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A new expression for harmonic oscillator brackets

J Dobeš

Institute of Nuclear Physics, Czechoslovak Academy of Sciences, CS 250 68 Řež, Czechoslovakia

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Abstract. An explicit formula for general harmonic oscillator brackets is derived. The formula is particularly useful and convenient in numerical computations.

1. Introduction

In many problems of nuclear physics we have to perform a transformation of the two-particle basis from the single-particle coordinates to the centre of mass and relative coordinates. This transformation is smoothly carried out in the harmonic oscillator basis where it is represented by the well known harmonic oscillator Talmi–Moshinsky brackets (TMB) (Talmi 1952, Moshinsky 1959, Smirnov 1961). In other bases the individual single-particle functions are often expanded in terms of the harmonic oscillator functions and then the Talmi–Moshinsky transformation is used. Such a procedure needs calculation of many TMB and is quite time-consuming. It is, therefore, desirable to try to derive simple and efficient formulae for TMB.

The closed form for TMB has been derived (Baranger and Davies 1966, Trlifaj 1972). Trlifaj's formula especially is very simple and the computer programs based on it (Sotona and Gmitro 1972) are the fastest ones for the computation of a single TMB to date. For the computation of the large set of TMB another procedure (Feng and Tamura 1975) using the formula of Baranger and Davies (1966) has also proved to be efficient. For the other formulae and techniques in the evaluation of TMB we refer to the discussion in the above mentioned papers.

In the present paper we give a new simple formula for TMB. Our procedure is somewhat similar to the procedure of Trlifaj (1972). It agrees with that of Trlifaj when the relative orbital momentum of the two particles $l = 0$. A self-evident fact that the Talmi–Moshinsky transformation also holds for a particular value of the coordinates, namely when the relative coordinate of the two particles $\boldsymbol{r} = 0$, was skilfully employed by Trlifaj. This method can be applied only when $l = 0$. For the other relative momenta Trlifaj uses the generalised relation between the general and $l = 0$ brackets (Baranger and Davies 1966).

We also use the approach of Trlifaj, but first we perform a complete decomposition of the angular part of the Talmi–Moshinsky transformation. We obtain an expression for the general TMB without employing the rather complicated relation between the general and $l = 0$ brackets. Our formula has proved to be more efficient and faster than the previous ones in the numerical computation, especially when large radial quantum numbers are involved.

2. Definitions

The harmonic oscillator brackets $\langle nlNL; \lambda | n_1 l_1 n_2 l_2; \lambda \rangle_D$ are defined through the relation

$$\sum_{m_1 m_2} (l_1 m_1 l_2 m_2 | \lambda \mu) \phi_{n_1 l_1}^{m_1}(\boldsymbol{r}_1) \phi_{n_2 l_2}^{m_2}(\boldsymbol{r}_2)$$
$$= \sum_{NLMnlm} (lmLM|\lambda\mu) \langle nlNL; \lambda | n_1 l_1 n_2 l_2; \lambda \rangle_D \phi_{nl}^{m}(\boldsymbol{r}) \phi_{NL}^{M}(\boldsymbol{R}), \tag{1}$$

where the quantities $(lmLM|\lambda\mu)$ are the Clebsch–Gordan coefficients. The harmonic oscillator functions ϕ_{nl}^m are given by

$$\phi_{nl}^m(\boldsymbol{r}) = c_{nl} r^l \exp(-\tfrac{1}{2}r^2) L_n^{l+\frac{1}{2}}(r^2) Y_l^m(\hat{\boldsymbol{r}}), \tag{2}$$

with the normalisation constant

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

and the Laguerre polynomials

$$L_n^{l+\frac{1}{2}}(x) = \sum_{m=0}^{n} (-1)^m \frac{\Gamma(n+l+\frac{3}{2})}{(n-m)!\Gamma(m+l+\frac{3}{2})} \frac{x^m}{m!}.$$

We use as an argument in (2) the vector $\boldsymbol{r}$ related to the usual position vector $\boldsymbol{x}$ by

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

with mass of the particle m and harmonic oscillator frequency ω. The single-particle coordinates $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ and the centre of mass and relative coordinates $\boldsymbol{R}$ and $\boldsymbol{r}$ in (1) are related by the orthogonal transformation

$$\boldsymbol{r}_1 = \left(\frac{D}{1+D} \right)^{1/2} \boldsymbol{R} + \left(\frac{1}{1+D} \right)^{1/2} \boldsymbol{r}$$
$$\boldsymbol{r}_2 = \left(\frac{1}{1+D} \right)^{1/2} \boldsymbol{R} - \left(\frac{D}{1+D} \right)^{1/2} \boldsymbol{r},$$

where D is the mass ratio $D = m_1/m_2$.

The conservation of the energy and parity leads to selection rules

$$2n + l + 2N + L = 2n_1 + l_1 + 2n_2 + l_2 \qquad (-1)^{l+L} = (-1)^{l_1+l_2}. \tag{3}$$

3. Derivation

We shall try to rewrite the left-hand side of (1) in terms of the variables $\boldsymbol{R}$ and $\boldsymbol{r}$. We start with a decomposition of the products $r_i^{l_i} Y_{l_i}^{m_i}(\hat{\boldsymbol{r}}_i)$ $(i = 1, 2)$ according to the well known formula (Varshalovich *et al* 1975)

$$|\boldsymbol{a}+\boldsymbol{b}|^l Y_l^m\left(\frac{\boldsymbol{a}+\boldsymbol{b}}{|\boldsymbol{a}+\boldsymbol{b}|} \right)$$
$$= \sqrt{[4\pi(2l+1)!]} \sum_{\lambda_1 \lambda_2} \delta(\lambda_1+\lambda_2, l) \frac{a^{\lambda_1} b^{\lambda_2}}{\sqrt{[(2\lambda_1+1)!(2\lambda_2+1)!]}} [Y_{\lambda_1}(\hat{\boldsymbol{a}}) Y_{\lambda_2}(\hat{\boldsymbol{b}})]_{lm},$$

where the end square brackets denote the composition of the angular momenta. The exponent part is simply given by

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

The Laguerre polynomials are rewritten as

$$L_{n_1}^{l_1+\frac{1}{2}}(r_1^2)L_{n_2}^{l_2+\frac{1}{2}}(r_2^2)$$
$$= \sum_{k_1k_2} \frac{(-1)^{k_1}}{k_1!k_2!}\left(\frac{2\sqrt{D}}{1+D}\boldsymbol{R}\,.\,\boldsymbol{r}\right)^{k_1+k_2} L_{n_1}^{l_1+k_1+\frac{1}{2}}\left(\frac{D}{1+D}R^2+\frac{1}{1+D}r^2\right)$$
$$\times L_{n_2}^{l_2+k_2+\frac{1}{2}}\left(\frac{1}{1+D}R^2+\frac{D}{1+D}r^2\right).$$

Here, we have used the formula (Gradshteyn and Ryzhik 1962, equation (8.977.2))

$$L_n^\alpha(x+y) = e^y \sum_{i=0}^{\infty} (-1)^i \frac{y^i}{i!} L_n^{\alpha+i}(x).$$

The scalar product $(\boldsymbol{R}\,.\,\boldsymbol{r})^{k_1+k_2}$ is expanded as (Varshalovich *et al* 1975):

$$(\boldsymbol{R}\,.\,\boldsymbol{r})^{k_1+k_2} = 4\pi R^{k_1+k_2} r^{k_1+k_2} \sum_k \frac{(-1)^k (k_1+k_2)!\sqrt{(2k+1)}}{(k_1+k_2-k)!!(k_1+k_2+k+1)!!}[Y_k(\hat{\boldsymbol{R}})Y_k(\hat{\boldsymbol{r}})]_{00},$$

where $k = k_1+k_2,\ k_1+k_2-2, \ldots, 1$ or 0.

Thus we have achieved a full separation of the radial and angular dependence in coordinates $\boldsymbol{R}$ and $\boldsymbol{r}$ on the left-hand side of (1). Now projecting (1) on the particular values of L and l, dividing it by r^l and equating $r = 0$, in the spirit of the method of Trlifaj (1972), we are left with

$$\sum_{\substack{\lambda_1\lambda_2\lambda_3\lambda_4\\ k_1k_2k}} \delta(\lambda_1+\lambda_2, l_1)\delta(\lambda_3+\lambda_4, l_2)\delta(\lambda_2+\lambda_4+k_1+k_2, l)(4\pi)^2$$
$$\times\left(\frac{(2l_1+1)!(2l_2+1)!}{(2\lambda_1+1)!(2\lambda_2+1)!(2\lambda_3+1)!(2\lambda_4+1)!}\right)^{1/2}$$
$$\times\frac{(-1)^{k_1}}{k_1!k_2!}\frac{(-1)^{\lambda_4}D^{(\lambda_1+\lambda_4)/2}}{(1+D)^{(l_1+l_2)/2}}\left(\frac{2\sqrt{D}}{1+D}\right)^{k_1+k_2}$$
$$\times\frac{(-1)^k\sqrt{(2k+1)}(k_1+k_2)!}{(k_1+k_2-k)!!(k_1+k_2+k+1)!!}c_{n_1l_1}c_{n_2l_2}$$
$$\times\langle (Ll)\lambda\,(kk)0, \lambda\,|(\lambda_1\lambda_2)l_1(\lambda_3\lambda_4)l_2, \lambda\rangle R^{\lambda_1+\lambda_3+k_1+k_2}$$
$$\times e^{-R^2/2} L_{n_1}^{l_1+k_1+\frac{1}{2}}\left(\frac{D}{1+D}R^2\right) L_{n_2}^{l_2+k_2+\frac{1}{2}}\left(\frac{1}{1+D}R^2\right)$$
$$= \sum_{Nn} \langle nlNL; \lambda\,|n_1l_1n_2l_2; \lambda\rangle_D c_{NL}c_{nl} R^L e^{-R^2/2} L_N^{L+\frac{1}{2}}(R^2)$$
$$\times L_n^{l+\frac{1}{2}}(0)(-1)^{l+L-\lambda}. \tag{4}$$

Here, we have got from the angular momenta recoupling (Varshalovich *et al* 1975)

$$\langle (Ll)\lambda(kk)0,\lambda|(\lambda_1\lambda_2)l_1(\lambda_3\lambda_4)l_2,\lambda\rangle$$

$$= \sum_{\lambda_{13}\lambda_{24}} \frac{1}{(4\pi)^2}(-1)^{l+L+\lambda}\begin{Bmatrix} l & \lambda_{24} & k \\ \lambda_{13} & L & \lambda \end{Bmatrix}\begin{Bmatrix} \lambda_1 & \lambda_3 & \lambda_{13} \\ \lambda_2 & \lambda_4 & \lambda_{24} \\ l_1 & l_2 & \lambda \end{Bmatrix}$$

$$\times(\lambda_1 0\lambda_3 0|\lambda_{13}0)(\lambda_2 0\lambda_4 0|\lambda_{24}0)(L0k0|\lambda_{13}0)(l0k0|\lambda_{24}0)[(2\lambda_1+1)$$

$$\times(2\lambda_2+1)(2\lambda_3+1)(2\lambda_4+1)(2l_1+1)(2l_2+1)(2L+1)(2l+1)(2k+1)]^{1/2}.$$

We introduce in (4) a new summation variable $m=\lambda_2+\lambda_4$ and instead of k_1+k_2 we write $l-m$.

We can slightly simplify the sum (see appendix)

$$\sum_{k_1k_2} \delta(k_1+k_2, l-m)\frac{(-1)^{k_1}}{k_1!k_2!}L_{n_1}^{l_1+k_1+\frac{1}{2}}\left(\frac{D}{1+D}R^2\right)L_{n_2}^{l_2+k_2+\frac{1}{2}}\left(\frac{1}{1+D}R^2\right)$$

$$= \sum_{k_1k_2} \delta(k_1+k_2, l-m)\frac{(-1)^{k_1}}{k_1!k_2!}L_{n_1-k_1}^{l_1+k_1+\frac{1}{2}}\left(\frac{D}{1+D}R^2\right)L_{n_2-k_2}^{l_2+k_2+\frac{1}{2}}\left(\frac{1}{1+D}R^2\right). \tag{5}$$

The summation variables N and n in (4) are dependent according to the energy relation (3). We use the orthogonality properties of the Laguerre polynomials, and project out the particular TMB. The integrals that follow:

$$\int dR\, R^{\lambda_1+\lambda_3+l-m+L+2}\, e^{-R^2}L_{n_1-k_1}^{l_1+k_1+\frac{1}{2}}\left(\frac{D}{1+D}R^2\right)L_{n_2-k_2}^{l_2+k_2+\frac{1}{2}}\left(\frac{1}{1+D}R^2\right)L_N^{L+\frac{1}{2}}(R^2)$$

we calculate in the same way as Trlifaj (1972); the Laguerre polynomials $L_{n_1-k_1}^{l_1+k_1+\frac{1}{2}}[D/(1+D)R^2]$ and $L_{n_2-k_2}^{l_2+k_2+\frac{1}{2}}[1/(1+D)R^2]$ are explicitly written down and formula (7.414.11) of Gradshteyn and Ryzhik (1962) is applied.

The final result for TMB is

$$\langle nlNL;\lambda|n_1l_1n_2l_2;\lambda\rangle_D = \sum_{m=0}^{l} Q_m T_m \tag{6}$$

with

$$Q_m = \tfrac{1}{2}\Gamma(l+\tfrac{3}{2})(2l_1+1)(2l_2+1)[(2L+1)(2l+1)(2l_1)!(2l_2)!]^{1/2}(-1)^m(l-m)!$$

$$\times\frac{D^{(l_1+l)/2}}{(1+D)^{\frac{1}{2}(l_1+l_2)-l-m}}\sum_{\lambda_{13}\lambda_{24}}\left(\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\delta(\lambda_1+\lambda_2, l_1)\delta(\lambda_3+\lambda_4, l_2)\delta(\lambda_2+\lambda_4, m)\right.$$

$$\left.\times\frac{(-1)^{\lambda_2}D^{-\lambda_2}}{((2\lambda_1)!(2\lambda_2)!(2\lambda_3)!(2\lambda_4)!)^{1/2}}(\lambda_1 0\lambda_3 0|\lambda_{13}0)(\lambda_2 0\lambda_4 0|\lambda_{24}0)\begin{Bmatrix} \lambda_1 & \lambda_3 & \lambda_{13} \\ \lambda_2 & \lambda_4 & \lambda_{24} \\ l_1 & l_2 & \lambda \end{Bmatrix}\right)$$

$$\times\left(\sum_k \frac{(-1)^k(2k+1)}{[\frac{1}{2}(l-m-k)]!\Gamma[\frac{1}{2}(l-m+k)+\frac{3}{2}]}(L0k0|\lambda_{13}0)(l0k0|\lambda_{24}0)\right.$$

$$\left.\times\begin{Bmatrix} \lambda_{24} & k & l \\ L & \lambda & \lambda_{13} \end{Bmatrix}\right) \tag{7}$$

and

$$T_m=(-1)^N\left(\frac{n_1!n_2!n!\Gamma(n_1+l_1+\frac{3}{2})\Gamma(n_2+l_2+\frac{3}{2})}{N!\Gamma(n+l+\frac{3}{2})\Gamma(N+L+\frac{3}{2})}\right)^{1/2}$$

$$\times\sum_{k_1k_2}\delta(k_1+k_2,l-m)\frac{(-1)^{k_1}}{k_1!k_2!}\sum_{j_1j_2}\frac{(-1)^{j_1+j_2}}{j_1!j_2!}\frac{D^{j_1}}{(1+D)^{j_1+j_2}}$$

$$\times\frac{\Gamma[\frac{1}{2}(l_1+l_2+l+L)-m+j_1+j_2+\frac{3}{2}][\frac{1}{2}(l_1+l_2+l-L)-m+j_1+j_2]!}{(n_1-k_1-j_1)!(n_2-k_2-j_2)!\Gamma(j_1+l_1+k_1+\frac{3}{2})\times\Gamma(j_2+l_2+k_2+\frac{3}{2})[\frac{1}{2}(l_1+l_2+l-L)-m-N+j_1+j_2]!} \tag{8}$$

Here, the summation variables are restricted by the usual angular momentum limitations and by the factorials in denominators.

4. Discussion

For the case $l=0$ our final formula for TMB agrees with that of Trlifaj (1972). This was to be expected, since the procedures of derivation are the same in this special case. For the general brackets we have not found any direct connection with the other formulae. There is no simple way of showing the equivalence with the other formulae.

Our formula is not symmetrical in all the quantum numbers involved. It is particularly convenient to have l as the lowest of the orbital angular momenta in TMB. This can be achieved using the symmetry relations for TMB (Aguilerra-Navarro *et al* 1970).

One can see from equations (6)–(8) that the quantities Q_m depend only on the orbital quantum numbers. Dependence of TMB on radial quantum numbers is contained in the quantities T_m. Such a separation of the orbital and radial parts is possible also in the previous formulae for TMB (Baranger and Davies 1966, Trlifaj 1972, Feng and Tamura 1975). In our case, however, the orbital and radial parts have only one common summation variable. This is useful in computation of large matrices of TMB with fixed orbital momenta since it is possible to compute the orbital part only once.

In the orbital part Q_m the 9-j symbol with two stretched configurations appears. It can be calculated conveniently as a single sum (Jucys and Bandzaitis 1965, Sharp 1967). In the formula of Trlifaj (1972) the 9-j symbol with one stretched configuration occurs, which may be expressed as a double sum.

We have ten independent summation indexes, including two from 9-j and 6-j symbols, in the present formula. At the same time, Trlifaj's formula contains seven independent summations, including two from the 9-j symbol. The summations are, however, more factorised in our expression. We have a larger number of summation variables, but the sums have a lower folding than those in the formula by Trlifaj (1972). In the final effect our formula is simpler to compute than that of Trlifaj. Moreover, the part depending on the radial quantum numbers appears in equations (6)–(8) in a fourfold sum, whereas in Trlifaj's formula it appears in a fivefold sum. Therefore, our expression will be efficient especially for large radial quantum numbers.

We have written a computer program based on equations (6)–(8) and compared results with the program of Sotona and Gmitro (1972) where Trlifaj's formula has been used. The time gain with our program has been a factor of about 1·5 and has reached a factor of 3 when the TMB with higher radial quantum numbers ($n \approx 8$) has been computed.

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Appendix

In this appendix we prove the relation (5)†. We rewrite the left-hand side of (5) in the form

$$\sum_{k_1 k_2} \delta(k_1+k_2,\lambda)\frac{(-1)^{k_1}}{k_1!k_2!} L_{n_1}^{\alpha_1+k_1}(x_1) L_{n_2}^{\alpha_2+k_2}(x_2), \tag{A.1}$$

which, after explicitly writing the Laguerre polynomials, is

$$\sum_{j_1 j_2} \frac{(-1)^{j_1+j_2} x_1^{j_1} x_2^{j_2}}{j_1! j_2! (n_1-j_1)!(n_2-j_2)!} \sum_{k_1 k_2} \delta(k_1+k_2,\lambda)\frac{(-1)^{k_1}}{k_1!k_2!} \frac{\Gamma(n_1+\alpha_1+k_1+1)\Gamma(n_2+\alpha_2+k_2+1)}{\Gamma(j_1+\alpha_1+k_1+1)\Gamma(j_2+\alpha_2+k_2+1)}.$$

Now we use the relation

$$\delta(k_1+k_2,\lambda) = \frac{1}{2\pi \mathrm{i}} \oint \mathrm{d}s\, s^{k_1+k_2-\lambda-1}$$

with the complex contour of integration around the origin. Noting the definition of the confluent hypergeometric function $\phi(\alpha,\beta;z)$ (Gradshteyn and Ryzhik 1962) we get

$$\sum_{j_1 j_2} \frac{(-1)^{j_1+j_2} x_1^{j_1} x_2^{j_2}}{j_1! j_2! (n_1-j_1)!(n_2-j_2)!} \frac{\Gamma(n_1+\alpha_1+1)\Gamma(n_2+\alpha_2+1)}{\Gamma(j_1+\alpha_1+1)\Gamma(j_2+\alpha_2+1)}$$
$$\times \frac{1}{2\pi \mathrm{i}} \oint \frac{\mathrm{d}s}{s^{\lambda+1}} \phi(n_1+\alpha_1+1, j_1+\alpha_1+1; -s)\phi(n_2+\alpha_2+1, j_2+\alpha_2+1; s). \tag{A.2}$$

Using the transformation formula

$$\phi(\alpha,\beta;z) = \mathrm{e}^z \phi(\beta-\alpha,\beta;z)$$

and the relation between the confluent hypergeometric function and Laguerre polynomial

$$L_n^\alpha(x) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)} \phi(-n,\alpha+1;x)$$

† The procedure of the proof has been suggested to us by L Trlifaj.

we rewrite (A.2) as

$$\sum_{j_1 j_2} \frac{(-1)^{j_1+j_2} x_1^{j_1} x_2^{j_2}}{j_1! j_2!} \frac{1}{2\pi i} \oint \frac{ds}{s^{\lambda+1}} L_{n_1-j_1}^{j_1+\alpha_1}(s) L_{n_2-j_2}^{j_2+\alpha_2}(-s).$$

This is simply equal to

$$\sum_{j_1 j_2} \frac{(-1)^{j_1+j_2} x_1^{j_1} x_2^{j_2}}{j_1! j_2!} \sum_{k_1 k_2} \delta(k_1+k_2, \lambda)$$

$$\times \frac{(-1)^{k_1}}{k_1! k_2!} \frac{\Gamma(n_1+\alpha_1+1)\Gamma(n_2+\alpha_2+1)}{(n_1-k_1-j_1)!(n_2-k_2-j_2)!\Gamma(k_1+j_1+\alpha_1+1)\Gamma(k_2+j_2+\alpha_2+1)}$$

or equivalent to

$$\sum_{k_1 k_2} \delta(k_1+k_2, \lambda) \frac{(-1)^{k_1}}{k_1! k_2!} L_{n_1-k_1}^{\alpha_1+k_1}(x_1) L_{n_2-k_2}^{\alpha_2+k_2}(x_2),$$

which proves the relation (5).

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