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A procedure to calculate the Talmi–Moshinsky coefficients for N-body systems with arbitrary masses†

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Abstract. A procedure is proposed to calculate the Talmi-Moshinsky coefficients of an N-body system with arbitrary masses by using those of its subsystems.

1. Introduction

The Talmi-Moshinsky coefficient (TMC) (Talmi 1952, Moshinsky 1959, Tobocman 1981) is a powerful tool in the calculation of few-body problems. The explicit expression of TMC is very complicated (Tobocman 1981, Gan *et al* 1985) and it becomes much more complicated when the number of particles increases. On the other hand, due to the great progress in computer science, the calculation of the N-body problem with $N \geqslant 5$ (Bao and Lim 1987) is gradually entering into the schedule of few-body physicists. Hence, it is desirable to find a relatively convenient way to obtain the TMC for N-body systems. Since a direct derivation of these coefficients is tedious, we will instead use an iterative procedure, i.e. to obtain the N-body TMC by using those of its subsystems. In this procedure, the three-body TMC will play a role as a basic building block. As a first step, we will show in the next section how the four-body TMC is calculated by using those of the three-body systems.

2. Three-body and four-body systems

The TMC are the transformation brackets which relate the harmonic oscillator (HO) product states having different sets of Jacobi coordinates (JCO) as arguments. In a three-body system, let $\boldsymbol{\xi}_1^\alpha$, $\boldsymbol{\xi}_2^\alpha$ be the mass-weighted JCO of the α set and let $\varphi_{nl}(\boldsymbol{\xi})$ denote the HO wavefunction. Then the HO product states which may be used as basis functions in solving three-body problems can be written as

$$(\varphi_{n_1 l_1}(\boldsymbol{\xi}_1^\alpha)\varphi_{n_2 l_2}(\boldsymbol{\xi}_2^\alpha))_l \tag{1}$$

where l_1 and l_2 are coupled to l. In this expression and also in this paper, the widths of the HO wavefunctions are the same.

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Let β denote another set of JCO. The ξ_1^α and ξ_2^α are related to those of the β set by an orthogonal transformation as

$$\begin{matrix}\xi_1^\alpha \\ \xi_2^\alpha\end{matrix} = \begin{pmatrix} \cos\eta & \sin\eta \\ -\sin\eta & \cos\eta \end{pmatrix} \begin{matrix}\xi_1^\beta \\ \xi_2^\beta\end{matrix}. \tag{2}$$

Then the three-body TMC are defined by the following equations:

$$(\varphi_{n_1l_1}(\xi_1^\alpha)\varphi_{n_2l_2}(\xi_2^\alpha))_l = \sum_{n_1'l_1'n_2'l_2'} a_{n_1'l_1'n_2'l_2'}^{n_1l_1n_2l_2l}(\eta)(\varphi_{n_1'l_1'}(\xi_1^\beta)\varphi_{n_2'l_2'}(\xi_2^\beta))_l. \tag{3}$$

In these equations, besides the total angular momentum l, the energy and the parity are conserved, i.e.

$$2(n_1+n_2)+l_1+l_2 = 2(n_1'+n_2')+l_1'+l_2'. \tag{4}$$

The explicit expression of the TMC $a_{n_1'l_1'n_2'l_2'}^{n_1l_1n_2l_2l}(\eta)$ and the program in FORTRAN for computing this coefficient can be found in the papers of Tobocman (1981) and Gan *et al* (1985).

Let ξ_i^α $(i=1,2,3)$ denote a set of mass-weighted JCO of a four-body system. Let the HO product states be denoted by

$$\Phi_{[k]}(\xi_i^\alpha) \equiv [\varphi_{n_1l_1}(\xi_1^\alpha)(\varphi_{n_2l_2}(\xi_2^\alpha)\varphi_{n_3l_3}(\xi_3^\alpha))_{l_0}]_L \tag{5}$$

where $[k]$ denotes a set of quantum number: n_1l_1 n_2l_2 n_3l_3 l_0 and L.

Let ξ_i^β belong to another set of JCO. These two sets are related to each other by a three-dimensional orthogonal matrix A_β^α.

Then the four-body TMC are defined by

$$\Phi_{[k]}(\xi_i^\alpha) = \sum_{[k']} \mathfrak{a}_{[k']}^{[k]}(A_\beta^\alpha)\Phi_{[k']}(\xi_i^\beta). \tag{6}$$

As before, the total angular momentum, the energy and the parity are conserved in (6).

It is evident that the Hamiltonian of the HO product states is conserved under a general orthogonal transformation. Thus, the concept of TMC can be generalised and can be considered as a representation of the O(3) group. A well known decomposition of the three-dimensional orthogonal matrix is

$$A_\beta^\alpha = \begin{pmatrix} \lambda & & \\ & \cos\eta_1 & \sin\eta_1 \\ & -\sin\eta_1 & \cos\eta_1 \end{pmatrix} \begin{pmatrix} \cos\eta_2 & \sin\eta_2 & \\ -\sin\eta_2 & \cos\eta_2 & \\ & & 1 \end{pmatrix} \begin{pmatrix} 1 & & \\ & \cos\eta_3 & \sin\eta_3 \\ & -\sin\eta_3 & \cos\eta_3 \end{pmatrix} \tag{7}$$

where $\lambda = \det|A_\beta^\alpha|$. Since A_β^α does not represent a real rotation, we call η_1, η_2 and η_3 the quasi-Euler angles. In short, (7) is rewritten as

$$A_\beta^\alpha = M_{\eta_1}M_{\eta_2}M_{\eta_3}. \tag{8}$$

With this decomposition, the TMC defined in equation (6) can be decomposed accordingly as

$$\mathfrak{a}_{[k']}^{[k]}(A_\beta^\alpha) = \sum_{[k''],[k''']} \mathfrak{a}_{[k'']}^{[k]}(M_{\eta_1})\mathfrak{a}_{[k''']}^{[k'']}(M_{\eta_2})\mathfrak{a}_{[k']}^{[k''']}(M_{\eta_3}). \tag{9}$$

The values of η_i can be easily obtained from (7) as

$$\begin{aligned} \sin\eta_1 &= \frac{a_{31}}{(1-a_{11}^2)^{1/2}} & \cos\eta_1 &= -\frac{a_{21}}{(1-a_{11}^2)^{1/2}} \\ \sin\eta_2 &= (1-a_{11}^2)^{1/2} & \cos\eta_2 &= \frac{a_{11}}{\lambda} \\ \sin\eta_3 &= \frac{a_{13}}{\lambda(1-a_{11}^2)^{1/2}} & \cos\eta_3 &= \frac{a_{12}}{\lambda(1-a_{11}^2)^{1/2}} \end{aligned} \tag{10}$$

where a_{ij} is an element of A_β^α.

Thus there is no ambiguity in this decomposition. TMC associated with M_{η_l} in fact mainly associates only with a three-body subsystem. Thus we have

$$\mathbb{a}^{[k]}_{[k'']}(M_{\eta_1}) = \varepsilon a^{n_2 l_2 n_3 l_3 l_0}_{n_2'' l_2'' n_3'' l_3''}(\eta_1) \tag{11a}$$

with

$$\varepsilon = 1 \qquad (\text{if } \lambda = 1)$$

$$\varepsilon = (-1)^{l_1} \qquad (\text{if } \lambda = -1)$$

$$\mathbb{a}^{[k'']}_{[k''']}(M_{\eta_2}) = \sum_{\tilde{l}_0 \tilde{\tilde{l}}_0} \hat{l}_0 \hat{\tilde{l}}_0 W(l_1 l_2'' L l_3''; \tilde{l}_0 l_0) \times a^{n_1 l_1 n_2'' l_2'' \tilde{l}_0}_{n_1''' l_1''' n_2''' l_2'''}(\eta_2) \hat{\tilde{l}}_0 \hat{\tilde{\tilde{l}}}_0 W(l_1''' l_2''' L l_3'', \tilde{l}_0 \tilde{\tilde{l}}_0) \tag{11b}$$

$$\mathbb{a}^{[k''']}_{[k']}(M_{\eta_3}) = a^{n_2''' l_2''' n_3'' l_3'' \tilde{\tilde{l}}_0}_{n_2' l_2' n_3' l_3'}(\eta_3). \tag{11c}$$

In (11b) the 6-j coefficients just arise from recoupling of angular momenta and $\hat{l}_0 = (2l_0 + 1)^{1/2}$.

Inserting (11a)–(11c) into (9) we have

$$\mathbb{a}^{[k]}_{[k']}(A^\alpha_\beta) = \sum_{n_2'' l_2'' n_3'' l_3''} \varepsilon a^{n_2 l_2 n_3 l_3 l_0}_{n_2'' l_2'' n_3'' l_3''}(\eta_1) \times \sum_{\tilde{l}_0 n_2''' l_2'''} \hat{l}_0 \hat{\tilde{l}}_0 W(l_1 l_2'' L l_3'', \tilde{l}_0 l_0) a^{n_1 l_1 n_2'' l_2'' \tilde{l}_0}_{n_1' l_1' n_2''' l_2'''}(\eta_2) \times \hat{\tilde{l}}_0 \hat{l}_0' W(l_1' l_2''' L l_3'', \tilde{l}_0 l_0') a^{n_2''' l_2''' n_3'' l_3'' l_0'}_{n_1' l_2' n_3' l_3'}(\eta_3) \tag{12}$$

where we succeed in expressing the four-body TMC by those of three-body systems.

In (12), the summations are restrained by the conservation of total angular momentum, energy and parity of each three-body TMC and by the rules of angular momentum coupling.

This procedure can be generalised to an N-body system as follows.

3. N-body system

Let the HO product state of N-body system be denoted by

$$\Phi_{[k]}(\boldsymbol{\xi}^\alpha_i) \qquad i = 1, 2, \ldots, N-1 \tag{13}$$

and the TMC are defined by

$$\Phi_{[k]}(\boldsymbol{\xi}^\alpha_i) = \sum_{[k']} \mathscr{A}^{[k]}_{[k']}(\mathbb{A}^\alpha_\beta) \Phi_{[k']}(\boldsymbol{\xi}^\beta_i) \tag{14}$$

where $\mathbb{A}^\alpha_\beta$ is an $(N-1)$-dimensional orthogonal matrix which is associated with a 'rotation' in a $(N-1)$-dimensional space. Suppose that in this 'rotation', the first base vector $\hat{n}_1$ is rotated to $\pm\hat{n}_1'$; then $\mathbb{A}^\alpha_\beta$ can be naturally decomposed as

$$\mathbb{A}^\alpha_\beta = \mathbb{M}_1 \cdot \mathbb{M}_2 \tag{15}$$

where $\mathbb{M}_2$ represents a 'rotation' moving $\hat{n}_1$ to $\pm\hat{n}_1'$ while $\mathbb{M}_1$ represents a successive 'rotation' around the $\hat{n}_1'$ axes (maybe together with a reflection of the $\hat{n}_1'$).

There are different ways to define $\mathbb{M}_2$; however a convenient way is to decompose $\mathbb{M}_2$ as a product of $N-2$ orthogonal matrices

$$\mathbb{M}_2 = \prod_{i=1}^{N-2} M_i(\theta_i) \tag{16}$$

where the elements of M_i denoted by m_{kl} is equal to zero when $k \neq l$, and equal to one when $k = l$, besides $m_{ii} = m_{i+1,i+1} = \cos\theta_i$ and $m_{i,i+1} = -m_{i+1,i} = \sin\theta_i$. The domain of the parameters θ_i is $(0, \pi)$; that of θ_{N-2} is $(0, 2\pi)$.

On the other hand, $\mathbb{M}_1$ can be written as

$$\mathbb{M}_1 = \begin{pmatrix} \lambda & \\ & \mathbb{B} \end{pmatrix} \tag{17}$$

where $\mathbb{B}$ is a $(N-2)$-dimensional orthogonal matrix with

$$\det|\mathbb{B}| = +1 \qquad \lambda = \det|\mathbb{A}_\beta^\alpha|.$$

In $\mathbb{M}_2$, we have introduced $N-2$ parameters; we also have $(N-2)(N-3)/2$ parameters in $\mathbb{B}$. In total we have $(N-1)(N-2)/2$ parameters; this is the right number to determine a $(N-1)$-dimensional orthogonal matrix. Now, we are going to prove that all these parameters can be uniquely determined without ambiguity if all elements a_{ij} in $\mathbb{A}_\beta^\alpha$ are known.

Equating the elements of the first row of both sides of (15), we have

$$\begin{aligned} a_{11} &= \lambda \cos\theta_1 \\ a_{12} &= \lambda \sin\theta_1 \cos\theta_2 \\ &\vdots \\ a_{1,N-2} &= \lambda \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{N-3} \cos\theta_{N-2} \\ a_{1,N-1} &= \lambda \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{N-3} \sin\theta_{N-2}. \end{aligned} \tag{18}$$

Since the domain of θ_i is $(0, \pi)$ for $i \leqslant N-3$, θ_1 can be firstly uniquely determined as

$$\theta_1 = \cos^{-1}\frac{a_{11}}{\lambda}. \tag{19a}$$

Then

$$\begin{aligned} \theta_2 &= \cos^{-1}\frac{a_{12}}{\lambda \sin\theta_1} \\ &\vdots\,. \end{aligned} \tag{19b}$$

When θ_1 to θ_{N-3} are all known, we can determine θ_{N-2} by the last two equations of (18). In this way, we can uniquely determine $\mathbb{M}_2$.

Once $\mathbb{M}_2$ is determined, we have

$$\begin{pmatrix} \lambda & 0 \\ 0 & \mathbb{B} \end{pmatrix} = \mathbb{A}_\beta^\alpha \mathbb{M}_2^{-1}. \tag{20}$$

This equation is sufficient to determine all unknowns in $\mathbb{B}$.

Now we have achieved a decomposition of $\mathbb{A}_\beta^\alpha$. Accordingly, the N-body TMC as a representation of $O(N-1)$ groups can be decomposed in a way like (9) as

$$\mathscr{A}^{[k]}_{[k']}(\mathbb{A}_\beta^\alpha) = \sum_{[k'']} \mathscr{A}^{[k]}_{[k'']}(\mathbb{M}_1)\mathscr{A}^{[k'']}_{[k']}(\mathbb{M}_2). \tag{21}$$

Since $\mathbb{M}_1$ is essentially an element belonging to the $O(N-2)$ subgroup; thus $\mathscr{A}^{[k]}_{[k'']}(\mathbb{M}_1)$ is associated with the TMC of an $N-1$ body system. Since $\mathbb{M}_2$ is a product of a series of elements each belonging to a O(2) subgroup. Thus $\mathscr{A}^{[k'']}_{[k']}(\mathbb{M}_2)$ is a product of a series of three-body TMC. Thus, in this way we can express the TMC of a N-body system by those of its subsystems. (It should be remembered that there will be some additional coefficients such as the 6-j and/or 9-j coefficients from angular momentum recouplings just as in equation (12) derived before).

4. Examples of application and conclusion

The N-body TMC can be extensively used in the calculation of few-body systems. Two examples of its application are given as follows.

4.1. Calculation of matrix elements

Let a state of channel α having the set $\boldsymbol{\xi}_i^\alpha$ as arguments be expanded by a set of HO product states. Let another state of channel β having $\boldsymbol{\xi}_i^\beta$ as arguments be likewise expanded. Let the operator $\hat{O}(\sigma_\gamma)$ be concerned with only the degrees of freedom of a subsystem σ_γ. Let γ denote a set of JCO where σ_γ can be isolated (this implies that there is a JCO in γ connecting the centre of mass of σ_γ with the rest). Then the general matrix element

$$\langle\Phi_{[k_\beta]}(\boldsymbol{\xi}_i^\beta)|\hat{O}(\sigma_\gamma)|\Phi_{[k_\alpha]}(\boldsymbol{\xi}_i^\alpha)\rangle \tag{22}$$

can be calculated by rewriting it in a form using TMC as

$$\sum_{[k_\gamma],[k'_\gamma]} \mathscr{A}^{[k_\beta]}_{[k'_\gamma]}(\mathbb{A}^\beta_\gamma)\mathscr{A}^{[k_\alpha]}_{[k_\gamma]}(\mathbb{A}^\alpha_\gamma)\langle\Phi_{[k'_\gamma]}(\boldsymbol{\xi}_i^\gamma)|\hat{O}(\sigma_\gamma)|\Phi_{[k_\gamma]}(\boldsymbol{\xi}_i^\gamma)\rangle. \tag{23}$$

In the RHS of (23), the same set of coordinates appears in the integrand, greatly simplifying the calculation.

4.2. To form basis functions with given symmetry

In the case of an identical particle system, TMC can be used to compose basis functions having given permutation symmetry. Let S_β denote a permutation of the particles which transforms the α set of JCO into the β set:

$$S_\beta(\boldsymbol{\xi}_i^\alpha) = (\boldsymbol{\xi}_i^\beta). \tag{24}$$

Accordingly, we have

$$S_\beta\Phi_{[k]}(\boldsymbol{\xi}_i^\alpha) = \Phi_{[k]}(\boldsymbol{\xi}_i^\beta) = \sum_{[k']} \mathscr{A}^{[k]}_{[k']}(\mathbb{A}^\beta_\alpha)\Phi_{[k']}(\boldsymbol{\xi}_i^\alpha). \tag{25}$$

Let $\Sigma_\beta\, C_\beta S_\beta$ be the associated projection operator of the given symmetry. Then the basis function having $\boldsymbol{\xi}_i^\alpha$ as arguments and having the desired symmetry is just

$$\sum_{[k']}\left(\sum_\beta C_\beta\mathscr{A}^{[k]}_{[k']}(\mathbb{A}^\beta_\alpha)\right)\Phi_{[k']}(\boldsymbol{\xi}_i^\alpha). \tag{26}$$

In conclusion, we have proposed a procedure to calculate the TMC of a N-body system by using those of its subsystems. In this way, we succeed in avoiding using very complicated formulae arising from a direct derivation of those coefficients. Furthermore, this procedure holds for all N-body systems with arbitrary masses.

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