RECURRENCE RELATIONS FOR HARMONIC OSCILLATOR BRACKETS*)

Jan Dobeš

Institute of Nuclear Physics, Czechosl. Acad. Sci., 250 68 Řež, Czechoslovakia

Received 26 January 1990

New recurrence relations for the harmonic oscillator Talmi-Moshinsky brackets are derived. The angular momenta are kept constant in these relations.

1. Introduction

In many problems of physics treated on the harmonic oscillator basis, one has to perform a transformation for two-body system from the single-particle coordinates to the centre-of-mass (c.m.) and relative coordinates. The coefficients of such a transformation are called the harmonic oscillator Talmi-Moshinsky brackets (TMB) [1–3]. They are of especial usefulness in nuclear structure and reaction theories. In fact, the harmonic oscillator basis is the only basis in which the transformation from the single-particle to the c.m. and relative coordinates is carried out in closed form. For a general single particle basis, one often uses an expansion in terms of the harmonic oscillator functions followed by the Talmi-Moshinsky transformation. Then, many TMB should be calculated with considerable computer-time demands. Efficient methods for computation of TMB are therefore of importance.

In this respect, a closed formula derived by Trlifaj [4] has been useful. Trlifaj employed skilfully the fact that the TM transformation also holds for a particular value of the coordinates, namely when the relative coordinate of the two particles is set to zero. A computer program based on that formula has been written [5]. The approach of Trlifaj has further been simplified by the present author [6, 7]. The closed formula of ref. [6] proved to be quite efficient especially in the cases of calculations of large matrices of TMB with the fixed angular momentum values. We note that such matrices appear in most of physical problems.

Another procedure which is offered for the calculation of large sets of TMB is the use of recurrence relations. The original recurrence relations [2, 8] combine TMB with different sets of angular momenta so that their application to the above-mentioned problem of fixed angular momenta is not convenient. The angular momentum variables are fixed in recurrence approach devised by Raynal [9], where the TMB is combined from the transformation coefficients of hyperspherical harmonics. For the latter, the recurrence relations have been derived. In practical calculations,

*) Dedicated to Ladislav Trlifaj on the occasion of his sixty-fifth birthday.

however, the Raynal method appears to be slightly less efficient than the use of closed formula [6].

In this paper, new recurrence relations for TMB are derived starting directly from the expression of ref. [6]. The angular momenta are fixed in the relations. As it was pointed out above, the TMB with fixed angular momenta are needed in most of applications. The present recurrence relations suggest themselves for efficient practical calculations.

2. Definitions

The tensor product of harmonic oscillator wave functions is expanded in the c.m. and relative coordinates as

$$(\phi_{n_1}^{l_1}(\boldsymbol{r}_1) \otimes \phi_{n_2}^{l_2}(\boldsymbol{r}_2))^{(\lambda)} = \sum \langle nlNL; \lambda \mid n_1 l_1 n_2 l_2; \lambda \rangle_D (\phi_n^l(\boldsymbol{r}) \otimes \phi_N^L(\boldsymbol{R}))^{(\lambda)} . \tag{1}$$

Here, the harmonic oscillator wave function is defined by

$$\phi_n^{lm}(\boldsymbol{r}) = c_{nl} r^l \exp\left(-\tfrac{1}{2}r^2\right) L_n^{l+1/2}(r^2)\, Y_l^m(\hat{\boldsymbol{r}}) ,$$

with the normalization constant

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

and the Laguerre polynomial

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

The harmonic oscillator bracket is denoted as $\langle nlNL; \lambda \mid n_1 l_1 n_2 l_2; \lambda \rangle_D$. The argument vector $\boldsymbol{r}$ of harmonic oscillator function is related to the usual position vector $\boldsymbol{x}$ by

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

with the mass of particle m and the harmonic oscillator frequency ω. The angular momentum coupling is denoted by $(\otimes)^{(j)}$ and the magnetic quantum numbers are not written explicitly in eq. (1). The single-particle coordinates $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ and the c.m. and relative coordinates $\boldsymbol{R}$ and $\boldsymbol{r}$ are related by

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

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

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

The TMB obeys the selection rules

$$2n + l + 2N + L = 2n_1 + l_1 + 2n_2 + l_2 ,$$

$$(-1)^{l+L} = (-1)^{l_1 + l_2} .$$

3. Recurrence relations

We start from the closed form expression given in refs. [6, 7]. Combining eqs. (11) and (12) of ref. [7], one writes TMB as

$$\begin{aligned}
&\langle nlNl; \lambda \mid n_1 l_1 n_2 l_2; \lambda \rangle_D = \\
&= (-1)^N \left(\frac{n!}{N!\, \Gamma(n + l + 3/2)\, \Gamma(N + L + 3/2)} \right)^{1/2} \\
&\times (n_1!\, n_2!\, \Gamma(n_1 + l_1 + 3/2)\, \Gamma(n_2 + l_2 + 3/2))^{1/2} \\
&\times \sum_{j_1 j} R_{j_1 j} \frac{1}{(n - n_1 - n_2 + j)!\, (n_1 - j_1)!\, (n_2 - j + j_1)!},
\end{aligned} \tag{2}$$

where the factor $R_{j_1 j}$ is given explicitly by eq. (13) of ref. [7]. This factor does not depend on the radial quantum numbers n, N, n_1, and n_2. An identity is easily proved

$$\begin{aligned}
&\frac{1}{(n - n_1 - n_2 + j)!\, (n_1 - j_1)!\, (n_2 - j + j_1)!} = \\
&= \frac{n + 1}{(n + 1 - n_1 - n_2 + j)!\, (n_1 - j_1)!\, (n_2 - j + j_1)!} \\
&- \frac{1}{(n + 1 - n_1 - n_2 + j)!\, (n_1 - j_1)!\, (n_2 - 1 - j + j_1)!} \\
&- \frac{1}{(n + 1 - n_1 - n_2 + j)!\, (n_1 - 1 - j_1)!\, (n_2 - j + j_1)!}.
\end{aligned}$$

Putting this identity into eq. (2), the recurrence relation is found after a simple manipulation

$$\begin{aligned}
&\langle nlNL; \lambda \mid n_1 l_1 n_2 l_2; \lambda \rangle_D \\
&= - \left(\frac{(n + 1)(n + l + 3/2)}{N(N + L + 1/2)} \right)^{1/2} \langle n + 1lN - 1L; \lambda \mid n_1 l_1 n_2 l_2; \lambda \rangle_D \\
&+ \left(\frac{n_2(n_2 + l_2 + 1/2)}{N(N + L + 1/2)} \right)^{1/2} \langle nlN - 1L; \lambda \mid n_1 l_1 n_2 - 1 l_2; \lambda \rangle_D \\
&+ \left(\frac{n_1(n_1 + l_1 + 1/2)}{N(N + L + 1/2)} \right)^{1/2} \langle nlN - 1L; \lambda \mid n_1 - 1 l_1 n_2 l_2; \lambda \rangle_D .
\end{aligned} \tag{3}$$

This relation can be used for successive computation of TMB with fixed angular momenta l, L, l_1, l_2 and λ. Knowing set of TMB for $2n + 2N + l + L = 2n_1 + 2n_2 + l_1 + l_2 = \varrho - 2$ and the starting value of TMB with $2n + l + L = 2n_1 + 2n_2 + l_1 + l_2 = \varrho, N = 0$, we obtain all TMB with $2n + 2N + l + L = \varrho$

recurrently. The starting TMB $\langle nl\,0L;\lambda\,|\,n_1l_1n_2l_2;\lambda\rangle_D$ is thus needed. To obtain this, we employ a symmetry relation [10]

$$\langle nl\,0L;\lambda\,|\,n_1l_1n_2l_2;\lambda\rangle_D = (-1)^{L-\lambda}\,\langle n_1l_1n_2l_2;\lambda\,|\,0Lnl;\lambda\rangle_{1/D}$$

and again eq. (2)

$$\begin{aligned}&\langle nl\,0L;\lambda\,|\,n_1l_1n_2l_2;\lambda\rangle_D\\&= (-1)^{L-\lambda+n_2}\left(\frac{n_1!}{n_2!\,\Gamma(n_1+l_1+3/2)\,\Gamma(n_2+l_2+3/2)}\right)^{1/2}\\&\times (n!\,\Gamma(n+l+3/2)\,\Gamma(L+3/2))^{1/2}\sum_j T_j\frac{1}{(n_1-n+j)!\,(n-j)!}\end{aligned}$$

with $T_j = R_{j0}(lL \leftrightarrow l_1l_2;1/D)$. Here, the notation in R_{j0} means that the actual values of angular momenta are interchanged and the inverse mass ratio is assumed. Employing the identity

$$\begin{aligned}\frac{1}{(n_1-n+j)!\,(n-j)!} &= \frac{n_1+1}{(n-j)!\,(n_1-n+1+j)!}\\&-\frac{1}{(n-1-j)!\,(n_1-n+1+j)!},\end{aligned}$$

we come to the recurrence relation

$$\begin{aligned}&\langle nl\,0L;\lambda\,|\,n_1l_1n_2l_2;\lambda\rangle_D\\&= -\left(\frac{(n_1+1)(n_1+l_1+3/2)}{n_2(n_2+l_2+1/2)}\right)^{1/2}\langle nl\,0L;\lambda\,|\,n_1+1l_1n_2-1l_2;\lambda\rangle_D\\&+\left(\frac{n(n+l+1/2)}{n_2(n_2+l_2+1/2)}\right)^{1/2}\langle n-1l\,0L;\lambda\,|\,n_1l_1n_2-1l_2;\lambda\rangle_D\,.\end{aligned}\tag{4}$$

The relation (4) suggests a successive calculation of $2n+l+L=\varrho$, $N=0$ TMB from the set of $2n+l+L=\varrho-2$, $N=0$ TMB and from the starting value $\langle nl\,0L;\lambda\,|\,n_1l_1\,0l_2;\lambda\rangle_D$. This starting value can be obtained simply by using directly the closed form expression of ref. [6].

The present recurrence relations thus provide a simple algorithm for obtaining TMB. Of course, its numerical stability remains to be investigated in practical computations.

References

[1] Talmi I.: Helv. Phys. Acta *25* (1952) 185.
[2] Moshinsky M.: Nucl. Phys. *13* (1959) 104.
[3] Smirnov Yu. F.: Nucl. Phys. *39* (1961) 346.

[4] Trlifaj L.: Phys. Rev. C *5* (1972) 1534.
[5] Sotona M., Gmitro M.: Comput. Phys. Commun. *3* (1972) 53.
[6] Dobeš J.: J. Phys. A: Math. Gen. *10* (1977) 2053; *11* (1978) 2131.
[7] Dobeš J.: Comput. Phys. Commun. *16* (1979) 373.
[8] Arima A., Terasawa T.: Prog. Theor. Phys. *23* (1960) 115.
Baranger M., Davies K. T. R.: Nucl. Phys. *79* (1966) 403.
Efros V. D.: Nucl. Phys. A *202* (1973) 180.
[9] Raynal J.: Nucl. Phys. A *259* (1976) 272.
[10] Brody T. A., Moshinsky M.: Tables of Transformation Brackets. Monografías del Instituto de Física, Mexico, 1960.