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Multipole moments of general ellipsoids with two polarized domains

M Schult, N Mikuszeit, E Y Vedmedenko and R Wiesendanger

Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

E-mail: nmikusze@physnet.uni-hamburg.de

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Abstract

The multipole moments of a homogeneously polarized ellipsoid and a homogeneously charged ellipsoidal disc are calculated. The resulting hypergeometric functions are expressed as finite polynomials of the semi-axes a, b and c of the ellipsoid. The polynomial form exists for any order of the multipole moments. It is shown that the solution also applies to a two-domain ellipsoid with antiparallel polarized domains and to a system with radially changing polarization density. The results allow us to calculate the potential as well as interaction energies within the framework of multipole expansion.

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1. Introduction

Expanding a Coulomb-like potential in terms of multipole moments is a classical tool of potential theory [1, 2]. The main purpose of a multipole expansion is the approximation of the potential outside a finite 'charged' body, which then can be used to calculate the stray field or the interaction energy with a second body exposed to this field. The approximation has, due to the scale invariance, a wide range of applications. On a very large scale, it can be utilized to describe the gravitational potential of galaxies [3, 4] and many body kinematics [5]. A typical example is the expansion of the Coulomb potential of charged particles as e.g. dielectric ellipsoids [6]. On the nanoscale, multipole expansion enables the fast calculation of interaction energies of magnetic particles with non-spherical geometry [7]. Even on the atomic scale it is utilized to calculate the interaction between atoms and molecules [8]. In contrast to the aforementioned direct tasks applications to inverse problems, i.e. the determination of internal effective properties of a system from its external potential, as well as a mathematical introduction to potential theory and multipole expansion are given in [9].

The evaluation of the interaction energy within the framework of the multipole expansion has several advantages: the calculation of the moments requires only 3-fold (2-fold) integrals while the exact integration of volume charge (surface charge) needs 6-fold (4-fold) integrals. The interaction is then handled via an interaction tensor, which does not change complexity—at least not in spherical coordinates [8, 10]—with increasing order of expansion. Furthermore, if the interacting particles change their relative orientation it is only necessary to rotate the moments in terms of Wigner-*D*-functions [11], while apart from a few trivial cases the exact integral has to be evaluated again, including a geometry specific coordinate transformation of the integration variables.

The calculations of multipole moments for simple and symmetric geometries are exercises of textbooks [12, 13], but only a few complex structures with analytical expressions are known. To calculate the potential of a polarized ellipsoid it is not necessary to utilize the multipole expansion. However, the solutions are complicated and for $a \neq b \neq c$ even require elliptic integrals [14]. Therefore, the exact calculation of the interaction energy via a 6-fold (4-fold) integral becomes a non-trivial task. Knowledge of the multipole moments would allow us to calculate easily the energies within one-, two- and three-dimensional systems of polarized elliptic particles under the influence of an external field. As ferromagnetic or ferroelectric particles are typically fixed in position the external field forces the polarization to change its orientation with respect to the particle geometry. Therefore, it changes the multipole moments and analytical expressions for the moments would be a very helpful and practical tool when calculating the interaction energy in such many particle systems.

In this study, analytical solutions for polarized general ellipsoids with semi-axes (a, b, c) and arbitrary polarization direction are derived. The polarization is assumed to be homogeneous, leaving uncompensated charges at the surface. In detail, the polarization has only to be homogeneous in one half of an ellipsoid, i.e. there may be two domains (figure 1) each homogeneously polarized. The resulting domain wall is symmetric in the (x, y)-plane[1]. To ensure a well-defined multipole expansion, it is required that the centre of charge and the origin coincide; obviously, this requirement is fulfilled by parallel or antiparallel polarization of the two halves[2]. The case of antiparallel domains is e.g. an approximation of spin domains in Bose–Einstein condensates, where the spin of the condensate is in general free to rotate and able to form domains in an external magnetic field [15]. In the case of parallel polarization of the two halves the moments just describe homogeneously polarized or magnetized nanoparticles [16–18].

The strategy to gain the multipole moments is as follows: first one has to integrate over the charge density, weighted by normalized spherical harmonic functions (section 2). The integration will be carried out in spherical coordinates. This requires us to express the charge density as well as the surface area element within this coordinate system. As a consequence the two integrals, over the polar and the azimuthal angles, couple in a non-trivial way (section 2.1). The coupling only vanishes in the case of a spheroid (section 2.1.3). It will be shown that the integration over the polar angle can be expressed in terms of Gaussian hypergeometric functions [19], where the arguments depend on the order of the multipolar expansion and on the azimuthal angle (section 2.1.1). These integrals have similarities with those emerging from calculating the demagnetizing tensor of an ellipsoid [1, 20, 21]. Indeed, it is possible to express the demagnetizing factors of a spheroid in terms of hypergeometric functions [22].

In the next step, it is shown that the azimuthal integration over each addend is of the same type as the polar integration (section 2.1.2). Consequently, each addend results in a hypergeometric function, which also can be expanded in finite polynomes. Accordingly,

[1] The (y, z)- and the (z, x)-plane can be realized by changing a, b and c plus a rotation of the system.

[2] Several other possibilities fulfilling the above condition exist, but in the case of arbitrary directions of polarization, centre of charge and origin do not coincide in general.

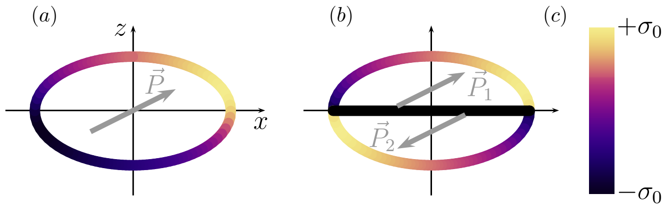

Figure 1. Two-dimensional sketch of two possible geometries, where centre of charge and origin coincide. In (*a*) the upper and lower domains are polarized in parallel resulting in a single domain with polarization $\vec{P}$; in (*b*) the polarization $\vec{P}_1$ of domain 1 ($z > 0$) is antiparallel to $\vec{P}_2$ of domain 2 ($z < 0$). Consequently, there is a negatively charged domain wall, the thick black line at $z = 0$. The circumferences of the ellipsoids are coloured with respect to the surface charge density σ (*c*), where the maximum surface charge density is $\sigma_0 = \kappa \parallel \vec{P} \parallel$ and κ either ϵ_0 or μ_0 (see the text for details).

(This figure is in colour only in the electronic version)

it is proved rigorously that, in contrast to the results of the demagnetizing factors, the hypergeometric functions emerging from integrating the multipole moments can be expressed as finite polynomials of a, b and c up to any order of the expansion.

With this scheme the multipole moments of polarized ellipsoids can be calculated easily by the sums of (15), (16) and (22). In the future, the results of the present investigation will be used for simulation of magnetic nanoparticles in arrays of arbitrary symmetry.

2. Integrating the charge density of a half ellipsoid (one domain)

Homogeneously polarized matter with polarization vector $\vec{P}$ in a volume V creates a surface charge $\sigma \propto \vec{n} \cdot \vec{P}$ on the surface S of a finite body (see figure 1), where $\vec{n} = \vec{S}/S$ is the surface normal. The integration of the multipole moments follows the definition given in [23]. In general the moments have the form

$$Q_{lm} = \kappa \int_S R_{lm}(\vec{S})\vec{P} \cdot \mathrm{d}\vec{S}, \tag{1}$$

where R is the regular normalized spherical harmonic function and κ is either ε_0 or μ_0, depending on whether the polarization is electric or magnetic. In the following the integrals are solved for one half—one domain—of the ellipsoids (figure 1(*b*)).

2.1. *The half shell of an ellipsoid*

The integrals over a half shell are not multipole moments in the common sense as the centre of charge and the origin of the coordinate system do not coincide; to emphasize this, these 'half moments' will be marked by a tilde. Giving the polarization in spherical coordinates as $\vec{P} = (P_0, \theta_\mathrm{p}, \phi_\mathrm{p})$ and introducing $\sigma_0 = \kappa P_0$ the half moments read

$$\tilde{Q}_{lm} = \sigma_0 \sqrt{\frac{(l-m)!}{(l+m)!}} \int_0^{\frac{\pi}{2}} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\; P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi} \sin\theta \\ \times \frac{\left(\frac{\cos\phi\cos\phi_\mathrm{p}}{a^2} + \frac{\sin\phi\sin\phi_\mathrm{p}}{b^2}\right)\sin\theta\sin\theta_\mathrm{p} + \frac{1}{c^2}\cos\theta\cos\theta_\mathrm{p}}{\left[\left(\frac{\cos^2\phi}{a^2} + \frac{\sin^2\phi}{b^2}\right)\sin^2\theta + \frac{1}{c^2}\cos^2\theta\right]^{\frac{l+4}{2}}}, \tag{2}$$

where the surface element of the general ellipsoid is expressed in spherical coordinates and P_l^m are the associated Legendre polynomials [19]. The numerator in (2) can be split into the sum of three terms $q_1 + q_2 + q_3$, which hold the proportionalities

$$\begin{aligned} q_1 &\propto P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}\cos\theta\sin\theta \\ q_2 &\propto P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}\cos\phi\sin^2\theta \\ q_3 &\propto P_l^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}\sin\phi\sin^2\theta. \end{aligned} \tag{3}$$

The exponential function can be expressed in terms of sine and cosine functions, $\exp(\mathrm{i}m\phi) = \cos m\phi + \mathrm{i}\sin m\phi$. Due to the symmetries of the trigonometric functions and the denominator the integration over $\sin m\phi$ of q_1 vanishes for all integer m. The integration over $\cos m\phi$ vanishes for all odd m. The terms q_2 and q_3, which contain additional trigonometric functions of ϕ, can be simplified further to four sums proportional to $G_i(m,\phi), i \in \{1,\ldots,4\}$ (see (A.1) in the appendix). In G_2 and G_3 only sine functions appear and the integral vanishes due to symmetry. In the case of G_1 and G_4 terms of $\cos(m \pm 1)\phi$ are nonzero only if m is odd. Consequently, two types of integrals must be evaluated,

$$q_1 \propto \int_0^{2\pi} \mathrm{d}\phi \frac{\cos m\phi}{c^2\left(\frac{\cos^2\phi}{a^2} + \frac{\sin^2\phi}{b^2}\right)^{\frac{l+4}{2}}} \int_0^{\frac{\pi}{2}} \mathrm{d}\theta \frac{P_l^m(\cos\theta)\cos\theta\sin\theta}{(1-\varepsilon(\phi)\cos^2\theta)^{\frac{l+4}{2}}} \tag{4}$$

$$q_{2,3} \propto \int_0^{2\pi} \mathrm{d}\phi \frac{\cos(m\pm 1)\phi}{2\left(\frac{\cos^2\phi}{a^2} + \frac{\sin^2\phi}{b^2}\right)^{\frac{l+4}{2}}} \int_0^{\frac{\pi}{2}} \mathrm{d}\theta \frac{P_l^m(\cos\theta)\sin^2\theta}{(1-\varepsilon(\phi)\cos^2\theta)^{\frac{l+4}{2}}}, \tag{5}$$

for even and odd m, respectively. To simplify matters $\varepsilon(\phi)$ with

$$\varepsilon(\phi) = 1 - \frac{1}{c^2\left(\frac{\cos\phi}{a^2} + \frac{\sin\phi}{b^2}\right)} \tag{6}$$

has been introduced.

2.1.1. Integrating over the polar angle. To integrate over θ a substitution of $\cos\theta$ by x is performed transforming the proportionality from above into

$$q_1 \propto \int_0^1 \mathrm{d}x \frac{P_l^m(x)x}{(1-\varepsilon(\phi)x^2)^{\frac{l+4}{2}}} \qquad q_{2,3} \propto \int_0^1 \mathrm{d}x \frac{P_l^m(x)\sqrt{1-x^2}}{(1-\varepsilon(\phi)x^2)^{\frac{l+4}{2}}}. \tag{7}$$

The associated Legendre polynomials $P_l^m(x)$ consist of a product of a polynomial of order $l - |m|$ and $(1-x^2)^{\frac{|m|}{2}}$, see (B.2). Hence, the integral over x can be separated into the addends of order n of this polynomial, resulting in

$$q_i \propto \sum_{n=0}^{l-|m|} \int_0^1 \mathrm{d}x \frac{p_n(l,m)x^{n-\tau+1}(1-x^2)^{\frac{|m|+\tau}{2}}}{(1-\varepsilon(\phi)x^2)^{\frac{l+4}{2}}}, \tag{8}$$

where $\tau = 0$ if m is even (q_1) and $\tau = 1$ if m is odd ($q_{2,3}$). Now substituting x^2 by t for each order n one gets the integral

$$q_i \propto I_{n,\tau}(l,m) = \frac{1}{2}\int_0^1 \mathrm{d}t \frac{t^{\frac{n-\tau}{2}}(1-t)^{\frac{|m|+\tau}{2}}}{(1-\varepsilon(\phi)t)^{\frac{l+4}{2}}} \tag{9}$$

which is an integral representation of the hypergeometric function (see appendix C). An additional linear transformation (see (C.2)) eventually gives

$$I_{n,\tau}(l,m) = \frac{1}{2}\frac{\Gamma\left(\frac{n-\tau+2}{2}\right)\Gamma\left(\frac{|m|+\tau+2}{2}\right)}{\Gamma\left(\frac{|m|+n+4}{2}\right)(1-\varepsilon(\phi))^{\frac{l-|m|-\tau+2}{2}}} \times {}_2F_1\left(-\frac{l-|m|-n}{2}, \frac{|m|+\tau+2}{2}; \frac{|m|+n+4}{2}; \varepsilon(\phi)\right) \tag{10}$$

for even m, $\tau = 0$, and for odd m, $\tau = 1$.

The boundary of n ensures that $(l-|m|-n)$ is a non-negative integer; due to the fact that every second $p_n(l,m)$ is zero it is also known that $(l-|m|-n)$ is even. Therefore, $(l-|m|-2)/2$ is a non-negative integer, which allows us to write the hypergeometric function in a polynomial form (see (C.3)). Inserting the results of (10) in (2) the integration over θ results in a polynomial

$$\tilde{Q}_{l,m} = \sigma_0\sqrt{\frac{(l-m)!}{(l+m)!}}\cos\theta_{\mathrm{p}}\sum_{n=0}^{l-|m|}\frac{p_n(l,m)}{2}\frac{\Gamma\left(\frac{n+2}{2}\right)\left(\frac{m}{2}\right)!}{\Gamma\left(\frac{|m|+n+4}{2}\right)}c^{l-|m|} \times \sum_{j=0}^{\frac{l-|m|-n}{2}}\frac{\left(-\frac{l-|m|-n}{2}\right)_j\left(\frac{|m|+2}{2}\right)_j}{j!\left(\frac{|m|+n+4}{2}\right)_j}\int_0^{2\pi}\mathrm{d}\phi\frac{\cos m\phi\,\varepsilon^j(\phi)}{\left(\frac{\cos^2\phi}{a^2}+\frac{\sin^2\phi}{b^2}\right)^{\frac{|m|+2}{2}}} \tag{11}$$

for even m[3] and

$$\tilde{Q}_{l,m} = \sigma_0\sqrt{\frac{(l-m)!}{(l+m)!}}\sin\theta_{\mathrm{p}}\sum_{n=0}^{l-|m|}\frac{p_n(l,m)}{2}\frac{\Gamma\left(\frac{n+1}{2}\right)\left(\frac{|m|+1}{2}\right)!}{\Gamma\left(\frac{|m|+n+4}{2}\right)}c^{l-|m|+1} \times \sum_{j=0}^{\frac{l-|m|-n}{2}}\frac{\left(-\frac{l-|m|-n}{2}\right)_j}{\left(\frac{|m|+n+4}{2}\right)_j}\frac{\left(\frac{|m|+3}{2}\right)_j}{j!}\int_0^{2\pi}\mathrm{d}\phi\,\varepsilon^j(\phi) \times \frac{\left(\frac{\cos\phi_{\mathrm{p}}}{a^2}+\mathrm{i}\frac{\sin\phi_{\mathrm{p}}}{b^2}\right)\cos(1-m)\phi+\left(\frac{\cos\phi_{\mathrm{p}}}{a^2}-\mathrm{i}\frac{\sin\phi_{\mathrm{p}}}{b^2}\right)\cos(1+m)\phi}{2\left(\frac{\cos^2\phi}{a^2}+\frac{\sin^2\phi}{b^2}\right)^{\frac{|m|+3}{2}}} \tag{12}$$

for odd m, while the more complicated integration over ϕ remains.

2.1.2. Integrating over the azimuthal angle. In the next step the technique already applied for the integration over θ will be applied to ϕ. To do so $\cos m\phi$ and $\cos(m\pm 1)\phi$ are expressed as polynomials of $\cos\phi$ (appendix A). The expansions of the cosine and of the factor $\varepsilon^j(\phi)$ each give an additional sum. Therefore, by introducing $\eta = 1-(b/a)^2$ and the binomial coefficient $\binom{j}{\kappa}$, it is possible to express the remaining integrals over ϕ in the form

$$\int_0^{2\pi}\mathrm{d}\phi\frac{\frac{\cos\phi_{\mathrm{p}}}{a^2}\pm\mathrm{i}\frac{\sin\phi_{\mathrm{p}}}{b^2}}{2}\sum_{k=0}^{\frac{m\mp 1}{2}}\sum_{\kappa=0}^{j}(-1)^\kappa\binom{j}{\kappa}\frac{\alpha_k(|m\mp 1|)(\cos^2\phi)^k}{(1-\eta\cos^2\phi)^{\kappa+\frac{|m|+3}{2}}}, \tag{13}$$

[3] It is worth noting that for even m the integrand $xP_l^m(x)$ may also be expressed as a polynomial of order $l+1$. This leads to a different expression of E_n with different $p_n(l,m)$. Expressing the integrand in this way simplifies the solution in the case of $m=0$ and odd l, which is interesting in the case of a monodomain spheroid, polarized along the axis of symmetry.

for odd m and in a similar way for even m. Due to symmetry the integral can be restricted to the interval $[0, \pi/2]$. By substituting $\cos^2\phi$ by t the integral can be transformed into a representation of the hypergeometric function

$$4\int_0^{\frac{\pi}{2}} \mathrm{d}\phi \frac{(\cos^2\phi)^k}{(1-\eta\cos^2\phi)^{\kappa+\frac{|m|+3}{2}}} = 2\int_0^1 \mathrm{d}t \frac{t^{k-\frac{1}{2}}}{\sqrt{1-t}\,(1-\eta t)^{\kappa+\frac{|m|+3}{2}}}, \tag{14}$$

which again can be expressed as a finite polynomial. With minor simplifications the final result for even m is

$$\begin{aligned}\tilde{Q}_{lm} = {}& \sigma_0\sqrt{\frac{(l-m)!}{(l+m)!}}\sqrt{\pi}\cos\theta_{\mathrm{p}}\sum_{n=0}^{l-|m|} p_n(l,m)\frac{\Gamma\left(\frac{n+2}{2}\right)\left(\frac{|m|}{2}\right)!}{\Gamma\left(\frac{n+|m|+4}{2}\right)}\\ &\times\sum_{j=0}^{\frac{l-|m|-n}{2}}\frac{\left(-\frac{l-|m|-n}{2}\right)_j\left(\frac{|m|+2}{2}\right)_j}{j!\left(\frac{|m|+n+4}{2}\right)_j}\sum_{k=0}^{\frac{|m|}{2}}\alpha_k(|m|)\sum_{\kappa=0}^{j}(-1)^\kappa\binom{j}{\kappa}\frac{\Gamma\left(k+\frac{1}{2}\right)}{k!}\\ &\times\sum_{u=0}^{\frac{|m|}{2}+\kappa-k}\frac{\left(k-\kappa-\frac{|m|}{2}\right)_u\left(\frac{1}{2}\right)_u}{u!(k+1)_u}\sum_{v=0}^{u}(-1)^v\binom{u}{v}a^{|m|+2\kappa-2v+1}b^{2v+1}c^{l-|m|-2\kappa},\end{aligned} \tag{15}$$

where two additional sums, over u and v, appear. The first sum is due to the expansion of the hypergeometric function, while the latter results from the expansion of η^u, the expansion parameter of the hypergeometric function. For odd m the polynomial has the form

$$\begin{aligned}\tilde{Q}_{lm} = {}& \sigma_0\sqrt{\frac{(l-m)!}{(l+m)!}}\frac{\sqrt{\pi}}{2}\sin\theta_{\mathrm{p}}\sum_{n=0}^{l-|m|} p_n(l,m)\frac{\Gamma\left(\frac{n+1}{2}\right)\left(\frac{|m|+1}{2}\right)!}{\Gamma\left(\frac{|m|+n+4}{2}\right)}\\ &\times\sum_{j=0}^{\frac{l-|m|-n}{2}}\frac{\left(-\frac{l-|m|-n}{2}\right)_j\left(\frac{|m|+3}{2}\right)_j}{j!\left(\frac{|m|+n+4}{2}\right)_j}\sum_{\kappa=0}^{j}(-1)^\kappa\binom{j}{\kappa}\\ &\times\left\{\left(\frac{\cos\phi_{\mathrm{p}}}{a^2}+\mathrm{i}\frac{\sin\phi_{\mathrm{p}}}{b^2}\right)\sum_{k=0}^{\frac{|m-1|}{2}}\alpha_k(|m-1|)\frac{\Gamma\left(k+\frac{1}{2}\right)}{k!}\sum_{u=0}^{\frac{|m|+1}{2}+\kappa-k}\frac{\left(\frac{1}{2}\right)_u}{u!}\right.\\ &\times\frac{\left(k-\kappa-\frac{|m|+1}{2}\right)_u}{(k+1)_u}\sum_{v=0}^{u}(-1)^v\binom{u}{v}a^{|m|+2\kappa-2v+2}b^{2v+1}c^{l-|m|-2\kappa+1}\\ &+\left(\frac{\cos\phi_{\mathrm{p}}}{a^2}-\mathrm{i}\frac{\sin\phi_{\mathrm{p}}}{b^2}\right)\sum_{k=0}^{\frac{|m+1|}{2}}\alpha_k(|m+1|)\frac{\Gamma\left(k+\frac{1}{2}\right)}{k!}\sum_{u=0}^{\frac{|m|+1}{2}+\kappa-k}\frac{\left(\frac{1}{2}\right)_u}{u!}\\ &\left.\times\frac{\left(k-\kappa-\frac{|m|+1}{2}\right)_u}{(k+1)_u}\sum_{v=0}^{u}(-1)^v\binom{u}{v}a^{|m|+2\kappa-2v+2}b^{2v+1}c^{l-|m|-2\kappa+1}\right\}.\end{aligned} \tag{16}$$

Hence, the two sums over k are almost identical; they can be combined leaving only the last addend from the second sum, where further simplification is possible as e.g. $\alpha_{\frac{m+1}{2}}(m+1) = 2^m$.

The lower order multipole moments calculated with (15) and (16) are listed in table 1.

2.1.3. Simplifications in the case of a spheroid. In the case of a spheroid, i.e. $a = b$, the rather complicated denominator of (2) becomes independent of ϕ. The remaining dependence in the numerator easily shows that the integral in (11) is nonzero only for $m = 0$ while (12) is

Table 1. Moments of a half shell of general ellipsoids with semi-axes a, b and c in x-, y- and z-direction, respectively, in units of the surface charge density σ_0 up to the order $l = 4$ calculated with (15) and (16). Remember that these are not multipole moments as the integration is not performed with respect to the centre of charge. Combining two shells (see the text) gives the true multipole moments. In the case of a two-domain ellipsoid also the moments of the domain wall have to be added. Solutions for negative m are easily obtained by the well-known relation $Q_{l-m} = (-1)^m Q_{lm}^*$.

l	m	$\tilde{Q}_{lm}\sigma_0^{-1}$
0	0	$\pi ab\cos\theta_{\mathrm{p}}$
1	0	$\frac{2\pi}{3}abc\cos\theta_{\mathrm{p}}$
	1	$-\frac{\sqrt{2}\pi}{3}abc\,\mathrm{e}^{\mathrm{i}\phi_{\mathrm{p}}}\sin\theta_{\mathrm{p}}$
2	0	$-\frac{\pi}{8}ab(a^2+b^2-4c^2)\cos\theta_{\mathrm{p}}$
	1	$-\sqrt{\frac{3}{32}}\pi abc^2\,\mathrm{e}^{\mathrm{i}\phi_{\mathrm{p}}}\sin\theta_{\mathrm{p}}$
	2	$\sqrt{\frac{3}{128}}\pi ab(a^2-b^2)\cos\theta_{\mathrm{p}}$
3	0	$-\frac{\pi}{5}abc(a^2+b^2-2c^2)\cos\theta_{\mathrm{p}}$
	1	$\frac{\pi}{10\sqrt{3}}abc(\cos\phi_{\mathrm{p}}(3a^2+b^2-4c^2)+\mathrm{i}\sin\phi_{\mathrm{p}}(a^2+3b^2-4c^2))\sin\theta_{\mathrm{p}}$
	2	$\frac{\pi}{\sqrt{30}}abc(a^2-b^2)\cos\theta_{\mathrm{p}}$
	3	$-\frac{\pi}{\sqrt{20}}abc(a^2-b^2)\,\mathrm{e}^{\mathrm{i}\phi_{\mathrm{p}}}\sin\theta_{\mathrm{p}}$
4	0	$\frac{\pi}{192}ab(9a^4+6a^2(b^2-8c^2)+(3b^2-8c^2)^2)\cos\theta_{\mathrm{p}}$
	1	$\frac{\sqrt{5}\pi}{96}abc^2(\cos\phi_{\mathrm{p}}(9a^2+3b^2-8c^2)+\mathrm{i}\sin\phi_{\mathrm{p}}(3a^2+9b^2-8c^2))\sin\theta_{\mathrm{p}}$
	2	$-\sqrt{\frac{5}{2}}\frac{\pi}{32}ab(a^2-b^2)(a^2+b^2-4c^2)\cos\theta_{\mathrm{p}}$
	3	$-\frac{\sqrt{35}\pi}{32}abc^2(a^2-b^2)\,\mathrm{e}^{\mathrm{i}\phi_{\mathrm{p}}}\sin\theta_{\mathrm{p}}$
	4	$\sqrt{\frac{35}{2}}\frac{\pi}{64}ab(a^2-b^2)^2\cos\theta_{\mathrm{p}}$

nonzero only if $|m| = 1$. The half moments then are

$$\tilde{Q}_{l0} = \sigma_0\pi\cos\theta_{\mathrm{p}}\sum_{n}^{l}p_n(l,0)\Gamma\left(\frac{n+2}{2}\right) \times \sum_{j=0}^{\frac{l-n}{2}}\frac{\left(-\frac{l-n}{2}\right)_j}{\Gamma\left(\frac{n+4}{2}+j\right)}\sum_{v=0}^{j}(-1)^v\binom{j}{v}a^{2v+2}c^{l-2v} \tag{17}$$

and

$$\tilde{Q}_{l\pm1} = \sigma_0\sqrt{\frac{(l\mp1)!}{(l\pm1)!}}\frac{\pi}{2}\sin\theta_{\mathrm{p}}\,\mathrm{e}^{\pm\mathrm{i}\phi_{\mathrm{p}}}\sum_{n}^{l-1}p_n(l,\pm1)\Gamma\left(\frac{n+1}{2}\right) \times \sum_{j=0}^{\frac{l-n-1}{2}}\frac{(j+1)\left(-\frac{l-n-1}{2}\right)_j}{\Gamma\left(\frac{n+5}{2}+j\right)}\sum_{v=0}^{j}(-1)^v\binom{j}{v}a^{2v+2}c^{l-2v}, \tag{18}$$

respectively.

2.2. The multipole moments of an ellipsoidal disc, the domain wall

If an ellipsoid possesses two domains, with a geometry described before, it also exhibits a disc-shaped charged domain wall. Due to homogeneously polarized domains, the disc has a

Table 2. Moments of an ellipsoidal disc with semi-axes a and b in x- and y-direction, respectively, in units of the surface charge density $\sigma_{\rm disc}$ up to the order $l = 4$ calculated with (22). Only even l and m are allowed.

l	m	$Q_{lm}^{\rm disc,ell}\sigma_{\rm disc}^{-1}$
0	0	$ab\pi$
2	0	$-\frac{\pi}{8}ab(a^2+b^2)$
	2	$\sqrt{\frac{3}{128}}\pi ab(a^2-b^2)$
4	0	$\frac{\pi}{64}(3a^5b+2a^3b^3+3ab^5)$
	2	$-\sqrt{\frac{5}{2}}\frac{\pi}{32}ab(a^4-b^4)$
	4	$\sqrt{\frac{35}{2}}\frac{\pi}{64}ab(a^2-b^2)^2$

homogeneous charge density. The given geometry automatically ensures that centre of charge and origin coincide and the integration over the surface directly gives the multipole moments of the disc. Defining polar coordinates as

$$\vec{r}(r,\phi) = \frac{r}{\sqrt{\frac{\cos^2\phi}{a^2}+\frac{\sin^2\phi}{b^2}}}\begin{pmatrix}\cos\phi\\ \sin\phi\end{pmatrix}, \tag{19}$$

where $r \in [0, 1]$ and introducing the charge density of the disc, $\sigma_{\rm disc} = -\sigma_0\cos\theta_{\rm p}$, the multipole moments have the integral form

$$Q_{lm}^{\rm disc,ell} = \sigma_{\rm disc}\sqrt{\frac{(l-m)!}{(l+m)!}}\int_0^{2\pi}{\rm d}\phi\int_0^1{\rm d}r\frac{P_l^m(0)r^{l+1}}{\left(\frac{\cos^2\phi}{a^2}+\frac{\sin^2\phi}{b^2}\right)^{\frac{l+2}{2}}}{\rm e}^{{\rm i}m\phi}. \tag{20}$$

For symmetry reasons it is obvious that m has to be even and as [19]

$$P_l^m(0) = 2^m\frac{\Gamma\left(\frac{l+m+1}{2}\right)}{\Gamma\left(\frac{l-m+2}{2}\right)}\cos\frac{\pi(l+m)}{2}, \tag{21}$$

it follows that also l must be even. Applying the same methods as before the moments eventually read

$$Q_{lm}^{\rm disc,ell} = 2\sqrt{\pi}\sigma_{\rm disc}\sqrt{\frac{(l-m)!}{(l+m)!}}\frac{P_l^m(0)}{l+2}\sum_{k=0}^{\frac{m}{2}}\alpha_k(m)\frac{\Gamma\left(k+\frac{1}{2}\right)}{k!}\sum_{j=0}^{\frac{l}{2}-k}\frac{\left(k-\frac{l}{2}\right)_j\left(\frac{1}{2}\right)_j}{j!\,(k+1)_j}$$
$$\times\sum_{v=0}^{j}(-1)^v\binom{j}{v}a^{l-2v+1}b^{2v+1}. \tag{22}$$

The lower order multipole moments of charged discs are listed in table 2. In the case of $a = b$ (22) simplifies to

$$Q_{l0}^{\rm disc} = (-1)^{\frac{m}{2}}2\pi\sigma_{\rm disc}\frac{P_l^0(0)}{l+2}a^{l+2}. \tag{23}$$

Hence, due to symmetry m has to be zero if $a = b$.

3. The multipole moments of the general ellipsoid

In the previous chapters the integrals over a half shell of an ellipsoid as well as a disc have been evaluated. As mentioned before, when combining two shells it is required that centre of charge and origin coincide. Combining the shells the parity of the integrand has to be considered. If the two shells have parallel polarization the parity of the charge distribution is negative and consequently the integral vanishes if the (regular normalized) spherical harmonics have positive parity. From this it follows that l has to be odd. Therefore, the multipole moments of a homogeneous polarized ellipsoid are twice the values given in table 1 if l is odd and zero otherwise. If, on the other hand, the two shells have antiparallel polarization the charge distribution has even parity and the normalized spherical harmonics must have the same symmetry. Hence, l must be even and the multipole moments are twice the results of table 1 plus—as both shells contribute to a domain wall—twice the result of table 2 if l is even and zero otherwise.

4. Summary and discussion

It has been shown that the multipole moments for ellipsoidal discs as well as general ellipsoids with homogenous polarization of arbitrary direction can be expressed as finite polynomials of the semi-axes (a, b, c). The results are valid for any order l of a multipole expansion. As the integrals for the ellipsoid are solved only for a half shell it is also possible to combine the results for a single domain as well as a two-domain ellipsoid with antiparallel polarization. Several other special cases of orientations of the polarization are possible, for instance in a spheroid where the angles ϕ_{p} can be chosen arbitrarily for each shell if $\theta_{\mathrm{p}} = \pi/2$.

One could argue that the restriction to a surface charge is an oversimplification. If e.g. the polarization density changes in space, a 'volume charge' emerges. The results given above easily can be extended to systems with a polarization density n changing with $n \propto f(t)$ and $t^2 = a^{-2}x^2 + b^{-2}y^2 + c^{-2}z^2$, i.e. the density is constant on an ellipsoid. If the direction of the polarization is constant and $f(t)$ is continuously differentiable all given results still hold as the required volume integral—after integrating over t—only differs from the surface integral (2) by a prefactor (see appendix D).

Therefore, the results are not only applicable to homogeneous polarization but also to systems where the polarization direction is constant but varies in intensity described by a function f with the aforementioned properties.

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Appendix A. Relations for trigonometric functions

The products of trigonometric functions, which appear in (3) are simplified to

$$
\begin{aligned}
G_1(m, \phi) &= \cos(m\phi)\cos\phi = \frac{1}{2}(\cos((1-m)\phi) + \cos((1+m)\phi) \\
G_2(m, \phi) &= \mathrm{i}\sin(m\phi)\cos\phi = \frac{\mathrm{i}}{2}(-\sin((1-m)\phi) + \sin((1+m)\phi) \\
G_3(m, \phi) &= \cos(m\phi)\sin\phi = \frac{1}{2}(\sin((1-m)\phi) + \sin((1+m)\phi) \\
G_4(m, \phi) &= \mathrm{i}\sin(m\phi)\sin\phi = \frac{\mathrm{i}}{2}(\cos((1-m)\phi) - \cos((1+m)\phi).
\end{aligned}
\tag{A.1}
$$

The function $\cos m\phi$, with m even, can be expressed as an even polynomial of $\cos\phi$ of order m,

$$\cos m\phi = \sum_{k=0}^{\frac{|m|}{2}} \alpha_k(|m|)\cos^{2k}\phi, \tag{A.2}$$

where the coefficients $\alpha_k(m)$ are given by

$$\alpha_k(m) = (-1)^{\frac{m}{2}-k}\frac{m}{2}\frac{2^{2k}\Gamma\left(k+\frac{m}{2}\right)}{\Gamma(2k+1)\,\Gamma\left(\frac{m}{2}-k+1\right)}, \tag{A.3}$$

and $\alpha_0(0) = 1$.

Appendix B. Coefficients of the associated Legendre functions

The associated Legendre functions can be expressed as [24]

$$P_l^m(x) = \sqrt{1-x^2}^m \sum_{k=0}^{\lfloor\frac{l-m}{2}\rfloor} \frac{(-1)^{k+m}}{2^l}\frac{(2l-2k)!}{k!(l-k)!(l-m-2k)!}x^{l-m-2k}, \tag{B.1}$$

where the floor function—denoted by the brackets—ensures that the upper limit of the sum is an integer value. Rearranging the sum the polynomial reads

$$\begin{aligned} P_l^m(x) &= \sqrt{1-x^2}^m \sum_{k=0}^{\frac{l-m-\tau}{2}} \frac{(-1)^{l+m-\tau+2k}}{2^l}\frac{(l+m+\tau+2k)!\,x^{2k+\tau}}{\left(\frac{l-m-\tau}{2}-k\right)!\left(\frac{l+m+\tau}{2}+k\right)!(2k+\tau)!} \\ &= \sqrt{1-x^2}^m \sum_{n=0}^{l-m} p_n(l,m)x^n, \end{aligned} \tag{B.2}$$

where $\tau = 0$ if $l+m$ is even and $\tau = 1$ if $l+m$ is odd. Eventually the coefficients for $m \geqslant 0$ have the form

$$\begin{aligned} p_n(l,m) &= \frac{1+(-1)^{l+m-n}}{2}\cdot\frac{(-1)^{\frac{l+m-n}{2}}}{2^l}\cdot\frac{(l+m+n)!}{\left(\frac{l-m-n}{2}\right)!\left(\frac{l+m+n}{2}\right)!n!} \\ p_n(l,-m) &= (-1)^m\frac{(l-m)!}{(l+m)!}p_n(l,m), \end{aligned} \tag{B.3}$$

where the first quotient is either zero or one and therefore ensures that the polynomial is either even or odd.

Appendix C. The hypergeometric function ${}_2F_1$

The properties of the hypergeometric function are given in [19]. The integral representation has the form

$$\frac{\Gamma(b)\Gamma(c-b)}{\Gamma(c)}{}_2F_1(a,b;c;z) = \int_0^1 \mathrm{d}t\, t^{b-1}(1-t)^{c-b-1}(1-zt)^{-a}. \tag{C.1}$$

Furthermore, the transformation

$${}_2F_1(a,b;c;z) = (1-z)^{c-a-b}{}_2F_1(c-a,c-b;c;z) \tag{C.2}$$

is applied several times in the text. The function is symmetric with respect to a and b. In the case of $a \in \mathbb{N}_0$ the hypergeometric function has a polynomial form

$${}_2F_1(-a,b;c;z) = \sum_{j=0}^{a}\frac{(-a)_j(b)_j}{(c)_j}\frac{z^j}{\Gamma(j+1)}, \tag{C.3}$$

utilizing for $x > 0$

$$(x)_j = \frac{\Gamma(x+j)}{\Gamma(x)} \qquad (-x)_j = (-1)^j \frac{\Gamma(1+x)}{\Gamma(1+x-j)} \quad (x \geqslant j). \tag{C.4}$$

All formulae required before have $j = 0$ if $x = 0$; in this case $(x)_0$ exists in the limit $x \to 0$ and is $(0)_0 = 1$.

Appendix D. Integration over volume charge

Assuming that the polarization density changes by a function f but has constant direction $\vec{p} = \vec{P}/P_0$ the volume charge is

$$\rho(\vec{r}) = -\sigma_0 \vec{p} \cdot \vec{\nabla} f(t(x, y, z)). \tag{D.1}$$

If the function $f(t)$ is of the form

$$f(t(x, y, z)) = f\left(\sqrt{\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}}\right) \tag{D.2}$$

the polarization density is constant on an ellipsoidal shell. The volume charge is given by

$$\begin{aligned}
\rho(\vec{r}) &= -\sigma_0 \begin{pmatrix} \sin\theta_{\rm p}\cos\phi_{\rm p} \\ \sin\theta_{\rm p}\sin\phi_{\rm p} \\ \cos\theta_{\rm p} \end{pmatrix} \cdot \begin{pmatrix} \frac{\rm d}{{\rm d}x} f(t(x, y, z)) \\ \frac{\rm d}{{\rm d}y} f(t(x, y, z)) \\ \frac{\rm d}{{\rm d}z} f(t(x, y, z)) \end{pmatrix} \\
&= -\sigma_0 \begin{pmatrix} \sin\theta_{\rm p}\cos\phi_{\rm p} \\ \sin\theta_{\rm p}\sin\phi_{\rm p} \\ \cos\theta_{\rm p} \end{pmatrix} \cdot \begin{pmatrix} \frac{x}{a^2} \\ \frac{y}{b^2} \\ \frac{z}{c^2} \end{pmatrix} \frac{1}{t} \frac{\partial}{\partial t} f(t) \\
&= -\sigma_0 r \begin{pmatrix} \sin\theta_{\rm p}\cos\phi_{\rm p} \\ \sin\theta_{\rm p}\sin\phi_{\rm p} \\ \cos\theta_{\rm p} \end{pmatrix} \cdot \begin{pmatrix} \frac{\sin\theta\cos\phi}{a^2} \\ \frac{\sin\theta\sin\phi}{b^2} \\ \frac{\cos\theta}{c^2} \end{pmatrix} \frac{1}{t} \frac{\partial}{\partial t} f(t) \\
&= -\sigma_0 t \frac{\left(\frac{\cos\phi\cos\phi_{\rm p}}{a^2} + \frac{\sin\phi\sin\phi_{\rm p}}{b^2}\right)\sin\theta\sin\theta_{\rm p} + \frac{1}{c^2}\cos\theta\cos\theta_{\rm p}}{\sqrt{\left(\frac{\cos^2\phi}{a^2} + \frac{\sin^2\phi}{b^2}\right)\sin^2\theta + \frac{1}{c^2}\cos^2\theta}} \frac{1}{t} \frac{\partial}{\partial t} f(t).
\end{aligned} \tag{D.3}$$

As the volume element has the form

$$\mathrm{d}V = \frac{t^2 \sin\theta}{\left(\left(\frac{\cos^2\phi}{a^2} + \frac{\sin^2\phi}{b^2}\right)\sin^2\theta + \frac{1}{c^2}\cos^2\theta\right)^{\frac{3}{2}}} \,\mathrm{d}t\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{D.4}$$

the integral over one half of an ellipsoid reads

$$\begin{aligned}
\tilde{Q}_{lm}^{\rm vol} &= -\sigma_0 \sqrt{\frac{(l-m)!}{(l+m)!}} \int_0^{2\pi} \mathrm{d}\phi \int_0^{\frac{\pi}{2}} \mathrm{d}\theta \int_0^1 \mathrm{d}t\, P_l^m(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\phi} \sin\theta \\
&\quad \times \frac{\left(\frac{\cos\phi\cos\phi_{\rm p}}{a^2} + \frac{\sin\phi\sin\phi_{\rm p}}{b^2}\right)\sin\theta\sin\theta_{\rm p} + \frac{1}{c^2}\cos\theta\cos\theta_{\rm p}}{\left[\left(\frac{\cos^2\phi}{a^2} + \frac{\sin^2\phi}{b^2}\right)\sin^2\theta + \frac{1}{c^2}\cos^2\theta\right]^{\frac{4}{2}}} t^2 r^l(t, \theta, \phi) \frac{\partial}{\partial t} f(t) \\
&= \left(-\int_0^1 \mathrm{d}t\, t^{l+2} \frac{\partial}{\partial t} f(t)\right) \sigma_0 \sqrt{\frac{(l-m)!}{(l+m)!}} \int_0^{2\pi} \mathrm{d}\phi \int_0^{\frac{\pi}{2}} \mathrm{d}\theta\; P_l^m(\cos\theta)\, \mathrm{e}^{\mathrm{i}m\phi} \sin\theta
\end{aligned}$$

$$\times \frac{\left(\frac{\cos\phi\cos\phi_{\mathrm{p}}}{a^2} + \frac{\sin\phi\sin\phi_{\mathrm{p}}}{b^2}\right)\sin\theta\sin\theta_{\mathrm{p}} + \frac{1}{c^2}\cos\theta\cos\theta_{\mathrm{p}}}{\left[\left(\frac{\cos^2\phi}{a^2} + \frac{\sin^2\phi}{b^2}\right)\sin^2\theta + \frac{1}{c^2}\cos^2\theta\right]^{\frac{l+4}{2}}}$$

$$= \left(-\int_0^1 \mathrm{d}t\, t^{l+2}\frac{\partial}{\partial t} f(t)\right)\tilde{Q}_{lm}, \tag{D.5}$$

where $\tilde{Q}_{lm}$ is given in (2). By means of distributions this result even contains the surface integral in the case of a constant polarization density that has a discontinuity at the surface. Differentiating $f(t) = H(1-t)$—the Heaviside step function—would lead to the Dirac delta $f'(t) = -\delta(1-t)$. Consequently, the result of the integral over t is $1^{l+2} = 1$ and eventually the solution for the volume integral is identical with the surface integral (2).

In an easy and similar way one shows that for the charged disc the angle-dependent integrals stay the same as well; only the prefactor $(l+2)^{-1}$ in (22) and (23) has to be replaced by an integral over $t^{l+1}f(t)$.

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