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A new expression for the Talmi–Moshinsky harmonic oscillator bracket

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Abstract. A simple analytic expression for the general Talmi–Moshinsky harmonic oscillator bracket is derived. This expression is expected to be more convenient, from the point of view of numerical computations, than the others available in the literature.

1. Introduction

In many nuclear physics problems one needs to perform a transformation on the two-particle system from single-particle coordinate basis to the centre-of-mass and the relative coordinate basis. When one expresses the single-particle wavefunctions in the harmonic oscillator basis, this transformation is represented in terms of the well-known Talmi–Moshinsky bracket (TMB) (Talmi 1952, Moshinsky 1959, Smirnov 1961). In general one tries to approximate the general wavefunction in terms of the harmonic oscillator wavefunctions and then uses this transformation. In such problems one requires the computation of a large number of TMBs.

Because of the history of the problem, many attempts have been made in the past to obtain for this bracket a simple, analytic expression which is also useful from the computational point of view. Various computer programs exist corresponding to these attempts. Mention can be made of at least two such programs, one by Sontona and Gmitro (1972), which is based on a formula from Trlifaj (1972), and the other by Feng and Tamura (1975), which is based on an expression obtained by Baranger and Davies (1966). From the point of view of analytic simplicity, the formula of Trlifaj (1972) is much better and generally it has also proved to be more useful computationally. In addition, various symmetrical analytical expressions also exist for this bracket which are, however, not very convenient for numerical computation (Bakri 1967, B Buck 1970, unpublished, quoted by Talman 1970, Talman 1970). The results of these attempts are essentially variants of a formula due to Kumar (1966).

Recently, Dobez (1977) has reattempted the problem following Trlifaj's procedure (1972) of skilfully specialising one vector. Dobez (1977) has arrived at a formula which has proved to be more efficient than that of Trlifaj (1972) *but it involves a larger number of summations.* The computational advantage is derived from the possibility of expressing the various expressions for the TMB as a sum of a quantity which factorises into a radial quantum number dependent (non-geometrical) part and a radial quantum number independent (geometrical) part. In Dobez' (1977) formula this sum has only

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one overlapping index of summation, whereas in Trlifaj's (1972) this number is three, which gives the computational advantage to Dobez'.

In this paper, we have also followed Trlifaj's (1972) procedure of fixing one of the momenta (Trlifaj used it for the $l=0$ case only, but we are using it for the general TMB). We have also used some angular momentum techniques to arrive at a still simpler expression. In our formula the total number of summations is seven, i.e. the same number as in Trlifaj's (1972) but three less than those in Dobez'; but when one expresses our formula as a sum of factorised expressions as described above, there is only one overlapping summation. Thus our formula, which combines the advantages of both Trlifaj's and Dobez', should be more advantageous computationally than the others under consideration. We hope to manifest this advantage *quantitatively* by actually writing a useful computer program.

One disturbing feature still remains. Except for the formulae of the type of Kumar's (1966), none of the others quoted above, including our own, manifest the obvious symmetries of the bracket. The procedure of Trlifaj is obviously not symmetrical and the results derived from it are thus also not so. We believe that it should be possible to derive a simpler expression for the TMB, which manifests its symmetries and is faster computationally. Though our attempt may prove to be a step in this direction, we have, unfortunately, not been able to achieve our final goal.

The plan of this paper is as follows: in the next section we present the notations for completeness and also derive a formula which we use in the last section to arrive at a useful, simple and analytic expression for the TMB. In the last section we also compare our expression with some of the previous results.

2. Notations and mathematical formulation

We write

$$A^{\mu}_{n_1l_1,n_2l_2;\lambda} = \sum_{m_1,m_2} \delta_{\mu,m_1+m_2}\langle l_1, m_1; l_2, m_2|\lambda, \mu\rangle \phi^{m_1}_{n_1l_1}(\boldsymbol{r}_1)\phi^{m_2}_{n_2l_2}(\boldsymbol{r}_2) \tag{1}$$

and

$$B^{\mu}_{nl,NL;\lambda} = \sum_{m,M} \delta_{\mu,m+M}\langle l, m; L, M|\lambda, \mu\rangle \phi^{m}_{nl}(\boldsymbol{r})\phi^{M}_{NL}(\boldsymbol{R}), \tag{2}$$

where

$$\phi^{m}_{nl}(\boldsymbol{r}) = c_{nl}r^l \exp(-\tfrac{1}{2}r^2)\mathrm{L}^{l+\frac{1}{2}}_n(r^2)\mathrm{Y}^m_l(\hat{\boldsymbol{r}}) \tag{3}$$

is the normalised three-dimensional harmonic oscillator wavefunction. In equation (3) the normalisation constant c_{nl} and the Laguerre polynomial $\mathrm{L}^{l+\frac{1}{2}}_n(r^2)$ are given by

$$c_{nl} = \left(\frac{2n!}{\Gamma(n+l+\frac{3}{2})}\right)^{1/2} \tag{4}$$

$$\mathrm{L}^{l+\frac{1}{2}}_n(r^2) = \sum_{m=0}^{n} (-1)^m \frac{\Gamma(n+l+\frac{3}{2})}{m!(n-m)!\Gamma(m+l+\frac{3}{2})} r^{2m}. \tag{5}$$

In the previous equations, in place of the position vector $\boldsymbol{x}$, we have used an argument $\boldsymbol{r}$ related to it by

$$\boldsymbol{r} = (m\omega/\hbar)^{1/2}\boldsymbol{x}.$$

Note that m_1, m_2, $m_\mu = (m_1 m_2)/(m_1+m_2)$, $m_{CM} = m_1 + m_2$ are the masses used in the above relation for $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}$ and $\boldsymbol{R}$ respectively.

The single-particle coordinates $\boldsymbol{r}_1$, $\boldsymbol{r}_2$ are related to the relative and the centre-of-mass coordinates $\boldsymbol{r}$, $\boldsymbol{R}$ by

$$\boldsymbol{r}_1 = \left(\frac{1}{1+D}\right)^{1/2} \boldsymbol{r} + \left(\frac{D}{1+D}\right)^{1/2} \boldsymbol{R}, \tag{6a}$$

$$\boldsymbol{r}_2 = -\left(\frac{D}{1+D}\right)^{1/2} \boldsymbol{r} + \left(\frac{1}{1+D}\right)^{1/2} \boldsymbol{R}, \tag{6b}$$

where $D = m_1/m_2$ is the mass ratio. Note that the transformation given in equations (6a) and (6b) is *orthogonal*. We can invert equations (1) and (2) to obtain

$$\phi_{n_1 l_1}^{m_1}(\boldsymbol{r}_1)\phi_{n_2 l_2}^{m_2}(\boldsymbol{r}_2) = \sum_\lambda \delta_{\mu, m_1+m_2}\langle l_1, m_1; l_2, m_2 | \lambda, \mu\rangle A^{\mu}_{n_1 l_1, n_2 l_2;\lambda}, \tag{1$'$}$$

$$\phi_{nl}^{m}(\boldsymbol{r})\phi_{NL}^{M}(\boldsymbol{R}) = \sum_\lambda \delta_{\mu, m+M}\langle l, m; L, M | \lambda, \mu\rangle B^{\mu}_{nl, NL;\lambda}. \tag{2$'$}$$

The transformation coefficient $\langle nl, NL; \lambda | n_1 l_1, n_2 l_2; \lambda\rangle$ known as the Talmi–Moshinsky bracket (TMB), which we wish to compute, is defined by

$$A^{\mu}_{n_1 l_1, n_2 l_2;\lambda} = \sum_{nl, NL} \langle nl, NL; \lambda | n_1 l_1, n_2 l_2; \lambda\rangle B^{\mu}_{nl, NL;\lambda}. \tag{7}$$

Evidently we can write

$$\phi_{n_1 l_1}^{m_1}(\boldsymbol{r}_1)\phi_{n_2 l_2}^{m_2}(\boldsymbol{r}_2) = \sum_{nlNLmM} \delta_{m_1+m_2, m+M} C^{m_1, m_2; m, M}_{n_1 l_1, n_2 l_2; nl, NL} \phi_{nl}^{m}(\boldsymbol{r})\phi_{NL}^{M}(\boldsymbol{R}) \tag{8}$$

which, on using equation (2$'$), becomes

$$\phi_{n_1 l_1}^{m_1}(\boldsymbol{r}_1)\phi_{n_2 l_2}^{m_2}(\boldsymbol{r}_2) = \sum_{nlNL\lambda} \delta_{\mu, m_1+m_2} B^{\mu}_{nl, N\lambda;\lambda} \sum_{mM} \delta_{\mu, m+M}\langle l, m; L, M | \lambda\mu\rangle C^{m_1, m_2; m, M}_{n_1 l_1, n_2 l_2; nl, NL}. \tag{9}$$

Alternatively, substituting for $A^{\mu}_{n_1 l_1, n_2 l_2;\lambda}$ from equation (7) in equation (1$'$), we find

$$\phi_{n_1 l_1}^{m_1}(\boldsymbol{r}_1)\phi_{n_2 l_2}^{m_2}(\boldsymbol{r}_2) = \sum_{nlNL\lambda} \delta_{\mu, m_1+m_2}\langle l_1, m_1; l_2, m_2 | \lambda, \mu\rangle\langle nl, NL; \lambda | n_1 l_1, n_2 l_2; \lambda\rangle B^{\mu}_{nl, NL}. \tag{10}$$

Comparing equations (9) and (10), we arrive at

$$\langle l_1, m_1; l_2, m_2 | \lambda, m_1+m_2\rangle\langle nl, NL; \lambda | n_1 l_1, n_2 l_2; \lambda\rangle = \sum_{mM} \delta_{m_1+m_2, m+M}\langle l, m; L, M | \lambda, m+M\rangle C^{m_1, m_2; m, M}_{n_1 l_1, n_2 l_2; nl, NL}. \tag{11}$$

Equations (8) and (11) define the procedure which we shall be following to obtain a simple analytic expression for the TMB represented by $\langle nl, NL; \lambda | n_1 l_1, n_2 l_2; \lambda\rangle$.

3. A simple expression for the general Talmi–Moshinsky bracket

In order to obtain the coefficients $C^{m_1, m_2; m, M}_{n_1 l_1, n_2 l_2; nl, NL}$ defined in equation (8), we must expand the product $\phi_{n_1 l_1}^{m_1}(\boldsymbol{r}_1)\phi_{n_2 l_2}^{m_2}(\boldsymbol{r}_2)$ in terms of the products $\phi_{nl}^{m}(\boldsymbol{r})\phi_{NL}^{M}(\boldsymbol{R})$. For this purpose, noting equation (6), we find

$$r_1^{l_1}\mathrm{Y}_{l_1}^{m_1}(\hat{\boldsymbol{r}}_1)=[4\pi(2l_1+1)!]^{1/2}\sum_{\lambda_1\mu_1}\frac{\langle\lambda_1,\mu_1;l_1-\lambda_1,m_1-\mu_1|l_1,m_1\rangle}{[(2\lambda_1+1)!(2l_1-2\lambda_1+1)!]^{1/2}}$$
$$\times\frac{D^{\frac{1}{2}(l_1-\lambda_1)}}{(1+D)^{\frac{1}{2}l_1}}r^{\lambda_1}\mathrm{Y}_{\lambda_1}^{\mu_1}(\hat{\boldsymbol{r}})R^{l_1-\lambda_1}\mathrm{Y}_{l_1-\lambda_1}^{m_1-\mu_1}(\hat{\boldsymbol{R}}) \tag{12}$$

and

$$r_2^{l_2}\mathrm{Y}_{l_2}^{m_2}(\hat{\boldsymbol{r}}_2)=[4\pi(2l_2+1)!]^{1/2}\sum_{\lambda_2\mu_2}\frac{\langle\lambda_2,\mu_2;l_2-\lambda_2,m_2-\mu_2|l_2,m_2\rangle}{[(2\lambda_2+1)!(2l_2-2\lambda_2+1)!]^{1/2}}$$
$$\times(-1)^{\lambda_2}\frac{D^{\frac{1}{2}\lambda_2}}{(1+D)^{\frac{1}{2}l_2}}r^{\lambda_2}\mathrm{Y}_{\lambda_2}^{\mu_2}(\hat{\boldsymbol{r}})R^{l_2-\lambda_2}\mathrm{Y}_{l_2-\lambda_2}^{m_2-\mu_2}(\hat{\boldsymbol{R}}), \tag{13}$$

using a well-known formula (Varshalovich *et al* 1975).

Further, using equations (5) and (6), we get

$$\mathrm{L}_{n_1}^{l_1+\frac{1}{2}}(r_1^2)\mathrm{L}_{n_2}^{l_2+\frac{1}{2}}(r_2^2)$$
$$=\sum_{t_1t_2}(-1)^{t_1+t_2}\frac{\Gamma(n_1+l_1+\frac{3}{2})\Gamma(n_2+l_2+\frac{3}{2})}{t_1!t_2!(n_1-t_1)!(n_2-t_2)!\Gamma(t_1+l_1+\frac{3}{2})\Gamma(t_2+l_2+\frac{3}{2})}r_1^{2t_1}r_2^{2t_2}$$
$$=\sum_{t_1t_2p_1p_2}(-1)^{t_1+t_2+p_2}\frac{\Gamma(n_1+l_1+\frac{3}{2})\Gamma(n_2+l_2+\frac{3}{2})}{(t_1-p_1)!(t_2-p_2)!(n_1-t_1)!(n_2-t_2)!\Gamma(t_1+l_1+\frac{3}{2})\Gamma(t_2+l_2+\frac{3}{2})p_1!p_2!}$$
$$\times\left(\frac{1}{1+D}r^2+\frac{D}{1+D}R^2\right)^{t_1-p_1}\left(\frac{D}{1+D}r^2+\frac{1}{1+D}R^2\right)^{t_2-p_2}\left(2\frac{\sqrt{D}}{1+D}\boldsymbol{r}\cdot\boldsymbol{R}\right)^{p_1+p_2} \tag{14}$$

and

$$\exp[-\tfrac{1}{2}(r_1^2+r_2^2)]=\exp[-\tfrac{1}{2}(r^2+R^2)]. \tag{15}$$

We shall also require

$$(2\boldsymbol{r}\cdot\boldsymbol{R})^p=2\pi^{3/2}(rR)^p\sum_{kq}\frac{(-1)^q}{[\frac{1}{2}(p-k)]!\Gamma(\frac{1}{2}(p+k+3))}\mathrm{Y}_k^q(\hat{\boldsymbol{r}})\mathrm{Y}_k^{-q}(\hat{\boldsymbol{R}}), \tag{16}$$

where $-k\leqslant q\leqslant k$ and the summation over k is such that k and $\frac{1}{2}(p-k)$ are both non-negative integers. This result can be obtained by using equation (5.8.3) in Edmonds (1960) with αk in place of k, differentiating p times with respect to α and replacing α finally by 0.

Now equations (3)–(5) and (12)–(16) give

$$\phi_{n_1l_1}^{m_1}(\boldsymbol{r}_1)\phi_{n_2l_2}^{m_2}(\boldsymbol{r}_2)$$
$$=8\pi^{5/2}c_{n_1l_1}c_{n_2l_2}\exp[-\tfrac{1}{2}(r^2+R^2)][(2l_1+1)!(2l_2+1)!]^{1/2}\Gamma(n_1+l_1+\tfrac{3}{2})\Gamma(n_2+l_2+\tfrac{3}{2})$$
$$\times\sum_{\substack{\lambda_1\mu_1\lambda_2\mu_2\\t_1t_2p_1p_2kq}}(-1)^{\lambda_2+t_1+t_2+p_2+q}$$
$$\times\frac{\langle\lambda_1,\mu_1;l_1-\lambda_1,m_1-\mu_1|l_1,m_1\rangle\langle\lambda_2,\mu_2;l_2-\lambda_2,m_2-\mu_2|l_2,m_2\rangle}{[(2\lambda_1+1)!(2l_1-2\lambda_1+1)!(2\lambda_2+1)!(2l_2-2\lambda_2+1)!]^{1/2}}$$
$$\times\frac{(p_1+p_2)!}{(n_1-t_1)!(n_2-t_2)!\Gamma(t_1+l_1+\frac{3}{2})\Gamma(t_2+l_2+\frac{3}{2})p_1!p_2!(t_1-p_1)!(t_2-p_2)!\times[\frac{1}{2}(p_1+p_2-k)]!\Gamma(\frac{1}{2}(p_1+p_2+k+3))}$$

$$\times \frac{D^{\frac{1}{2}(l_1-\lambda_1+\lambda_2+p_1+p_2)}}{(1+D)^{\frac{1}{2}(l_1+l_2)+p_1+p_2}}\left(\frac{1}{1+D}r^2+\frac{D}{1+D}R^2\right)^{t_1-p_1}$$
$$\times\left(\frac{D}{1+D}r^2+\frac{1}{1+D}R^2\right)^{t_2-p_2}$$
$$\times r^{\lambda_1+\lambda_2+p_1+p_2}Y_{\lambda_1}^{\mu_1}(\hat{r})Y_{\lambda_2}^{\mu_2}(\hat{r})Y_k^q(\hat{r})$$
$$\times R^{l_1+l_2-\lambda_1-\lambda_2+p_1+p_2}Y_{l_1-\lambda_1}^{m_1-\mu_1}(\hat{\boldsymbol{R}})Y_{l_2-\lambda_2}^{m_2-\mu_2}(\hat{\boldsymbol{R}})Y_k^{-q}(\hat{\boldsymbol{R}}). \tag{17}$$

From the above, it is easy to project out the angular part $Y_l^m(\hat{r})Y_L^M(\hat{\boldsymbol{R}})$, where $m=\mu_1+\mu_2+q$ and $M=m_1+m_2-\mu_1-\mu_2-q$ (so that $m_1+m_2=m+M$) by making use of standard angular momentum techniques. Indeed $0\leqslant l\leqslant\lambda_1+\lambda_2+k$ and $0\leqslant L\leqslant l_1+l_2-\lambda_1-\lambda_2+k$ in the projection from the term

$$Y_{\lambda_1}^{\mu_1}(\hat{r})Y_{\lambda_2}^{\mu_2}(\hat{r})Y_k^q(\hat{r})Y_{l_1-\lambda_1}^{m_1-\mu_1}(\hat{\boldsymbol{R}})Y_{l_2-\lambda_2}^{m_2-\mu_2}(\hat{\boldsymbol{R}})Y_k^{-q}(\hat{R}),$$

where the lower bounds on l and L may not be achieved. (Note that

$$Y_{l_1}^{m_1}(\hat{r})Y_{l_2}^{m_2}(\hat{r})Y_{l_3}^{m_3}(\hat{r})=\sum_l C_{l_1l_2l_3,l}^{m_1m_2m_3}Y_l^{m_1+m_2+m_3}(\hat{r})$$

where if, e.g. $l_1=\max(l_1,l_2,l_3)$, $l_{\min}\leqslant l_1\leqslant l+l_2+l_3$, where $l_{\min}$ is defined as $\max(0,l_1-l_2-l_3,|m_1+m_2+m_3|)$.)

The coefficient of this term is $r^{\lambda_1+\lambda_2+p_1+p_2}R^{l_1+l_2-\lambda_1-\lambda_2+p_1+p_2}$ times a multinomial in r, R. Since $p_1+p_2-k\geqslant 0$, the powers of both r and R are no less than the upper bounds of l and L respectively. Thus we have the possiblity of having in our expression for $\phi_{n_1l_1}^{m_1}(\boldsymbol{r}_1)\phi_{n_2l_2}^{m_2}(\boldsymbol{r}_2)$ all values of l and L allowed by the angular momentum consideration in any term.

Next we project out $\exp[-\frac{1}{2}(r^2+R^2)]r^lY_l^m(\hat{r})R^LY_L^M(\hat{\boldsymbol{R}})$. Then the coefficient C of $\exp[-\frac{1}{2}(r^2+R^2)]r^lY_l^m(\hat{r})R^LY_L^M(\hat{\boldsymbol{R}})$ in $\phi_{n_1l_1}^{m_1}(\boldsymbol{r}_1)\phi_{n_2l_2}^{m_2}(\boldsymbol{r}_2)$ is given by

$$C=8\pi^{5/2}c_{n_1l_1}c_{n_2l_2}[(2l_1+1)!(2l_2+1)!]^{1/2}\Gamma(n_1+l_1+\tfrac{3}{2})\Gamma(n_2+l_2+\tfrac{3}{2})$$
$$\times\sum_{\substack{\lambda_1\mu_1\lambda_2\mu_2\\ t_1t_2p_1p_2k}}(-1)^{\lambda_2+t_1+t_2+p_2+m-\mu_1-\mu_2}$$
$$\times\frac{\langle\lambda_1,\mu_1;l_1-\lambda_1,m_1-\mu_1|l_1,m_1\rangle\langle\lambda_2,\mu_2;l_2-\lambda_2,m_2-\mu_2|l_2,m_2\rangle}{[(2\lambda_1+1)!(2l_1-2\lambda_1+1)!(2\lambda_2+1)!(2l_2-2\lambda_2+1)!]^{1/2}}$$
$$\times\frac{1}{(n_1-t_1)!(n_2-t_2)!\Gamma(t_1+l_1+\frac{3}{2})\Gamma(t_2+l_2+\frac{3}{2})p_1!p_2!(t_1-p_1)!(t_2-p_2)![\frac{1}{2}(p_1+p_2-k)]!}$$
$$\times\frac{(p_1+p_2)!}{\Gamma(\frac{1}{2}(p_1+p_2+k+3))}r^{\lambda_1+\lambda_2+p_1+p_2-l}R^{l_1+l_2-\lambda_1-\lambda_2+p_1+p_2-L}$$
$$\times\left(\frac{1}{1+D}r^2+\frac{D}{1+D}R^2\right)^{t_1-p_1}\left(\frac{D}{1+D}r^2+\frac{1}{1+D}R^2\right)^{t_2-p_2}$$
$$\times\text{coefficeint of }Y_l^m(\hat{r})Y_L^M(\hat{R})\text{ in }Y_{\lambda_1}^{\mu_1}(\hat{r})Y_{\lambda_2}^{\mu_2}(\hat{r})Y_k^q(\hat{r})Y_{l_1-\lambda_1}^{m_1-\mu_1}(\hat{\boldsymbol{R}})Y_{l_2-\lambda_2}^{m_2-\mu_2}(\hat{\boldsymbol{R}})Y_k^{-q}(\hat{\boldsymbol{R}}). \tag{18}$$

From equation (8), we see that the same coefficient C is also given by

$$C=\sum_{nN}C_{n_1l_1,n_2l_2;nl,NL}^{m_1,m_2;m,M}c_{nl}c_{NL}L_n^{l+\frac{1}{2}}(r^2)L_N^{L+\frac{1}{2}}(R^2). \tag{19}$$

Because of the energy conservation requirement

$$2n_1+2n_2+l_1+l_2=2n+2N+l+L, \tag{20}$$

and the fact that n_1, l_1, n_2, l_2, l, L are fixed in equation (19), the sum in this equation is over only one *independent* variable. Henceforth, we shall indicate only one such variable in our summations.

At this stage we use a generalisation of the $r\to 0$ technique previously used by Trlifaj(1972) specifically for the $l=0$ case. Essentially the same method was also used by Dobez (1977) though after following some expansions of the products of Laguerre polynomials in a manner different from (and more complicated than) ours. In equation (19), it is trivial to calculate the $r\to 0$ limit. Indeed

$$C(r\to 0)=\sum_n C^{m_1,m_2;m,M}_{n_1l_1,n_2l_2;nl,NL}c_{nl}c_{NL}\mathrm{L}_n^{l+\frac{1}{2}}(0)\mathrm{L}_N^{L+\frac{1}{2}}(R^2). \tag{21}$$

In equation (18), however, when we approach this limit, only those terms with

$$l=\lambda_1+\lambda_2+p_1+p_2 \tag{22}$$

survive. Since also $l\leqslant\lambda_1+\lambda_2+k$ from angular momentum considerations where $k\leqslant p_1+p_2$ we are forced to take

$$k=p_1+p_2. \tag{23}$$

(Note that k is to be such that both k and $\frac{1}{2}(p_1+p_2-k)$ are non-negative integers. The special choice $k=p_1+p_2$ satisfies both these requirements.) Thus l is obtained from the three angular momenta λ_1, λ_2 and k in the *most stretched* configuration. The outcome of the above analysis is that in order to obtain $C(r\to 0)$ from equation (18), we may take p_2 and λ_2 as dependent upon other summation indices, as given in equations (22) and (23) above. Subsequently we shall explicitly eliminate p_2 and add a delta function $\delta_{l,\lambda_1+\lambda_2+k}$ in the equations to remind us of the condition $l=\lambda_1+\lambda_2+k$.

Now since

$$\begin{aligned}\mathrm{Y}^{m_1}_{l_1}(\hat{r})\mathrm{Y}^{m_2}_{l_2}(\hat{r})&=\sum_l\left(\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}\right)^{1/2}\langle l_1,0;l_2,0|l,0\rangle\\&\times\langle l_1,m_1;l_2,m_2|l,m_1+m_2\rangle\mathrm{Y}^{m_1+m_2}_l(\hat{r})\end{aligned} \tag{24}$$

(equation (4.6.8) in Edmonds (1960)), we find the coefficient of $\mathrm{Y}^m_l(\hat{r})\mathrm{Y}^M_L(\hat{\boldsymbol{R}})$ in

$$\mathrm{Y}^{\mu_1}_{\lambda_1}(\hat{r})\mathrm{Y}^{\mu_2}_{\lambda_2}(\hat{r})\mathrm{Y}^{m_1-\mu_1}_{l_1-\lambda_1}(\hat{\boldsymbol{R}})\mathrm{Y}^{m_2-\mu_2}_{l_2-\lambda_2}(\hat{\boldsymbol{R}})\mathrm{Y}^{-q}_k(\hat{\boldsymbol{R}}),$$

as

$$\begin{aligned}&\frac{1}{16\pi^2}(2k+1)\left(\frac{(2\lambda_1+1)(2l_1-2\lambda_1+1)(2\lambda_2+1)(2l_2-2\lambda_2+1)}{(2l+1)(2L+1)}\right)^{1/2}\\&\quad\times\langle\lambda_1,\mu_1;\lambda_2,\mu_2|\lambda_1+\lambda_2,\mu_1+\mu_2\rangle\langle\lambda_1+\lambda_2,\mu_1+\mu_2;k,q|l,m\rangle\\&\quad\times\langle\lambda_1,0;\lambda_2,0|\lambda_1+\lambda_2,0\rangle\langle\lambda_1+\lambda_2,0;k,0|l,0\rangle\\&\quad\times\sum_{\lambda_{12}}\langle l_1-\lambda_1,m_1-\mu_1;l_2-\lambda_2,m_2-\mu_2|\lambda_{12},m_1+m_2-\mu_1-\mu_2\rangle\\&\quad\times\langle\lambda_{12},m_1+m_2-\mu_1-\mu_2;k,-q|L,M\rangle\\&\quad\times\langle l_1-\lambda_1,0;l_2-\lambda_2,0|\lambda_{12},0\rangle\langle\lambda_{12},0;k,0|L,0\rangle.\end{aligned}$$

The computation of the coefficients $C^{m_1,m_2;m,M}_{n_1l_1,n_2l_2;nl,NL}$ now only requires comparison of the $C(r\to 0)$ obtained from equation (18) and that given in equation (21), and equating the coefficient of $L_N^{L+1/2}(R^2)$ in both of these results. This comparison is possible on account of the orthogonality of $L_N^{l+1/2}(x)$ given explicitly by

$$\int_0^\infty x^{l+\frac{1}{2}}e^{-x}L_n^{l+\frac{1}{2}}(x)L_{n'}^{l+\frac{1}{2}}\,dx=\delta_{nn'}\frac{\Gamma(n+l+\frac{3}{2})}{n!}$$

and the equation

$$\int_0^\infty x^{\gamma-1}e^{-x}L_n^{\mu}(x)\,dx=(-1)^n\frac{\Gamma(\gamma)\Gamma(\gamma-\mu)}{n!\Gamma(\gamma-\mu-n)},\tag{25}$$

which are equations (7.414 (3,11)) in Gradshteyn *et al* (1965). Substituting the value of $C^{m_1,m_2;m,M}_{n_1l_1,n_2l_2;nl,NL}$ thus calculated into equation (11), we finally arrive at

$$\begin{aligned}
&\langle l_1,m_1;l_2,m_2|\lambda,m_1+m_2\rangle\langle nl,NL;\lambda|n_1l_1,n_2l_2;\lambda\rangle\\
&=\tfrac{1}{2}\pi^{1/2}(-1)^N\left(\frac{n_1!n_2!n!}{N!}\,\frac{(2l_1+1)(2l_2+1)}{(2l+1)(2L+1)}\,\frac{\Gamma(n_1+l_1+\frac{3}{2})\Gamma(n_2+l_2+\frac{3}{2})}{\Gamma(n+l+\frac{3}{2})\Gamma(N+L+\frac{3}{2})}\right)^{1/2}\Gamma(l+\tfrac{3}{2})\\
&\quad\times\sum_{\lambda_1\lambda_2t_1t_2k}(-1)^{\lambda_2+t_1+t_2+k+p_1}\delta_{l,\lambda_1+\lambda_2+k}\\
&\quad\times\frac{D^{\frac{1}{2}(l_1-\lambda_1+\lambda_2+k)+t_1-p_1}}{(1+D)^{\frac{1}{2}(l_1+l_2)+t_1+t_2}}\\
&\quad\times\frac{(t_1+t_2+(l_1+l_2-l-L)/2)!\Gamma(t_1+t_2+(l_1+l_2-l+L+3)/2)}{p_1!(k-p_1)!(t_1-p_1)!(t_2-k+p_1)!(n_1-t_1)!(n_2-t_2)!\times\Gamma(t_1+l_1+\frac{3}{2})\Gamma(t_2+l_2+\frac{3}{2})(t_1+t_2+(l_1+l_2-l-L)/2-N)!}\\
&\quad\times\frac{(2k+1)!k!}{\Gamma(k+\frac{3}{2})[(2\lambda_1)!(2\lambda_2)!(2l_1-2\lambda_1+1)!(2l_2-2\lambda_2+1)!]^{1/2}}\\
&\quad\times\langle\lambda_1,0;\lambda_2,0|\lambda_1+\lambda_2,0\rangle\langle\lambda_1+\lambda_2,0;k,0|l,0\rangle\\
&\quad\times\sum_{\lambda_{12}\mu_1\mu_2q}\langle\lambda_1,\mu_1;l_1-\lambda_1,m_1-\mu_1|l_1,m_1\rangle\langle\lambda_2,\mu_2;l_2-\lambda_2,m_2-\mu_2|l_2,m_2\rangle\\
&\quad\times\langle\lambda_1,\mu_1;\lambda_2,\mu_2|\lambda_1+\lambda_2,\mu_1+\mu_2\rangle\langle\lambda_1+\lambda_2,\mu_1+\mu_2;k,q|l,m\rangle\\
&\quad\times\langle l_1-\lambda_1,m_1-\mu_1;l_2-\lambda_2,m_2-\mu_2|\lambda_{12},m_1+m_2-\mu_1-\mu_2\rangle\\
&\quad\times\langle\lambda_{12},m_1+m_2-\mu_1-\mu_2;k,-q|L,M\rangle\\
&\quad\times\langle l_1-\lambda_1,0;l_2-\lambda_2,0|\lambda_{12},0\rangle\langle\lambda_{12},0;k,0|L,0\rangle\langle l,m;L,M|\lambda,m+M\rangle,
\end{aligned}\tag{26}$$

where $m=\mu_1+\mu_2+q$, $M=m_1+m_2-\mu_1-\mu_2-q$ (and therefore $m_1+m_2=m+M$) and many of the Clebsch–Gordan coefficients appearing in this equation correspond to stretched configurations. Note that we have replaced the m-summation appearing in equation (11) by a summation over q, which can be done since the two are not independent.

Next we wish to perform the summations over the three *magnetic* quantum numbers μ_1, μ_2, q appearing on the right-hand side of the above equation, in such a manner as to be able to *factorise the magnetic quantum numbers dependent part* $\langle l_1,m_1;l_2,m_2|\lambda,m_2+m_2\rangle$. Then we shall be left with an *invariant* expression for the TMB which we are interested in.

First note that

$$\sum_q (-1)^q \langle \lambda_1+\lambda_2, \mu_1+\mu_2; k, q \,|\, l, m\rangle \langle \lambda_{12}, m_1+m_2-\mu_1-\mu_2; k, -q \,|\, L, M\rangle$$
$$\times \langle l, m; L, M \,|\, \lambda, m_1+m_2\rangle$$
$$= (-1)^k \left(\frac{(2L+1)}{(2\lambda_{12}+1)}\right)^{1/2} \sum_q \langle \lambda_1+\lambda_2, \mu_1+\mu_2; k, q \,|\, l, m\rangle$$
$$\times \langle k, q; L, M \,|\, \lambda_{12}, m_1+m_2-\mu_1-\mu_2\rangle \langle l, m; L, M \,|\, \lambda, m_1+m_2\rangle,$$

using equation (3.5.16), p 42, in Edmonds (1960). Now we can perform the q-summation using equation (6.2.7), p 95, in Edmonds (1960) with $j_1=\lambda_1+\lambda_2$, $j_2=k$, $j_3=L$, $j_{12}=l$, $j=\lambda$, $j_{23}=\lambda_{12}$ to arrive at

$$\sum_q (-1)^q \langle \lambda_1+\lambda_2, \mu_1+\mu_2; k, q \,|\, l, m\rangle$$
$$\times \langle \lambda_{12}, m_1+m_2-\mu_1-\mu_2; k, -q \,|\, L, M\rangle \langle l, m; L, M \,|\, \lambda, m_1+m_2\rangle$$
$$= (-1)^{L+\lambda_1+\lambda_2+\lambda}[(2l+1)(2L+1)]^{1/2}$$
$$\times \langle \lambda_1+\lambda_2, \mu_1+\mu_2; \lambda_{12}, m_1+m_2-\mu_1-\mu_2 \,|\, \lambda, m_1+m_2\rangle$$
$$\times \begin{Bmatrix} \lambda_1+\lambda_2 & k & l \\ L & \lambda & \lambda_{12} \end{Bmatrix}. \qquad (28)$$

Next we examine the μ_1-, μ_2-summations. For this purpose, we use

$$(-1)^{2j_{11}-2j_{22}-j_{13}+j_{31}+j_{23}-j_{32}-2m_{33}}[(2j_{13}+1)(2j_{23}+1)(2j_{31}+1)(2j_{32}+1)]^{1/2}$$
$$\times \langle j_{13}, m_{13}; j_{23}, m_{23} \,|\, j_{33}, m_{33}\rangle \begin{Bmatrix} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{Bmatrix}$$
$$= \sum_{m_{11}m_{21}} \langle j_{11}, m_{11}; j_{12}, m_{12} \,|\, j_{13}, m_{13}\rangle \langle j_{21}, m_{21}; j_{22}, m_{22} \,|\, j_{23}, m_{23}\rangle$$
$$\times \langle j_{31}, m_{31}; j_{32}, m_{32} \,|\, j_{33}, m_{33}\rangle$$
$$\times \langle j_{11}, m_{11}; j_{21}, m_{21} \,|\, j_{31}, m_{31}\rangle \langle j_{12}, m_{12}; j_{22}, m_{22} \,|\, j_{32}, m_{32}\rangle, \qquad (29)$$

with $j_{11}=\lambda_1$, $j_{12}=l_1-\lambda_1$, $j_{13}=l_1$, $j_{21}=\lambda_2$, $j_{22}=l_2-\lambda_2$, $j_{23}=l_2$, $j_{31}=\lambda_1+\lambda_2$, $j_{32}=\lambda_{12}$, $j_{33}=j$ (the above is a variant of equation (6.4.4), p 101, in Edmonds (1960)), to obtain

$$\sum_{\mu_1,\mu_2} \langle \lambda_1, \mu_1; l_1-\lambda_1, m_1-\mu_1 \,|\, l_1, m_1\rangle \langle \lambda_2, \mu_2; l_2-\lambda_2, m_2-\mu_2 \,|\, l_2, m_2\rangle$$
$$\times \langle \lambda_1+\lambda_2, \mu_1+\mu_2; \lambda_{12}, m_1+m_2-\mu_1-\mu_2 \,|\, \lambda, m_1+m_2\rangle$$
$$\times \langle \lambda_1, \mu_1; \lambda_2, \mu_2 \,|\, \lambda_1+\lambda_2, \mu_1+\mu_2\rangle$$
$$\times \langle l_1-\lambda_1, m_1-\mu_1; l_2-\lambda_2, m_2-\mu_2 \,|\, \lambda_{12}, m_1+m_2-\mu_1-\mu_2\rangle$$
$$= (-1)^{l_1+l_2+\lambda_1+\lambda_2+\lambda_{12}}[(2l_1+1)(2l_2+1)(2\lambda_1+2\lambda_2+1)(2\lambda_{12}+1)]^{1/2}$$
$$\times \langle l_1, m_1; l_2, m_2 \,|\, \lambda, m_1+m_2\rangle \begin{Bmatrix} \lambda_1 & l_1-\lambda_1 & l_1 \\ \lambda_2 & l_2-\lambda_2 & l_2 \\ \lambda_1+\lambda_2 & \lambda_{12} & \lambda \end{Bmatrix}. \qquad (30)$$

On substituting from equations (28) and (30) in equation (26) and cancelling the factor $\langle l_1, m_1; l_2, m_2|\lambda, m_1+m_2\rangle$ on both sides, we finally arrive at

$$\begin{aligned}
&\langle nl, NL; \lambda\,|n_1l_1, n_2l_2; \lambda\rangle \\
&\quad=\tfrac{1}{2}\pi^{1/2}(-1)^N\left(\frac{n_1!n_2!n!}{N!}\,\frac{\Gamma(n_1+l_1+\frac{3}{2})\Gamma(n_2+l_2+\frac{3}{2})}{\Gamma(n+l+\frac{3}{2})\Gamma(N+L+\frac{3}{2})}\right. \\
&\qquad\left.\times(2l_1+1)(2l_1+1)!(2l_2+1)(2l_2+1)!\right)^{1/2}\Gamma(l+\tfrac{3}{2}) \\
&\qquad\times\sum_{\lambda_1\lambda_2t_1t_2p_1\lambda_{12}k}(-1)^{L+\lambda_1+t_1+t_2+k+p_1+\lambda}\delta_{l,\lambda_1+\lambda_2+k}\frac{D^{\frac{1}{2}(l_1-\lambda_1+\lambda_2+k)+t_1-p_1}}{(1+D)^{\frac{1}{2}(l_1+l_2)+t_1+t_2}} \\
&\qquad\times\frac{[t_1+t_2+(l_1+l_2-l-L)/2]!\Gamma(t_1+t_2+(l_1+l_2-l+L+3)/2)}{p_1!(k-p_1)!(t_1-p_1)!(t_2-k+p_1)!(n_1-t_1)!(n_2-t_2)!\times\Gamma(t_1+l_1+\frac{3}{2})\Gamma(t_2+l_2+\frac{3}{2})[t_1+t_2+(l_1+l_2-l-L)/2-N]!} \\
&\qquad\times\langle\lambda_1, 0; \lambda_2, 0|l-k, 0\rangle\langle l-k, 0; k, 0|l, 0\rangle \\
&\qquad\times\langle l_1-\lambda_1, 0; l_2-\lambda_2, 0|\lambda_{12}, 0\rangle\langle\lambda_{12}, 0; k, 0|L, 0\rangle \\
&\qquad\times\frac{(2k+1)k![(2\lambda_1+2\lambda_2+1)(2\lambda_{12}+1)]^{1/2}}{\Gamma(k+\frac{3}{2})[(2\lambda_1)!(2\lambda_2)!(2l_1-2\lambda_1)!(2l_2-2l_2)!]^{1/2}} \\
&\qquad\times\begin{Bmatrix} l-k & k & l \\ L & \lambda & \lambda_{12}\end{Bmatrix}\begin{Bmatrix}\lambda_1 & l_1-\lambda_1 & l_1 \\ \lambda_2 & l_2-\lambda_2 & l_2 \\ l-k & \lambda_{12} & \lambda\end{Bmatrix},
\end{aligned}\tag{31}$$

where, to simplify the phase, we have used the fact that $l_1-\lambda_1+l_2-\lambda_2+\lambda_{12}$ is an *even* integer.

In the above equation we have our expression for the TMB bracket, which contains only seven summations, since the stretched 6-j symbol has none, whereas the doubly stretched (row-wise) 9-j symbol has only one summation (Jucys and Bandzaitis 1965, Sharp 1967). Again, *all* the Clebsch–Gordan coefficients appearing in this equation can be explicitly given without any summation. These various quantities are given below:

$$\langle\lambda_1, 0; l_2, 0|l-k, 0\rangle=\left(\frac{(2\lambda_1)!(2\lambda_2)!}{(2l-2k)!}\right)^{1/2}\frac{(l-k)!}{\lambda_1!\lambda_2!},\tag{32}$$

$$\langle l-k, 0; k, 0|l, 0\rangle=\left(\frac{(2l-2k)!(2k)!}{(2l)!}\right)^{1/2}\frac{l!}{(l-k)!k!},\tag{33}$$

$$\begin{aligned}
&\langle l_1-\lambda_1, 0; l_2-\lambda_2, 0|\lambda_{12}, 0\rangle \\
&\quad=(-1)^{\frac{1}{2}(l_1+l_2-\lambda_1-\lambda_2-\lambda_{12})} \\
&\qquad\times\frac{(2\lambda_{12}+1)(l_1+l_2-\lambda_1-\lambda_2-\lambda_{12})!(l_1-l_2-\lambda_1+\lambda_2+\lambda_{12})!\times(l_1-l_2-\lambda_1+\lambda_2+\lambda_{12})!(-l_1+l_2+\lambda_1-\lambda_2+\lambda_{12})!}{(l_1+l_2-\lambda_1-\lambda_2+\lambda_{12}+1)!} \\
&\qquad\times\frac{[\frac{1}{2}(l_1+l_2-\lambda_1-\lambda_2+\lambda_{12})]!}{[\frac{1}{2}(l_1+l_2-\lambda_1-\lambda_2-\lambda_{12})]![\frac{1}{2}(l_1-l_2-\lambda_1+\lambda_2+\lambda_{12})]!\times[\frac{1}{2}(-l_1+l_2+\lambda_1-\lambda_2+\lambda_{12})]!},
\end{aligned}\tag{34}$$

$$\langle\lambda_{12},0;k,0|L,0\rangle$$

$$=(-1)^{\frac{1}{2}(-L+k+\lambda_{12})}\left(\frac{(2L+1)(L+k-\lambda_{12})!(L-k+\lambda_{12})!(-L+k+\lambda_{12})!}{(L+k+\lambda_{12}+1)!}\right)^{1/2}$$

$$\times\frac{[\frac{1}{2}(L+k+\lambda_{12})]!}{[\frac{1}{2}(L+k-\lambda_{12})]![\frac{1}{2}(L-k+\lambda_{12})]![\frac{1}{2}(-L+k+\lambda_{12})]!},\qquad(35)$$

$$\begin{Bmatrix} l-k & k & l \\ L & \lambda & \lambda_{12}\end{Bmatrix}$$

$$=\begin{Bmatrix} L & \lambda & l \\ l-k & k & \lambda_{12}\end{Bmatrix}$$

$$=(-1)^{l+L+\lambda}$$

$$\times\left(\frac{(2k)!(2l-2k)!(l+L+\lambda+1)!(l+L-\lambda)!(l-L+\lambda)!(L-k+\lambda_{12})!}{(2l+1)!(-l+L+\lambda)!(L+k-\lambda_{12})!(-L+k+\lambda_{12})!(L+k+\lambda_{12}+1)!}\right)^{1/2}$$

$$\times\left(\frac{(-l+k+\lambda+\lambda_{12})!}{(l-k+\lambda-\lambda_{12})!(l-k-\lambda+\lambda_{12})!(l-k+\lambda+\lambda_{12}+1)!}\right)^{1/2},\qquad(36)$$

$$\begin{Bmatrix} \lambda_1 & l_1-\lambda_1 & l_1 \\ \lambda_2 & l_2-\lambda_2 & l_2 \\ l-k & \lambda_{12} & \lambda\end{Bmatrix}$$

$$=(-1)^{\lambda+l-k+\lambda_{12}}\begin{Bmatrix} l_1-\lambda_1 & \lambda_1 & l_1 \\ l_2-\lambda_2 & \lambda_2 & l_2 \\ \lambda_{12} & l-k & \lambda\end{Bmatrix}$$

$$=\left(\frac{(2l_1-2\lambda_1)!(2l_2-2\lambda_2)!}{(2l_1+1)!(2l_2+1)!(2l-2k+1)!}\right.$$

$$\left.\times\frac{(l_1+l_2+\lambda+1)!(l_1+l_2-\lambda)!(l_1-l_2+\lambda)!}{(-l_1+l_2+\lambda)!}\right)^{1/2}$$

$$\times\left(\frac{(l-k+\lambda_{12}+\lambda+1)!(l-k-\lambda_{12}+\lambda)!(l-k+\lambda_{12}-\lambda)!}{(-l+k+\lambda_{12}+\lambda)!}\right)^{1/2}$$

$$\times\left(\frac{(-l_1+l_2+\lambda_1-\lambda_2+\lambda_{12})!}{(l_1+l_2-l+k+\lambda_{12}+1)!(l_1-l_2-\lambda_1+\lambda_2+\lambda_{12})!(l_1+l_2-l+k-\lambda_{12})!}\right)^{1/2}$$

$$\times\sum_z(-1)^z$$

$$\times\frac{(-l+k+\lambda_{12}+\lambda+z)!(-l_1+l_2+\lambda+z)!}{z!(l-k+\lambda_{12}-\lambda-z)!(-l_1+l_2+\lambda_1-\lambda_2-l+k+\lambda+z)!(2\lambda+1+z)!}\qquad(37)$$

(equations (3.7.17) and (6.3.1) in Edmonds (1960) and equation (A2) in註Ališauskas and Jucys (1971)).

Using the duplication formula

$$\Gamma(2z)=\frac{1}{\sqrt{\pi}}2^{2z-1}\Gamma(z)\Gamma(z+\tfrac{1}{2}),\qquad(38)$$

we find

$$\frac{(2k+1)!\Gamma(l+\frac{3}{2})l!}{k!\Gamma(k+\frac{3}{2})(2l+1)!}=2^{2k-2l}. \tag{39}$$

Thus we finally arrive at

$$\begin{aligned}
\langle nl, NL; \lambda \,|\, n_1 l_1, n_2 l_2; \lambda \rangle
&= \tfrac{1}{2}\pi^{1/2}[(2l_1+1)(2l_2+1)(2l+1)(2L+1)]^{1/2} \\
&\times \frac{(l_1+l_2+\lambda+1)!(l_1+l_2-\lambda)!(l_1-l_2+\lambda)! \times (l+L+\lambda+1)!(l+L-\lambda)!(l-L+\lambda)!}{(-l_1+l_2+\lambda)!(-l+L+\lambda)!} \\
&\times (-1)^N \left(\frac{n_1!n_2!n!}{N!}\,\frac{\Gamma(n_1+l_1+\frac{3}{2})\Gamma(n_2+l_2+\frac{3}{2})}{\Gamma(n+l+\frac{3}{2})\Gamma(N+L+\frac{3}{2})}\right)^{1/2} \\
&\times \sum_k \Bigg[\Bigg(\sum_{\lambda_1\lambda_2\lambda_{12}z} \delta_{l,\lambda_1+\lambda_2+k}(-1)^{\frac{1}{2}(l_1+l_2+l-L)+\lambda_1+z} \\
&\times \frac{D^{\frac{1}{2}(l_1-\lambda_1+\lambda_2+k)}}{(1+D)^{\frac{1}{2}(l_1+l_2)}}\,\frac{2^{2k-2l}(2\lambda_{12}+1)}{\lambda_1!\lambda_2!} \\
&\times \frac{k!(-l_1+l_2+\lambda_1-\lambda_2+\lambda_{12})![\frac{1}{2}(l_1+l_2-l+k+\lambda_{12})]!}{(l_1+l_2-l+k+\lambda_{12}+1)![\frac{1}{2}(l_1+l_2-l+k-\lambda_{12})]! \times [\frac{1}{2}(l_1-l_2-\lambda_1+\lambda_2+\lambda_{12})]![\frac{1}{2}(-l_1+l_2+\lambda_1-\lambda_2+\lambda_{12})]!} \\
&\times \frac{(L-k+\lambda_{12})![\frac{1}{2}(L+k+\lambda_{12})]!}{(L+k+\lambda_{12}+1)![\frac{1}{2}(L+k-\lambda_{12})]![\frac{1}{2}(L-k+\lambda_{12})]![\frac{1}{2}(-L+k+\lambda_{12})]!} \\
&\times \frac{(-l+k+\lambda_{12}+\lambda+z)!(-l_1+l_2+\lambda+z)!}{z!(l-k+\lambda_{12}-\lambda-z)!(-l_1+l_2+\lambda_1-\lambda_2-l+k+\lambda+z)!(2\lambda+1+z)!}\Bigg) \\
&\times \Bigg(\sum_{t_1t_2p_1} (-1)^{t_1+t_2+p_1} \frac{D^{t_1-p_1}}{(1+D)^{t_1+t_2}}\,\frac{1}{p_1!(k-p_1)!(t_1-p_1)!(t_2-k+p_1)!} \\
&\times \frac{[t_1+t_2+(l_1+l_2-l-L)/2]!\Gamma(t_1+t_2+(l_1+l_2-l+L+3)/2)}{(n_1-t_1)!(n_2-t_2)!\Gamma(t_1+l_1+\frac{3}{2})\Gamma(t_2+l_2+\frac{3}{2}) \times (t_1+t_2+(l_1+l_2-l-L)/2-N)!}\Bigg)\Bigg].
\end{aligned} \tag{40}$$

Above we have attempted to write the TMB as a *single* sum of products of a geometrical (radial quantum number independent) and a non-geometrical (radial quantum number dependent) part; each of these parts involves only *three* summations. If we compare our result with Trlifaj's (1972) we note that we have only one *overlapping* summation between these parts, whereas the formula of Trlifaj contains three such summations, though the total number of summations is the same (seven) as in our formula. The non-geometrical part in our formula agrees with that in Dobez' and the number of overlapping summations is also the same (one). However, in our formula the geometrical part contains only three summations, whereas in Dobez' (1977) formula there are six. Naturally, our expression, which combines the advantages of both Trlifaj's and Dobez' formulae, should be more useful from the computational point of view. It is also hoped that the simplicity of our expression will provide guidance in arriving at (possibly) a simpler expression for the TMB with manifest well-known symmetries.

4. Special cases

4.1. $D=0$

In this case, evidently, $\lambda_1=l_1$, $\lambda_2=k=p_1=t_1=0$, $l=l_1$, $\lambda_{12}=l_2=L$; then summing over the remaining z and t_2, we arrive at

$$\langle nl, NL; \lambda \,|\, n_1l_1, n_2l_2; \lambda\rangle \xrightarrow[D\to 0]{} \delta_{nn_1}\delta_{Nn_2}\delta_{ll_1}\delta_{Ll_2}.$$

4.2. $D=\infty$

In this case, evidently, $\lambda_2=l_2$, $\lambda_1=k=p_1=t_2=0$; $l=l_2$, $\lambda_{12}=l_1=L$; then summing over the remaining z and t_1, we arrive at

$$\langle nl, NL; \lambda \,|\, n_1l_1, n_2l_2; \lambda\rangle \xrightarrow[D\to \infty]{} (-1)^{L+\lambda}\delta_{nn_2}\delta_{Nn_1}\delta_{ll_2}\delta_{Ll_1}.$$

4.3. $l=0$

In this case, $\lambda_1=\lambda_2=k=0$, which results in $p_1=0$ and $\lambda_{12}=\lambda=L$, which then gives $z=0$. Thus we are left with the t_1, t_2 summations only. Indeed

$$\begin{aligned}\langle n0, NL; \lambda \,|\, n_1l_1, n_2l_2; \lambda\rangle &= \tfrac{1}{2}\pi^{1/2}(-1)^N\langle l_1,0; l_2, 0 \,|\, L, 0\rangle \\ &\quad\times\left(\frac{n_1!n_2!n!}{N!}\cdot\frac{(2l_1+1)(2l_2+1)}{(2L+1)}\cdot\frac{\Gamma(n_1+l_1+\frac{3}{2})\Gamma(n_2+l_2+\frac{3}{2})}{\Gamma(n+\frac{3}{2})\Gamma(N+L+\frac{3}{2})}\right)^{1/2} \\ &\quad\times\sum_{t_1t_2}(-1)^{t_1+t_2}\frac{D^{\frac{1}{2}l_1+t_1}}{(1+D)^{\frac{1}{2}(l_1+l_2)+t_1+t_2}} \\ &\quad\times\frac{[t_1+t_2+(l_1+l_2-L)/2]!\,\Gamma(t_1+t_2+(l_1+l_2+L+3)/2)}{t_1!t_2!(n_1-t_1)!(n_2-t_2)!\Gamma(t_1+l_1+\frac{3}{2})\times\Gamma(t_2+l_2+\frac{3}{2})[t_1+t_2+(l_1+l-L/2)-N]!},\end{aligned} \qquad (41)$$

where

$$\begin{aligned}\langle l_1,0; l_2,0 \,|\, L,0\rangle &= (-1)^{\frac{1}{2}(l_1+l_2-L)}\left(\frac{(2L+1)(l_1+l_2-L)!(l_1-l_2+L)!(-l_1+l_2+L)!}{(l_1+l_2+L+1)!}\right)^{1/2} \\ &\quad\times\frac{[\frac{1}{2}(l_1+l_2+L)]!}{[\frac{1}{2}(l_1+l_2-L)]![\frac{1}{2}(l_1-l_2+L)]![\frac{1}{2}(-l_1+l_2+L)]!}.\end{aligned} \qquad (42)$$

The expression in equation (41) is the same as that appearing in equation (11) in Trlifaj (1972).

Finally, we wish to remark that the transformation in equation (6) is an orthogonal transformation, since if

$$\mathbf{T}=\begin{pmatrix}[1/(1+D)]^{1/2} & [D/(1+D)]^{1/2} \\ -[D/(1+D)]^{1/2} & [1/(1+D)]^{1/2}\end{pmatrix},$$

$\mathbf{TT}^t = \mathbf{1}$. In fact, this is also a unitary unimodular transformation since $\mathbf{T}$ is real and $\det \mathbf{T} = 1$. The computation of the TMB for a general SU(2) transformation

$$\mathbf{T} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

with

$$\mathbf{TT}^+ = 1, \qquad \det \mathbf{T} = 1,$$

is essentially identical to that given in this paper.

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Note added in proof. Professor J Dobez has informed the author that he also has arrived at the same expression for the TMB and has written a computer programme (Dobez J 1979 *Comput. Phys. Commun.* **16** 373–81) for the evaluation of such brackets.

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