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Elementary Hyper-Trigonometry of the Particle Triangle

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Abstract. In the hyperspherical treatment of three-body rotational states we introduced earlier two special subsets of body-fixed hyperspherical harmonics. With their help elementary trigonometry-like identities are derived, interconnecting the familiar geometric angles of the triangle, the hyperspherical angles which intermix the geometric angles and the particle masses, and the so-called angles of the kinematic rotation which are purely mass-dependent. One set represents stringent constraints to be observed in any calculation using at the same time hyperspherical coordinates belonging to different fragmentations of the particles. The other one supports the conjecture of the nonexistence of simple coordinate transformation laws between hyperspherical angles belonging to different fragmentations.

1 Introduction

Hyperspherical coordinates are very useful, and hence popular, for solving problems with several particles in physics and chemistry, although analytic results are scarce. This paper intends to contribute to this latter point.

The hyperspherical method is based on the fact that the $D-$dimensional Laplacian has the alternative Cartesian and polar forms [1, 2, 3]

$$\sum_{i=1}^{D} \frac{\partial^2}{\partial x_i^2} = \frac{1}{R^{D-1}} \frac{\partial}{\partial R} R^{D-1} \frac{\partial}{\partial R} - \frac{\Lambda_D^2}{R^2}, \tag{1}$$

with $R^2 = \sum_i x_i^2$ defining the hyperradius R. The grand angular momentum operator Λ_D^2, expressed through the pair angular momenta, and its eigenvalue equation are

$$\Lambda_D^2 = \sum_{i,k} l_{ik}^2, \quad i,k = 1,2,\cdots,D, \tag{2}$$

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$$\Lambda^2_D \; Y_{K\{\widetilde{\mu}\}}(\Omega) = K(K + D - 2)Y_{K\{\widetilde{\mu}\}}(\Omega). \tag{3}$$

Here, $\{\widetilde{\mu}\}$ stands for a set of quantum numbers characterizing the degenerate hyperspherical harmonics (HH) $Y_{K\{\widetilde{\mu}\}}(\Omega)$ for each K, and Ω denotes the additional $D - 1$ variables.[1]

Since the HH can be given in terms of classical polynomials, and since the corresponding kinetic energy operator (1) looks rather simple and elegant, many authors exploited them in their studies of nuclear, atomic and chemical few-body systems, see e.g. [4, 5]. Disadvantages are, however, that the degeneracy of the $Y_{K\{\widetilde{\mu}\}}(\Omega)$,

$$dim(D, K) = (D + 2K - 2)(D + K - 3)!/(K!(D - 2)!), \tag{4}$$

is very high and that the HH are solutions of the free Schrödinger equation only. Hence the standard expansion of a physical wave function

$$\Psi^D(R, \Omega) = \sum_{K,\{\widetilde{\mu}\}} \psi_{K\{\widetilde{\mu}\}}(R)Y_{K\{\widetilde{\mu}\}}(\Omega) \tag{5}$$

often suffers from slow convergence so that usually special tricks must be devised to make the results reliable [6, 7, 8, 9].

1.1 Three-Body Rotational States

For a system of three particles with masses m_k, $k = (1, 2, 3)$, any one of the three pairs of Jacobi vectors $\{\mathbf{x}_k, \mathbf{y}_k\}$ suffices to fix the kinematics in the center of mass coordinate system, Fig 1. In our treatment of three-body rotational states we use a body-fixed frame so that the HH in each Jacobi channel k can be factorized into an external part depending on three Euler-rotation angles $\{\widetilde{\gamma}, \widetilde{\beta}, \widetilde{\alpha}\}$ which define the orientation of the body-fixed frame, and an internal one that depends on two internal variables Ω_k [10],

$$Y^{J\pi m_J}_{Kl_xl_y}(\Omega_k, \widetilde{\gamma}, \widetilde{\beta}, \widetilde{\alpha}) = \sum_{m=0(1)}^{J} u^{J\pi}_{Kl_xl_ym}(\Omega_k)B^{J\pi\, m_J}_{m}(\widetilde{\gamma}, \widetilde{\beta}, \widetilde{\alpha}). \tag{6}$$

The parity preserving combinations of the Wigner $D-$functions [10, 11],

$$B^{J\pi\, m_J}_{m}(\widetilde{\gamma}, \widetilde{\beta}, \widetilde{\alpha}) = \frac{(-\mathrm{i})^m}{4\pi}\sqrt{\frac{2J + 1}{1 + \delta_{0m}}} \times \left[D^J_{-m,-m_J}(\widetilde{\gamma}, \widetilde{\beta}, \widetilde{\alpha}) + \pi\,(-)^J D^J_{m,-m_J}(\widetilde{\gamma}, \widetilde{\beta}, \widetilde{\alpha})\right], \tag{7}$$

represent the partial wave components of the HH (6). Here, J stands for the total angular momentum and π for the total parity quantum number, $m_J(m)$ is the quantum number of the space(body)-fixed projection of $\mathbf{J}$; l_x and l_y are the orbital angular momentum quantum numbers connected with the k-th Jacobi vector pair. The coefficients in (6) are conveniently arranged as a column matrix $\mathbf{u}^{J\pi}_{Kl_xl_y}(\widetilde{\Omega}_k)$ of dimension J or $(J + 1)$ for normal and abnormal parity states,

[1] Obviously, for the three dimensional case of two particles in the center of mass system Λ^2_3 will be just the familiar orbital angular momentum operator l^2.

resp., and serve to expand the internal part of the total wave function of the physical system.

In applications, this expansion can be dramatically simplified [12, 13] if the analysis can be restricted to special minimal subsets of HH. The internal parts of those subsets will be called intrinsic hyperspherical harmonics (*IHH*), see the next Section for their formal definition. Specifically we present the basis already used in our variational adiabatic treatment of the $(J = 31, \pi = -1)$-symmetry states of the hydrogen molecular ion H_2^+ [14] and utilize it now for analytic work. Besides it is also instructive to compare it with more famous basis sets [6, 7, 8, 9]. The manipulations with the *IHH* are straightforward since for each K the corresponding degenerate *IHH*-set can be represented as a triangular solution matrix. Simple formulae interconnecting the *IHH* in different channels can be derived, some of them to be given in this paper. The usefulness of the *IHH* has already been demonstrated by a derivation of a new representation of the Wigner parity-projected rotation matrices in [15] and of new identities for the Legendre polynomials in [12] [2].

In the same way, relations have been found in [17, 18] between the *IHH* solution matrices in different Jacobi channels which depend on internal hyperspherical angles and involve in addition a Raynal-Revai orthogonal transformation matrix (depending on the masses of the particles) [19] and a Wigner rotation matrix accounting for a change of the body-fixed quantization axis (the latter depends on the internal angles of the triangle). These results will be generalized in the present paper by utilizing for the *IHH* alternative choices of the body-fixed quantization axis.

1.2 Kinematic relations

Let the Jacobi coordinate $\mathbf{x}_k$ be the vector pointing from particle i to particle j, with the corresponding reduced mass M_k, while the Jacobi coordinate $\mathbf{y}_k$ points from the center-of-mass of $(i+j)$ to particle k, with the reduced mass μ_k, $i \neq j \neq k \in (1,2,3)$. Unit vectors are characterized by a hat. For the reduced masses we have the standard expressions

$$M_k^{-1} = m_i^{-1} + m_j^{-1}, \quad \mu_k^{-1} = m_k^{-1} + (m_i + m_j)^{-1}. \tag{8}$$

In this paper and for numerical tests we use three mass-depending parameters, namely $\mu = \mu_3, M = M_3$, and $\kappa = (m_1 - m_2)/(m_2 + m_3)$. Thus, for example, the $\{k = 2\}$ and the $\{k = 3\}$ Jacobi pairs are related via

$$\begin{pmatrix} c_2\mathbf{x}_2 \\ c_2^{-1}\mathbf{y}_2 \end{pmatrix} = \mathbf{R}^{1,-1}(\phi_{23}) \begin{pmatrix} c_3\mathbf{x}_3 \\ c_3^{-1}\mathbf{y}_3 \end{pmatrix}, \tag{9}$$

where

$$\mathbf{R}^{1,-1}(\phi) = \begin{pmatrix} -\cos\phi & -\sin\phi \\ \sin\phi & -\cos\phi \end{pmatrix}, \tag{10}$$

$$c_2^4 = 4c/\rho_2^2, \ c_3^4 = 1/4c, \ \sin^2\phi_{23} = 1/\rho_2, \tag{11}$$

[2] This same idea was used in [16] to derive the threshold laws for three-body recombination.

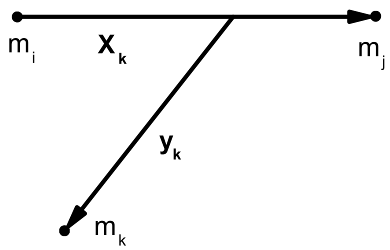

Figure 1. The Jacobi vectors for fragmentation k of three bodies.

with $c = \mu/4M$ and $\rho_2 = 1 + c(1+\kappa)^2$. The transformation (9) is written for mass-weighted coordinates and introduces the orthogonal matrix of the so-called kinematic rotation (also used later) with angle ϕ_{23} [19].

The hyperspherical coordinates $\{R, \Omega_k\}$ allow for a natural treatment of different fragmentation channels $(i+j)+k$ of a three-body system. Note that R, defined as

$$R = (x_3^2 + \mu_3 y_3^2/M_3)^{1/2}, \tag{12}$$

is, up to constant scaling factors, independent of the Jacobi index and, therefore, called "global" variable. In contrast, the $\{\Omega_k\}$ are channel-dependent. For this reason it is useful to have at hand for each k a set of hyperspherical angles and hyperspherical harmonics. The most frequently used internal hyperspherical angles $\{\Omega_k\} \equiv \{\alpha_k, \theta_k\}$ are defined as

$$\cos\theta_k = (\hat{\mathbf{x}}_k \cdot \hat{\mathbf{y}}_k), \quad \tan\alpha_k = M_k^{1/2}\ x_k/(\mu_k^{1/2}\ y_k). \tag{13}$$

1.3 Plan of the Paper

The structure of the paper is close to that of [18] but now we draw important conclusions by concretizing the general identities obtained there and present several new results. Generally speaking, elementary trigonometric functions of $\{\alpha_i, \theta_i\}$ are found to be expressible through elementary trigonometric functions of $\{\alpha_j, \theta_j\}, j \neq i$, of the corresponding angle of kinematic rotation and of the geometric angle accounting for the change of the quantization axis. The next section introduces the classical three-body HH in the laboratory and body-fixed coordinate frames. Also an example of the relations to be considered later on is given. The *IHH* are defined for arbitrary total angular momentum J and parity π. For illustration the case $(J = 1, \pi = -1)$ is described explicitly. The detailed forms of the *IHH* and the corresponding solution matrices are presented in the subsequent section. The following two sections contain the new results. In the first one we derive two independent expressions for the angle of the kinematic rotation in terms of the basic hyperspherical angles. They are expected to serve as stringent analytic checks of any numerical work that makes use of hypespherical angles in different channels, which is generally the case. The other section describes alltogether eight simple identities, four of them new. Here we argue as to the completeness of this list of simple equations. The last section contains our conclusions.

2 Classical HH and Intrinsic HH (*IHH*)

For three particles in the c.m. system ($D = 6$) the hyperangular momentum operator (2) reads (note that whenever an expression holds for any index k, the latter will be omitted to keep the notation concise)

$$\Lambda^2 = -\frac{1}{\sin^2 2\alpha}\frac{\partial}{\partial\alpha}\sin^2 2\alpha\frac{\partial}{\partial\alpha} + \frac{\mathbf{l}_y^2}{\cos^2\alpha} + \frac{\mathbf{l}_x^2}{\sin^2\alpha}. \tag{14}$$

The volume element is given by $dv = R^5 dR d\hat{o}$, with $d\hat{o} = (\sin\alpha\cos\alpha)^2 d\alpha d\hat{\mathbf{x}} d\hat{\mathbf{y}}$. The eigenfunctions $Y_{K\{\widetilde{\mu}\}}$ of (14) (HH) depend now on five hyperangles $\{\Omega\}$, with the degeneracy $\sim K^4 (K = 0, 1, 2, \cdots)$, as given by (4).

2.1 Classical Case

The most commonly used laboratory set of five hyperangles is $\{\Omega\} = \{\alpha_i, \hat{\mathbf{x}}_i, \hat{\mathbf{y}}_i\}$, where $\hat{\mathbf{x}}_i$ and $\hat{\mathbf{y}}_i$ stand for the polar angles of the corresponding unit vectors. The non-normalized eigenfunctions of (14) have the known analytic form [2, 3]

$$Y^{J\pi M_J}_{Kl_xl_y}(\alpha, \hat{\mathbf{x}}, \hat{\mathbf{y}}) = \cos^{l_x}\alpha\, \sin^{l_y}\alpha\; F(-n_\alpha, a, b; \sin^2\alpha)\mathcal{Y}^{J\pi M_J}_{l_xl_y}(\hat{\mathbf{x}}, \hat{\mathbf{y}}), \tag{15}$$

with the bipolar harmonics defined by

$$\mathcal{Y}^{J\pi M_J}_{l_xl_y}(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = \left[1 + \pi\,(-1)^{l_x+l_y}\right] \sum_{m,m'} Y_{l_xm}(\hat{\mathbf{x}}) Y_{l_ym'}(\hat{\mathbf{y}})(l_x, l_y, m, m'|J, M_J). \tag{16}$$

The first parameter $n_\alpha = (K - l_x - l_y)/2$ of the hypergeometric function F should be non-negative, $a = (K + l_x + l_y + 4)/2$ and $b = l_y + 3/2$.

2.2 Intrinsic HH (IHH)

In what follows, we shall work with the subsets of HH satisfying either the condition $K = J$ or $K = J + 1$, depending on the parity [12]. They can most directly be introduced by making use of a familiar relation for the grand angular momentum [1, 2, 3]

$$K = 2n_\alpha + l_x + l_y, \tag{17}$$

which illustrates the fact that six-dimensional rotations are composed of physical and "quasiradial" (internal) ones. Indeed,

$$n_\alpha = 0 \tag{18}$$

isolates the subspace of the purely rotational HH [3]. For fixed K, condition (18) allows one to simplify the notation as the quantum numbers K and l_x can be omitted, leaving $l_y \equiv l$. Define

$$\epsilon \equiv K - J = 0(1) \text{ for } \pi = -1(+1). \tag{19}$$

[3] It is easy to see that the restriction (18) is equivalent to the conditions derived by Schwartz in his successful variational use of bipolar spherical harmonics [20].

Then it proves advantageous to introduce for each $l = (\epsilon, \epsilon+1, \cdots, J)$ a column matrix HH, referenced to as *IHH* and with elements enumerated by the magnetic quantum number $m = (\epsilon, \cdots, l)$, that depends on two internal hyperspherical angles,

$$\mathbf{u}_l^{J\pi}(\alpha_i, \theta_i)|_{\hat{\boldsymbol{\omega}}} \equiv \mathbf{u}_{Kl_xl_y}^{J\pi}(\alpha_i, \theta_i)|_{\hat{\boldsymbol{\omega}}}. \tag{20}$$

The subscript $\hat{\boldsymbol{\omega}}$ characterizes the direction of the quantization axis. It is obvious that using relations like (9) one can form scalar products of vectors from different Jacobi sets leading to identities which include the usual internal angles of the triangle, a kinematic angle like ϕ_{23}, and the hyperspherical angles. Indeed, we were able to derive an infinite series of matrix equalities of that kind. A typical example of one that interconnects two pairs of hyperspherical angles reads as

$$\mathbf{d}^{1,-1}(\theta_{23})\mathbf{P}^{1,-1}(\alpha_2, \theta_2) = \mathbf{P}^{1,-1}(\alpha_3, \theta_3)\mathbf{R}^{1,-1}(\phi_{23}), \tag{21}$$

with $\mathbf{R}^{1,-1}(\phi)$ given by (10), $\cos\theta_{23} = (\hat{\mathbf{x}}_2 \cdot \hat{\mathbf{x}}_3)$ and

$$\mathbf{d}^{1,-1}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \tag{22}$$

$$\mathbf{P}^{1,-1}(\alpha, \theta) = \begin{pmatrix} \sin\alpha & \cos\alpha\cos\theta \\ 0 & -\cos\alpha\sin\theta \end{pmatrix}. \tag{23}$$

The geometric background of (21) is as follows. The triangular solution matrix of the intrinsic hyperspherical harmonics (see next section for details) in channel $\{k = 2\}$ (utilizing $\hat{\boldsymbol{\omega}} = \hat{\mathbf{x}}_2$ as the quantization axis), if multiplied from left by the rotation matrix, equals the equivalent solution matrix but in channel $\{k = 3\}$ (quantized with respect to $\hat{\mathbf{x}}_3$) multiplied from right by the matrix of the kinematic rotation. It is exactly the generalized Raynal-Revai transformation relation used in the subspace of the *IHH* (20), except that an additional rotation matrix occurs since different quantization axes are used simultaneously. In [17] we have shown that the matrix identity (21) is just the specialization to $(J = 1, \pi = -1)$ of the general result interconnecting *IHH*'s in the $\{2\}-$ and $\{3\}-$channels

$$\mathbf{d}^{J\pi}(\theta_{23})\mathbf{P}^{J\pi}(\alpha_2, \theta_2) = \mathbf{P}^{J\pi}(\alpha_3, \theta_3)\mathbf{R}^{J\pi}(\phi_{23}), \tag{24}$$

where the auxiliary matrix $\mathbf{P}^{J\pi}(\alpha_i, \theta_i)$ is defined in the next section, $\mathbf{R}^{J\pi}(\phi)$ is the matrix of the kinematic rotation (also given later). The elements of the parity-projected Wigner matrices $\mathbf{d}^{J\pi}(\theta)$ were introduced in [10] as

$$d_{mm'}^{J\pi}(\theta) = \frac{d_{mm'}^J(\theta) + \pi\,(-1)^{J+m'} d_{m,-m'}^J(\theta))}{(1+\delta_{m0})(1+\delta_{m'0})}, \tag{25}$$

with $d_{mm'}^J(\theta)$ denoting the usual Wigner-rotation matrix elements [11].

3 Explicit Form of the *IHH* and the Solution Matrices

The column matrix *IHH* solves, for each l, the matrix differential equation [12]

$$\left\{[\Lambda_i^2]^{J\pi}|_{\hat{\boldsymbol{\omega}}} - (J+\epsilon)(J+\epsilon+4)\right\}\ \mathbf{u}_l^{J\pi}(\alpha_i, \theta_i)|_{\hat{\boldsymbol{\omega}}} = 0, \tag{26}$$

where $[\Lambda_i^2]^{J\pi}|_{\hat{\boldsymbol{\omega}}}$ is the hyperangular part of the total three-body kinetic energy operator projected onto the states of fixed total angular momentum J and parity π, with quantization axis $\hat{\boldsymbol{\omega}}$. This eigenvalue equation holds for states of any parity. After introducing for each possible $l = (\epsilon, \cdots, J)$ and $L = J - l + \epsilon$ the auxiliary column matrix[4] $\mathbf{p}_l^{J\pi}(\alpha_i, \theta_i)$ with elements $p_{lm}^{J\pi}(\alpha_i, \theta_i), m = \epsilon, \cdots, l$,

$$\mathbf{p}_l^{J\pi}(\alpha_i, \theta_i) = \frac{\sin^L \alpha_i \cos^l \alpha_i}{\sqrt{l!!\ L!!}} \begin{pmatrix} (-1)^\epsilon U_{\epsilon L}^{J\pi l}\ P_l^\epsilon(\theta_i) \\ \vdots \\ (-1)^m U_{mL}^{J\pi l}\ P_l^m(\theta_i) \\ \vdots \\ (-1)^l U_{lL}^{J\pi l}\ P_l^l(\theta_i) \end{pmatrix}, \tag{27}$$

we are ready to write down the basic entity of the approach, which is the column matrix *IHH* $\mathbf{u}_l^{J\pi}(\alpha_i, \theta_i)|_{\hat{\boldsymbol{\omega}}}$, in the factorized form

$$\mathbf{u}_l^{J\pi}(\alpha_i, \theta_i)|_{\hat{\boldsymbol{\omega}}} = \mathbf{d}^{J\pi}(\omega_i)\ \mathbf{p}_l^{J\pi}(\alpha_i, \theta_i), \tag{28}$$

where the quantization axis is arbitrarily located within the particle plain with direction $\hat{\boldsymbol{\omega}}$. Here $\cos\omega_i = \hat{\boldsymbol{\omega}} \cdot \hat{\mathbf{x}}_i$, and the matrix elements of $\mathbf{d}^{J\pi}(\omega_i)$ are given by (24). In (27) $P_l^m(\theta_i)$ are the normalized associated Legendre polynomials. Note that the length of the column matrices $\mathbf{p}_l^{J\pi}$, i.e. the number of rows, differs for different l.

We now construct the solution matrix $\mathbf{P}^{J\pi}(\alpha_i, \theta_i)|_{\hat{\boldsymbol{\omega}}}$ whose columns are just the column vectors $\mathbf{u}_l^{J\pi}(\alpha_i, \theta_i)|_{\hat{\boldsymbol{\omega}}}$, starting with the smallest value $l = \epsilon$,

$$\mathbf{P}^{J\pi}(\alpha_i, \theta_i) = \left(\mathbf{u}_\epsilon^{J\pi}|_{\hat{\mathbf{x}}_i}, \mathbf{u}_{\epsilon+1}^{J\pi}|_{\hat{\mathbf{x}}_i}, \cdots, \mathbf{u}_J^{J\pi}|_{\hat{\mathbf{x}}_i}\right). \tag{29}$$

Herein, we have already fixed the quantisation axis $\hat{\boldsymbol{\omega}}$ to lie in the direction $\hat{\mathbf{x}}_i$. Since, as mentioned before, the column matrices $\mathbf{u}_l^{J\pi}|_{\hat{\mathbf{x}}_i}$ differ in length, they are to be filled with zeroes up to the maximal length $l = J$. Consequently, the matrix $\mathbf{P}^{J\pi}(\alpha_i, \theta_i)$ is of right-upper triangular form. The corresponding degeneracies of the specified subsets are easily seen to be:

$$dim(6, K = J) = J + 1 \text{ and } \ dim(6, K = J + 1) = J \tag{30}$$

for states of the normal and abnormal parity, respectively.

Comparison of the degree of degeneracy (30) of the *IHH* with the much higher initial one (4) of the HH is instructive. The reason for such a dramatic reduction is that the internal rotations, see (17), are frozen by condition (18). Therefore, only so many HH's are needed as to describe the rotation of the physical system.

As discussed in [15], for each Jacobi channel there exists one more "natural" body-fixed coordinate system, namely the one with quantization axis $\hat{\boldsymbol{\omega}} = \hat{\mathbf{y}}_i$.

[4] The Chang-Fano coefficients $U_{mL}^{J\pi l} = p(-)^{J+l+m}\sqrt{2-\delta_{0m}}(l, J, -m, m|L, 0)\Big(\sum_{m=0}^{l}\ (U_{mL}^{J\pi l})^2 = 1\Big)$ were defined earlier [21]. The peculiar form of the *IHH* (28) reflects the fact that the space- to body-fixed coordinate transformation was carried out in two steps. First, two space-fixed unit vectors are brought into the plane of the particle triangle with the z'-axis pointing along $\mathbf{x}_3$. Then, the rotation in the particle-plane about the angle ω_3 is performed: $\hat{D}^{J\pi}(\widetilde{\gamma}, \widetilde{\beta}, \widetilde{\alpha}) = \hat{D}^{J\pi}(0, \omega_3, 0)\hat{D}^{J\pi}(\phi_3, \hat{\mathbf{x}}_3)$.

Also in this case the solution matrix is simple again, namely of a left-upper triangular form (triangular with respect to the second diagonal). To stress its close analogy but also its difference to (29) we shall use the notation $\bar{\mathbf{P}}^{J\pi}(\alpha_i, \theta_i)$:

$$\bar{\mathbf{P}}^{J\pi}(\alpha_i, \theta_i) = \left(\mathbf{u}_J^{J\pi}|_{\hat{\mathbf{y}}_i}, \mathbf{u}_{J-1}^{J\pi}|_{\hat{\mathbf{y}}_i}, \cdots, \mathbf{u}_{\epsilon}^{J\pi}|_{\hat{\mathbf{y}}_i}\right). \tag{31}$$

It can be calculated from its geometric definition[5]

$$\mathbf{d}^{J\pi}(\theta_i)\mathbf{P}^{J\pi}(\alpha_i, \theta_i) = \bar{\mathbf{P}}^{J\pi}(\alpha_i, \theta_i), \tag{32}$$

which for $(J = 1, \pi = -1)$ yields, by using (22) and (23),

$$\bar{\mathbf{P}}^{1,-1}(\alpha_i, \theta_i) = \begin{pmatrix} \sin\alpha_i \cos\theta_i & \cos\alpha_i \\ \sin\alpha_i \sin\theta_i & 0 \end{pmatrix}. \tag{33}$$

As an alternative to derive $\bar{\mathbf{P}}^{J\pi}(\alpha_i, \theta_i)$ the following simple prescription applies: starting from the solution matrix $\mathbf{P}^{J\pi}(\alpha_i, \theta_i)$ we first interchange its columns by reflection on the central vertical line, and substitute α_i by $\alpha_i - \pi/2$ and θ_i by $-\theta_i$. Note that by multiplying relation (32) from the right with the inverse of $\mathbf{P}^{J\pi}(\alpha_i, \theta_i)$ one arrives at a useful method for calculating the parity-projected Wigner matrices $\mathbf{d}^{J\pi}(\theta_i)$ in terms of Legendre polynomials and Clebsch-Gordon coefficients.

In analogy to relation (21), the matrix identity for $\bar{\mathbf{P}}^{J\pi}(\alpha_i, \theta_i)$, connecting the Jacobi channels 2 and 3, reads for the special case $(J = 1, \pi = -1)$ as [18]

$$\begin{pmatrix} \cos\vartheta_{23} & \sin\vartheta_{23} \\ -\sin\vartheta_{23} & \cos\vartheta_{23} \end{pmatrix} \begin{pmatrix} \sin\alpha_2 \cos\theta_2 & \cos\alpha_2 \\ \sin\alpha_2 \sin\theta_2 & 0 \end{pmatrix} = \begin{pmatrix} \sin\alpha_3 \cos\theta_3 & \cos\alpha_3 \\ \sin\alpha_3 \sin\theta_3 & 0 \end{pmatrix} \begin{pmatrix} -\cos\phi_{23} & \sin\phi_{23} \\ -\sin\phi_{23} & -\cos\phi_{23} \end{pmatrix}. \tag{34}$$

Here the matrices (10), (22), and (33) were used and $\cos\vartheta_{23} = (\hat{\mathbf{y}}_2 \cdot \hat{\mathbf{y}}_3)$. Thus, on the left-hand side the Jacobi vector $\hat{\mathbf{y}}_2$ serves as quantization axis (before the rotation) and on the right-hand side of the identity $\hat{\mathbf{y}}_3$ (after the rotation). Generalizing (34) for the *IHH* of arbitrary $(J\pi)$-symmetry we have the matrix identity [18]

$$\mathbf{d}^{J\pi}(\vartheta_{23})\bar{\mathbf{P}}^{J\pi}(\alpha_2, \theta_2) = \bar{\mathbf{P}}^{J\pi}(\alpha_3, \theta_3)\mathbf{R}^{J\pi}(\phi_{23}). \tag{35}$$

4 Angular Form-Factor and New Identities

In the body-fixed reference frame the operator $[\Lambda_i^2]^{J\pi}|_{\hat{\boldsymbol{\omega}}}$ is the only complicated part of the three-body kinetic energy operator as it is a $(J+1-\epsilon) \times (J+1-\epsilon)$ matrix differential operator depending on the parity of the state. In [13] we have

[5] The theory described and used in the paper is not typical for the HH approach and we refer to the content of [18] where all the matrices needed for the simple but non-trivial case $(J = 1, \pi = -1)$ were written down.

introduced a new column matrix variational basis that includes the *IHH* as its angular part, [6]

$$\boldsymbol{\psi}_l^{(i)J\pi}(R,\xi,\eta) = \tilde{\mathcal{R}}_l^{(i)}(R,\sin\alpha_i)\mathbf{u}_l^{J\pi}(\alpha_i,\theta_i) \tag{36}$$

$(l=\epsilon,\cdots,J; i=1,2,3)$. Since the functions $\tilde{\mathcal{R}}_l^{(i)}(R,\sin\alpha_i)$ are arbitrary for any allowed value of the pair angular momentum l and any possible Jacobi channel i, this ansatz is rather general.

The primitives (36) diagonalize the Coriolis couplings (i.e., the operator $[\Lambda_i^2]^{J\pi}|_{\hat{\boldsymbol{\omega}}}$). This fact allows one to treat rotational states numerically as easily as nonrotational ones. Actually, in order to calculate the matrix elements of the Hamiltonian between the basis functions (36), integration must be performed over three internal variables and summation over the magnetic quantum numbers. It turns out that the latter summation can be carried out analytically [13], by factorizing out the scalar product of the two column matrix *IHH*'s as

$$\sigma_{ll'}^{ij}(\xi,\eta) = \sum_{mm'} p_{lm}^{J\pi}(\alpha_i,\theta_i)p_{l'm'}^{J\pi}(\alpha_j,\theta_j)d_{mm'}^{J\pi}(\theta_{ij}), \tag{37}$$

with $p_{lm}^{J\pi}(\alpha,\theta)$ denoting the elements of the column matrix (27) and $\cos\theta_{ij} = \hat{\mathbf{x}}_i\cdot\hat{\mathbf{x}}_j$.

It can easily be seen that $\sigma_{ll'}^{ij}$ is an element of the angular "form factor matrix"

$$\boldsymbol{\Sigma}_{ij}^{J\pi}(\xi,\eta) = \left[\mathbf{P}^{J\pi}(\alpha_i,\theta_i)\right]^T\mathbf{P}^{J\pi}(\alpha_j,\theta_j) \tag{38}$$

which, owing to (24), can be calculated by using any of two alternative expressions

$$\mathbf{R}^{J\pi}(\phi_{ij})\left[\mathbf{P}^{J\pi}(\alpha_i,\theta_i)\right]^T\mathbf{P}^{J\pi}(\alpha_i,\theta_i) = \left[\mathbf{P}^{J\pi}(\alpha_j,\theta_j)\right]^T\mathbf{P}^{J\pi}(\alpha_j,\theta_j)\mathbf{R}^{J\pi}(\phi_{ij}), \tag{39}$$

where for the *IHH* solution matrices the definition (29) is to be used.

This identity demonstrates the fact that the "form factors" (38), being "measurable" quantities, do not depend on the choice of the body-fixed quantization axis $\hat{\boldsymbol{\omega}}$. It is worth noticing that for our choice of hyperspherical harmonics (18), i.e. for the *IHH*, the orthogonal matrices of the Raynal-Revai transformation $\mathbf{R}^{J\pi}(\phi_{ij})$ can be simply given in terms of the regular Wigner rotation matrices [23]

$$\mathbf{R}^{J\pi}(\phi) = \mathbf{d}^{(J-\epsilon)/2}_{-(J+\epsilon)/2+l,-(J+\epsilon)/2+l'}(2\phi), \quad \epsilon\le l,l'\le J. \tag{40}$$

Indeed, the identity (39) has been used in our variational calculations of the adiabatic state with $(J=31,\pi=-1)$ of the molecular ion H_2^+ [14].

Specializing (39) for the states of $(J=1,\pi=-1)$-symmetry yields

$$\mathbf{R}^{1,-1}(\phi_{ij})\begin{pmatrix} 2\sin^2\alpha_i & \sin 2\alpha_i\cos\theta_i \\ \sin 2\alpha_i\cos\theta_i & 2\cos^2\alpha_i\end{pmatrix} = \tag{41}$$

[6] In the following we introduce an unspecified pair of global hyperspherical angles $\{\xi,\eta\}$ which are independent of the Jacobi channel index i. In our calculations [14] we used prolate spheroidal coordinates [22].

$$\begin{pmatrix} 2\sin^2\alpha_j & \sin 2\alpha_j \cos\theta_j \\ \sin 2\alpha_j \cos\theta_j & 2\cos^2\alpha_j \end{pmatrix} \mathbf{R}^{1,-1}(\phi_{ij}).$$

With (10) it is easily verified that from (41) only two different scalar identities follow. From the diagonal matrix elements one obtains

$$\tan\phi_{ij} = \frac{1}{2}\frac{\sin 2\alpha_j \cos\theta_j + \sin 2\alpha_i \cos\theta_i}{\sin^2\alpha_i - \sin^2\alpha_j}, \tag{42}$$

and from nondiagonal ones

$$\tan\phi_{ij} = \frac{1}{2}\frac{\sin 2\alpha_j \cos\theta_j - \sin 2\alpha_i \cos\theta_i}{\sin^2\alpha_i - \cos^2\alpha_j}. \tag{43}$$

Both expressions (42) and (43) are highly nontrivial since the kinematic angle ϕ_{ij} is defined by the particle masses, while the right-hand sides depend on both the coordinates and the masses of the particles.[7] Equation (41) can be rewritten in a simpler form which could be of practical use. For this purpose, instead of α_i and θ_i, new channel-dependent hyperspherical variables are introduced as

$$\zeta_i = \sin^2\alpha_i, \quad \tau_i = \sin\alpha_i \cos\alpha_i \cos\theta_i. \tag{44}$$

Then, using (41), we easily find that the pairs (44) in different channels are interconnected by the linear transformation

$$\mathbf{W}(\phi_{ij}) \begin{pmatrix} \zeta_i \\ \tau_i \end{pmatrix} = \begin{pmatrix} \sin^2\phi_{ij} \\ \sin\phi_{ij}\cos\phi_{ij} \end{pmatrix} + \begin{pmatrix} \zeta_j \\ \tau_j \end{pmatrix}, \tag{45}$$

with

$$\mathbf{W}(\phi_{ij}) = \begin{pmatrix} \cos\phi_{ij} & \sin\phi_{ij} \\ \sin\phi_{ij} & -\cos\phi_{ij} \end{pmatrix}. \tag{46}$$

The peculiar matrix $\mathbf{W}$ is orthogonal, coincides with its inverse and satisfies the antigroup property $\mathbf{W}(\phi_1)\mathbf{W}(\phi_2) = \mathbf{W}(\phi_1 - \phi_2)$. We point out that the hyperspherical variables (44) were introduced in [10] where they were found to be most appropriate for calculating the HH with $J = 0$ since their use disposes of the dummy singularity in the well-known analytic expression for the HH.

5 New Relations Connecting *IHH*'s from Different Jacobi Channels

In this section we generalize the matrix identities (24) and (32) that correlate the solution matrices composed of *IHH*'s having either the Jacobi vectors $\mathbf{x}_i$ and $\mathbf{x}_j$, or $\mathbf{y}_i$ and $\mathbf{y}_j$, as quantization axes. The derivation is straightforward if (24) is rewritten as

$$\mathbf{d}^{J\pi}(\vartheta_{23})\mathbf{d}^{J\pi}(\theta_2)\mathbf{d}^{J\pi}(-\theta_2)\mathbf{P}^{J\pi}(\alpha_2,\theta_2) = \mathbf{P}^{J\pi}(\alpha_3,\theta_3)\mathbf{R}^{J\pi}(\phi_{23}). \tag{47}$$

Use of the geometric definition (32) of $\bar{\mathbf{P}}^{J\pi}(\alpha_i,\theta_i)$ and the group property of the parity-preserving rotation matrices $\mathbf{d}^{J\pi}(\theta)$ then finally leads to the first of the sought-after matrix identities

$$\mathbf{d}^{J\pi}(\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{x}}_3})\bar{\mathbf{P}}^{J\pi}(\alpha_2,\theta_2) = \mathbf{P}^{J\pi}(\alpha_3,\theta_3)\mathbf{R}^{J\pi}(\phi_{23}). \tag{48}$$

[7] For $\alpha_i = \alpha_j$ only (43) can be used while for $\alpha_i = \alpha_j = \pi/4$ both expressions fail.

Here, the angle $\theta_{\hat{\mathbf{y}}_i\hat{\mathbf{x}}_j}$ between the vectors $\hat{\mathbf{y}}_i$ and $\hat{\mathbf{x}}_j$ has been introduced. Geometrically (48) means that the *IHH*'s quantized with respect to $\hat{\mathbf{y}}_2$ can be expressed in terms of the *IHH*'s quantized in the frame having $\hat{\mathbf{x}}_3$ as the $z'-$axis. For the $(J = 1, \pi = -1)$-symmetry the general result (48) reduces, when the matrices (10), (22), (23), and (33) are used, to a (2×2)-matrix identity

$$\begin{pmatrix} \cos\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{x}}_3} & \sin\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{x}}_3} \\ -\sin\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{x}}_3} & \cos\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{x}}_3} \end{pmatrix} \begin{pmatrix} \sin\alpha_2\cos\theta_2 & \cos\alpha_2 \\ \sin\alpha_2\sin\theta_2 & 0 \end{pmatrix} = \begin{pmatrix} \sin\alpha_3 & \cos\alpha_3\cos\theta_3 \\ 0 & -\cos\alpha_3\sin\theta_3 \end{pmatrix} \begin{pmatrix} -\cos\phi_{23} & \sin\phi_{23} \\ -\sin\phi_{23} & -\cos\phi_{23} \end{pmatrix}. \tag{49}$$

In a similar manner we derive the second matrix identity for an alternative choice of the quantization axis:

$$\mathbf{d}^{J\pi}(\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{y}}_3})\mathbf{P}^{J\pi}(\alpha_2,\theta_2) = \bar{\mathbf{P}}^{J\pi}(\alpha_3,\theta_3)\mathbf{R}^{J\pi}(\phi_{23}). \tag{50}$$

Specialization to the case $(J = 1, \pi = -1)$ yields

$$\begin{pmatrix} \cos\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{y}}_3} & \sin\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{y}}_3} \\ -\sin\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{y}}_3} & \cos\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{y}}_3} \end{pmatrix} \begin{pmatrix} \sin\alpha_2 & \cos\alpha_2\cos\theta_2 \\ 0 & -\cos\alpha_2\sin\theta_2 \end{pmatrix} = \begin{pmatrix} \sin\alpha_3\cos\theta_3 & \cos\alpha_3 \\ \sin\alpha_3\sin\theta_3 & 0 \end{pmatrix} \begin{pmatrix} -\cos\phi_{23} & \sin\phi_{23} \\ -\sin\phi_{23} & -\cos\phi_{23} \end{pmatrix}, \tag{51}$$

with (2×2)-matrices $\mathbf{d}^{1,-1}$, $\mathbf{P}^{1,-1}$, $\bar{\mathbf{P}}^{1,-1}$, and $\mathbf{R}^{1,-1}$ given by (22), (23), (33), and (10), respectively. In the case of (50) and (51) the *IHH* are to be quantized with respect to $\hat{\mathbf{x}}_2$ before and with respect to $\hat{\mathbf{y}}_3$ after the rotation.

6 Simple Hyper-Trigonometric Identities

Here is a "complete list" of simple hyper-trigonometric relations:

$$\sin\alpha_2\sin\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{x}}_3} = -\sin\phi_{23}\cos\alpha_3\sin\theta_3, \tag{52}$$
$$\cos\alpha_2\sin\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{y}}_3} = -\sin\phi_{23}\sin\alpha_3\sin\theta_3, \tag{53}$$
$$\cos\alpha_2\sin\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{x}}_3} = -\cos\phi_{23}\cos\alpha_3\sin\theta_3, \tag{54}$$
$$\sin\alpha_2\sin\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{y}}_3} = \cos\phi_{23}\sin\alpha_3\sin\theta_3, \tag{55}$$

and [8]

$$\sin\alpha_2\cos\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{x}}_3} = -(\sin\alpha_3\cos\phi_{23} + \cos\alpha_3\cos\theta_3\sin\phi_{23}), \tag{56}$$
$$\cos\alpha_2\cos\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{y}}_3} = -\cos\alpha_3\cos\phi_{23} + \sin\alpha_3\cos\theta_3\sin\phi_{23}, \tag{57}$$
$$\cos\alpha_2\cos\theta_{\hat{\mathbf{y}}_2\hat{\mathbf{x}}_3} = \sin\alpha_3\sin\phi_{23} - \cos\alpha_3\cos\theta_3\cos\phi_{23}, \tag{58}$$
$$\sin\alpha_2\cos\theta_{\hat{\mathbf{x}}_2\hat{\mathbf{y}}_3} = -(\cos\alpha_3\sin\phi_{23} + \sin\alpha_3\cos\theta_3\cos\phi_{23}). \tag{59}$$

[8] The next four relations can be easily produced by making use of (9) and forming the corresponding scalar product of two Jacobi vectors.

The first two identities of each sublist can be easily extracted from our earlier papers [17, 18] or from (21) and (34), the other four following from (49) and (51) are new. We believe that this list is "complete" since, if we consider the abnormal parity case of $(J = 2, \pi = -1)$-symmetry, we arrive at four similar (2×2)-matrix identities with columns belonging now to $l = 1$ and 2 in (29) - but no new result appears. Moreover, in order to derive the above list of eight independent identities, we have used four (2×2)-matrix identities with eight extra relations just fixing the kinematics of the adopted Jacobi vector description.

7 Conclusions

Different Jacobi fragmentation channels $k = 1, 2$, and 3 are needed in order to account for the complex dynamics of a three-body system. Hyperspherical coordinates allow for a fairly "democratic" treatment since they include the "global" hyperradius R. Formulae that interconnect the channel-dependent hyperspherical angles should be of practical use. We have presented several of them. All simple identities were derived using *IHH*'s (27) of $(J = 1, \pi = -1)$-symmetry where the associated Legendre polynomials occurring in the column matrices $\mathbf{p}_l^{J\pi}(\alpha_i, \theta_i)$ are trivial, and the solution matrices (29) for $\hat{\boldsymbol{\omega}} = \hat{\mathbf{x}}_i$, or (31) for $\hat{\boldsymbol{\omega}} = \hat{\mathbf{y}}_i$, are elementary (2×2) matrices, with columns belonging to $l = 0$ and 1. It is obvious that one cannot have too many simple identities of similar structure since only two independent scalar identities follow from each (2×2) matrix equation. We, therefore, believe that set of simple identities which include only elementary trigonometry functions of geometric and hypergeometric angles is "complete".

Two important consequences follow from our results:
(i) Both relations (42) and (43) consist on the left-hand side of a constant (for a given physical system) while the right-hand side interconnects hyperspherical angles from two different Jacobi channels. This provides stringent constraints in calculations which, in order to account for the physical existence of more than one fragmentation channel, use for each of them the appropriate hyperspherical angles. The existence of such constraints was, in fact, to be expected since only two variables, in addition to the hyperradius, are needed for the complete specification of the kinematics.
(ii) Relations of the type (52) to (59) provide support for the long-standing conjecture that no simple coordinate transformations exist between hyperspherical angles belonging to different Jacobi indices though formally we should have $\alpha_2 = \alpha_2(\alpha_3, \theta_3)$ and $\theta_2 = \theta_2(\alpha_3, \theta_3)$ variable transformation. The reason can now be traced to the occurrence of the angles between different quantization axes.

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