figure 1, Tables 1 and 2.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Trabecular Vector n $(x,y,z)$</th>
<th>Center T $(x,y,z)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>left/top</td>
<td>$\sin 10^\circ, 0, \cos 10^\circ$</td>
<td>0, $\sin 95^\circ, \cos 95^\circ$</td>
</tr>
<tr>
<td>middle</td>
<td>1, 0, 0</td>
<td>0, 0, 1</td>
</tr>
<tr>
<td>right/bottom</td>
<td>$\sin 15^\circ, 0, \cos 15^\circ$</td>
<td>0, $\sin 95^\circ, \cos 95^\circ$</td>
</tr>
</tbody>
</table>

Table 1: Parameters of the oblate ellipsoids utilized in Model I. Units of the centres are given in $\mu$m. The susceptibility of the trabecular bone and the bone marrow were set to $\chi_1 = -0.62 \times 4\pi \times 10^{-6}$ and $\chi_2 = -0.9 \times 4\pi \times 10^{-6}$, respectively (Hopkins and Wehrli, 1997). A main magnetic induction of $B_0z = 3$ T, $\alpha = 5^\circ$ and $\beta = 0^\circ$ was applied.

### 5.2.4 Simulating bone loss

In this subsection the results of the analysis studying the effect of loss of bone mass on the field distribution and the resulting relaxation constant $T_2'$ are presented. The resulting histograms are reflecting the impact of decreasing $\varsigma$ on the field distribution of the reaction fields, see Figure 2. Depending on the fraction the reaction fields varied approximately between -0.6 and -0.05 A/m. As a consequence of the bone loss the field distribution became more homogeneous.

<table>
<thead>
<tr>
<th>Dimensions</th>
<th>ellipsoids $a/b_{c,h}$</th>
<th>3000/100 $\mu$m</th>
</tr>
</thead>
<tbody>
<tr>
<td>unit cell</td>
<td>volume</td>
<td>3.92 mm$^3$</td>
</tr>
<tr>
<td>initial BV/TV</td>
<td>$\varsigma_0$</td>
<td>0.482</td>
</tr>
</tbody>
</table>

Table 2: Dimensions of the ellipsoids, the unit cells and the initial bone volume fractions BV/TV.
Figure 2: Resulting field distributions of the reaction field $H_{r1,z}$ induced by the susceptibility effect between bone and bone marrow. The fields were computed within the entire volume of Model I as a function of $\varsigma$. A main magnetic field $B_0 = 3$ T, respective $H_0 = 2.38732 \cdot 10^6$ A/m with $\alpha = 5^\circ$ and $\beta$ parallel z-axes, and values of $\chi_1 = -0.62 \cdot 4 \cdot \pi \cdot 10^{-6}$ and $\chi_2 = -0.9 \cdot 4 \cdot \pi \cdot 10^{-6}$ were applied. Hence the broadness of the histogram narrowed, whereby its maxima was shifted in the direction of a more positive field strength.

The simulated signal curves as a function of $\varsigma$ are presented in Figure 3 together with the estimated relaxation times. The estimated parameters of the least-squares approximation are given in Table 3. During the decrease of $\varsigma$ the applied Gaussian signal model responded with a moderate increase of $T_2'$. Further, the Gaussian approach exhibited an almost linear relation between the loss of bone mass and the increase of $T_2'$, as can be concluded from Table 3.
Table 3: Resulting parameter estimates of the non-linear least-squares approximation of the simulated signal decay to a Gaussian function. The approximations were performed for various $\varsigma$.

<table>
<thead>
<tr>
<th>BV/TV</th>
<th>$A_{pca}$</th>
<th>$B_{pca}$</th>
<th>$T'_2$ (ms)</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.530</td>
<td>-0.021</td>
<td>1.021</td>
<td>36.10</td>
<td>0.12 \cdot 10^{-3}</td>
</tr>
<tr>
<td>0.505</td>
<td>-0.029</td>
<td>1.030</td>
<td>38.86</td>
<td>0.10 \cdot 10^{-3}</td>
</tr>
<tr>
<td>0.482</td>
<td>-0.035</td>
<td>1.035</td>
<td>42.12</td>
<td>0.07 \cdot 10^{-3}</td>
</tr>
<tr>
<td>0.457</td>
<td>-0.035</td>
<td>1.035</td>
<td>45.78</td>
<td>0.05 \cdot 10^{-3}</td>
</tr>
<tr>
<td>0.431</td>
<td>-0.038</td>
<td>1.038</td>
<td>49.99</td>
<td>0.03 \cdot 10^{-3}</td>
</tr>
<tr>
<td>0.406</td>
<td>-0.035</td>
<td>1.035</td>
<td>54.88</td>
<td>0.02 \cdot 10^{-3}</td>
</tr>
</tbody>
</table>

5.3 Discussion

The novel analytical solutions of the three-dimensional Laplacian potential problem of spheroids were successfully applied in the area of MR-Osteodensitometry. Especially coordinate transformations became unnecessary, thus simplifying the modelling of arbitrary orientated trabecular bones in an arbitrary orientated main magnetic field.

To the authors best knowledge for the first time oblate ellipsoids were used to mimic the field effects of plate-like structures more realistically. Such structures made it possible to study the effects of bone mass loss in a basic model of osteous bone. In principle there are no restrictions concerning the amount and orientation of the used oblate spheroids, hence even complex architectures are accessible for modelling.

In the case of bone disorders such as osteoporosis annual changes of the bone mass between 2–5 % were reported (Harris and Dawson-Hughes, 1992; Davis et al., 1991). Applying the presented novel analytical field expressions, such realistic alterations in conjunction with their effects on the MR relaxation parameter $T'_2$ can be studied. In the current simulations minor alterations of $\Delta \varsigma = 0.025$ were successfully modelled, yielding variations of the MR relaxation parameter $T'_2$ in a measurable range of ms. The presented results are qualitatively comparable with previously reported studies, whereby either a different size of the volume of interest or different trabecular elements, rod-like structures, were utilized (Selby et al., 1996; Chung et al., 1996).

In general, the use of the analytical field expression of the prolate case enables the investigation of induced field distortions in the surrounding of the trabecular microcracks. This has been studied in a second application described in the report given by (Kraiger and Schnizer, 2011). In an additional study using a more realistic 3D bone model the variations of the reaction fields along the progression of pathological bone remodelling are under investigation. The results of the ongoing study will be published elsewhere.

6 Conclusions

1. Expressions for the potential and field of a prolate spheroid in a homogeneous external field of arbitrary direction have been derived in prolate spheroidal coordinates. These expressions have been transformed to
Cartesian coordinates. The resulting expressions have been generalized to an arbitrary direction of the symmetry axis while the external field axis may still have another arbitrary direction.

2. The same has been done for an oblate spheroid with arbitrary symmetry axis and an other arbitrary field axis.

3. Since the magnetic susceptibilities of biological tissues are small (volume susceptibility $\approx -10^{-6}$) (Schenck, 1996) it is easy to construct models of trabecular bone structures by arrays of spheroids as described in the previous item. The total magnetic induction is that of the primary field plus that of all the spheroids in the array to a very good approximation which disregards the small magnetic interaction of the spheroids among themselves.

4. This modelling is particularly easy since all field dependences may be expressed in the same general Cartesian coordinate system.

5. As an example of the method the following configuration is treated: Oblate spheroids are used in a 3D model to study the impact of trabecular bone loss on the MR signal decay characteristic.

6. In the present work just one application of the analytical expressions, the modelling of bone disorders in the area of MR-Osteodensitometry, was given. For example in the field of functional MRI the developed toolbox eases the analysis of the BOLD (blood oxygenation level-dependent) contrast, where induced reaction fields in the surrounding of vascular networks are of great interest (Ogawa et al., 1990). A fast and precise computation of the magnetic distortion is essential for improving the precision of the temperature determination in techniques using the proton resonance frequency (PRF) shift method (Hindmann, 1966; Rieke and Pauly, 2008). Temperature mapping in the vicinity of the needle electrode is a crucial determinant of MRI guided interventional radiofrequency ablations (Boss et al., 2005). Further, in the field of metabolism studies using NMR spectroscopy (MRS) the expressions can be used in order to model specific cells introduced in solutes differing in magnetic susceptibility (Kuchel, 1983).

7. The authors believe that the novel formulation of solutions depending solely on the Cartesian coordinates will facilitate the modelling of countless magnetostatic problems.

Not added in proof:

A very concise compilation of the formulas of this paper together with some new formulas for the coefficients $L_0, L_1, ..., M_1$ have been given in Kraiger and Schnizer (2112).

References


22


Schenck, J.F. (1996), "The role of magnetic susceptibility in magnetic res-


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