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Transformation properties of spheroidal multipole moments and potentials

Georg Jansen

Institut für Theoretische Chemie, Heinrich-Heine-Universität Düsseldorf, Universitätsstrasse 1, D-40225 Düsseldorf, Germany

E-mail: georg@theochem.uni-duesseldorf.de

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Abstract. Introducing definitions of solid spheroidal harmonics which contain those of solid spherical harmonics as special cases for vanishing ellipticity it is shown that the formalism of the multipole expansion of a $1/R$-potential can be consistently extended to incorporate prolate and oblate spheroidal multipole moments. For finite ellipticity one can transform between regular solid spheroidal and spherical harmonics and multipole moments through simple relations given before and independently proven here. Corresponding relations between irregular solid spheroidal and spherical harmonics are presented for the first time, together with an investigation of the convergence properties of the resulting series expansions. Explicit formulae are derived for the transformations between spheroidal multipoles calculated in coordinate systems of different ellipticity, origin and orientation. These fromulae can be utilized to calculate the energy of interaction between two arbitrarily oriented spheroidal charge or mass distributions of different ellipticity. The performance of spheroidal multipole expansions is illustrated with some numerical examples.

1. Introduction

One of the most useful series expansions in physics is certainly that of the inverse of a distance between two points in space into a Taylor series around one of the points, or, more elegantly, into products of corresponding regular and irregular solid spherical harmonics. For example, if all of the members of a set of particles interact with a separate single particle via an inverse distance energy law, as is the case for electrostatic or gravitational interactions, this series expansion can be used to express the energy of interaction in powers of the inverse distance between the single particle and an appropriate point within the particle distribution, resulting in the multipole expansion of the potential of the charge distribution. Similarly, the energy of interaction between two separate sets of particles can be expanded in powers of the inverse distance between chosen centres of the two charge distributions. Using the multipole expansion for the calculation of potentials or interaction energies one can replace the detailed knowledge of the individual positions of the particles within the distributions by a set of multipole moments. This is particularly useful when considering continuous charge or mass distributions. The multipole moments are computed once and for all, and it is often the case that either only a finite number of them do not vanish or that higher multipole moments can be safely neglected.

The multipole expansion of an interaction energy will converge to the exact result when each of the separate charge or mass distributions can be enclosed in a sphere and the respective spheres do not overlap or touch. This does preclude its application to problems such as that of computing the electrostatic interaction between, for example, a long rod-like and a

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spherical charge distribution, when the latter is located on a place at the side of the former which is closer than half of the rod length. Similarly, the conventional multipole expansion in general will not converge when the spherical charge distribution is placed on top of a disc-like charge distribution at a distance smaller than the radius of the disc. Problems of this type are frequently encountered in the theory of intermolecular interactions [1], for example when one wants to study the interaction of a water molecule with an extended polymer chain or with a flat polycyclic aromatic system. These situations can be more appropriately described when using prolate or oblate spheroidal instead of spherical coordinates. It is well known that in these coordinates one can give a series expansion of the inverse of a distance between two points in a similar way as in the case of spherical coordinates, replacing spherical with prolate or oblate spheroidal harmonics [2, 3]. Some time ago Stiles and Buchdahl [4–6] derived formulae which relate regular solid spherical harmonics to their spheroidal counterparts, showing explicitly how the latter can be obtained as linear combinations of the former and vice versa. Unfortunately, these results and related work on the ellipsoidal case [7, 8] seem to have gone largely unnoticed—perhaps due to the complications connected with the occurence of associated Legendre functions of the second kind in the spheroidal series expansion. Yet, for numerical calculations this plays hardly any role, and the development of a systematic formalism dealing with spheroidal multipoles appears to be worthwhile, mainly, but not exclusively, with applications in the theory of intermolecular interactions in mind.

Some basic ingredients of such a theory of spheroidal multipole expansions will be presented in this paper. First of all, since spherical coordinates can be obtained as a special case of the spheroidal coordinates for vanishing ellipticity, it is desirable that regular and irregular solid spherical harmonics can be obtained as special cases of corresponding spheroidal harmonics as well. Such a consistent definition of regular and irregular solid prolate spheroidal harmonics is given in section 2, which also contains the formulae for transformation between the regular harmonics (a new proof of which is given in appendix B) and, for the first time, the formulae for transformation between the irregular harmonics. The latter have the form of an infinite series expansion whose convergence properties will be briefly investigated, elucidating some advantages of an expansion into spheroidal multipole potentials. An important feature of the theory of spherical harmonics is the availability of formulae for their transformations under translation and rotation of the coordinate system, making it easy to shift or rotate spherical multipoles. These transformations are of particular value in those cases where the charge or mass distribution deviates from an idealized spherical shape, so that one may wish to 'readjust' a known set of multipoles to a rotated or displaced coordinate system. Furthermore, they play a crucial role in the derivation of formulae for the interaction between arbitrarily oriented multipoles [1]. For prolate spheroidal multipole moments there is an additional transformation to be considered, namely that due to a readjustment of the distance between the confocal points of the spheroid. The corresponding transformation formulae for scaling, translation, and rotation of regular solid prolate spheroidal harmonics can easily be derived from their relation to the spherical harmonics. Explicit formulae which apply directly to prolate spheroidal multipole moments are given in section 3, along with some basic properties of the transformation coefficients. The definition of regular and irregular solid oblate spheroidal harmonics and the modifications of the transformation relations necessary to handle oblate spheroidal multipole moments are presented in section 4. In the concluding section 5 it is indicated how these relations can be exploited to determine the energy of interaction between arbitrarily oriented or scaled spheroidal multipole moments and some numerical comparisons of the performance of spheroidal and spherical multipole expansions will be shown.

2. Prolate spheroidal multipole expansion

2.1. Regular and irregular solid spherical harmonics

The Laplace expansion of the inverse distance between two points $\boldsymbol{r}$ and $\boldsymbol{R}$ in a three-dimensional real space

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{R}|} = \sum_{l=0}^{\infty} \frac{r^l}{R^{l+1}} P_l(s) P_l(S) + 2 \sum_{l=1}^{\infty} \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} \frac{r^l}{R^{l+1}} P_l^m(s) P_l^m(S) \cos m(\varphi - \phi) \tag{1}$$

where (r, s, φ) and (R, S, ϕ) are the spherical coordinates (cf appendix A (i)) of the points $\boldsymbol{r}$ and $\boldsymbol{R}$, respectively, is one of the most frequently used series expansions in physics. It converges absolutely for $R > r$. Introducing regular and irregular solid spherical harmonics defined through the Racah spherical harmonics $C_{lm}(s, \varphi)$ as [1, 9, 10]

$$R_{lm}^s(\boldsymbol{r}) = r^l C_{lm}(s, \varphi) = r^l \sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(s) \mathrm{e}^{\mathrm{i}m\varphi} \tag{2}$$

$$I_{lm}^s(\boldsymbol{R}) = R^{-l-1} C_{lm}(S, \phi) = R^{-l-1} \sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(S) \mathrm{e}^{\mathrm{i}m\phi} \tag{3}$$

respectively, the Laplace expansion can conveniently be rewritten in the form

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{R}|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} I_{lm}^{s*}(\boldsymbol{R}) R_{lm}^s(\boldsymbol{r}). \tag{4}$$

The numerical factors in the definitions (2), (3) are chosen such that $R_{l(-m)}^s = (-1)^m R_{lm}^{s*}$ and $I_{l(-m)}^s = (-1)^m I_{lm}^{s*}$. Employing, for simplicity, atomic units ($e = 1 = 4\pi\epsilon_0$) the electric potential $\Phi(\boldsymbol{R}) = \int_{\mathcal{V}} \mathrm{d}\tau \rho(\boldsymbol{r})/|\boldsymbol{r}-\boldsymbol{R}|$ generated by a charge distribution can now be calculated from the spherical multipole expansion

$$\begin{aligned}\Phi(\boldsymbol{R}) &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} I_{lm}^{s*}(\boldsymbol{R}) \int_{\mathcal{V}} \mathrm{d}\tau\, R_{lm}^s(\boldsymbol{r}) \rho(\boldsymbol{r}) \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} I_{lm}^{s*}(\boldsymbol{R}) Q_{lm}^s \end{aligned} \tag{5}$$

where the integration has to be carried out over the volume $\mathcal{V}$ occupied by the charge distribution and $\boldsymbol{R}$ must be outside the smallest sphere enclosing $\mathcal{V}$. Equation (5) contains the definition of the spherical multipole moments Q_{lm}^s.

2.2. Regular and irregular solid prolate spheroidal harmonics

Using prolate spheroidal coordinates (t, u, φ) and (T, U, ϕ) to describe the points $\boldsymbol{r}$ and $\boldsymbol{R}$ (cf appendix A (i)) one obtains the Neumann expansion

$$\begin{aligned}\frac{1}{|\boldsymbol{r}-\boldsymbol{R}|} &= \sum_{l=0}^{\infty} \frac{2l+1}{c} \mathcal{P}_l(t) \mathcal{Q}_l(T) P_l(u) P_l(U) + 2 \sum_{l=1}^{\infty} \sum_{m=1}^{l} \frac{2l+1}{c} (-1)^m \left(\frac{(l-m)!}{(l+m)!}\right)^2 \\ &\quad \times \mathcal{P}_l^m(t) \mathcal{Q}_l^m(T) P_l^m(u) P_l^m(U) \cos m(\varphi - \phi). \end{aligned} \tag{6}$$

It converges absolutely for $T > t$ (cf [3], volume I, p 90 ff). Introducing the definitions

$$R_{lm}^p(\boldsymbol{r}; c) = c^l \frac{(l-m)!}{(2l-1)!!} \sqrt{\frac{(l-m)!}{(l+m)!}} \mathcal{P}_l^m(t) P_l^m(u) \mathrm{e}^{\mathrm{i}m\varphi} \tag{7}$$

$$I^p_{lm}(\boldsymbol{R}; c) = c^{-l-1}(-1)^m \frac{(2l+1)!!}{(l+m)!}\sqrt{\frac{(l-m)!}{(l+m)!}}\,\mathcal{Q}^m_l(T)P^m_l(U)\mathrm{e}^{\mathrm{i}m\phi} \tag{8}$$

for regular and irregular solid prolate spheroidal harmonics, equation (6) can be recast into the simple form

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{R}|} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} I^{p*}_{lm}(\boldsymbol{R}; c)R^p_{lm}(\boldsymbol{r}; c). \tag{9}$$

The definitions (7), (8) imply that $c^{-l}R^p_{lm}(\boldsymbol{r}; c) = R^p_{lm}(\boldsymbol{r}/c; 1)$ and $c^{l+1}I^p_{lm}(\boldsymbol{r}; c) = I^p_{lm}(\boldsymbol{r}/c; 1)$. As for the spherical harmonics, the spheroidal harmonics are of parity $(-1)^l$, $R^p_{lm}(-\boldsymbol{r}; c) = (-1)^l R^p_{lm}(\boldsymbol{r}; c)$ and $I^p_{lm}(-\boldsymbol{r}; c) = (-1)^l I^p_{lm}(\boldsymbol{r}; c)$. The numerical factors in definitions (7), (8) are chosen such that $R^p_{l(-m)} = (-1)^m R^{p*}_{lm}$ and $I^p_{l(-m)} = (-1)^m I^{p*}_{lm}$. Furthermore, as it will be seen in sections 2.3 and 2.4, they ensure that

$$\lim_{c\to 0} R^p_{lm}(\boldsymbol{r}; c) = R^s_{lm}(\boldsymbol{r}) \tag{10}$$

$$\lim_{c\to 0} I^p_{lm}(\boldsymbol{R}; c) = I^s_{lm}(\boldsymbol{R}). \tag{11}$$

Using this the electric potential generated by a charge distribution can now alternatively be calculated from the prolate spheroidal multipole expansion

$$\begin{aligned}\Phi(\boldsymbol{R}) &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} I^{p*}_{lm}(\boldsymbol{R}; c)\int_{\mathcal{V}} \mathrm{d}\tau\, R^p_{lm}(\boldsymbol{r}; c)\rho(\boldsymbol{r}) \\ &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} I^{p*}_{lm}(\boldsymbol{R}; c)Q^p_{lm}(c) \end{aligned}\tag{12}$$

where $\boldsymbol{R}$ must be outside the smallest prolate spheroid enclosing the volume $\mathcal{V}$ occupied by the charge distribution. Equation (12) defines the prolate spheroidal multipole moments $Q^p_{lm}(c)$. The transformation and limiting formulae for the regular solid prolate spheroidal harmonics derived in the following sections apply immediately to the corresponding multipole moments as well.

2.3. Relation to regular solid spherical harmonics

The spherical harmonic $r^l P^m_l(s)$ contains products and powers of $r^2 = c^2(t^2 - u^2 - 1)$, $rs = ctu$, and $r^m(1-s^2)^{m/2} = c(t^2-1)^{m/2}(1-u^2)^{m/2}$. Therefore, it is clear that it can be expanded in products of associated Legendre functions $\mathcal{P}^m_i(t)P^m_j(u)$, with i and j ranging down from l to $|m|$ or $|m|+1$ in steps of two. As it turns out (cf appendix B.1) only terms with $j = i$ occur in the expansion:

$$\left(\frac{r}{c}\right)^l P^m_l(s) = \sum_{i=|m|}^{l} a^{li}_m \mathcal{P}^m_i(t)P^m_i(u). \tag{13}$$

An explicit form for the expansion coefficients has first been given by Stiles and Buchdahl [5,6]. It can be written as

$$a^{li}_m = \frac{(2i+1)(l+m)!}{(l-i)!!(l+i+1)!!}\,\frac{(i-m)!}{(i+m)!}\Delta^{li}_m \tag{14}$$

where, for convenience, the range of definition has been extended to arbitrary combinations of l, i and m using

$$\Delta^{li}_m = \begin{cases} 1 & (l-i)\ \text{even}, \quad l \geqslant i \geqslant |m| \\ 0 & \text{else.}\end{cases} \tag{15}$$

Appendix B.1 presents an elementary proof. Considering the inverse relation to equation (13) it is clear that one can expand

$$\mathcal{P}_l^m(t)P_l^m(u) = \sum_{i=|m|}^{l} \tilde{a}_m^{li} \left(\frac{r}{c}\right)^i P_i^m(s). \tag{16}$$

The explicit form of the expansion coefficients now reads [5, 6]:

$$\tilde{a}_m^{li} = \frac{(-1)^{(l-i)/2}(l+i-1)!!}{(l-i)!!(i+m)!} \frac{(l+m)!}{(l-m)!} \Delta_m^{li}. \tag{17}$$

Equations (16), (17) can be shown by inserting equations (13), (14) into (16) and using the sum rule

$$\sum_{i=k}^{l} \tilde{a}_m^{li} a_m^{ik} = \delta_{lk} \tag{18}$$

derived in appendix B.2. It is clear then that

$$\sum_{i=k}^{l} a_m^{li} \tilde{a}_m^{ik} = \delta_{lk} \tag{19}$$

must also hold.

Combining the definitions (2) and (7) with the above relations one obtains the formulae for the transformation between regular solid spherical harmonics and their prolate spheroidal counterparts:

$$R_{lm}^s(\boldsymbol{r}) = \sum_{i=|m|}^{l} c^{l-i}[s:p]_m^{li} R_{im}^p(\boldsymbol{r}; c) \tag{20}$$

$$R_{lm}^p(\boldsymbol{r}; c) = \sum_{i=|m|}^{l} c^{l-i}[p:s]_m^{li} R_{im}^s(\boldsymbol{r}) \tag{21}$$

with

$$[s:p]_m^{li} = [s:p]_{-m}^{li} = \sqrt{\frac{(l+m)!(l-m)!}{(i+m)!(i-m)!}} \frac{(2i+1)!!}{(l-i)!!(l+i+1)!!} \Delta_m^{li} \tag{22}$$

$$[p:s]_m^{li} = [p:s]_{-m}^{li} = \sqrt{\frac{(l+m)!(l-m)!}{(i+m)!(i-m)!}} \frac{(-1)^{(l-i)/2}(l+i-1)!!}{(l-i)!!(2l-1)!!} \Delta_m^{li} \tag{23}$$

and

$$\sum_{i=k}^{l} [p:s]_m^{li} [s:p]_m^{ik} = \sum_{i=k}^{l} [s:p]_m^{li} [p:s]_m^{ik} = \delta_{lk}. \tag{24}$$

Noting that $[s:p]_m^{ii} = [p:s]_m^{ii} = 1$, one obtains (10) immediately from (21). It is easy to calculate the transformation coefficients numerically by employing the simple forward recursions

$$[s:p]_m^{(l+2)i} = \frac{\sqrt{((l+2)^2-m^2)((l+1)^2-m^2)}}{(l+2-i)(l+i+3)} [s:p]_m^{li} \tag{25}$$

$$[p:s]_m^{(l+2)i} = -\frac{(l+i+1)\sqrt{((l+2)^2-m^2)((l+1)^2-m^2)}}{(l+2-i)(2l+3)(2l+1)} [p:s]_m^{li} \tag{26}$$

or similar backward recursions for $[s:p]_m^{l(i-2)}$ and $[s:p]_m^{l(i-2)}$. Figure 1 shows some of the low-rank transformation coefficients, which, for large l, decrease inversely proportional to l in case of the $[s:p]_m^{li}$ and exponentially in case of the $[p:s]_m^{li}$.

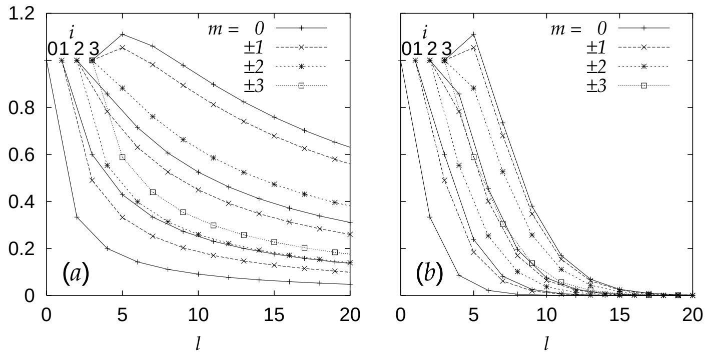

Figure 1. Some coefficients for transformation from solid prolate spheroidal to spherical harmonics, $[s:p]^{li}_m$ (*a*), and the absolute values of the back-transformation coefficients, $|[p:s]^{li}_m|$ (*b*), as a function of l.

2.4. Relation to irregular solid spherical harmonics

Let us assume that $r < R$ and $t < T$ for the points $\boldsymbol{r}$ and $\boldsymbol{R}$. Inserting (16) into the Neumann expansion (6), comparing it with the Laplace expansion (1), and making use of the orthogonality of $\cos m(\varphi - \phi)$ and $P^m_i(s)$ shows

$$\left(\frac{c}{R}\right)^{l+1} P^m_l(S) = \sum_{i=l}^{\infty} \mathcal{Q}^m_i(T) P^m_i(U) b^{il}_m \tag{27}$$

where

$$b^{il}_m = \frac{(-1)^{(i-l+2m)/2}(2i+1)(i+l-1)!!}{(i-l)!!(l-m)!} \frac{(i-m)!}{(i+m)!} \Delta^{il}_m. \tag{28}$$

From the addition theorem for the associated Legendre functions it follows:

$$|P^m_i(S)| \leqslant \sqrt{\frac{(i+m)!}{(i-m)!}} \frac{1}{\sqrt{2-\delta_{m0}}} \qquad -1 \leqslant S \leqslant 1 \tag{29}$$

while a slightly tightened version of the inequality (87-7) of [3], volume II, p 273, may be written as

$$|\mathcal{Q}^m_i(T)| < \frac{2^{i+1}(i+m)!}{(2i+1)!!} \left(\frac{1}{T+\sqrt{T^2-1}}\right)^{i+1} \mathcal{F}_m(T) \qquad T > 1 \tag{30}$$

$$\mathcal{F}_m(T) = \frac{1}{2}\left(\sqrt{\frac{T+1}{T-1}}^{\,m} + \sqrt{\frac{T-1}{T+1}}^{\,m}\right)\left(\frac{T+\sqrt{T^2-1}}{2\sqrt{T^2-1}}\right)^{\frac{1}{2}} \tag{31}$$

wherein a factor of $(2\pi/(2l+1))^{1/2}$ has been replaced by the original factor of $2^{l+1}l!/(2l+1)!!$. These inequalities allow one to see that the absolute values of the terms on the rhs of (27) are smaller than those of the series

$$\sum_{i=l}^{\infty} \frac{\mathcal{F}_m(T)2^{i+1}(i+l-1)!!\sqrt{(i-m)!(i+m)!}}{\sqrt{2-\delta_{m0}}(l-m)!(i-l)!!(2i-1)!!} \Delta^{il}_m \left(\frac{1}{T+\sqrt{T^2-1}}\right)^{i+1}.$$

Employing the quotient criterium it is easily verified that this series has a convergence radius of one, so that (27) is found to be absolutely convergent for $T > 1$. On the other hand, it is clear that (27) loses its sense for any point $(T, S) = (1, S)$ on the line between the focal points, since $\mathcal{Q}_i^m(T) \to \infty$ for $T \to 1$. Similarly to equation (27), the relation inverse to it is obtained as

$$\mathcal{Q}_l^m(T)P_l^m(U) = \sum_{i=l}^{\infty} \left(\frac{c}{R}\right)^{i+1} P_i^m(S)\tilde{b}_m^{il} \tag{32}$$

where

$$\tilde{b}_m^{il} = \frac{(-1)^m(i-m)!}{(i-l)!!(i+l+1)!!}\frac{(l+m)!}{(l-m)!}\Delta_m^{il}. \tag{33}$$

Employing (29) the series

$$\sum_{i=l}^{\infty} \frac{(l+m)!\sqrt{(i-m)!(i+m)!}}{\sqrt{2-\delta_{m0}}(l-m)!(i-l)!!(i+l+1)!!}\Delta_m^{il}\left(\frac{c}{R}\right)^{i+1}$$

is seen to majorize the series formed by the absolute values of the terms in (32). The convergence radius of this series is found to be one, so that (32) is absolutely convergent for $R > c$. For $R \leqslant c$, on the other hand, in general it will not converge, as it can be deduced from the special case $(R, S) = (c, 1)$, $l = m = 0$, for which the rhs of equation (32) becomes the divergent subseries $\sum_{i=0}^{\infty} \Delta_0^{i0}/(i+1) = 1 + \frac{1}{3} + \frac{1}{5} + \cdots$ of the harmonic series.

Introducing the irregular solid harmonics (3) and (8) the above transformation formulae can be stated as:

$$I_{lm}^s(\boldsymbol{R}) = \sum_{i=l}^{\infty} c^{i-l} I_{im}^p(\boldsymbol{R}; c)[p : s]_m^{il} \tag{34}$$

$$I_{lm}^p(\boldsymbol{R}; c) = \sum_{i=l}^{\infty} c^{i-l} I_{im}^s(\boldsymbol{R})[s : p]_m^{il} \tag{35}$$

which, using $[s : p]_m^{ll} = 1$ in (35), shows the validity of equation (11). Figure 2 visualizes the convergence/divergence behaviour of these expansions for the special case $l = m = 0$. The expansion (34) is seen to converge reasonably fast to $I_{00}^s(\boldsymbol{R}) = 1/R$, except for points close to the axis between the focal points of the prolate spheroidal coordinates. On the other hand, while (35) converges to $I_{00}^p(\boldsymbol{R}; c) = (1/c)$ arcoth T outside a sphere with radius c, it can even alternate within that sphere. Note that $I_{lm}^s(\boldsymbol{R})$ is the electric potential of the spherical multipole Q_{lm}^s and $I_{lm}^p(\boldsymbol{R}; c)$ that of the prolate multipole $Q_{lm}^p(c)$. Loosely speaking, figure 2 demonstrates that it is 'safer' to expand the potential of a spherical multipole into prolate multipole potentials than the other way round, since the convergence domain is larger in the first case.

3. Transformations of regular solid prolate spheroidal harmonics

3.1. Scaling of the distance between the confocal points

The transformation between regular solid prolate spheroidal harmonics defined in a coordinate system with confocal points $\pm c_1$ and those with confocal points $\pm c_2$ can easily be obtained by inserting equation (20) for c_2 into equation (21) for c_1. This yields

$$R_{lm}^p(\boldsymbol{r}; c_1) = \sum_k c_1^{l-k} \mathcal{S}_m^{lk}(c_2/c_1) R_{km}^p(\boldsymbol{r}; c_2) \tag{36}$$

where

$$\mathcal{S}_m^{lk}(x) = \Delta_m^{lk}\left(\delta_{lk} + (1-\delta_{lk})\frac{(-1)^{(l-k)/2}}{l-k}\sqrt{\frac{(l+m)!(l-m)!}{(k+m)!(k-m)!}}\frac{(2k+1)!!}{(2l-1)!!}\right.$$

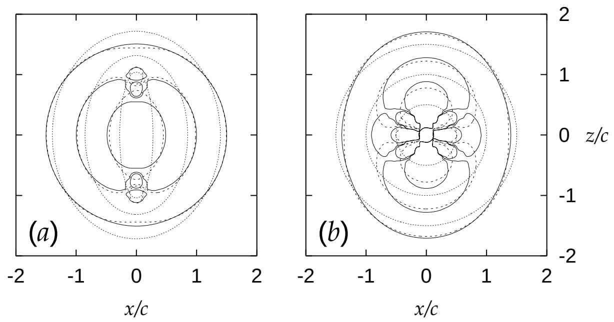

Figure 2. Contour lines of $\sum_{i=0}^{i_{\max}} c^{i-l} I_{im}^{p}(\boldsymbol{R}; c)[p:s]_{m}^{il}$ (a), and $\sum_{i=0}^{i_{\max}} c^{i-l} I_{im}^{s}(\boldsymbol{R})[s:p]_{m}^{il}$ (b), for $l = m = 0$ and $i_{\max} = 0$ (dotted curves), 2 (broken curves), and 4 (solid curves). The isocontour values are $2/3c$ (outermost contour), $1/c$, and $2/c$ (innermost contour).

$$\times \sum_{j=0}^{(l-k)/2} (-1)^{j} \binom{\frac{l-k}{2}}{j} \binom{\frac{l+k-1}{2} + j}{\frac{l-k}{2} - 1} x^{2j} \Bigg) \tag{37}$$

and a simple generalization of the results of appendix B.2 has been used. Note that the presence of Δ_m^{lk} in (37) allows one to supress the summation limits in (36). Whenever possible this simplified notation will also be employed in the following. Some basic properties of the scale transformation coefficients which ensure consistency of (36) with equations (20), (21) and (24) are

$$\mathcal{S}_m^{lk}(0) = [p:s]_m^{lk} \tag{38}$$

$$\mathcal{S}_m^{lk}(1) = \delta_{lk} \tag{39}$$

$$\lim_{x\to\infty} \mathcal{S}_m^{lk}(x) = [s:p]_m^{lk} x^{l-k}. \tag{40}$$

Furthermore, with the help of the sum rule (24) it is easy to show that

$$\mathcal{S}_m^{lk}(x_1 \cdot x_2) = \sum_i \mathcal{S}_m^{li}(x_1) x_1^i \mathcal{S}_m^{ik}(x_2) x_2^k \tag{41}$$

which specializes to a sum rule between scaling and 'rescaling' coefficients:

$$\sum_i \mathcal{S}_m^{li}(x) x^{i-k} \mathcal{S}_m^{ik}(1/x) = \delta_{lk}. \tag{42}$$

A set of multipoles $Q_{km}^{p}(c_2)$ which were evaluated in a prolate spheroidal coordinate system with distance $2c_2$ between the confocal points can now easily be transformed into corresponding multipoles defined with respect to another prolate spheroidal coordinate system, as long as the underlying cartesian axis systems are identical. The general transformation equation

$$Q_{lm}^{p}(c_1) = \sum_k c_1^{l-k} \mathcal{S}_m^{lk}(c_2/c_1) Q_{km}^{p}(c_2) \tag{43}$$

encloses the cases of transformation to or from spherical multipole moments, i.e., $c_1 = 0$ or $c_2 = 0$. Please note that when there is a c for which $Q_{km}^{p}(c) = 0$ for all $k > k_0$, this will not be the case for any other c'.

3.2. Translation

Let us now examine what will happen to the spheroidal multipole moments under a parallel transportation of the axis system. For spherical multipole moments the corresponding transformation law follows from the addition theorem for regular solid spherical harmonics:

$$R^s_{lm}(\boldsymbol{a}+\boldsymbol{b}) = \sum_{i_1,i_2}\sum_{m_1,m_2} \delta_{i_1+i_2,l}\delta_{m_1+m_2,m}\sqrt{\binom{l+m}{i_1+m_1}\binom{l-m}{i_1-m_1}}R^s_{i_1m_1}(\boldsymbol{a})R^s_{i_2m_2}(\boldsymbol{b}) \tag{44}$$

where a Clebsch–Gordon coefficient has already been evaluated [1,10]. For prolate spheroidal harmonics expanding $R^p_{lm}(\boldsymbol{a}+\boldsymbol{b};c)$ in spherical harmonics, using (44) and re-expanding $R^s_{i_2m_2}(\boldsymbol{b})$ in prolate spheroidal harmonics yields the 'mixed' addition theorem

$$R^p_{lm}(\boldsymbol{a}+\boldsymbol{b};c) = \sum_{i_1,j_2}\sum_{m_1,m_2} c^{l-i_1-j_2} u^{\,i_1\,j_2\,l}_{\,m_1\,m_2\,m} R^s_{i_1m_1}(\boldsymbol{a})R^p_{j_2m_2}(\boldsymbol{b};c) \tag{45}$$

where the coupling coefficient is found to be

$$u^{\,i_1\,j_2\,l}_{\,m_1\,m_2\,m} = \tilde{\Delta}^{\,i_1\,j_2\,l}_{\,m_1\,m_2\,m}\left(\delta_{i_10}\delta_{j_2l} + (1-\delta_{i_10})\sqrt{\frac{(l+m)!(l-m)!}{(i_1+m_1)!(i_1-m_1)!(j_2+m_2)!(j_2-m_2)!}}\right.$$
$$\left.\times\frac{(2j_2+1)!!(l+i_1-j_2-2)!!(l+i_1+j_2-1)!!}{(2l-1)!!(2i_1-2)!!(l-i_1-j_2)!!(l-i_1+j_2+1)!!}\right) \tag{46}$$

with

$$\tilde{\Delta}^{\,i_1\,j_2\,l}_{\,m_1\,m_2\,m} = \begin{cases} 1 & (l+i_1+j_2) \text{ even} \qquad m = m_1+m_2 \\ & l \geqslant i_1+j_2 \geqslant |m| \qquad i_1 \geqslant |m_1| \qquad j_2 \geqslant |m_2| \\ 0 & \text{else.} \end{cases} \tag{47}$$

The derivation of equation (46) for the mixed coupling coefficients makes use of

$$\sum_{i_2=j_2}^{(l-i_1)}{}' \frac{(-1)^{(l-i_1-i_2)/2}(l+i_1+i_2-1)!!}{(l-i_1-i_2)!!(i_2-j_2)!!(i_2+j_2+1)!!}$$
$$= (-1)^{(l-i_1-j_2)/2}\frac{(l+i_1-j_2-2)!!}{(l-i_1-j_2)!!}\sum_{k=0}^{(l-i_1-j_2)/2}(-1)^k$$
$$\times\binom{\frac{l-i_1-j_2}{2}}{k}\binom{\frac{l+i_1+j_2-1}{2}+k}{\frac{l+i_1-j_2}{2}-1} \tag{48}$$

where the prime at the summmation sign on the lhs indicates that i_2 varies in steps of two, and of equation (B2), the rhs of which has been rewritten in terms of double factorials. From equation (46) we see

$$u^{\,i_1\,j_2\,l}_{\,-m_1\,-m_2\,-m} = u^{\,i_1\,j_2\,l}_{\,m_1\,m_2\,m}. \tag{49}$$

Substituting also $R^s_{i_1m_1}(\boldsymbol{a})$ in the mixed addition theorem (45) by its expansion in prolate spheroidal harmonics one obtains the 'full' addition theorem

$$R^p_{lm}(\boldsymbol{a}+\boldsymbol{b};c) = \sum_{j_1,j_2}\sum_{m_1,m_2} c^{l-j_1-j_2} t^{\,j_1\,j_2\,l}_{\,m_1\,m_2\,m} R^p_{j_1m_1}(\boldsymbol{a};c)R^p_{j_2m_2}(\boldsymbol{b};c). \tag{50}$$

The corresponding full coupling coefficients can be obtained by transforming expression (46) for the mixed coupling coefficients with $[s:p]^{i_1j_1}_{m_1}$ which results in

$$t^{\,j_1\,j_2\,l}_{\,m_1\,m_2\,m} = \tilde{\Delta}^{\,j_1\,j_2\,l}_{\,m_1\,m_2\,m}\left(\delta_{j_10}\delta_{j_2l} + \sqrt{\frac{(l+m)!(l-m)!}{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!}}\right.$$
$$\times\frac{(2j_1+1)!!(2j_2+1)!!}{(2l-1)!!}$$
$$\left.\times\sum_{i_1=J_1}^{(l-j_2)}{}'\frac{(l+i_1-j_2-2)!!(l+i_1+j_2-1)!!}{(l-i_1-j_2)!!(l-i_1+j_2+1)!!(2i_1-2)!!(i_1-j_1)!!(i_1+j_1+1)!!}\right) \tag{51}$$

where the sum starts at $J_1 = 2$ for $j_1 = 0$ and at $J_1 = j_1$ else. An alternative expression in the form of a double sum can be found directly from equation (44) as

$$t\,{}^{j_1}_{m_1}\,{}^{j_2}_{m_2}\,{}^{l}_{m} = \tilde{\Delta}\,{}^{j_1}_{m_1}\,{}^{j_2}_{m_2}\,{}^{l}_{m}\,\frac{(2j_1+1)!!(2j_2+1)!!}{(2l-1)!!}\sqrt{\frac{(l+m)!(l-m)!}{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!}}$$
$$\times \sum_{i_1=j_1}^{i_1+i_2\leqslant l}{}' \sum_{i_2=j_2}{}' \frac{(-1)^{(l-i_1-i_2)/2}(l+i_1+i_2-1)!!}{(l-i_1-i_2)!!(i_1-j_1)!!(i_1+j_1+1)!!(i_2-j_2)!!(i_2+j_2+1)!!} \tag{52}$$

where i_1 and i_2 vary in steps of 2 and their sum has to be smaller or equal to l. Equation (52) clearly displays the symmetry relations

$$t\,{}^{j_2}_{m_2}\,{}^{j_1}_{m_1}\,{}^{l}_{m} = t\,{}^{j_1}_{m_1}\,{}^{j_2}_{m_2}\,{}^{l}_{m} = t\,{}^{j_1}_{-m_1}\,{}^{j_2}_{-m_2}\,{}^{l}_{-m}. \tag{53}$$

With the help of the addition theorems one can now express the translation of a regular solid prolate spherical harmonic to a new origin $\boldsymbol{a}$ as

$$R^p_{lm}(\boldsymbol{r}-\boldsymbol{a};c) = \sum_{k,m'} c^{l-k} R^p_{km'}(\boldsymbol{r};c)\mathcal{T}\,{}^{k}_{m'}\,{}^{l}_{m}(\boldsymbol{a}/c). \tag{54}$$

When the scaled shift vector $\boldsymbol{a}/c$ is expressed in terms of spherical coordinates the translation coefficients introduced in this equation can be calculated using the mixed addition theorem as

$$\mathcal{T}\,{}^{k}_{m'}\,{}^{l}_{m}(\boldsymbol{a}/c) = (-1)^{l-k}\sum_i u\,{}^{i}_{m-m'}\,{}^{k}_{m'}\,{}^{l}_{m} R^s_{i(m-m')}(\boldsymbol{a}/c) \tag{55}$$

where $c^{-i}R^s_{im}(-\boldsymbol{a}) = (-1)^i R^s_{im}(\boldsymbol{a}/c)$ has been used along with the fact that the only non-zero contributions to the sum over i all have parity $(-1)^i = (-1)^{l-k}$. Expressing $\boldsymbol{a}/c$ in terms of prolate spheroidal coordinates from equation (50) and $c^{-l}R^p_{lm}(-\boldsymbol{a};c) = (-1)^l R^p_{lm}(\boldsymbol{a}/c;1)$, one obtains

$$\mathcal{T}\,{}^{k}_{m'}\,{}^{l}_{m}(\boldsymbol{a}/c) = (-1)^{l-k}\sum_i t\,{}^{i}_{m-m'}\,{}^{k}_{m'}\,{}^{l}_{m} R^p_{i(m-m')}(\boldsymbol{a}/c;1). \tag{56}$$

Applying equation (54) twice yields

$$\mathcal{T}\,{}^{k}_{m'}\,{}^{l}_{m}((\boldsymbol{a}+\boldsymbol{b})/c) = \sum_{i,m''}\mathcal{T}\,{}^{k}_{m'}\,{}^{i}_{m''}(\boldsymbol{a}/c)\mathcal{T}\,{}^{i}_{m''}\,{}^{l}_{m}(\boldsymbol{b}/c). \tag{57}$$

Since $\mathcal{T}\,{}^{i}_{m''}\,{}^{l}_{m}(-\boldsymbol{a}/c) = (-1)^{l-i}\mathcal{T}\,{}^{i}_{m''}\,{}^{l}_{m}(\boldsymbol{a}/c)$, this specializes to the sum rule

$$\sum_{i,m''}(-1)^{l-i}\mathcal{T}\,{}^{k}_{m'}\,{}^{i}_{m''}(\boldsymbol{a}/c)\mathcal{T}\,{}^{i}_{m''}\,{}^{l}_{m}(\boldsymbol{a}/c) = \delta_{lk}\delta_{mm'}. \tag{58}$$

Note also that (49) or (53) lead to $(\mathcal{T}\,{}^{k}_{m'}\,{}^{l}_{m}(\boldsymbol{a}/c))^* = (-1)^{m-m'}\mathcal{T}\,{}^{k}_{-m'}\,{}^{l}_{-m}(\boldsymbol{a}/c)$.

By equation (54) a set of shifted multipoles $Q^p_{lm}(\boldsymbol{a};c)$, referred to the origin $\boldsymbol{a}$, is obtained from the original multipoles $Q^p_{lm}(\boldsymbol{0};c)$ as

$$Q^p_{lm}(\boldsymbol{a};c) = \sum_{k,m'} c^{l-k} Q^p_{km'}(\boldsymbol{0};c)\mathcal{T}\,{}^{k}_{m'}\,{}^{l}_{m}(\boldsymbol{a}/c). \tag{59}$$

As it is the case for spherical multipole moments as well, the translated prolate spheroidal multipole moments depend on unshifted moments of lower degree only. Thus, using $t\,{}^{0}_{0}\,{}^{l}_{m}\,{}^{l}_{m} = u\,{}^{0}_{0}\,{}^{l}_{m}\,{}^{l}_{m} = 1$ in equations (56), (59) the first non-vanishing multipole moment is seen to be independent on the origin, while the values of all multipole moments of higher degree depend on the origin. A single shifted multipole of degree l will be described through an infinite series of multipoles of degree $\geqslant l$ in the original coordinate system.

3.3. Rotation

Spherical harmonics of degree l transform under rotations as

$$R^s_{lm}(\boldsymbol{r}') = \sum_{m'=-l}^{l} R^s_{lm'}(\boldsymbol{r})\mathcal{D}^l_{m'm}(\alpha,\beta,\gamma) \tag{60}$$

where (α,β,γ) are Euler angles leading from the original to the rotated axis system.

$$\mathcal{D}^l_{m'm}(\alpha,\beta,\gamma) = \mathrm{e}^{-\mathrm{i}(\alpha m'+\gamma m)} d^l_{m'm}(\beta) \tag{61}$$

is a Wigner rotation matrix [10]. Using the explicit form for the reduced rotation matrix $d^l_{m'm}(\beta)$ along with (20) and (21) one can generalize this to describe rotation of regular solid prolate spheroidal harmonics

$$R^p_{lm}(\boldsymbol{r}';c) = \sum_k \sum_{m'} c^{l-k} R^p_{lm'}(\boldsymbol{r};c)\mathcal{D}^{kl}_{m'm}(\alpha,\beta,\gamma). \tag{62}$$

The rotation coefficients in this formula are given as

$$\mathcal{D}^{\,k\ l}_{\,m'\ m}(\alpha,\beta,\gamma) = \mathrm{e}^{-\mathrm{i}(\alpha m'+\gamma m)} d^{\,k\ l}_{\,m'\ m}(\beta) \tag{63}$$

and the explicit form of the reduced rotation coefficients reads

$$\begin{aligned} d^{\,k\ l}_{\,m'\ m}(\beta) = \Delta^{lk}_m \Delta^{kk}_{m'} \sqrt{\frac{(l+m)!(l-m)!}{(k+m')!(k-m')!}} \frac{(2k+1)!!}{(2l-1)!!} {\sum_{i=I_1}^{l}}' \frac{(-1)^{(l-i)/2}(l+i-1)!!}{(l-i)!!(i-k)!!(i+k+1)!!} \\ \times \sum_{t=T_1}^{T_2} (-1)^t \binom{i+m'}{t}\binom{i-m'}{t+m-m'} (\cos\beta/2)^{2i+m'-m-2t}(\sin\beta/2)^{2t+m-m'} \end{aligned} \tag{64}$$

where $I_1 = \max(k,|m|)$ for $(l-m)$ even and $I_1 = \max(k,|m|+1)$ else, while the sum over t runs from $T_1 = \max(0, m'-m)$ to $T_2 = \min(i+m', i-m)$. From the symmetry relations for the reduced rotation matrices $d^i_{m'm}(\beta)$ and equations (20) and (21) it is seen that the reduced rotation coefficients fulfil

$$\begin{aligned} d^{\,k\ l}_{\,m'\ m}(\beta) &= (-1)^{m'-m} d^{\,k\ \ \ l}_{\,-m'\ -m}(\beta) = (-1)^{m'-m} d^{\,k\ l}_{\,m'\ m}(-\beta) \\ &= (-1)^{l-m'} d^{\,k\ \ l}_{\,m'\ -m}(\pi-\beta) = (-1)^{l+m} d^{\,k\ \ l}_{\,m'\ -m}(\pi+\beta). \end{aligned} \tag{65}$$

Twofold application of (62) shows

$$\mathcal{D}^{\,k\ l}_{\,m'\ m}(\alpha,\beta,\gamma) = \sum_{i,m''} \mathcal{D}^{\,k\ i}_{\,m'\ m''}(\alpha_2,\beta_2,\gamma_2)\mathcal{D}^{\,i\ l}_{\,m''\ m}(\alpha_1,\beta_1,\gamma_1) \tag{66}$$

where (α,β,γ) is the result of first rotating by $(\alpha_1,\beta_1,\gamma_1)$ and then by $(\alpha_2,\beta_2,\gamma_2)$. This can be specialized to

$$d^{\,k\ l}_{\,m'\ m}(\beta_1+\beta_2) = \sum_{i,m''} d^{\,k\ i}_{\,m'\ m''}(\beta_2) d^{\,i\ l}_{\,m''\ m}(\beta_1). \tag{67}$$

Furthermore, with $\mathcal{D}^{\,k\ l}_{\,m'\ m}(-\gamma,-\beta,-\alpha) = (-1)^{m'-m}(\mathcal{D}^{\,k\ l}_{\,m'\ m}(\alpha,\beta,\gamma))^*$ and $d^{\,k\ l}_{\,m'\ m}(0) = \delta_{lk}\delta_{m'm}$ we see

$$\sum_{i,m''} (-1)^{m'-m''} (\mathcal{D}^{\,k\ i}_{\,m'\ m''}(\gamma,\beta,\alpha))^* \mathcal{D}^{\,i\ l}_{\,m''\ m}(\alpha,\beta,\gamma) = \delta_{lk}\delta_{mm'}. \tag{68}$$

While the spherical harmonics of degree l form the basis of an irreducible representation of the three-dimensional rotation group $O^+(3)$, this is not the case for the spheroidal harmonics, which form a basis of the two-dimensional rotation group $O^+(2) \equiv C_\infty$ only, where the axis of rotation is that joining the two confocal points. According to the formula describing rotation of a prolate spheroidal multipole of degree l

$$\tilde{Q}^p_{lm}(c) = \sum_k \sum_{m'} c^{l-k} Q^p_{lm'}(c) \mathcal{D}^{kl}{}_{m'}{}^{k}{}_{m}^{l}(\alpha, \beta, \gamma) \tag{69}$$

a rotation about any other axis will 'mix in' multipoles of degree $(l-2)$, $(l-4)$, and so on. Inversly, a single rotated multipole in general will be described by an infinite series of multipoles with degree $\geqslant l$ in the original coordinate system.

4. Modifications for solid oblate spheroidal harmonics

If oblate spheroidal coordinates (v, w, φ) and (V, W, ϕ) are used to describe the points $\boldsymbol{r}$ and $\boldsymbol{R}$ (cf appendix A (i)) the the Neumann expansion reads

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{R}|} = \mathrm{i} \sum_{l=0}^{\infty} \frac{2l+1}{c} \mathcal{P}_l(\mathrm{i}v) \mathcal{Q}_l(\mathrm{i}V) P_l(w) P_l(W) + 2\mathrm{i} \sum_{l=1}^{\infty} \sum_{m=1}^{l} \frac{2l+1}{c} (-1)^m \left(\frac{(l-m)!}{(l+m)!} \right)^2$$
$$\times \mathcal{P}^m_l(\mathrm{i}v) \mathcal{Q}^m_l(\mathrm{i}V) P^m_l(w) P^m_l(W) \cos m(\varphi - \phi). \tag{70}$$

It converges absolutely for $V > v$ (cf [3], volume III, p 102 ff). In analogy to definitions (7), (8) it will be found that the most useful definitions of regular and irregular solid oblate spheroidal harmonics reads:

$$R^o_{lm}(\boldsymbol{r}; c) = (-\mathrm{i}c)^l \frac{(l-m)!}{(2l-1)!!} \sqrt{\frac{(l-m)!}{(l+m)!}} \mathcal{P}^m_l(\mathrm{i}v) P^m_l(w) \mathrm{e}^{\mathrm{i}m\varphi} \tag{71}$$

$$I^o_{lm}(\boldsymbol{R}; c) = (-\mathrm{i}c)^{-l-1} (-1)^m \frac{(2l+1)!!}{(l+m)!} \sqrt{\frac{(l-m)!}{(l+m)!}} \mathcal{Q}^m_l(\mathrm{i}V) P^m_l(W) \mathrm{e}^{\mathrm{i}m\phi} \tag{72}$$

which allows one to rewrite (70) in a similar form as in equations (4) or (9). With the help of the explicit expressions of $\mathcal{P}^m_l(\mathrm{i}v)$ and $\mathcal{Q}^m_l(\mathrm{i}V)$ (cf [11]) it is easily verified that these definitions guarantee real valued representations of multipole moments and potentials—except for the phase factors $\mathrm{e}^{\mathrm{i}m\varphi}$ and $\mathrm{e}^{\mathrm{i}m\phi}$. Furthermore, they have the same symmetry properties as the prolate solid spherical harmonics, they also become spherical harmonics for $c \to 0$ (cf equations (10), (11)), and they obey $c^{-l} R^o_{lm}(\boldsymbol{r}; c) = R^o_{lm}(\boldsymbol{r}/c; 1)$ and $c^{l+1} I^o_{lm}(\boldsymbol{r}; c) = I^o_{lm}(\boldsymbol{r}/c; 1)$.

It is not difficult to modify the proofs given in appendix B to show

$$\left(\frac{\mathrm{i}r}{c}\right)^l P^m_l(s) = \sum_{i=|m|}^{l} a^{li}_m \mathcal{P}^m_i(\mathrm{i}v) P^m_i(w) \tag{73}$$

$$\mathcal{P}^m_l(\mathrm{i}v) P^m_l(w) = \sum_{i=|m|}^{l} \tilde{a}^{li}_m \left(\frac{\mathrm{i}r}{c}\right)^i P^m_i(s). \tag{74}$$

From that one finds

$$R^s_{lm}(\boldsymbol{r}) = \sum_{i=|m|}^{l} (-\mathrm{i}c)^{l-i} [s:p]^{li}_m R^o_{im}(\boldsymbol{r}; c) = \sum_{i=|m|}^{l} c^{l-i} [s:o]^{li}_m R^o_{im}(\boldsymbol{r}; c) \tag{75}$$

$$R^o_{lm}(\boldsymbol{r}; c) = \sum_{i=|m|}^{l} (-\mathrm{i}c)^{l-i} [p:s]^{li}_m R^s_{im}(\boldsymbol{r}) = \sum_{i=|m|}^{l} c^{l-i} [o:s]^{li}_m R^s_{im}(\boldsymbol{r}) \tag{76}$$

which demonstrates that the transformation coefficients are real valued:

$$[s:o]^{li}_m = (-1)^{(l-i)/2} [s:p]^{li}_m \tag{77}$$

$$[o:s]^{li}_m = (-1)^{(l-i)/2} [p:s]^{li}_m. \tag{78}$$

Naturally, they obey sum rules strictly analogous to (24).

Let us assume that $r < R$ and $v < V$ for the points $\boldsymbol{r}$ and $\boldsymbol{R}$. Following similar considerations as in section 2.4 we obtain from equation (70) and equations (73), (74)

$$\left(\frac{c}{\mathrm{i}R}\right)^{l+1} P_l^m(S) = \sum_{i=l}^{\infty} \mathcal{Q}_i^m(\mathrm{i}V) P_i^m(W) b_m^{il} \tag{79}$$

$$\mathcal{Q}_l^m(\mathrm{i}V) P_l^m(W) = \sum_{i=l}^{\infty} \left(\frac{c}{\mathrm{i}R}\right)^{i+1} P_i^m(S) \tilde{b}_m^{il}. \tag{80}$$

From (29) and

$$|\mathcal{Q}_i^m(\mathrm{i}V)| < \frac{2^{i+1}(i+m)!}{(2i+1)!!} \left(\frac{1}{V+\sqrt{V^2+1}}\right)^{i+1} \left(\frac{V+\sqrt{V^2+1}}{2V}\right)^{\frac{1}{2}} \qquad V > 0 \tag{81}$$

which is a slightly tightened version of the inequality (87-5) of [3], volume II, p 272, one sees that the series of the absolute values of the terms in (79) is majorized by

$$\sum_{i=l}^{\infty} \frac{2^{i+1}(i+l-1)!!\sqrt{(i-m)!(i+m)!}}{\sqrt{2-\delta_{m0}}(l-m)!(i-l)!!(2i-1)!!} \Delta_m^{il} \left(\frac{1}{V+\sqrt{V^2+1}}\right)^{i+1} \left(\frac{V+\sqrt{V^2+1}}{2V}\right)^{\frac{1}{2}}$$

showing that (79) is absolutely convergent for $V > 0$. For $V = 0$, on the other hand, the series (79) in general will not converge absolutely. This is easily verified for the special case $l = m = 0$, $W = 0$, by utilizing $|\mathcal{Q}_i^0(\mathrm{i}0)| = (\pi/2)(i-1)!!/i!!$ for i even together with $P_i^0(0)b_0^{i0} = (2i-1)((i-1)!!/i!!)^2$, and observing that their product is larger than $(\pi/2)/(i+1)$. Remember that the choice of parameters $(V, W) = (0, W)$ describes the points of the disc surrounded by the circle of the confocal points (for which $W = 0$), while $V > 0$ for the points outside this disc of radius c. Naturally, expansion (80), the reverse to (79), is absolutely convergent under the same conditions as already discussed for (32), i.e., for $R > c$, and in general not for $R \leqslant c$. This clarifies the range of validity of the transformation formulae between the irregular solid harmonics:

$$I_{lm}^s(\boldsymbol{R}) = \sum_{i=l}^{\infty} (-\mathrm{i}c)^{i-l} I_{im}^o(\boldsymbol{R}; c)[p:s]_m^{il} = \sum_{i=l}^{\infty} c^{i-l} I_{im}^o(\boldsymbol{R}; c)[o:s]_m^{il} \tag{82}$$

$$I_{lm}^o(\boldsymbol{R}; c) = \sum_{i=l}^{\infty} (-\mathrm{i}c)^{i-l} I_{im}^s(\boldsymbol{R})[s:p]_m^{il} = \sum_{i=l}^{\infty} c^{i-l} I_{im}^s(\boldsymbol{R})[s:o]_m^{il}. \tag{83}$$

Figure 3 visualizes the convergence/divergence behaviour of these expansions for the special case $l = m = 0$. Expansion (82) is seen to converge reasonably fast to $I_{00}^s(\boldsymbol{R}) = 1/R$, except for points close to the disc surrounded by the confocal ring, while expansion (83) of the electric potential of an oblate multipole into spherical multipole potentials is obviously of no use inside a sphere with radius c.

Finally, comparing equation (76) with (21) makes clear that the regular solid oblate spheroidal harmonics formally result from their prolate counterparts when replacing c with $-\mathrm{i}c$. Therefore, their transformation properties and those of the oblate spheroidal multipoles under scaling, translation and rotation can easily be derived from the results of section 3 by replacing c with $-\mathrm{i}c$ as well. Note that this does not introduce any imaginary terms into the resulting formulae but only sign changes in the appropriate places. From the real valuedness of the coefficients $\mathcal{S}_m^{lk}(x)$ for purely imaginary arguments this is seen to also hold true for the most general case of the scaling transformation from prolate to oblate spheroidal multipole moments and vice versa.

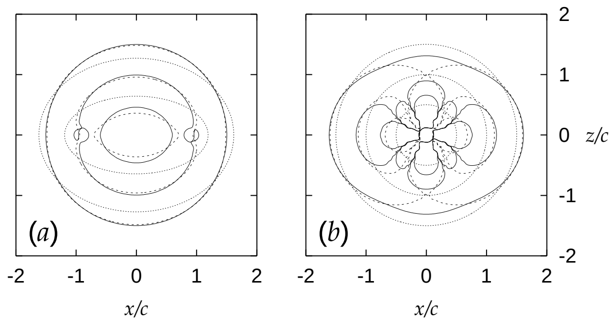

Figure 3. Contour lines of $\sum_{i=0}^{i_{\max}} c^{i-l} I^{o}_{im}(\boldsymbol{R}; c)[o:s]^{il}_{m}$ (*a*), and $\sum_{i=0}^{i_{\max}} c^{i-l} I^{s}_{im}(\boldsymbol{R})[s:o]^{il}_{m}$ (*b*), for $l = m = 0$ (cf figure 2).

5. Discussion and conclusions

In sections 3 and 4 it has been shown that the regular solid spheroidal harmonics and, in consequence, spheroidal multipole moments can be handled with nearly the same ease as their conventional spherical counterparts. A translated spheroidal multipole will depend on the untranslated multipoles of the same and lower degrees, exactly as it is the case for the spherical multipoles, even if the calculation of the translation coefficients is a little more involved. The main complication is that a rotated spheroidal multipole in general will not only depend on unrotated multipoles of the same degree, but also on those of lower degrees—except for rotation around the symmetry axis of the spheroid, of course. If the charge distribution under consideration does possess a rotation axis, only rotations around and translations along this axis will be of interest. Yet, in those cases where the charge distribution has only an approximate spheroidal shape the general formulae will help to transform the mutipole moments obtained in one coordinate system to another, readjusted coordinate system. A similar remark applies to the scaling of spheroidal multipoles.

The addition theorem for regular spherical harmonics is often used to derive a formula for the multipole–multipole interactions between two 'spherical' charge distributions [1], i.e., two separate non-overlapping charge distributions enclosed in spheres which do not touch. That can easily be achieved by inserting (44) for $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ into (4), where $\boldsymbol{R}$ is interpreted as the distance vector between the centres of the two spheres, $\boldsymbol{r}_1$ as the distance vector between a charge located in the first sphere and its centre, and $\boldsymbol{r}_2$ as the distance vector between a charge located in the second sphere and its centre. In principle, utilizing the mixed addition theorem (45) this can also be performed for the interaction between a spheroidal and a spherical charge distribution, and similarly from the full addition theorem (50) for the interaction between two non-overlapping spheroidal charge distributions. However, in both cases there is an important difference to the purely spherical case: the degrees of the spherical harmonics entering the product terms in (44) are restricted to $i_1 + i_2 = l$, while in (45) products with $i_1 + j_2 \leqslant l$ do occur, and similarly products with $j_1 + j_2 \leqslant l$ in (50). As a consequence, an interaction potential $I^{p*}_{lm}(\boldsymbol{R}; c)$ will also couple multipoles with $i_1 + j_2 < l$ (or $j_1 + j_2 < l$). So, even if all multipoles higher than a certain degree $i_{\max}$ or $j_{\max}$ should vanish the series expansion in general will not terminate after $l_{\max} = i_{\max} + j_{\max}$, in contrast to what is found for the conventional spherical multipole expansion. The only exception is the interaction between spheroidal multipoles and purely monopolar spherical charge distributions, of course.

Nevertheless, the series expansion of the interaction between prolate (or oblate) spheroidal and spherical mutlipoles will be preferred over the conventional multipole expansion when one

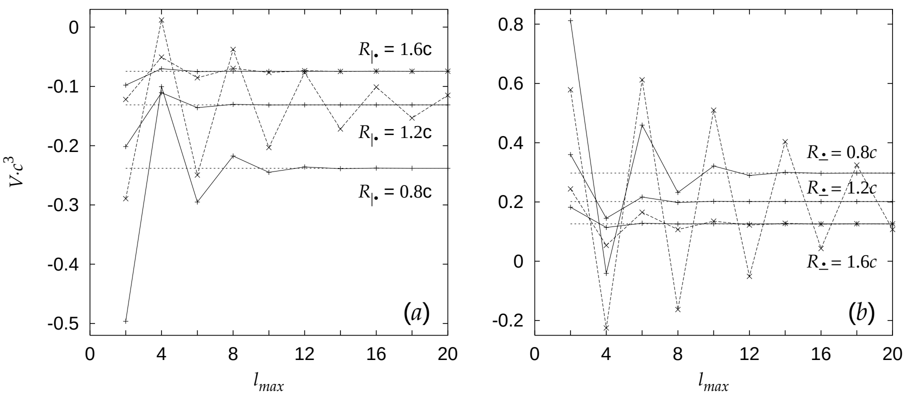

Figure 4. The energy V of interaction between a point-quadrupole and monopolar line- (*a*), and disc-charges (*b*), respectively, as a function of the expansion length $l_{\max}$ for various distances R between them. Energies from the spheroidal expansions are connected by solid lines, those from the spherical expansion by dashed lines, and exact values are represented by dotted lines.

of the charge distributions has a shape more closely resembling a rod (or a disc, respectively) than a sphere. This is demonstrated by figure 4 which contains a comparison between spherical and spheroidal multipole expansions for the energy of interaction between a spherical quadrupole and prolate and oblate spheroidal monopoles, respectively. The potential of a prolate spheroidal monopole is $I_{00}^{p}(\boldsymbol{R}; c) = (1/c)$ arcoth T, which is also the potential of a uniformly charged line of length $2c$ (cf [12], p 154 f), showing that this charge distribution plays the role of the spatially smallest possible multipole in the theory of prolate spheroidal multipoles, i.e. a 'line monopole', in analogy to the role of the point charge as smallest monopole in the theory of spherical multipoles. The interaction energies shown in the figure were calculated for three distances $R_{|\bullet}$ of a Q_{20}^{s} unit quadrupole from the centre of the line charge, with the quadrupole in a symmetrical position to both ends of the line. At the largest distance considered of $R_{|\bullet} = 1.6c$ the prolate spheroidal multipole expansion is close to converged at $l_{\max} = 6$, while in the spherical case one needs to go up to $l_{\max} = 12$ to achieve a similar accuracy. The advantages of the prolate spheroidal multipole expansion become even more evident for $R_{|\bullet} = 1.2c$, i.e., somewhat outside the smallest sphere containing the line charge, and in particular for $R_{|\bullet} = 0.8c$, where the spherical multipole expansion diverges so badly that not a single interaction energy from it is found within the plot ranges. Similar remarks apply to the oblate spheroidal case shown in the second half of figure 4. The potential of an oblate spheroidal monopole is $I_{00}^{o}(\boldsymbol{R}; c) = (1/c)$ arcot V. This is also the potential of an infinitely thin disc of radius c with a surface charge which is radially distributed according to $1/\sqrt{1 - (\rho/c)^2}$ (cf [12], p 254 f). The interaction energies shown in the figure were calculated for three distances $R_{\underline{\bullet}}$ of a Q_{20}^{s} unit quadrupole from the centre of this disc monopole, with the quadrupole located on the rotation axis.

While the above considerations demonstrate that the infinite series expansion of the energy of interaction between a spheroidal and a point multipole is much more successful than its purely spherical counterpart, there is a way to calculate that energy without a series expansion. This way, suggested by Stiles [4, 5], makes use of the fact that point dipoles interact with the electric field at their location only, point quadrupoles with the field gradient only, and so on. Thus, knowledge of the derivatives of the spheroidal multipole potentials is all what is needed to calculate spheroidal–spherical multipole interactions without having to resort to a series expansion—and this was how the exact interaction energies displayed in figure 4 have been

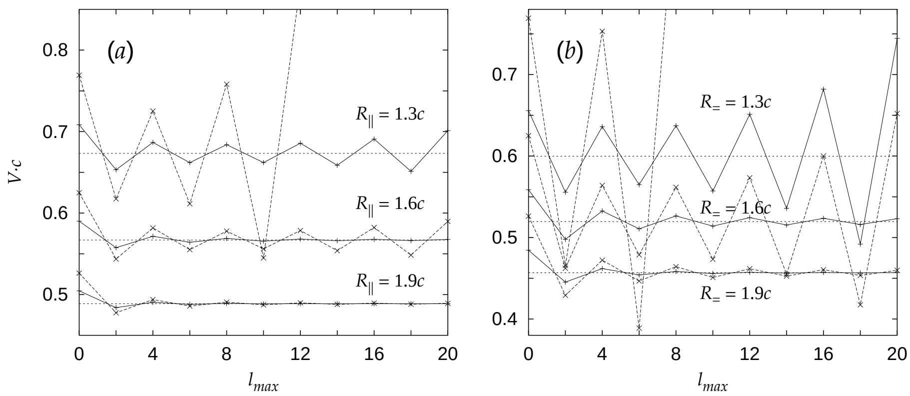

Figure 5. The energy V of interaction between two parallel monopolar line- (*a*), and disc-charges (*b*), respectively, as a function of the expansion length $l_{\max}$ for various distances R between them (cf figure 4).

computed. Nevertheless, the series expansions may turn out to have a certain practical value: while the derivatives of spherical multipole potentials are simply other spherical multipole potentials of a higher degree, this is not the case for the spheroidal multipole potentials. The analytic differentiation of the spheroidal multipole potentials may become so tedious for higher derivatives that it is more convenient to use the first few members of their expansions in terms of irregular solid spheroidal harmonics—which leads us back to the series expansion considered above.

The spheroidal and spherical multipole expansions of the energy of interaction between two non-overlapping parallel spheroidal charge distributions are compared in figure 5. In the prolate case, both line monopoles are contained in the same plane and at a rectangular angle to the line joining their centres, while similarly the two disc monopoles are centred around a common rotation axis in the oblate case. In the figure we considered only distances $R_\parallel$ or $R_=$ between the line or disc monopoles, respectively, which are smaller than the sum $2c$ of the radii of the smallest spheres containing them, so that the spherical multipole expansion does not necessarily converge any more. Yet, it performs quite well at a distance of $1.9c$, at least when cut at relatively low values of $l_{\max}$. For smaller values of $R_\parallel$ or $R_=$ its divergence becomes obvious already for $l_{\max} \leqslant 20$. The spheroidal multipole expansions, on the other hand, seem to be useful down to a distance of about $1.6c$, though in absence of any formal proof of convergence one cannot be sure wether for even larger values of $l_{\max}$ they will start to show a similar divergence pattern as the spherical multipole expansion. The 'exact' interaction energies displayed in the figure were obtained from (one-dimensional) numerical integrations of the product of one charge distribution with the electric potential of the other. This is easily done for the case of the two uniform line charges, while it requires some care in the second case due to the singularity of the surface charge distribution at the edge of the disc.

While in the examples discussed above it was assumed that both charge distributions had the same orientation and the same length or radius, respectively, the general case of the interaction between arbitrary spheroidal charge distributions can be considered with the help of the scaling and rotation transformations. To that end one can first scale the mutipole moments of the second charge distribution to meet the ellipticity of the first, followed by a rotation of the resulting multipole moments so as to align the coordinate systems and finally employing the translation formula as indicated above. Clearly, the result will not depend on the order of these operations, yet the larger of the two parameters c_1 and c_2 coming into play should be chosen for the calculation of the interaction potentials $I_{lm}^{p/o}(\boldsymbol{R};c)$ in order to achieve the best convergence properties. Let us finally remark that in practice the best way to treat the interaction between two arbitrary spheroidal charge distributions is perhaps another one: it is possible to cut one of the charge distributions formally into pieces, to calculate the spherical multipole moments of each of these domains, and finally the potential, field, field gradient etc, of the other charge distribution at the locations of these 'distributed multipole moments'. For molecules there is a number of different schemes which generate, for example, multipole moments and polarizabilities of individual atoms within the molecule in order calculate interaction energies from them [1,13,14]. This procedure overcomes the limits of the spherical multipole expansion, yet, it requires calculation of the interactions between all atoms of one and all atoms of the other molecule. Using spheroidal multipole expansions one can either completely avoid to partition one of the molecules into domains or one can use much larger domains, thus drastically scaling down the computational effort. Work along these lines is in progress.

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Appendix A. Notation

(i) Let (x,y,z) be the cartesian coordinates of a point in $\mathbb{R}^3$. Its *spherical coordinates* (r,s,φ) as used here are related to the cartesian coordinates by the formulae:

$$x = r\sqrt{1-s^2}\cos\varphi \qquad y = r\sqrt{1-s^2}\sin\varphi \qquad z = rs \tag{A1}$$

where $0 \leqslant r < \infty$, $-1 \leqslant s \leqslant 1$, and $0 \leqslant \varphi < 2\pi$. The reverse transformation is given by

$$r = \sqrt{x^2+y^2+z^2} \qquad s = \frac{z}{r} \qquad \varphi = \arctan\frac{y}{x}. \tag{A2}$$

Note that the usual definition of the spherical coordinates replaces s by $\theta = \arccos s$.

The *prolate spheroidal coordinates* (t,u,φ) are related to cartesian coordinates by

$$x = c\sqrt{(t^2-1)(1-u^2)}\cos\varphi \qquad y = c\sqrt{(t^2-1)(1-u^2)}\sin\varphi \qquad z = ctu \tag{A3}$$

where $1 \leqslant t < \infty$, $-1 \leqslant u \leqslant 1$, $0 \leqslant \varphi < 2\pi$, and $c > 0$ is half of the distance of the two focal points located at the z-axis. The reverse transformation is given by

$$\begin{aligned} t &= \frac{1}{2c}\left(\sqrt{x^2+y^2+(z+c)^2} + \sqrt{x^2+y^2+(z-c)^2}\right) \\ u &= \frac{1}{2c}\left(\sqrt{x^2+y^2+(z+c)^2} - \sqrt{x^2+y^2+(z-c)^2}\right) \\ \varphi &= \arctan\frac{y}{x}. \end{aligned} \tag{A4}$$

Thus, the distance of a point from the focal point $z = -c$ is given by $r_1 = c(t+u)$ while its distance from the other focal point $z = +c$ is $r_2 = c(t-u)$. Another definition of the prolate spheroidal coordinates replaces t by $\alpha = \operatorname{arccosh} t$ and u by $\beta = \arccos u$.

The *oblate spheroidal coordinates* (v,w,φ) are related to cartesian coordinates by

$$x = c\sqrt{(v^2+1)(1-w^2)}\cos\varphi \qquad y = c\sqrt{(v^2+1)(1-w^2)}\sin\varphi \qquad z = cvw \tag{A5}$$

where $0 \leqslant v < \infty$, $-1 \leqslant w \leqslant 1$, $0 \leqslant \varphi < 2\pi$, and $c > 0$ is the radius of the focal circle around the z-axis. The reverse transformation is given by

$$v = \frac{1}{\sqrt{2}c}\left(x^2 + y^2 + z^2 - c^2 + \sqrt{(x^2 + y^2 + z^2 - c^2)^2 + 4c^2z^2}\right)^{\frac{1}{2}}$$
$$w = \frac{z}{cv} \qquad \varphi = \arctan\frac{y}{x}. \tag{A6}$$

Another definition of the prolate spheroidal coordinates replaces v by $\alpha = \operatorname{arcsinh} v$ and w by $\beta = \arccos w$. Note that $\lim_{c\to 0} ct = r = \lim_{c\to 0} cv$ and $\lim_{c\to 0} u = s = \lim_{c\to 0} w$.

(ii) Let $l \in \mathbb{N}_0$, $[-1, 1] := \{x \in \mathbb{R}; -1 \leqslant x \leqslant 1\}$, $x \in [-1, 1]$, $z \in \mathbb{C}\backslash[-1, 1]$, and $\mu \in \mathbb{C}$. The *Legendre functions of the first kind* may then be defined employing Rodrigues' formula as ([2], p 18):

$$P_l(\mu) = \frac{1}{(2l)!!}\frac{\mathrm{d}^l}{\mathrm{d}\mu^l}\left(\mu^2 - 1\right)^l \tag{A7}$$

while the *Legendre functions of the second kind* may be defined as ([2], p 63):

$$\mathcal{Q}_l(z) = \frac{1}{2}\int_{-1}^{+1}\mathrm{d}x\,\frac{P_l(x)}{z - x}. \tag{A8}$$

Now let $m \in \{\mathbb{N}_0; 0 \leqslant m \leqslant l\}$. The *associated Legendre functions of the first kind* are then defined by ([2], p 89 ff):

$$P_l^m(x) = (-1)^m(1 - x^2)^{m/2}\frac{\mathrm{d}^m P_l(x)}{\mathrm{d}x^m} \tag{A9}$$

$$\mathcal{P}_l^m(z) = (z^2 - 1)^{m/2}\frac{\mathrm{d}^m P_l(z)}{\mathrm{d}z^m} \tag{A10}$$

while the *associated Legendre functions of the second kind* are given as ([2], p 89 ff):

$$\mathcal{Q}_l^m(z) = (z^2 - 1)^{m/2}\frac{\mathrm{d}^m \mathcal{Q}_l(z)}{\mathrm{d}z^m} \tag{A11}$$

where it is to be understood that $P_l^0 = \mathcal{P}_l^0 = P_l$ and $\mathcal{Q}_l^0 = \mathcal{Q}_l$. Finally, the definition of associated Legendre functions may be extended to all $m \in \{\mathbb{Z}; -l \leqslant m \leqslant l\}$ using ([2], pp 99 and 109):

$$P_l^{-m}(x) = (-1)^m\frac{(l - m)!}{(l + m)!}P_l^m(x) \tag{A12}$$

$$\mathcal{P}_l^{-m}(z) = \frac{(l - m)!}{(l + m)!}\mathcal{P}_l^m(z) \tag{A13}$$

$$\mathcal{Q}_l^{-m}(z) = \frac{(l - m)!}{(l + m)!}\mathcal{Q}_l^m(z). \tag{A14}$$

Note that some workers supress the phase factor $(-1)^m$ in equation (A9). Explicit expressions for the associated Legendre functions of first and second kind may be found in [11], p 115 ff.

(iii) Let $n \in \mathbb{N}_0 \cup \{-1\}$. The *double factorial* is defined as:

$$n!! = n(n - 2)(n - 4)\cdots(2 \text{ or } 1) \tag{A15}$$

with the special values $(-1)!! = 0!! = 1$.

Appendix B. Proof of some relations

B.1. Proof of relations (13) and (14)

To show (13) and (14) for $m \geqslant 0$ first note that

$$r^m P_m^m(s) = r^m(2m-1)!!(1-s^2)^{m/2}$$
$$= c^m(2m-1)!!(t^2-1)^{m/2}(1-u^2)^{m/2} = O_m^m(t,u)$$

and

$$r^{m+1} P_{m+1}^m(s) = r^{m+1}(2m+1)!!s(1-s^2)^{m/2}$$
$$= c^{m+1}(2m+1)!!t(t^2-1)^{m/2}u(1-u^2)^{m/2} = O_{m+1}^m(t,u)$$

where $O_l^m(t,u)$ denotes $r^l P_l^m(s)$ expressed in prolate spheroidal coordinates. This leads to $a_{mm}^m = 1/(2m-1)!!$ and $a_{(m+1)(m+1)}^m = 1/(2m+1)!!$, in accordance with (14). The proof for $l \geqslant m+2$ then proceeds by complete induction, using the well known recursion relation

$$P_l^m(s) = \frac{2l-1}{l-m} s P_{l-1}^m(s) - \frac{l+m-1}{l-m} P_{l-2}^m(s) \tag{B1}$$

which, after multiplication with r^l and introducing prolate spheroidal coordinates yields

$$O_l^m(t,u) = \frac{2l-1}{l-m} ctu O_{l-1}^m(t,u) + \frac{l+m-1}{l-m} c^2(1-t^2-u^2) O_{l-2}^m(t,u).$$

Using (B1) for $P_l^m(u)$ and an analogous recursion relation for $\mathcal{P}_l^m(t)$ one finds that

$$tu\mathcal{P}_i^m(t)P_i^m(u) = \left(\frac{i+m}{2i+1}\right)^2 \mathcal{P}_{i-1}^m(t)P_{i-1}^m(u) + \left(\frac{i-m+1}{2i+1}\right)^2 \mathcal{P}_{i+1}^m(t)P_{i+1}^m(u)$$
$$+\frac{(i+m)(i-m+1)}{(2i+1)^2}(\mathcal{P}_{i-1}^m(t)P_{i+1}^m(u) + \mathcal{P}_{i+1}^m(t)P_{i-1}^m(u))$$

and

$$(1-t^2-u^2)\mathcal{P}_i^m(t)P_i^m(u)$$
$$= \left(1 - 2\frac{(i+m)(i-m)}{(2i+1)(2i-1)} - 2\frac{(i+m+1)(i-m+1)}{(2i+3)(2i+1)}\right)\mathcal{P}_i^m(t)P_i^m(u)$$
$$-\frac{(i+m)(i+m-1)}{(2i+1)(2i-1)}(\mathcal{P}_i^m(t)P_{i-2}^m(u) + \mathcal{P}_{i-2}^m(t)P_i^m(u))$$
$$-\frac{(i-m+1)(i-m+2)}{(2i+1)(2i+3)}(\mathcal{P}_{i+2}^m(t)P_i^m(u) + \mathcal{P}_i^m(t)P_{i+2}^m(u)).$$

It follows that

$$O_l^m(t,u) = c^l \sum_{i=m}^{l} a_{li}^m \mathcal{P}_i^m(t)P_i^m(u) + c^l \sum_{i=m+1}^{l-1} \alpha_m^{li}(\mathcal{P}_{i+1}^m(t)P_{i-1}^m(u) + \mathcal{P}_{i-1}^m(t)P_{i+1}^m(u)).$$

The coefficients in the first sum are given by

$$a_m^{li} = \frac{2l-1}{l-m}\left(\frac{(i+m+1)^2}{(2i+3)^2}a_m^{(l-1)(i+1)} + \frac{(i-m)^2}{(2i-1)^2}a_m^{(l-1)(i-1)}\right)$$
$$+\frac{l+m-1}{l-m}\frac{4m^2-1}{(2i+3)(2i-1)}a_m^{(l-2)i}$$

which upon assuming relation (14) for the $a_m^{(l-1)k}$ and $a_m^{(l-2)i}$ results back in equation (14) for a_m^{li}. Furthermore, one finds that the coefficients

$$\alpha_m^{li} = \frac{2l-1}{l-m}\frac{(i+m)(i-m+1)}{(2i+1)^2}a_m^{(l-1)i} - \frac{l+m-1}{l-m}\left(\frac{(i+m+1)(i+m)}{(2i+3)(2i+1)}a_m^{(l-2)(i+1)} + \frac{(i-m)(i-m+1)}{(2i+1)(2i-1)}a_m^{(l-2)(i-1)}\right)$$

in the second sum vanish for all admissible values of i.

Finally, the theorem which has up to now only been proven for $m \geqslant 0$ can readily be extended to all m in the range $-l \leqslant m \leqslant l$ by inserting equations (A12) and (A13) into (13), (14).

B.2. Proof of relation (18)

Equation (18) is trivially fulfilled for $(l-k)$ odd. For $(l-k)$ even one has

$$\sum_{i=k}^{l} \tilde{a}_m^{li} a_m^{ik} = (2k+1)\frac{(l+m)!}{(l-m)!}\frac{(k-m)!}{(k+m)!}\sum_{i=k}^{l}{}' \frac{(-1)^{(l-i)/2}(l+i-1)!!}{(l-i)!!(i-k)!!(i+k+1)!!}$$

where the prime at the summmation sign on the rhs indicates that i varies in steps of two. It is easy to see that $\tilde{a}_m^{ll} a_m^{ll} = 1$. For $k = (l-2), (l-4), \ldots$ the sum on the rhs can be expressed as a sum over binominal coefficients

$$\frac{(-1)^{(l-k)/2}}{l-k}\sum_{j=0}^{(l-k)/2}(-1)^j \binom{\frac{l-k}{2}}{j}\binom{\frac{l+k-1}{2}+j}{\frac{l-k}{2}-1}$$

where i has been replaced by $2j+k$. Using the identity

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{a+j}{m} = (-1)^n\binom{a}{m-n} \qquad 0 \leqslant m \leqslant n \qquad \text{(B2)}$$

with $n = (l-k)/2$ (and thus $m < n$) this sum is seen to vanish (cf [15], p 619, 47/55).

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