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# On a relation between spherical and spheroidal harmonics 

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#### Abstract

Expressions are found for the coefficients in the relations which exhibit spheroidal harmonics as linear combinations of spherical harmonics and vice versa. In particular it is shown that in the case of prolate spheroidal harmonics the non-vanishing coefficients $k_{L M 1}$ in the relation


$$
\hat{P}_{L}^{M}(u) P_{L}^{M}(v)=\sum_{l} k_{L M I} r^{l} P_{l}^{M}(\cos \theta)
$$

are given by

$$
k_{L M l}=\frac{(-1)^{(L-l) / 2} 2^{-L} a^{-l}(L+M)!(L+l)!}{(L-M)!(l+M)!\left(\frac{1}{2} L+\frac{1}{2} l\right)!\left(\frac{1}{2} L-\frac{1}{2} l\right)!}
$$

where $l=L, L-2, L-4, \ldots, M^{\prime}$ with $M^{\prime}=M$ or $M+1$ according as $L-M$ is even or odd, respectively.

## 1. Introduction

In certain physical applications, for instance the problem of magnetic shielding outside molecules having approximately spheroidal shape (Stiles 1975), one needs to know the coefficients of expansion $k_{L M}$ of spheroidal harmonics as linear combinations of spherical harmonics:

$$
\begin{equation*}
\hat{P}_{L}^{M}(u) P_{L}^{M}(v)=\sum_{l} k_{L M} r^{\prime} P_{l}^{M}(\cos \theta), \tag{1.1}
\end{equation*}
$$

prolate spheroidal harmonics being contemplated for the time being. In (1.1) $P_{L}^{M}(x)$, $x^{2} \leqslant 1$, is the associated Legendre function

$$
\begin{equation*}
P_{L}^{M}(x)=\frac{1}{2^{L} L!}\left(1-x^{2}\right)^{M / 2} \frac{\mathrm{~d}^{L+M}}{\mathrm{~d} x^{L+M}}\left(x^{2}-1\right)^{L} \tag{1.2}
\end{equation*}
$$

whilst, for $x^{2} \geqslant 1$, the function $\hat{P}_{L}^{M}(x)$ is given by the right-hand member of (1.2) provided the initial factor on the right be replaced by $\left(x^{2}-1\right)^{M / 2} . u, v, \phi$ are prolate
spheroidal coordinates and $r, \theta, \phi$ spherical polar coordinates so that, if $x, y, z$ are Cartesian coordinates,

$$
\begin{align*}
& x=a\left(u^{2}-1\right)^{1 / 2}\left(1-v^{2}\right)^{1 / 2} \cos \phi=r \sin \theta \cos \phi \\
& y=a\left(u^{2}-1\right)^{1 / 2}\left(1-v^{2}\right)^{1 / 2} \sin \phi=r \sin \theta \sin \phi  \tag{1.3}\\
& z=a u v=r \cos \theta
\end{align*}
$$

$2 a$ is the distance between the foci of the spheroidal coordinate surfaces $u=$ constant, their eccentricity being $u^{-1}$. The angle $\phi$ does not occur in (1.1) since it enters into both kinds of harmonics through the same factor $\exp (i M \phi)$ which has been removed.

Although the problem of expanding spheroidal in terms of spherical harmonics forms part of a more general investigation by Boyer et al (1976) we have been unable to locate a simple explicit expression for the required coefficients $k_{L M}$ in the literature. It is therefore obtained by elementary means in § 2, as is, in §3, an expression for the coefficients $\kappa_{L M}$ which occur in the relation inverse to (1.1). The modifications which arise when the spheroidal harmonics are oblate are dealt with in $\S 4$.

## 2. The coefficients $\boldsymbol{k}_{\text {LM }}$

If

$$
\begin{equation*}
p_{L}^{M}(x)=\frac{1}{2^{L} L!} \frac{\mathrm{d}^{L+M}}{\mathrm{~d} x^{L+M}}\left(x^{2}-1\right)^{L}=\sum_{n} p_{L M n} x^{L-M-2 n}, \tag{2.1}
\end{equation*}
$$

say, (1.1) may be written in the form

$$
\begin{align*}
p_{L}^{M}(u) P_{L}^{M}(v) & =\sum_{l} k_{L M I}\left(u^{2}-1\right)^{-M / 2} r^{l} \sin ^{M} \theta p_{l}^{M}(\cos \theta) \\
& =\sum_{l} k_{L M I} a^{M} r^{l-M}\left(1-v^{2}\right)^{M / 2} p_{l}^{M}(\cos \theta) \tag{2.2}
\end{align*}
$$

Now set $u=1$ and write $p_{L}^{M}(1)=p_{L M}$. Then (2.2) becomes

$$
\begin{equation*}
p_{L M} p_{L}^{M}(v)=\sum_{l} k_{L M} a^{l} p_{I M} v^{l-M} \tag{2.3}
\end{equation*}
$$

Comparison of (2.3) with (2.1) now yields, with $n=\frac{1}{2} L-\frac{1}{2} l$,

$$
k_{L M}= \begin{cases}a^{-l} p_{L M} p_{L M n} / p_{l M} & \text { when } L-l \text { is even }  \tag{2.4}\\ 0 & \text { when } L-l \text { is odd }\end{cases}
$$

A well known representation (Gradshteyn and Ryzhik 1965, p 1015) of $P_{L}^{M}(x)$ as a (hypergeometric) series in ascending powers of $\frac{1}{2}(1-x)$ shows that

$$
\begin{equation*}
p_{L M}=\frac{2^{-M}(L+M)!}{M!(L-M)!} \tag{2.5}
\end{equation*}
$$

and from (2.1), virtually by inspection,

$$
\begin{equation*}
p_{L M n}=\frac{(-1)^{n} 2^{-L}(2 L-2 n)!}{n!(L-n)!(L-M-2 n)!} \tag{2.6}
\end{equation*}
$$

Using (2.5) and (2.6) in (2.4) it finally follows that the non-vanishing coefficients $k_{\text {LM }}$ are given by

$$
\begin{equation*}
k_{L M}=\frac{(-1)^{(L-l) / 2} 2^{-L} a^{-l}(L+M)!(L+l)!}{(L-M)!(l+M)!\left(\frac{1}{2} L+\frac{1}{2} l\right)!\left(\frac{1}{2} L-\frac{1}{2} l\right)!} \tag{2.7}
\end{equation*}
$$

where $l=L, L-2, L-4, \ldots, M^{\prime}$ with $M^{\prime}=M$ when $L-M$ is even and $M^{\prime}=M+1$ when $L-M$ is odd.

## 3. The coefficients $\kappa_{L M}$

Let

$$
\begin{equation*}
r^{L} P_{L}^{M}(\cos \theta)=\sum_{l} \kappa_{L M} \hat{P}_{l}^{M}(u) P_{l}^{M}(v) \tag{3.1}
\end{equation*}
$$

be the relation inverse to (1.1). Proceeding as in § 2, this may be written in the form

$$
\begin{equation*}
a^{M} r^{L-M}\left(1-v^{2}\right)^{M / 2} p_{L}^{M}(\cos \theta)=\sum_{l} \kappa_{L M l} p_{l}^{M}(u) P_{l}^{M}(v) \tag{3.2}
\end{equation*}
$$

As before, set $u=1$, so that (3.2) becomes

$$
\begin{equation*}
a^{L} p_{L M} v^{L-M}\left(1-v^{2}\right)^{M / 2}=\sum_{l^{\prime}} \kappa_{L M M^{\prime}} p_{l^{\prime} M} P_{l^{\prime}}^{M}(v) \tag{3.3}
\end{equation*}
$$

Multiply throughout by $P_{l}^{M}(v)$ and integrate from -1 to 1 . On the left one has the integral

$$
\begin{equation*}
\int_{-1}^{1} v^{L-M}\left(1-v^{2}\right)^{M / 2} P_{l}^{M}(v) \mathrm{d} v=i_{L M l} \tag{3.4}
\end{equation*}
$$

say, while on the right on account of the orthogonality of the Legendre functions

$$
\begin{equation*}
\int_{-1}^{1} P_{l}^{M}(v) P_{l}^{M}(v) \mathrm{d} v=c_{l M} \delta_{l l}, \tag{3.5}
\end{equation*}
$$

say. Therefore

$$
\begin{equation*}
\kappa_{L M I}=a^{L} p_{L M} i_{L M} / c_{I M} p_{I M} \tag{3.6}
\end{equation*}
$$

Now the integrand on the left of (3.4) is an odd function of $v$ when $L-l$ is odd so that $i_{L M}$ then vanishes. When $L-l$ is even one has (Gradshteyn and Ryzhik 1965, p 799 )

$$
\begin{equation*}
i_{L M}=\frac{2^{l+1}(l+M)!(L-M)!\left(\frac{1}{2} L+\frac{1}{2} l\right)!}{(l-M)!(L+l+1)!\left(\frac{1}{2} L-\frac{1}{2} l\right)!} \tag{3.7}
\end{equation*}
$$

where the duplication formula for the factorial function has been used to cast the result given in the preceding reference into a more convenient form. Also (Gradshteyn and Ryzhik 1965, p 794)

$$
\begin{equation*}
c_{l M}=\frac{(l+M)!}{\left(l+\frac{1}{2}\right)(l-M)!} \tag{3.8}
\end{equation*}
$$

and upon using (2.5), (3.7) and (3.8) in (3.6) there emerges the result

$$
\begin{equation*}
\kappa_{L M l}=\frac{2^{\prime} a^{L}(2 l+1)(L+M)!(l-M)!\left(\frac{1}{2} L+\frac{1}{2} l\right)!}{(L+l+1)!(l+M)!\left(\frac{1}{2} L-\frac{1}{2} l\right)!} \tag{3.9}
\end{equation*}
$$

for the non-vanishing coefficients, the relevant values of $l$ being again as given after (2.7). It is not difficult to verify directly that the matrices whose elements are, for any given value of $M, k_{L M}$ and $\kappa_{L M}$ respectively are inverse to each other.

## 4. The case of oblate spheroidal harmonics

The relation of oblate spheroidal coordinates to spherical polar coordinates is given by (1.3) after the factors $\left(u^{2}-1\right)^{1 / 2}$ which appear in them have been replaced by $\left(u^{2}+1\right)^{1 / 2}$. In place of (1.1) one now has to consider the relation

$$
\begin{equation*}
\hat{P}_{L}^{M}(\mathrm{i} u) P_{L}^{M}(v)=\sum_{l} \tilde{k}_{L M I} r^{l} P_{l}^{M}(\cos \theta) \tag{4.1}
\end{equation*}
$$

To avoid possible difficulties with phase factors it is wise to write

$$
\begin{equation*}
\hat{P}_{L}^{M}(\mathrm{i} u)=\mathrm{i}^{M}\left(u^{2}+1\right)^{M / 2} p_{L}^{M}(\mathrm{i} u) \tag{4.2}
\end{equation*}
$$

One may now proceed much as before except that it is appropriate this time to assign the special value unity to $v$ rather than to $u$. It is not worth spelling out the details of the work which leads to the result

$$
\begin{equation*}
\tilde{k}_{L M l}=\mathrm{i}^{\prime} k_{L M I} . \tag{4.3}
\end{equation*}
$$

Finally, as regards the coefficients $\tilde{\kappa}_{L M I}$ in the relation inverse to (4.1) (cf equation (3.1))

$$
\begin{equation*}
\tilde{\kappa}_{L M I}=\mathrm{i}^{-L} \kappa_{L M I} . \tag{4.4}
\end{equation*}
$$

## References

[^0]
[^0]:    Boyer C P, Kalnins E G and Miller W Jr 1976 Nagoya Math. J. 6035
    Gradshteyn I S and Ryzhik I M 1965 Tables of Integrals, Series and Products (New York: Academic)
    Stiles P J 1975 Proc. R. Soc. A 346209

