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COMMENT

Comment on Witschel's operator method for the calculation of Gaunt's coefficients

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Abstract. Witschel's operator method for the calculation of spherical harmonic matrix elements yields in some cases an incorrect result. A correct derivation of the operator formulae is given.

The full theory of angular momentum in the framework of boson calculus was developed by Schwinger (1952). Quite recently Witschel (1974) has used the factorization method of Infeld and Hull (1951) to relate Schwinger's bilinear operator expressions of the two-dimensional isotropic oscillator with the differential operators raising and lowering j and m of the spherical harmonics $Y_{j,m}(\theta, \varphi)$. It has been shown that matrix elements of spherical harmonics can be written down without using $3j$-symbols. Therefore, one has made use of the equations of Infeld and Hull, § 9. However these equations are not generally valid since they depend on the definition of the spherical harmonics and especially on the phase convention adopted.

To evaluate spherical harmonic matrix elements it is only necessary to have $\cos\theta\, Y_{j,m}(\theta, \varphi)$ and $\sin\theta \exp(\pm i\varphi) Y_{j,m}(\theta, \varphi)$, expressed as linear combinations of contiguous solutions. These relations are closely related to the corresponding relations for the normalized associated Legendre polynomials $\mathrm{P}_{j,m}(\cos\theta)$ (Bethe 1933):

$$\cos\theta\, \mathrm{P}_{j,m}(\cos\theta) = \left(\frac{(j+m+1)(j-m+1)}{(2j+1)(2j+3)}\right)^{1/2} \mathrm{P}_{j+1,m}(\cos\theta) + \left(\frac{(j+m)(j-m)}{(2j+1)(2j-1)}\right)^{1/2} \mathrm{P}_{j-1,m}(\cos\theta) \tag{1}$$

and

$$\sin\theta\, \mathrm{P}_{j,m}(\cos\theta) = \pm\left(\frac{(j\pm m+1)(j\pm m+2)}{(2j+1)(2j+3)}\right)^{1/2} \mathrm{P}_{j+1,m\pm 1}(\cos\theta) \mp \left(\frac{(j\mp m)(j\mp m-1)}{(2j+1)(2j-1)}\right)^{1/2} \mathrm{P}_{j-1,m\pm 1}(\cos\theta). \tag{2}$$

There are, *inter alia*, two conventions in common use for defining $Y_{j,m}(\theta, \varphi)$ in terms of $\mathrm{P}_{j,m}(\cos\theta)$:

(i) $Y^{(\mathrm{I})}_{j,m}(\theta, \varphi) = 1/(2\pi)^{1/2}\mathrm{P}_{j,m}(\cos\theta)\exp(\mathrm{i}m\varphi).$ (3)

This is the definition used by Bethe (1933) and also by Infeld and Hull (1951). Further in this paper we shall call this definition the Bethe convention, although it is not certain at all that Bethe was the first one to introduce it.

(ii) $Y^{(\mathrm{II})}_{j,m}(\theta, \varphi) = (-1)^m 1/(2\pi)^{1/2}\mathrm{P}_{j,m}(\cos\theta)\exp(\mathrm{i}m\varphi).$ (4)

This corresponds to the well known Condon–Shortley (1935) convention.

Inserting equations (3) or (4) into (1) gives the following result for $i = \mathrm{I}$ or II:

$$\begin{aligned}\cos\theta\, Y^{(i)}_{j,m}(\theta, \varphi) &\\ = \left(\frac{(j+m+1)(j-m+1)}{(2j+1)(2j+3)}\right)^{1/2} Y^{(i)}_{j+1,m}(\theta, \varphi) &\\ + \left(\frac{(j+m)(j-m)}{(2j+1)(2j+3)}\right)^{1/2} Y^{(i)}_{j-1,m}(\theta, \varphi). &\qquad (5)\end{aligned}$$

Substituting equations (3) or (4) into (2) gives different results:

$$\begin{aligned}\sin\theta\exp(\pm\mathrm{i}\varphi) Y^{(\mathrm{I})}_{j,m}(\theta, \varphi) &\\ = \pm\left(\frac{(j\pm m+1)(j\pm m+2)}{(2j+1)(2j+3)}\right)^{1/2} Y^{(\mathrm{I})}_{j+1,m\pm1}(\theta, \varphi) &\\ \mp\left(\frac{(j\mp m)(j\mp m-1)}{(2j+1)(2j+3)}\right)^{1/2} Y^{(\mathrm{I})}_{j-1,m\pm1}(\theta, \varphi) &\qquad (6)\end{aligned}$$

and

$$\begin{aligned}\sin\theta\exp(\pm\mathrm{i}\varphi) Y^{(\mathrm{II})}_{j,m}(\theta, \varphi) &\\ = \mp\left(\frac{(j\pm m+1)(j\pm m+2)}{(2j+1)(2j+3)}\right)^{1/2} Y^{(\mathrm{II})}_{j+1,m\pm1}(\theta, \varphi) &\\ \pm\left(\frac{(j\mp m)(j\mp m-1)}{(2j+1)(2j+3)}\right)^{1/2} Y^{(\mathrm{II})}_{j-1,m\pm1}(\theta, \varphi). &\qquad (7)\end{aligned}$$

Translation into Witschel's operator language for both of these conventions is straightforward and is given in table 1. All symbols used have been defined by Witschel.

Table 1. The translation of equations (5)–(7) into Witschel's operator language. The expressions in θ, φ are applied either on $Y^{(\mathrm{I})}_{j,m}$ (left-hand column) or on $Y^{(\mathrm{II})}_{j,m}$ (right-hand column), whereas the combined operator expressions are applied to $|jm\rangle$.

Bethe convention	Condon–Shortley convention
$\cos\theta \to \hat{c}_j\hat{R}_+ + \hat{c}_j^*\hat{R}_-$	$\cos\theta \to \hat{c}_j\hat{R}_+ + \hat{c}_j^*\hat{R}_-$
$\sin\theta\exp(\mathrm{i}\varphi) \to \hat{c}_j\hat{M}_+ - \hat{g}_j\hat{M}_-$	$\sin\theta\exp(\mathrm{i}\varphi) \to -\hat{c}_j\hat{M}_+ + \hat{g}_j\hat{M}_-$
$\sin\theta\exp(-\mathrm{i}\varphi) \to -\hat{c}_j\hat{N}_+ + \hat{g}_j^*\hat{N}_-$	$\sin\theta\exp(-\mathrm{i}\varphi) \to \hat{c}_j\hat{N}_+ - \hat{g}_j^*\hat{N}_-$

The spherical harmonic matrix elements or Gaunt's coefficients (Gaunt 1929), which are given in terms of $3j$-symbols by

$$\langle j_1 m_1 | Y_{j_2 m_2} | j_3 m_3 \rangle = \int Y^*_{j_1, m_1} Y_{j_2, m_2} Y_{j_3, m_3} \, \mathrm{d}\Omega$$
$$= (-1)^{m_1} \left(\frac{(2j_1+1)(2j_2+1)(2j_3+1)}{4\pi} \right)^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix},$$

are independent of the convention used for the definition of the $Y_{j,m}(\theta, \varphi)$. In order to obtain the correct result from Witschel's operator formulae one has to combine the expression of Y_{j_2, m_2} with the operator form deduced in the same convention. However, Witschel derived the operator forms in the Bethe convention yet used the $Y_{j_2 m_2}$ expressions deduced in the Condon–Shortley convention. Such a mixture leads to the wrong sign for the Gaunt coefficients for odd m_2 values. As an example consistent use of either convention yields the following operator form for $Y_{2,1}$:

$$Y_{2,1} = (15/8\pi)^{1/2} (\hat{c}_j \hat{K}_+ + \hat{c}_j^* \hat{K}_-)(\hat{c}_j \hat{M}_+ - \hat{g}_j \hat{M}_-)$$

in contrast with Witschel's incorrect expression (24).

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