

Hypergeometric Polynomials, Hyperharmonic Discrete and Continuous Expansions: Evaluations, Interconnections, Extensions

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Abstract. The important mathematical subject of special functions and orthogonal polynomials found in the last decades a systematization regarding those of hypergeometric type. The growth of these developments are due to interconnections with quantum angular momentum theory which is basic to that of spin-networks, of recent relevance in various branches of physics. Here we consider their power as providing expansion basis sets such as specifically are needed in chemistry to represents potential energy surfaces, the achievements being discussed and illustrated. A novel visualization of key members of the polynomial sets attributes a central role to the Kravchuk polynomials: its relationship with Wigner's rotation matrix elements are here emphasized and taken as exemplary for computational and analytical features. The sets are considered regarding progress on the formulation of a discretization technique, the hyperquantization, which allows to efficiently deal with physical problems where quantum mechanical operators act on continuous manifolds, to yield discrete grids suitable for computation of matrix elements without need of multidimensional integration.

Keywords: Quantum angular momentum · Spin networks · Hyperquantization

1 Introduction

A survey has been recently presented [1] on the connection between atomic and molecular orbitals to be used as basis sets in applied quantum chemistry and those advances in the mathematics of special functions and orthogonal polynomials, not commonly explicitly related in the numerous expositions of the quantum theory of angular momentum.

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We restricted the list to nine functions, some defined on discrete grids and others spanning ranges of continuous variables. In discrete cases, the Sturm-Liouville theory of differential equations, to which Schrödinger equations belong, has its counterpart in the theory of difference equations, of recurrence relationships, of Jacobi (tridiagonal and symmetric) matrices.

Here we focus on features of these sets of orthogonal polynomials, as expansion basis sets. When properly normalized, they constitute archetypal complete sets for expanding, for example as far quantum chemistry is concerned, atomic orbitals, or in case of molecules, in terms of orthogonal polynomials centered in different space points: in general, even for molecular systems under the effect of fields where the possibility of expanding the fields themselves in the same sets of orthogonal polynomials at the end makes analytical the calculations of all the involved integrals turns out analytically advantageous and eventually also computationally.

The main mathematical ideas actually were developed also in connection with one of the pillars of theoretical physics: the quantum theory of angular momentum. In the quantum theory of angular momentum, the group theoretical aspects led to discrete sets of orthogonal objects, differently called vector coupling or recoupling coefficients, or, in equivalent language, $3j$, $6j$, …, $3nj$ symbols of quantum angular momentum theory.

The connection between the two areas became clear in the Thirties when the one-century old Jacobi theory of orthogonal polynomials reached its maturity (see [1] and references therein). At that point it was clear that Jacobi polynomials were playing a leading role and all the rest of orthogonal polynomials, depending on a smaller number of parameters, could be arranged in a way that one could in essence solve all the problems in second order ordinary differential equations, which could be reconducted to the Gaussian hypergeometric series. Wigner established the connection between Jacobi polynomials and his reduced rotation matrix elements, so the road was open to discover discrete polynomials, such as the Meixner and in particular the Kravchuk set as simple connected by explicit duality operations.

In Fig. 1, we report the 3×3 matrix partial representation of the Askey scheme with duality relations and the asymptotic connection from discrete to continuous representations. Figure 2 gives visually an impression of the content of the paper. The double arrow shows the connection of the Kravchuk polynomials with Jacobi and Meixner that proceed toward continuous type polynomials toward Laguerre and Charlier polynomials, leading to the analytical solution of the Schrödinger equation for the hydrogen atom and on the other side discrete representations, toward the Hahn and Racah polynomials, related to the theory of angular momentum to $3j$ and $6j$ respectively.

Next section gives exemplary computational illustrations for the key Kravchuk polynomials and their discrete representations [2–11]. They are functions of two variables and span a square manifold, the screen: this two-dimensional approach gives interesting insights, being a natural extension to exhibit the role of these discrete functions as matrix elements. The screen has demonstrated to be versatile and applicable to various fields that go from the theory of angular momentum to the geometrical features of molecules and the four-bar linkage mechanism in kinematics.

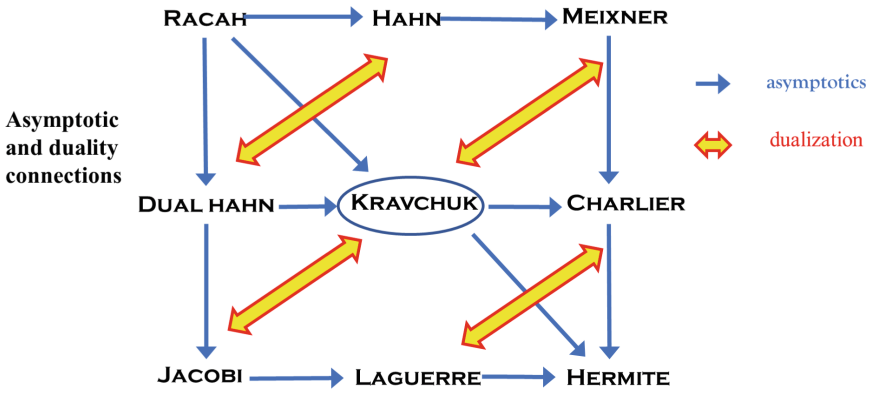

Fig. 1. The nine polynomial sets in the 3 × 3 matrix representation, adapted from [1], as a modification of a portion of the Askey scheme, emphasizing that dualization, namely exchange of role of polynomial degree and variable, appears as a reflection with respect to the main diagonal; asymptotic connections physically correspond to semiclassical limits.

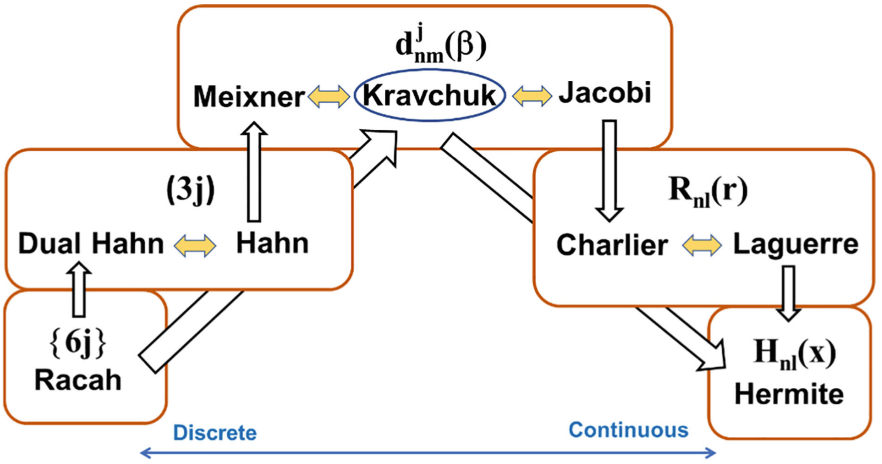

Fig. 2. The stepping stones of Fig. 1 consolidated as a bridge, where arrangement was given as a staircase, to be contrasted to the corresponding Fig. 1 in [1]. Details on the connections and emphasis of central role for the Kravchuk polynomial given in the text.

Section 3 summarizes the ingredients developed for quantum chemistry, hyperspherical harmonics [12–19] and Sturmian orbitals [20–29], applied to the methods of theoretical chemistry (see also [1]), and present conclusions.

In an Appendix we deal with use of expansions, both in continuous and in discrete sets: the sets of orthogonal polynomials [30–32] described in [1] are connected with the theory of angular momentum, specifically with the spin networks [3–5, 29, 33–45]. The hyperquantization algorithm [46–55], has been introduced to solve the reactive scattering Schrödinger equation. It employs a symmetric version of hyperspherical

coordinates, and a discretization procedure based on the special properties of the Hahn orthogonal polynomials [56]. Connections to stereodynamics [57–59] and alignment are also reported [60–68]. Spherical and hyperspherical harmonics have been employed to expand analytical expressions of potential energy surfaces of systems. The method, initially applied to treat the case of atom (p orbital) – atom (s orbital), has been extended to systems of increasing complexity including singlet-states atoms and molecules such as atom – diatom, diatom – diatom, water – atom, water – diatom, and floppy-molecule – atom [69–84].

2 Kravchuk Polynomials: Features, Computational, Caustics, Asymptotics

Section 2 of this paper presents the quantitative connections between the Kravchuk polynomials ($d^{j}_{mm'}(\beta)$ functions) with the Dual Hahn polynomials (Wigner 3j symbols) and the Racah polynomials (Wigner 6j symbols). The qualitative relationships are shown on the left side of Fig. 2, and the resulting screens are naturally on a square grid. This section illustrates the exemplary case of Kravchuk polynomials (the equations in this first paragraph are taken from [85]); the orthogonality relation is

$$\sum_{x=0}^{N}\binom{N}{x}p^{x}(1-p)^{N-x}K_m(x;p,N)K_n(x;p,N)=\binom{N}{n}^{-1}\left(\frac{1-p}{p}\right)^{n}\delta_{mn},\quad 0\le p\le 1$$

The transformation [85]

$$U_{pN}(x,n)=\sqrt{\frac{p^{x}(1-p)^{N-x}}{x!(N-x)!}}K_n(x;p,N)$$

leads to the symmetric three-term recurrence relation

$$\varsigma r_{+}(x)U_{pN}(x+1,n)+\varsigma_0 r_0(x,N)U_{pN}(x,n)+\varsigma r_{-}(x)U_{pN}(x-1,n)=\varsigma_0\lambda(n)U_{pN}(x,n)$$

where

$$r_{-}(x)=\sqrt{x(N-x+1)},\quad r_{+}(x)=r_{-}(x+1)=\sqrt{(x+1)(N-x)}$$
$$r_0(x)=x(2p-1)-pN,\qquad \lambda(n)=-n.$$

We solve the eigenvalue/eigenvector equation using double precision arithmetic. To assure the correct number of nodes and eigenvalue order we choose $\varsigma=\varsigma_0=-1$. Figure 3 shows the screen for $\left|U_{pN}(x,n)\right|$, where $N = 201$ and $p = 0.25$.

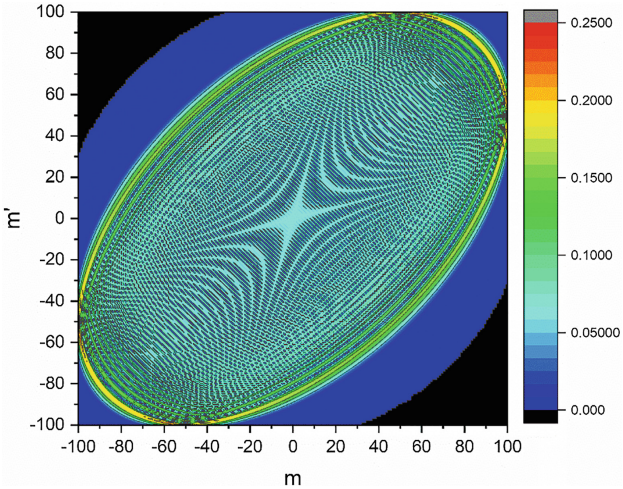

Fig. 3. Screen for Kravchuk polynomial, $UpN\,(x,\,n), j = 100$ and $p = 0.25$. The axes are labeled with m and m', but an alternative uses x and n with ranges 0 to N.

Nikiforov *et al.* [86] states in Eq. 5.1.27a (p. 236) that:

$$d^{j}_{mm'}(\beta) = (-1)^{\varphi}\frac{\sqrt{\rho(x)}}{d_n}K_n(x;p,N) = (-1)^{\varphi}U_{pN}(x,n)$$

with $\sin^2\beta/2 = p,\ \ j = N/2,\quad m = x - N/2,\quad$ and $m' = n - N/2$. The identity $cos\,\beta = 1 - 2p$ is also useful. The equation indicates that $d^{j}_{mm'}(\beta)$ and $U_{pN}(x,n)$ are identical apart from a phase factor. We have independently calculated $d^{j}_{mm'}(\beta)$ for $j = 100$ and $cos\,\beta = 0.5$ with multi-precision arithmetic, and the values of $\left|d^{j}_{mm'}(\beta)\right|$ and $\left|U_{pN}(x,n)\right|$ are identical with an absolute error less than 5×10^{-14}. With $\varsigma = \varsigma_0 = -1$ and a requirement that $K_n(x;p,N)$ is positive for $x = N$, all of the phases for $d^{j}_{mm'}(\beta)$ and $U_{pN}(x,n)$ are correct. We find that diagonalization of the tridiagonal matrix for $U_{pN}(x,n)$ is an accurate, fast method for calculation of many $d^{j}_{mm'}(\beta)$. For the computer used in this work the diagonalization method is thousands of times faster than the multiple arithmetic method. The caustics of $d^{j}_{mm'}(\beta)$ are determined by an ellipse given in [87] $j^2 sin^2\beta - m^2 - m'^2 + 2mm' cos\,\beta = 0$. The ellipse touches the left boundary of the square at the point $(m,m') = (-j,-j\cos\beta)$. The right, bottom, and top boundaries are $(j,jcos\,\beta)(-jcos\,\beta,-j)(jcos\,\beta,j)$. The caustics for $U_{pN}(x,n)$ are given by the same ellipse with the equivalencies for p, N, x, and n given above.

2.1 Representation of $d^{j}_{mm'}(\beta)$ with 6*j* Symbols. Caustics for 6*j* Symbols: $\begin{Bmatrix} a & b & x \\ c & d & y \end{Bmatrix}$

Setting $A = a + \frac{1}{2},\ B = b + \frac{1}{2},\ C = c + \frac{1}{2},\ D = d + \frac{1}{2},\ X = x + \frac{1}{2}, Y = y + 1/2,$ we can calculate the ridges:

$$X^{*2} = \frac{\left[(B^2 - C^2)(D^2 - A^2) + J_t^2 Y^2 - Y^4\right]}{2Y^2},$$
$$Y^{*2} = \frac{\left[(A^2 - B^2)(C^2 - D^2) + J_t^2 X^2 - X^4\right]}{2X^2}$$

$$\text{and } J_t^2 = A^2 + B^2 + C^2 + D^2.$$

The maximum tetrahedron volume along the X* and Y* curves:

$$V_{max,X^*} = 2F(A,D,Y)F(B,C,Y)/3Y, \qquad V_{max,Y^*} = 2F(A,B,X)F(D,C,X)/3X$$

Then the caustic becomes $X_z^2 = X^{*2} \pm 12V_{max,X^*}/Y$ and $Y_z^2 = Y^{*2} \pm 12V_{max,Y^*}/X$.

To have 6*j* coefficients in Canonical order there must be some restrains on *a, b*, c and *d*. Then $N = 2a + 1$ and *k, m,* and *n* are non-negative integers.

$$\begin{Bmatrix} a & b & x \\ c & d & y \end{Bmatrix} = \begin{Bmatrix} a & a + \frac{n}{2} & x \\ a + \frac{|m-n|}{2} + k & a + \frac{m}{2} & y \end{Bmatrix} 0 \le k \le m + n - |m - n|,$$

$$n/2 \le x \le 2a + n/2, m/2 \le y \le 2a + m/2$$

We find the 6*j* symbols that correspond to $d^{j}_{mm'}$ functions by investigating the caustic curves for both 6*j* and $d^{j}_{mm'}$. For the 6*j* caustics we have:

Consider $Y^{*2} = \left[(A^2 - B^2)(C^2 - D^2) + J_t^2 X^2 - X^4\right]/2X^2$ which becomes for $B = D$: $Y^{*2} = \left[(A^2 - B^2)(C^2 - B^2) + J_t^2 X^2 - X^4\right]/2X^2$. We have $X = B - A$ the bottom of the screen, so $Y^{*2} = [A^2 B - AB^2 - B^3 + AC^2]/[A - B]$.

The location of the gate on the west side corresponding to $X = B - A$ is given by $y = \sqrt{[A^2 B - AB^2 - B^3 + AC^2]/[A - B]} - (B - A)$. We put this expression into a more tractable form by introducing: $r = A/B$. Since A will be much smaller than B, r is much less than unity. Keeping terms of first order in r we have: $Y^* \approx 2A(1 - C^2/4B^2)$ and from the limitations for Canonical form we have $a \le c \le 2(b - a)$. Comparing the gate position for $d^{j}_{mm'}$, we see that the parameter, p, in the Kravchuk polynomials is $p = 1 - \frac{C^2}{4B^2},\ \sin^2\frac{\beta}{2} = 1 - \frac{C^2}{4B^2},\ \cos\frac{\beta}{2} = \frac{C}{2B}$. Figure 4a shows the caustic curves for $c = \sqrt{3} \times 10^8$, and $b = 10^8$. Fig. 4b and c show caustics for c = 1000000 and c = 99000000.

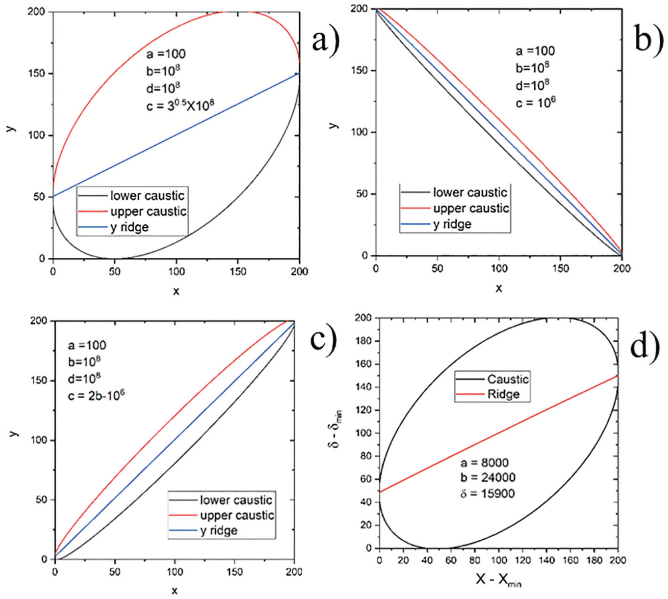

Fig. 4. Caustic curves for (a) $p = 0.25$; (b) $p = 0.999975$; (c) $p = 0.009975$; (d) 3*j* approximation to *d* function with $p = 0.25$

2.2 Representation of $d^{j}_{mm'}(\beta)$ with 3j Symbols 3j Caustics for $\begin{pmatrix} a & b & x \\ \sigma+\delta & \sigma-\delta & -2\sigma \end{pmatrix}$

Now we consider correspondence between 3*j* symbols and d functions. Neglecting the difference between *A, B, X* and *a, b, x*; where $A = a + ½$, $B = b + ½$, and $X = x + ½$ we have:

Ridges:

$$\delta^*(x) = \frac{\sigma(a^2 - b^2)}{x^2}, \qquad x^*(\delta) = \sqrt{a^2 + b^2 + 2\left(\sigma^2 - \delta^2\right)}$$

$$max(|a - b|, |2\sigma|) \le x \le a + b,$$

$$\max(-a - \sigma, -b + \sigma) \le \delta \le \min(a - \sigma, b + \sigma)$$

$$\delta = (\alpha - \beta)/2, \qquad \sigma = -\gamma/2 = (\alpha + \beta)/2$$

Upper and lower caustics are given by

$$\delta_{\pm}(x) = \delta^*(x) \pm \frac{2F(a, b, x)\sqrt{x^2 - 4\sigma^2}}{x^2},$$

Where

$$F(a,b,x) = \sqrt{(a+b+x)(-a+b+x)(a-b+x)(a+b-x)}/4$$

In our analysis, we will have large values for *a, b, x* and σ. We note that on the right $x_{\max} = a + b$ and on the left side of the screen that $x_{\min} = |2\sigma|$. Hence the number of intervals, n, is given by $n = x_{\max} - x_{\min} = a + b - |2\sigma|$, or $|\sigma| = (a + b - n)/2$. We see that n is much smaller than *a, b, x,* and σ. We also assume that b is greater than a, or that $b = ay$ where $y \geq 1$.

To proceed further we must consider whether σ is positive or negative. When s is positive, the bottom of the screen corresponds to $\delta_{\min} = -b + \sigma$ and the top of the screen corresponds to $\delta_{\max} = a - \sigma$. (Note that $n = \delta_{\max} - \delta_{\min}$, so the screen is square.). Now we relate y and p, and we see on the right side of the screen that:

$$\begin{aligned}\delta^*(x_{\max}) - \delta_{\min} &= \sigma\left(a^2 - b^2\right)/(a+b)^2 + b - \sigma = (1-p)n \\ &= \sigma(1-y)/(1+y) + ay - \sigma = (1-p)n\end{aligned}$$

After substitution with $|\sigma| = (a + b - n)/2$, we can easily find that $y = \frac{1-p}{p}$ for $0 \leq p \leq 1/2$. Now we can calculate

$$\begin{aligned}\delta^*(x_{\min}) - \delta_{\min} &= \sigma\left(a^2 - b^2\right)/(2\sigma)^2 + b - \sigma = p'n \\ &= a^2\left(1 - y^2\right)/(2\sigma) + ay - \sigma = p'n\end{aligned}$$

We can now prove that $p' \to p$ for large a. Solving the last equation for p', we find that $p' = \frac{(2a-n)p}{2n-2np} \approx p\left(1 + \frac{n}{2a} + \cdots\right)$. For large a, $p' \to p$.

Figure 4d shows a *3j* approximation to d for p = ¼. The figure is drawn with calculations based on A, B, and X. Hence the small difference with expected results from the simplified theory in this paper.

To obtain *3j* approximations to d functions with $1/2 < p \leq 1$, we must consider negative σ. Now $\delta_{\min} = -a - \sigma$, and $\delta_{\max} = b + \sigma$. Repeating the above derivation, we find that $y = p/(1-p)$ and $p' \to p$.

3 Summarizing and Concluding Remarks

In a recent paper [1] we provided an overview from an orthogonal polynomial set perspective on the quantum mechanics of hydrogen-like atom, augmented by the Fock's projection (1935) initiating use of hyperspherical harmonics as orbitals for the solution of atomic and molecular structure problems. Only recently the search started on exploiting unique properties and computational advantages leading to the development of Sturmian basis sets (see also [22]) which are essentially orthogonal polynomials of the classical series, and also to highlight how the orbitals in the reciprocal (momentum) space are hyperspherical harmonics. Not only they are continuous sets of hypergeometric polynomials, but also the connections between different representations

(or of different systems of separable coordinates) can be all written as orthogonal polynomials of discrete type, of the Hahn and Racah series. To complete picture, we found it useful to generalize to the multidimensional hydrogenic Coulomb orbitals in dimensions higher than physical. They are also useful in quantum cosmology, quantum field theory, quantum information science, not to mention that the dimensional dependence of the entropic properties for the stationary states of the multidimensional quantum systems is extensively studied for the large content in quantum information not available from the standard representation [33–36].

Sturmian basis sets in configuration space can be obtained as a product of Laguerre polynomials (one of our nine players) and a multidimensional hyperspherical harmonic, or, according to the chosen coordinate system, as the product of two Laguerre polynomials (as in parabolic coordinates) and a lower dimensional hyperspherical harmonic. These hyperspherical harmonics can, in turn, in the most general case, be written as the set of Jacobi polynomials (another player in our scheme), and, in case of special values of the parameters down to Gegenbauer, or further to Legendre, polynomials, or even to the Wigner d - matrix (*e.g.* occurring in the four dimensional symmetric harmonics on the sphere S^3).

When we move to the momentum space perspective, Coulomb Sturmian basis sets can be Fourier transformed to hyperspherical harmonics (or Jacobi polynomials), for which it is easy to explicitly work out the superposition coefficients allowing the passage from one coordinate system to another (or, alternatively, from one spatial quantization scheme to a different one, *i.e.* to different sets of quantum numbers). Indeed, such coefficients are multidimensional integrals over a product of continuous orthogonal polynomials, which, in the most general case, corresponds to discrete Racah polynomials (the upper level of our scheme), or generalized 6j coefficients. Again, upon simplification down to lower dimensionality, these coefficients asymptotically reduce to either Hahn (or dual Hahn) discrete polynomial sets, that are essentially Clebsch-Gordan or 3j coefficients, or to the Wigner d rotation matrices starting as our cornerstone in the conceptual scheme that we have come to describe as the bridge of Fig. 2.

Our survey of current advances in quantum chemistry, especially as far as the expansion of atomic and molecular orbitals is concerned as a function of mathematically and physically motivated basis sets, involved combined observations of relationships of this area with other related ones. In particular, from the mathematical point of view, it is expedient to present the important connections as far as concerning the widely investigated area of recent mathematics: they involve special functions and orthogonal polynomials, in turn related to the theory of representation of groups, specifically continuous groups, and therefore the Lie theory.

In our current work and in this paper, we have tried to provide a picture of what is our appreciation of this aspect. The presentation started with an adaptation of the current general scheme for orthogonal polynomials of hypergeometrical type as a ladder that goes from Hermite up to Racah polynomials, immediately bringing inside further connections with the theory of angular momentum: in turn, this feature has been more and more intimately connected to the area of investigation of spin-networks. Individuating the main characters of the play were restricted to nine orthogonal

polynomial sets of discrete variable and arranging them as a matrix is a compact way of putting the pieces of the mosaic into a unified scheme.

What we analyzed in this paper is limited to some aspects, essentially focused on the leading role of the polynomial of Kravchuk type and its equivalent in quantum mechanical language, the d-matrix.

A further survey will also consider well known important features: however still needing compactness. For instance, the explicit expression of the objects as truncated converging terminating series, needing some care for computation, are put into reference within the theory of hypergeometric generalized series. Regarding computation, the direct sums often present calculation difficulties, often dealt with, in modern research, by using the property that all these functions, being orthogonal polynomials, obey recurrence relationships. These relationships offer an important computational tool: they are seen to be also in connection with the fact that they are always in the scheme associated by duality with difference equation, or, in the case of the lower steps of the ladder, with differential equations of Schrödinger type, the fundamental tool in quantum theory.

The concept of special duality that involves the underlying theory is often usefully represented as a bidimensional plot, that we define as the screen that has been illustrated elsewhere for the crucial member of the set, the Kravchuk polynomials. The centrality of this function was the theme of the paper and it involved as mirror modification of the sequences in the Askey scheme, interchanging position with the Jacobi polynomial.

On the other hand the scheme has extremely important amplifications when including passage from spherical to elliptic or parabolic manifolds. The literature on q-hypergeometrical polynomials is a subject of wide interest in modern mathematics, but they are less developed as tools for expansion basis sets in quantum mechanics. Some steps were undertaken recently [4].

Appendix: Discrete and Continuous Harmonic Expansions of Intermolecular Interaction

Experiments carried out by the Stern-Gerlach magnet in the early 1990s, shown that under supersonic conditions seeded O_2 would undergo variation in speed and redistribution of the internal states (for the case of oxygen rotational and vibrational cooling), producing as additional effect the molecular alignment, *i.e.* the possibility of forcing the molecule to rotate in a preferential plane. Alignment was initially induced to various diatomic molecules and linear hydrocarbons, then extended to disk-shaped molecules like benzene. Current developments are attempting to exploit the helicoidal motion of chiral molecules. The technique determined significant advances in the area of the molecular beam scattering, especially for what concerns the phenomenology of anisotropies related to van der Waals interactions.

A conceptually important advance of the asymptotic (semiclassical) discretization of continuous function exemplified in this work lead to hyperquantization algorithms.

They are based on the observation that discrete analogues of hyperspherical harmonics can be defined by means of the 3nj symbols. The method was initially employed to solve the Schrödinger equation for the prototypical reaction F + H_2 and generalized to include other triatomic systems and various quantum effects. Exact representations have been also employed to describe steric effects in quantum mechanics, such as the interpretation of reactive scattering resonances. Tools refined for the quantum mechanical treatment of few body systems have been employed to give a reformulation of the classical mechanics protocol, to be applied in many-body problems characterizing atomic and molecular clusters.

More conventionally, spherical and hyperspherical harmonics are implemented in quantum chemical calculations to compute energy as a function of a properly defined distance and of one or more angles, according to the complexity of the system. This approach is inspired by the open-shell – closed-shell atom–atom interactions, where the angle θ defines a minimal model for collinear ($\theta = 0$) and perpendicular ($\theta = \pi/2$) configurations and had been initially to the atom – diatom case [60, 69, 88]. The method consists in an exact transformation of quantum chemical (or experimental) input data related to a minimum set of configurations, the "leading configurations", whose choice relies upon geometrical and physical characteristics of the system, by a multipolar expansion [89].

Extension of the simplest case, the abovementioned triatomic system, have been done for four- and five- body problems. For example, systems formed by two diatomic molecules can be described by two Jacobi vectors lying along the chemical bonds and a third vector which joins the centers-of-mass of the two molecules. Hyperspherical harmonics have also been applied to describe interactions of floppy molecules, characterized by having an active torsional motion, as a prototype of enantiomeric change in chiral molecules [71, 73].

References

1. Coletti, C., Aquilanti, V., Palazzetti, F.: Hypergeometric orthogonal polynomials as expansion basis sets for atomic and molecular orbitals: the Jacobi ladder. Adv. Quantum Chem. https://doi.org/10.1016/bs.aiq.2019.05.002
2. Anderson, R.W., Aquilanti, V., Cavalli, S., Grossi, G.: Stereodirected discrete bases in hindered rotor problems: atom-diatom and pendular states. J. Phys. Chem. **97**, 2443–2452 (1993). https://doi.org/10.1021/j100112a053
3. Anderson, R.W., Aquilanti, V.: The discrete representation correspondence between quantum and classical spatial distributions of angular momentum vectors. J. Chem. Phys. **124**, 214104 (9 p.) (2006)
4. Anderson, R.W., Aquilanti, V., da S. Ferreira, C.: Exact computation and large angular momentum asymptotics of 3nj symbols: semiclassical disentangling of spin networks. J. Chem. Phys. **129**, 161101 (5 p.) (2008)
5. Anderson, R.W., Aquilanti, V., Marzuoli, A.: 3nj morphogenesis and semiclassical disentangling. J. Phys. Chem. A **113**, 15106–15117 (2009). https://doi.org/10.1021/jp905212a

6. Aquilanti, V., Caglioti, C., Lombardi, A., Maciel, Glauciete S., Palazzetti, F.: Screens for displaying chirality changing mechanisms of a series of peroxides and persulfides from conformational structures computed by quantum chemistry. In: Gervasi, O., et al. (eds.) ICCSA 2017. LNCS, vol. 10408, pp. 354–368. Springer, Cham (2017). https://doi.org/10.1007/978-3-319-62404-4_26
7. Caglioti, C., Santos, R.F.D., Aquilanti, V., Lombardi, A., Palazzetti, F.: Screen mapping of structural and electric properties, chirality changing rates and racemization times of chiral peroxides and persulfides. In: AIP Conference Proceedings, vol. 2040, p. 020021 (2018). https://doi.org/10.1063/1.5079063
8. Aquilanti, V., et al.: Quadrilaterals on the square screen of their diagonals: Regge symmetries of quantum mechanical spin networks and Grashof classical mechanisms of four-bar linkages. Rend. Lincei **30**, 67–81 (2019). https://doi.org/10.1007/s12210-019-00776-x
9. Anderson, R.W., Aquilanti, V., Bitencourt, A.C.P., Marinelli, D., Ragni, M.: The screen representation of spin networks: 2D recurrence, eigenvalue equation for 6*j* symbols, geometric interpretation and Hamiltonian dynamics. In: Murgante, B., et al. (eds.) ICCSA 2013. LNCS, vol. 7972, pp. 46–59. Springer, Heidelberg (2013). https://doi.org/10.1007/978-3-642-39643-4_4
10. Bitencourt, A.C.P., Ragni, M., Littlejohn, R.G., Anderson, R., Aquilanti, V.: The screen representation of vector coupling coefficients or Wigner 3*j* symbols: exact computation and illustration of the asymptotic behavior. In: Murgante, B., et al. (eds.) ICCSA 2014. LNCS, vol. 8579, pp. 468–481. Springer, Cham (2014). https://doi.org/10.1007/978-3-319-09144-0_32
11. Aquilanti, V., et al.: The astrochemical observatory: computational and theoretical focus on molecular chirality changing torsions around O - O and S - S bonds. In: AIP Conference Proceedings, vol. 1906, p. 030010 (2017). https://doi.org/10.1063/1.5012289
12. Aquilanti, V., Cavalli, S.: Coordinates for molecular dynamics: orthogonal local systems. J. Chem. Phys. **85**, 1355–1361 (1986). https://doi.org/10.1063/1.451223
13. Aquilanti, V., Cavalli, S., Grossi, G.: Hyperspherical coordinates for molecular dynamics by the method of trees and the mapping of potential energy surfaces for triatomic systems. J. Chem. Phys. **85**, 1362–1375 (1986). https://doi.org/10.1063/1.451224
14. Aquilanti, V., Capecchi, G., Cavalli, S.: Hyperspherical coordinates for chemical reaction dynamics. Adv. Quantum Chem. **36**, 341–363 (2000). https://doi.org/10.1016/S0065-3276(08)60491-8
15. Aquilanti, V., Tonzani, S.: Three-body problem in quantum mechanics: hyperspherical elliptic coordinates and harmonic basis sets. J. Chem. Phys. **120**, 4066–4073 (2004). https://doi.org/10.1063/1.1644098
16. Aquilanti, V., Ascenzi, D., Fedeli, R., Pirani, F., Cappelletti, D.: Molecular beam scattering of nitrogen molecules in supersonic seeded beams: a probe of rotational alignment. J. Phys. Chem. A **101**, 7648–7656 (2002). https://doi.org/10.1021/jp971237t
17. Aquilanti, V., Lombardi, A., Littlejohn, R.G.: Hyperspherical harmonics for polyatomic systems: basis set for collective motions. Theoret. Chem. Acc. **111**, 400–406 (2004). https://doi.org/10.1007/s00214-003-0526-3
18. Aquilanti, V., Lombardi, A., Sevryuk, M.B.: Phase-space invariants for aggregates of particles: hyperangular momenta and partitions of the classical kinetic energy. J. Chem. Phys. **121**, 5579 (2004). https://doi.org/10.1063/1.1785785
19. Sevryuk, M.B., Lombardi, A., Aquilanti, V.: Hyperangular momenta and energy partitions in multidimensional many-particle classical mechanics: the invariance approach to cluster dynamics. Phys. Rev. A - At. Mol. Opt. Phys. **72**, 033201 (2005). https://doi.org/10.1103/PhysRevA.72.033201

20. Aquilanti, V., Cavalli, S., Coletti, C., Grossi, G.: Alternative Sturmian bases and momentum space orbitals: an application to the hydrogen molecular ion. Chem. Phys. **209**, 405–419 (1996). https://doi.org/10.1016/0301-0104(96)00162-0
21. Aquilanti, V., Cavalli, S., Coletti, C.: The d-dimensional hydrogen atom: hyperspherical harmonics as momentum space orbitals and alternative Sturmian basis sets. Chem. Phys. **214**, 1–13 (1997). https://doi.org/10.1016/S0301-0104(96)00310-2
22. Aquilanti, V., Capecchi, G.: Regular article Harmonic analysis and discrete polynomials. From semiclassical angular momentum theory to the hyperquantization algorithm. Theoret. Chem. Acc. **104**, 183–188 (2000). https://doi.org/10.1007/s002140000148
23. Aquilanti, V., Cavalli, S., Coletti, C., Di Domenico, D., Grossi, G.: Hyperspherical harmonics as Sturmian orbitals in momentum space: a systematic approach to the few-body Coulomb problem. Int. Rev. Phys. Chem. **20**, 673–709 (2010). https://doi.org/10.1080/01442350110075926
24. Aquilanti, V., Caligiana, A., Cavalli, S.: Hydrogenic elliptic orbitals. Coulomb Sturmian sets, and recoupling coefficients among alternative bases. Int. J. Quantum Chem. **92**, 99–117 (2003)
25. Aquilanti, V., Caligiana, A.: Sturmian approach to one-electron many-center system: integrals and iteration schemes. Chem. Phys. Lett. **366**, 157–164 (2002)
26. Aquilanti, V., Caligiana, A., Cavalli, S., Coletti, C.: Hydrogen orbitals in momentum space and hyperspherical harmonics: elliptic Sturmian basis sets. Int. J. Quantum Chem. **92**, 212–228 (2003)
27. Calderini, D., Cavalli, S., Coletti, C., Grossi, G., Aquilanti, V.: Hydrogenoid orbitals revisited: from Slater orbitals to Coulomb Sturmians. J. Chem. Sci. **124**, 187–192 (2012). https://doi.org/10.1007/s12039-012-0215-7
28. Coletti, C., Calderini, D., Aquilanti, V.: D-dimensional Kepler-Coulomb Sturmians and hyperspherical harmonics as complete orthonormal atomic and molecular orbitals. Adv. Quantum Chem. **67**, 73–127 (2013). https://doi.org/10.1016/B978-0-12-411544-6.00005-4
29. Calderini, D., Coletti, C., Grossi, G., Aquilanti, V.: Continuous and discrete algorithms in quantum chemistry: polynomial sets, spin networks and Sturmian orbitals. In: Murgante, B., et al. (eds.) ICCSA 2013. LNCS, vol. 7972, pp. 32–45. Springer, Heidelberg (2013). https://doi.org/10.1007/978-3-642-39643-4_3
30. Aquilanti, V., Cavalli, S., Coletti, C.: Angular and hyperangular momentum recoupling, harmonic superposition and Racah polynomials: a recursive algorithm. Chem. Phys. Lett. **344**, 587–600 (2001)
31. Aquilanti, V., Coletti, C.: 3nj-symbols and harmonic superposition coefficients: an icosahedral abacus. Chem. Phys. Lett. **344**, 601–611 (2001). https://doi.org/10.1016/S0009-2614(01)00757-6
32. De Fazio, D., Cavalli, S., Aquilanti, V.: Orthogonal polynomials of a discrete variable as expansion basis sets in quantum mechanics the hyperquantization algorithm. Int. J. Quantum Chem. **93**, 91–111 (2003)
33. Aquilanti, V., Marinelli, D., Marzuoli, A.: Symmetric coupling of angular momenta, quadratic algebras and discrete polynomials. J. Phys: Conf. Ser. **482**, 012001 (2014). https://doi.org/10.1088/1742-6596/482/1/012001
34. Dos Santos, R.F., et al.: Couplings and recouplings of four angular momenta: alternative 9j symbols and spin addition diagrams. J. Mol. Model. **23**, 147 (2017). https://doi.org/10.1007/s00894-017-3320-1
35. Arruda, M.S., Santos, R.F., Marinelli, D., Aquilanti, V.: Spin-coupling diagrams and incidence geometry: a note on combinatorial and quantum-computational aspects. In: Gervasi, O., et al. (eds.) ICCSA 2016. LNCS, vol. 9786, pp. 431–442. Springer, Cham (2016). https://doi.org/10.1007/978-3-319-42085-1_33

36. Dos Santos, R.F., et al.: Quantum angular momentum, projective geometry and the networks of seven and ten spins: Fano, Desargues and alternative incidence configurations. J. Mol. Spectrosc. **337**, 153–162 (2017). https://doi.org/10.1016/j.jms.2017.05.005
37. Aquilanti, V., Marzuoli, A.: Projective Ponzano-Regge spin networks and their symmetries. J. Phys: Conf. Ser. **965**, 012005 (2018). https://doi.org/10.1088/1742-6596/965/1/012005
38. Coletti, C., Dos Santos, R.F., Arruda, M.S., Bitencourt, A.C.P., Ragni, M., Aquilanti, V.: Spin networks and Sturmian orbitals: orthogonal complete polynomial sets in molecular quantum mechanics. In: AIP Conference Proceedings, vol. 1906, p. 030013 (2017). https://doi.org/10.1063/1.5012292
39. Anderson, R.W., Aquilanti, V.: Spherical and hyperbolic spin networks: the *q*-extensions of Wigner-Racah 6*j* coefficients and general orthogonal discrete basis sets in applied quantum mechanics. In: Gervasi, O., et al. (eds.) ICCSA 2017. LNCS, vol. 10408, pp. 338–353. Springer, Cham (2017). https://doi.org/10.1007/978-3-319-62404-4_25
40. Aquilanti, V., Haggard, H.M., Littlejohn, R.G., Yu, L.: Semiclassical analysis of Wigner 3 j-symbol. J. Phys. A **40**, 5637–5674 (2007)
41. Aquilanti, V., Bitencourt, A.C.P., da S. Ferreira, C., Marzuoli, A., Ragni, M.: Quantum and semiclassical spin networks: from atomic and molecular physics to quantum computing and gravity. Phys. Scr. **78**, 058103 (2008)
42. Aquilanti, V., Bitencourt, A.C.P., da S. Ferreira, C., Marzuoli, A., Ragni, M.: Combinatorics of angular momentum recoupling theory: spin networks, their asymptotics and applications. Theoret. Chem. Acc. **123**, 237 (2009)
43. Aquilanti, V., Haggard, H.M., Hedeman, A., Jeevangee, N., Littlejohn, R., Yu, L.: Semiclassical mechanics of the Wigner 6j-symbol. J. Phys. A **45**, 065209 (2012)
44. Bitencourt, A.C.P., Marzuoli, A., Ragni, M., Anderson, R.W., Aquilanti, V.: Exact and asymptotic computations of elementary spin networks: classification of the quantum–classical boundaries. In: Murgante, B., et al. (eds.) ICCSA 2012. LNCS, vol. 7333, pp. 723–737. Springer, Heidelberg (2012). https://doi.org/10.1007/978-3-642-31125-3_54
45. Aquilanti, V., Marinelli, D., Marzuoli, A.: Hamiltonian dynamics of a quantum of space: hidden symmetries and spectrum of the volume operator, and discrete orthogonal polynomials. J. Phys. A Math. Theor. **46** (2013). https://doi.org/10.1088/1751-8113/46/17/175303
46. Aquilanti, V., Grossi, G.: Discrete representations by artificial quantization in the quantum mechanics of anisotropic interactions. Lett. Al Nuovo Cimento Ser. **2**(42), 157–162 (1985). https://doi.org/10.1007/BF02739563
47. Aquilanti, V., Cavalli, S., Grossi, G.: Discrete analogs of spherical harmonics and their use in quantum mechanics: the hyperquantization algorithm. Theoret. Chim. Acta **79**, 283–296 (1991). https://doi.org/10.1007/BF01113697
48. Aquilanti, V., Cavalli, S., De Fazio, D.: Hyperquantization algorithm. I. Theory for triatomic systems. J. Chem. Phys. **109**, 3792–3804 (1998)
49. Aquilanti, V., et al.: Hyperquantization algorithm. II. Implementation for the $F + H_2$ reaction dynamics including open-shell and spin-orbit interactions. J. Chem. Phys. **109**, 3805–3818 (1998). https://doi.org/10.1063/1.476980
50. Aquilanti, V., Cavalli, S., De Fazio, D., Volpi, A., Aguilar, A.: Probabilities for the F + H = HF + H reaction by the hyperquantization algorithm: alternative sequential diagonalization schemes. The Hamiltonian matrix. Phys. Chem. Chem. Phys. **1**, 1091–1098 (1999)
51. Aquilanti, V., et al.: Exact reaction dynamics by the hyperquantization algorithm: integral and differential cross sections for $F + H_2$, including long-range and spin – orbit effects. **4**, 401–415 (2002). https://doi.org/10.1039/b107239k

52. Aquilanti, V., Cavalli, S., De Fazio, D., Volpi, A., Aguilar, A., Lucas, J.M.: Benchmark rate constants by the hyperquantization algorithm. The F + H_2 reaction for various potential energy surfaces: features of the entrance channel and of the transition state, and low temperature reactivity. Chem. Phys. **308**, 237–253 (2005). https://doi.org/10.1016/j.chemphys.2004.03.027
53. Aquilanti, V., Cavalli, S., De Fazio, D., Simone, A., Tscherbul, T.V.: Direct evaluation of the lifetime matrix by the hyperquantization algorithm: narrow resonances in the reaction dynamics and their splitting for nonzero angular momentum. J. Chem. Phys. **123**, 054314 (2005). https://doi.org/10.1063/1.1988311
54. Aquilanti, V., Cavalli, S., Simoni, A., Aguilar, A., Lucas, J.M., De Fazio, D.: Lifetime of reactive scattering resonances: Q-matrix analysis and angular momentum dependence for the F + H_2 reaction by the hyperquantization algorithm. J. Chem. Phys. **121**, 11675–11690 (2004). https://doi.org/10.1063/1.1814096
55. Aquilanti, V., Cavalli, S., De Fazio, D., Volpi, A.: Theory of electronically nonadiabatic reactions: rotational, coriolis, spin – orbit couplings and the hyperquantization algorithm. Int. J. Quantum Chem. **85**, 368–381 (2001)
56. Aquilanti, V., Cavalli, S., De Fazio, D.: Angular and hyperangular momentum coupling coefficients as Hahn polynomials. J. Phys. Chem. **99**, 15694–15698 (1995)
57. Littlejohn, R.G., Mitchell, K.A., Reinsch, M., Aquilanti, V., Cavalli, S.: Internal spaces, kinematic rotations, and body frames for four-atom systems. Phys. Rev. A - At. Mol. Opt. Phys. **58**, 3718–3738 (1998). https://doi.org/10.1103/PhysRevA.58.3718
58. Alvarino, J.M.M., et al.: Stereodynamics from the stereodirected representation of the exact quantum S matrix: the Li + HF = LiF + H reaction. J. Phys. Chem. A **102**, 9638–9644 (1998)
59. Aldegunde, J., Alvariño, J.M., De Fazio, D., Cavalli, S., Grossi, G., Aquilanti, V.: Quantum stereodynamics of the F + H_2 → HF + H reaction by the stereodirected S-matrix approach. Chem. Phys. **301**, 251–259 (2004). https://doi.org/10.1016/j.chemphys.2004.02.002
60. Aquilanti, V., Liuti, G., Pirani, F., Vecchiocattivi, F.: Orientational and spin-orbital dependence of interatomic forces. J. Chem. Soc. Faraday Trans. 2 Mol. Chem. Phys. **85**, 955–964 (1989). https://doi.org/10.1039/F29898500955
61. Kasai, T., et al.: Directions of chemical change: experimental characterization of the stereodynamics of photodissociation and reactive processes. Phys. Chem. Chem. Phys. **16**, 9776–9790 (2014). https://doi.org/10.1039/c4cp00464g
62. Lombardi, A., Palazzetti, F., Aquilanti, V., Grossi, G.: Collisions of chiral molecules theoretical aspects and experiments. In: AIP Conference Proceedings, vol. 2040, p. 020020 (2018). https://doi.org/10.1063/1.5079062
63. Lombardi, A., Palazzetti, F.: Chirality in molecular collision dynamics. J. Phys.: Condens. Matter **30**, 063003 (2018). https://doi.org/10.1088/1361-648X/aaa1c8
64. Albernaz, A.F., Barreto, P.R.P., Aquilanti, V., Lombardi, A., Palazzetti, F., Pirani, F.: The astrochemical observatory: the interaction between helium and the chiral molecule propylene oxide. In: AIP Conference Proceedings, vol. 2040, p. 020018 (2018). https://doi.org/10.1063/1.5079060
65. Lombardi, A., Palazzetti, F., Aquilanti, V., Pirani, F., Casavecchia, P.: The astrochemical observatory: experimental and computational focus on the chiral molecule propylene oxide as a case study. In: Gervasi, O., et al. (eds.) ICCSA 2017. LNCS, vol. 10408, pp. 267–280. Springer, Cham (2017). https://doi.org/10.1007/978-3-319-62404-4_20
66. Palazzetti, F., Maciel, G.S., Lombardi, A., Grossi, G., Aquilanti, V.: The astrochemical observatory: molecules in the laboratory and in the cosmos. J. Chin. Chem. Soc. **59** (2012). https://doi.org/10.1002/jccs.201200242

67. Che, D.-C., Kanda, K., Palazzetti, F., Aquilanti, V., Kasai, T.: Electrostatic hexapole state-selection of the asymmetric-top molecule propylene oxide: rotational and orientational distributions. Chem. Phys. **399**, 180–192 (2012). https://doi.org/10.1016/j.chemphys.2011.11.020
68. Che, D.-C., Palazzetti, F., Okuno, Y., Aquilanti, V., Kasai, T.: Electrostatic hexapole state-selection of the asymmetric-top molecule propylene oxide. J. Phys. Chem. A **114**, 3280–3286 (2010). https://doi.org/10.1021/jp909553t
69. Aquilanti, V., Beneventi, L., Grossi, G., Vecchiocattivi, F.: Coupling schemes for atom-diatom interactions and an adiabatic decoupling treatment of rotational temperature effects on glory scattering. J. Chem. Phys. **89**, 751–761 (1988). https://doi.org/10.1063/1.455198
70. Barreto, P.R.P., Albernaz, A.F., Palazzetti, F., Lombardi, A., Grossi, G., Aquilanti, V.: Hyperspherical representation of potential energy surfaces: intermolecular interactions in tetra-atomic and penta-atomic systems. Phys. Scr. **84**, 28111 (2011). https://doi.org/10.1088/0031-8949/84/02/028111
71. Barreto, P.R.P., Vilela, A.F.A., Lombardi, A., Maciel, G.S., Palazzetti, F., Aquilanti, V.: The hydrogen peroxide-rare gas systems: quantum chemical calculations and hyperspherical harmonic representation of the potential energy surface for atom-floppy molecule interactions. J. Phys. Chem. A **111**, 12754–12762 (2007). https://doi.org/10.1021/jp076268v
72. Maciel, G.S., Barreto, P.R.P., Palazzetti, F., Lombardi, A., Aquilanti, V.: A quantum chemical study of H_2S_2: intramolecular torsional mode and intermolecular interactions with rare gases. J. Chem. Phys. **129**, 164302 (2008). https://doi.org/10.1063/1.2994732
73. Barreto, P.R.P., Palazzetti, F., Grossi, G., Lombardi, A., Maciel, G.S., Vilela, A.F.A.: Range and strength of intermolecular forces for van der Waals complexes of the type H_2X_n-Rg, with X = O, S and n = 1, 2. Int. J. Quantum Chem. **110**, 777–786 (2010). https://doi.org/10.1002/qua.22127
74. Lombardi, A., Palazzetti, F., Maciel, G.S., Aquilanti, V., Sevryuk, M.B.: Simulation of oriented collision dynamics of simple chiral molecules. Int. J. Quantum Chem. **111**, 1651–1658 (2011). https://doi.org/10.1002/qua.22816
75. Lombardi, A., Palazzetti, F., Peroncelli, L., Grossi, G., Aquilanti, V., Sevryuk, M.B.: Few-body quantum and many-body classical hyperspherical approaches to reactions and to cluster dynamics. Theoret. Chem. Acc **117**, 709–721 (2007). https://doi.org/10.1007/s00214-006-0195-0
76. Lombardi, A., Palazzetti, F., Grossi, G., Aquilanti, V., Castro Palacio, J.C., Rubayo Soneira, J.: Hyperspherical and related views of the dynamics of nanoclusters. Phys. Scr. **80**, 048103 (2009). https://doi.org/10.1088/0031-8949/80/04/048103
77. Lombardi, A., et al.: Spherical and hyperspherical harmonics representation of van der Waals aggregates. In: AIP Conference Proceedings, vol. 1790, pp. 020005 (2016). https://doi.org/10.1063/1.4968631
78. Aquilanti, V., Bartolomei, M., Cappelletti, D., Carmona-Novillo, E., Pirani, F.: The N_2–N_2 system: an experimental potential energy surface and calculated rotovibrational levels of the molecular nitrogen dimer. J. Chem. Phys. **117**, 615 (2002)
79. Aquilanti, V., et al.: Molecular beam scattering of aligned oxygen molecules. The nature of the bond in the O_2-O_2 dimer. J. Am. Chem. Soc. **121**, 10794–10802 (1999). https://doi.org/10.1021/ja9917215
80. Aquilanti, V., Bartolomei, M., Carmona-Novillo, E., Pirani, F.: The asymmetric dimer N_2–O_2: characterization of the potential energy surface and quantum mechanical calculation of rotovibrational levels. J. Chem. Phys. **118**, 2214 (2003)

81. Barreto, P.R.P., et al.: The spherical-harmonics representation for the interaction between diatomic molecules: the general case and applications to CO–CO and CO–HF. J. Mol. Spectrosc. **337**, 163–177 (2017). https://doi.org/10.1016/j.jms.2017.05.009
82. Barreto, P.R.P., Ribas, V.W., Palazzetti, F.: Potential energy surface for the H_2O-H_2 system. J. Phys. Chem. A **113**, 15047–15054 (2009). https://doi.org/10.1021/jp9051819
83. Barreto, P.R.B., et al.: Potential energy surfaces for interactions of H_2O with H_2, N_2 and O_2: a hyperspherical harmonics representation, and a minimal model for the H_2O-rare-gas-atom systems. Comput. Theoret. Chem. **990**, 53–61 (2012). https://doi.org/10.1016/j.comptc.2011.12.024
84. Barreto, P.R.P., Albernaz, A.F., Palazzetti, F.: Potential energy surfaces for van der Waals complexes of rare gases with H_2S and H_2S_2: extension to xenon interactions and hyperspherical harmonics representation. Int. J. Quantum Chem. **112**, 834–847 (2012). https://doi.org/10.1002/qua.23073
85. Anderson, R.: Discrete orthogonal transformations corresponding to the discrete polynomials of the Askey scheme. In: Murgante, B., et al. (eds.) ICCSA 2014. LNCS, vol. 8579, pp. 490–507. Springer, Cham (2014). https://doi.org/10.1007/978-3-319-09144-0_34
86. Nikiforov, A.F., Suslov, S.K., Uvarov, V.B.: Classical Orthogonal Polynomials of a Discrete Variable. Springer, Berlin (1991). https://doi.org/10.1007/978-3-642-74748-9_2
87. Braun, P.A., Gewinski, F., Haake, H., Schomerus, H.: Semiclassics of rotation and torsion. Z. Phys. B **100**, 115–127 (1996)
88. Aquilanti, V., Grossi, G.: Angular momentum coupling schemes in the quantum mechanical treatment of P-state atom collisions. J. Chem. Phys. **73**, 1165–1172 (1980). https://doi.org/10.1063/1.440270
89. Palazzetti, F., Munusamy, E., Lombardi, A., Grossi, G., Aquilanti, V.: Spherical and hyperspherical representation of potential energy surfaces for intermolecular interactions. Int. J. Quantum Chem. **111**, 318–332 (2011). https://doi.org/10.1002/qua.22688