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Quantum Spin Networks and their Applications:
Illustration of Classical and Non-Classical Borderlines

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Spin Networks in Atomic and Molecular Physics, Quantum Chemistry and Quantum Computing

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Quantum and semiclassical spin networks

The traditional ingredients of quantum mechanical **angular momentum coupling**, which were developed to explain spectroscopic phenomena in atomic, molecular and molecular physics, are now embedded in modern algebraic frameworks which emphasize the underlying combinational aspects. What were previously known only as **3nj-symbols** (together with the related problems of their calculations, their general properties, their asymptotic limits for large entries) are now among the protagonists of modern quantum gravity and quantum computing applications under the general name of "**spin networks**".

Further progress has also to be recorded on the established connections with the theory of orthogonal polynomials, of great relevance for a wide spectrum of applications. For quantum chemistry, the relevance lies in the development and classification of complete orthogonal basis sets in atomic and molecular problems, either in configuration space (**Sturmian orbitals**) or in momentum space.

The connection with the theory of orthogonal polynomials (**Askey scheme**) allows us to develop powerful tools based on asymptotic expansions – physically corresponding to the various levels of the **semi-classical limits**. Results are of use in molecular physics and also in motivating algorithms for the computationally demanding problems of chemical reaction theory, where large angular momenta are involved—our **hyperquantization algorithm**.

The talk lists and discusses some aspects of further developments.

Spin networks

for quantum computation and quantum gravity

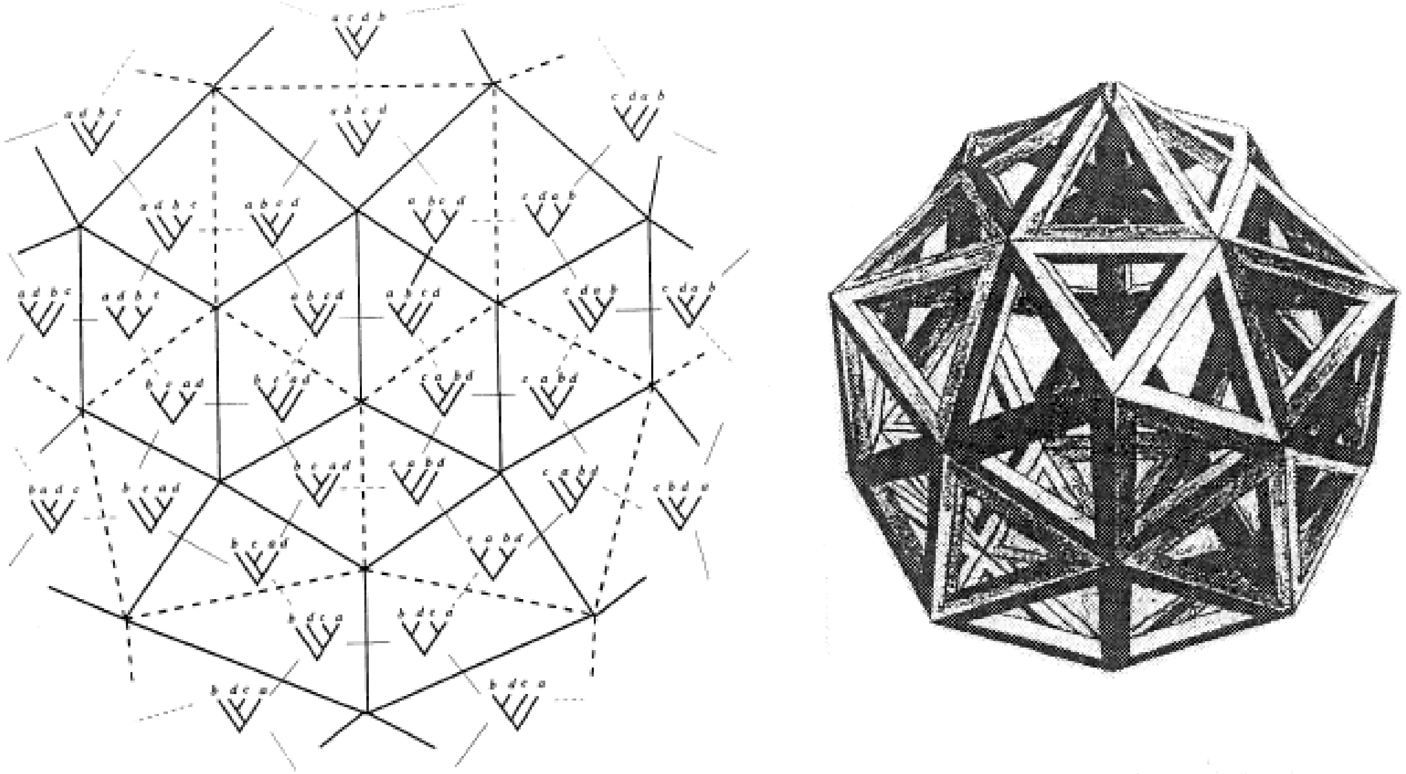

Fig. 4. The tree scheme can be obtained by 'dualizing' the graph of Fig. 3. One should consider as a guide the dual of the truncated icosahedron, the elevated pentagonododecahedron illustrated again by a drawing by Leonardo. Exchanging vertices and centers of faces one obtains 60 triangular faces. In the corresponding graph, the new lines are orthogonal to the previous ones and form triangles each of which represents a tree (a coupling scheme).

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Angular and hyperangular momentum recoupling, harmonic superposition and Racah polynomials: a recursive algorithm

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Abstract

Generalized 6j symbols are defined in terms of orthonormalized Racah polynomials of a discrete variable and given explicitly as hypergeometric ${}_4F_3(1)$ series. They extend the recoupling coefficients of ordinary angular momentum algebra, including multiples of 1/4 as quantum numbers. A three-term recurrence relationship is exploited for extensive calculations and illustration of their properties. Their role is outlined as matrix elements for superpositions (or overlaps) both between alternative spherical and hyperspherical harmonics and between alternative Sturmian sets, an important case being that of four-dimensional harmonics of S^3, which apply to the momentum-space hydrogen atom orbitals. © 2001 Elsevier Science B.V. All rights reserved.

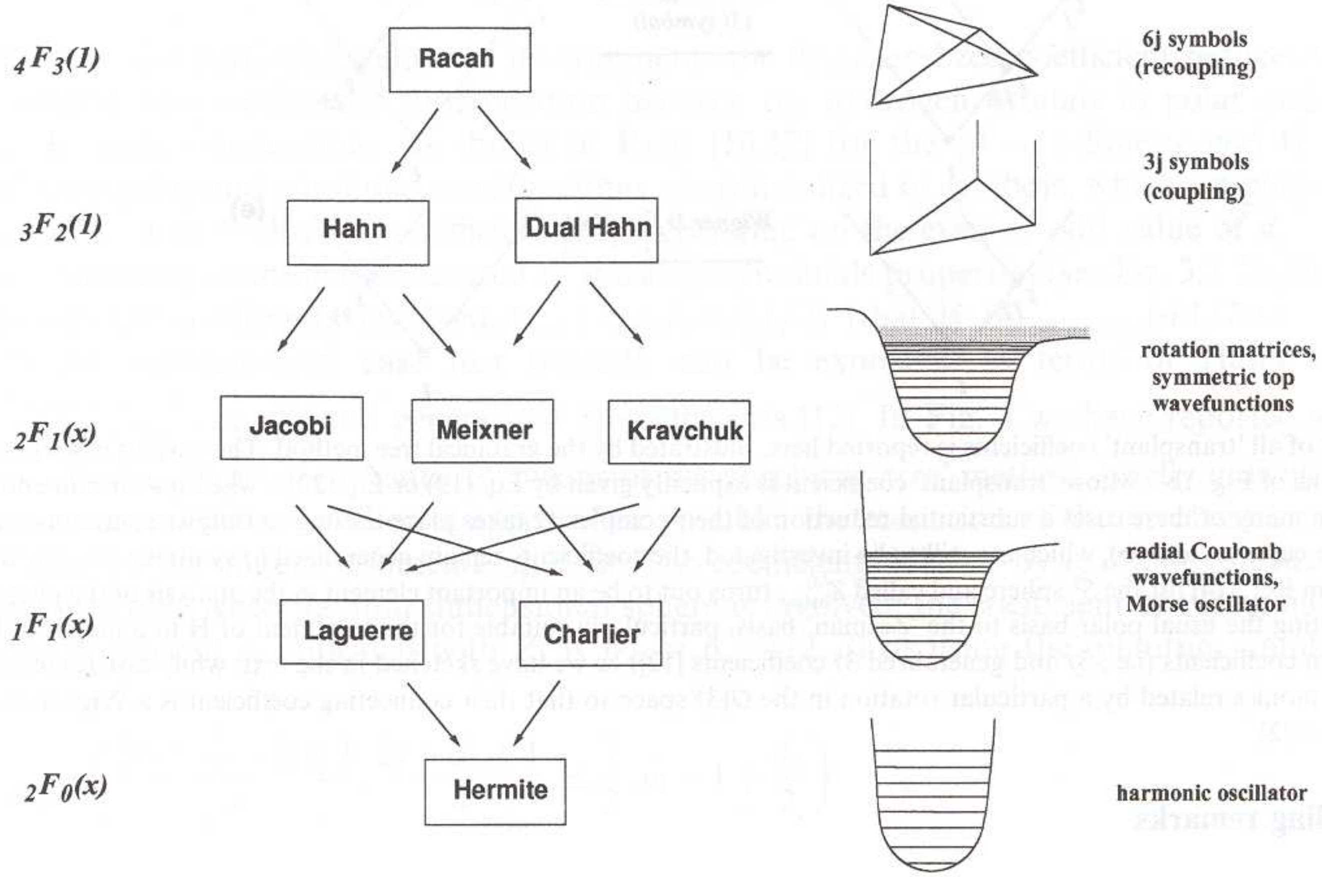
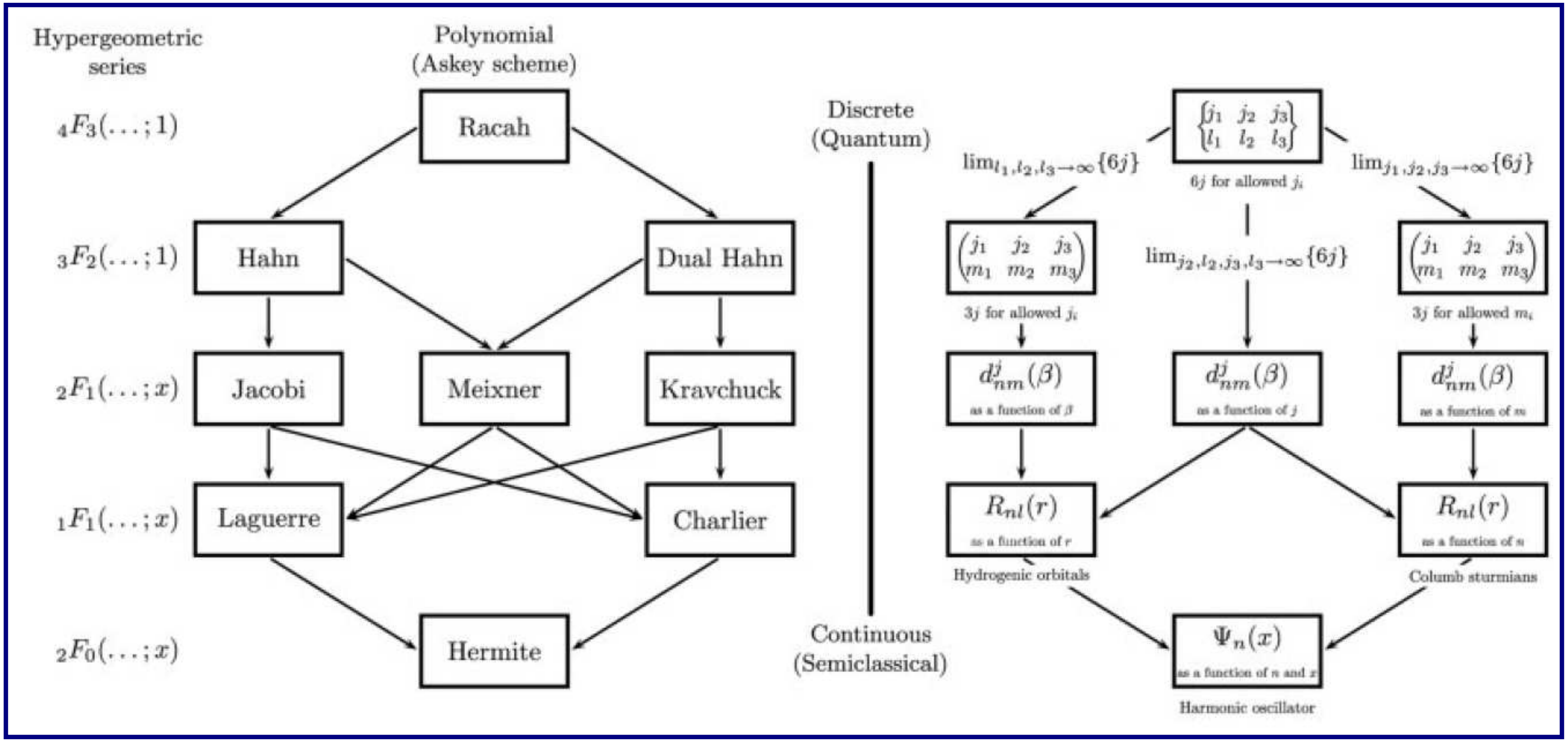


Fig. 5. Comparison between a classification of orthogonal hypergeometric polynomials (a partial view of schemes in [5,6]) and their current occurrence in quantum mechanics. The first two downward connections are limiting relationships which physically correspond to semiclassical limits [13], while the remaining ones are progressive confinements in space due to the form of the potential. Polynomials at the same level are identical, but the role of the three-term recurrence relation and of the finite difference equation varies – Hahn and dual Hahn differ in the role played by the 'degree' and the 'variable' parameters, which correspond to the dual role that angular momentum and projection quantum numbers play in vector coupling coefficients [12]. Similarly for the Jacobi polynomials, where the Meixner and Kravchuk polynomials are the 'discrete' counterparts, and the Charlier polynomials are the 'discrete' dual of Laguerre polynomials.

Comparative classifications of orthogonal hypergeometric polynomials and of ingredients of quantum theory of angular momentum and wave-functions.



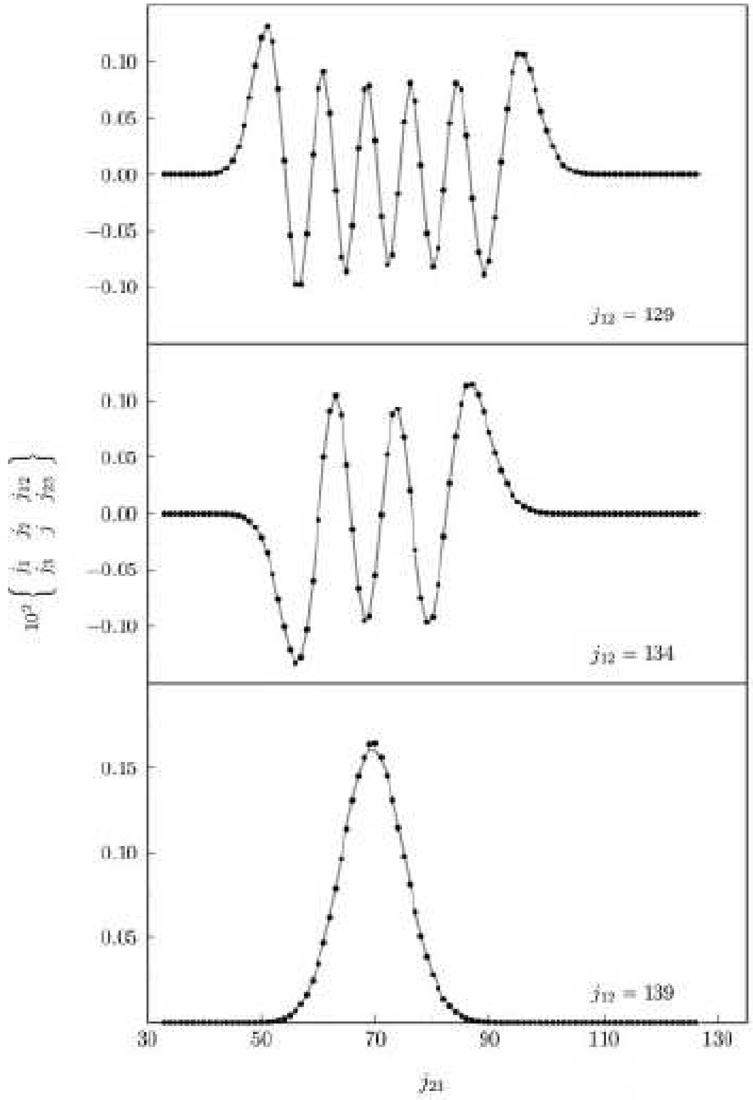


FIGURE 5. 6*j* values as a function of allowed j_{23} for $j_1 = 92$, $j_2 = 47$, $j_3 = 80$, $j = 121$ and the indicated j_{12} values for the three panels. The lines connect the points evaluated by the hypergeometric series of Section 2. The dots are evaluated by the Schulten-Gordon formulas of Section 3. Data available from the authors. Comparison should be made with Figure 3 of Ref. [3].

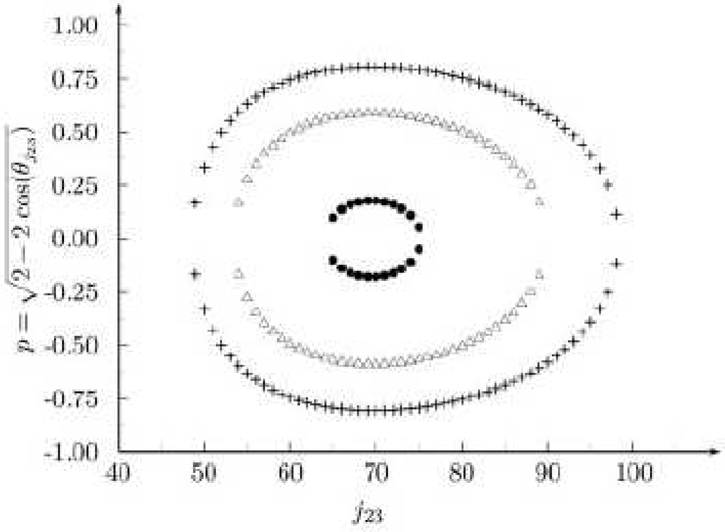


FIGURE 6. Illustration of phase space for semiclassical quantization for $j_1 = 92$, $j_2 = 47$, $j_3 = 80$, $j = 121$, and $j_{12} = 139$ (dots), 134 (triangles), and 129 (plus signs), i.e., the three cases of Figure 5.

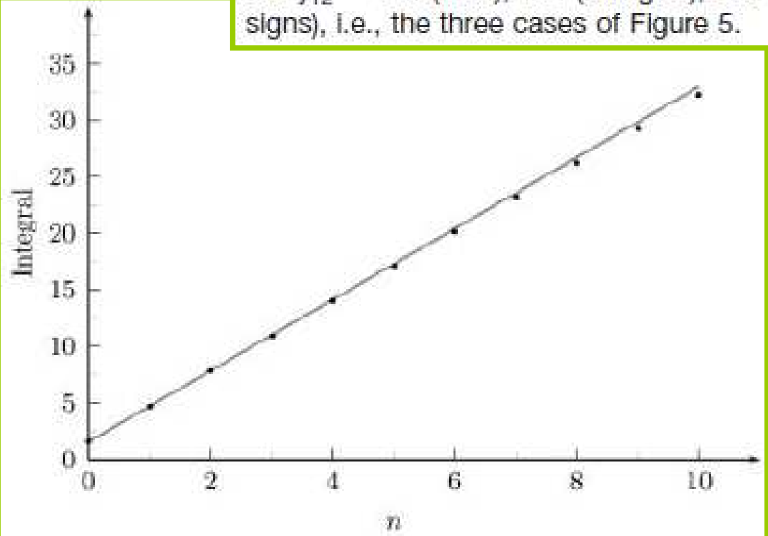


FIGURE 7. Values for the integral of Eq. (29) for different number of nodes *n*. $j_{12} = 139 \rightarrow n = 0$, $j_{12} = 134 \rightarrow n = 5$, $j_{12} = 129 \rightarrow n = 10$. The values of the integrals are connected by the line while the dots are evaluated with *p* given by Eq. (28).

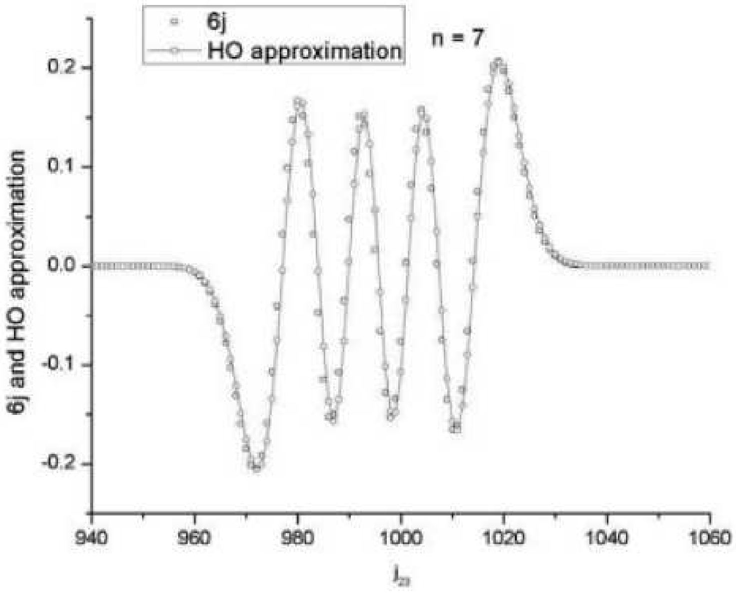


FIGURE 10. As in Figure 8, for $j_1 = 1000$, $j_2 = 1000$, $j_{12} = 193$, $j_3 = 100$, $j = 100$.

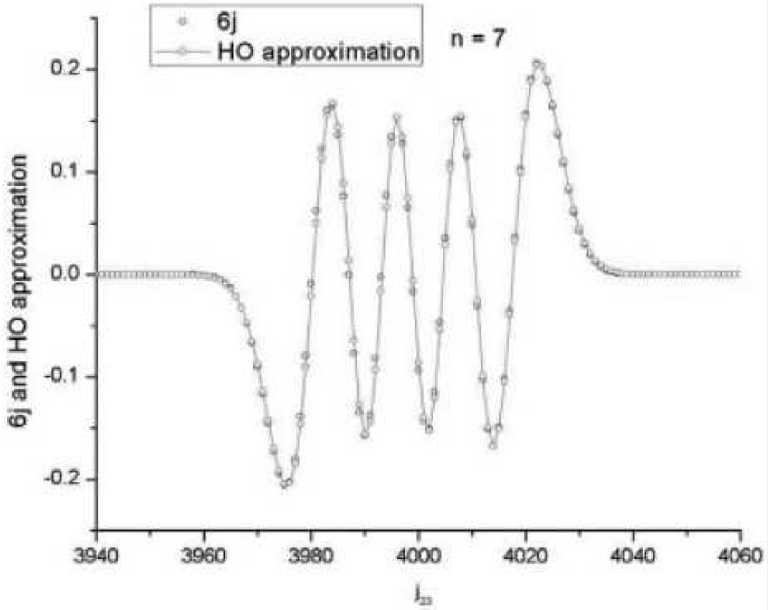


FIGURE 11. As in Figure 8, for $j_1 = 4000$, $j_2 = 4000$, $j_{12} = 200$, $j_3 = 100$, $j = 100$.

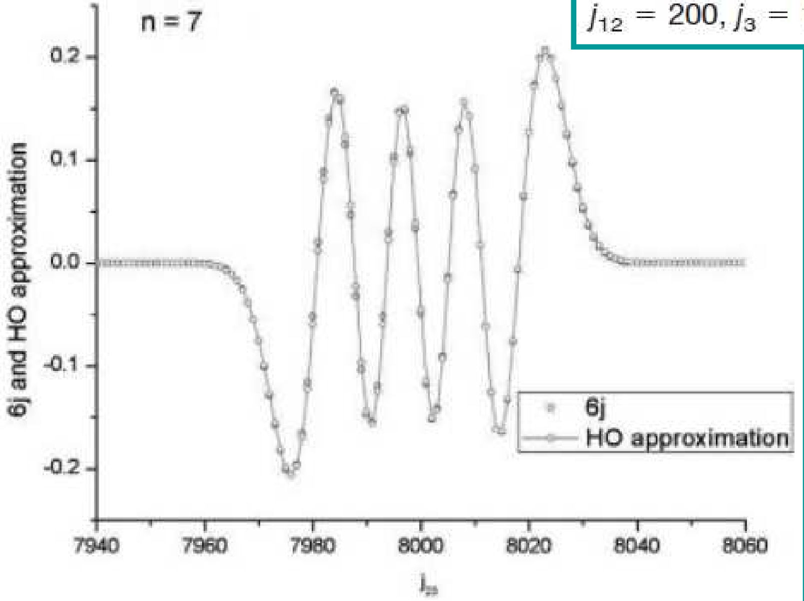


FIGURE 12. As in Figure 8, for $j_1 = 8000$, $j_2 = 8000$, $j_{12} = 200$, $j_3 = 100$, $j = 100$.

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Uniform Semiclassical Approximation for the Wigner 6*j*-Symbol in Terms of Rotation Matrices[†]

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A new uniform asymptotic approximation for the Wigner 6*j*-symbol is given in terms of Wigner rotation matrices (*d*-matrices). The approximation is uniform in the sense that it applies for all values of the quantum numbers, even those near caustics. The derivation of the new approximation is not given, but the geometrical ideas supporting it are discussed and numerical tests are presented, including comparisons with the exact 6*j*-symbol and with the Ponzano−Regge approximation.

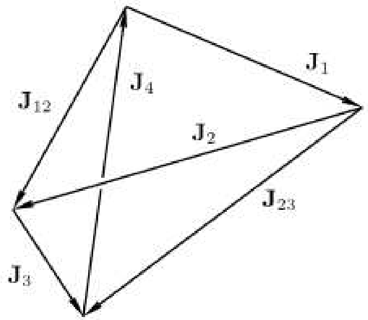

Figure 2. A tetrahedron of positive volume with conventional labeling of edges by angular momentum vectors.

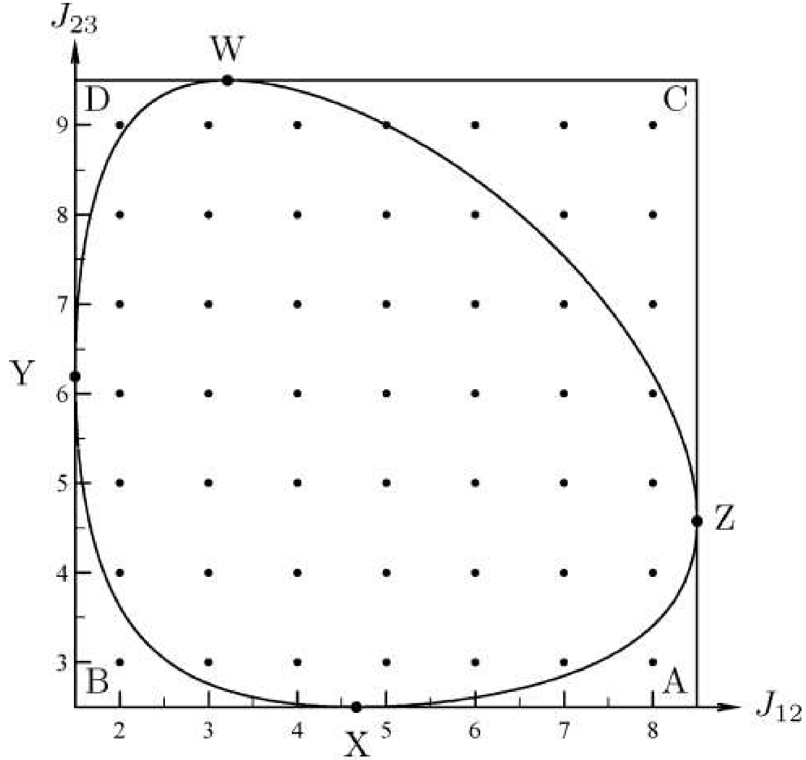

Figure 3. The J_{12}−J_{23} plane for $j_1 = 9/2$, $j_2 = 3$, $j_3 = 11/2$, $j_4 = 6$. The classical bounds are $J_{12,\,\mathrm{min}} = 3/2$, $J_{12,\,\mathrm{max}} = 17/2$, $J_{23,\,\mathrm{min}} = 5/2$, $J_{23,\,\mathrm{max}} = 19/2$. The dimension of the matrix $\langle j_{12}|j_{23}\rangle$ is $D = \mathrm{dim}Z = 7$. The point $J_{12} = 5$, $J_{23} = 9$ ($j_{12} = 9/2$, $j_{23} = 17/2$) is very close to the caustic line, but lies just inside. The Ponzano−Regge approximation is too large by a factor of 7 at this point.

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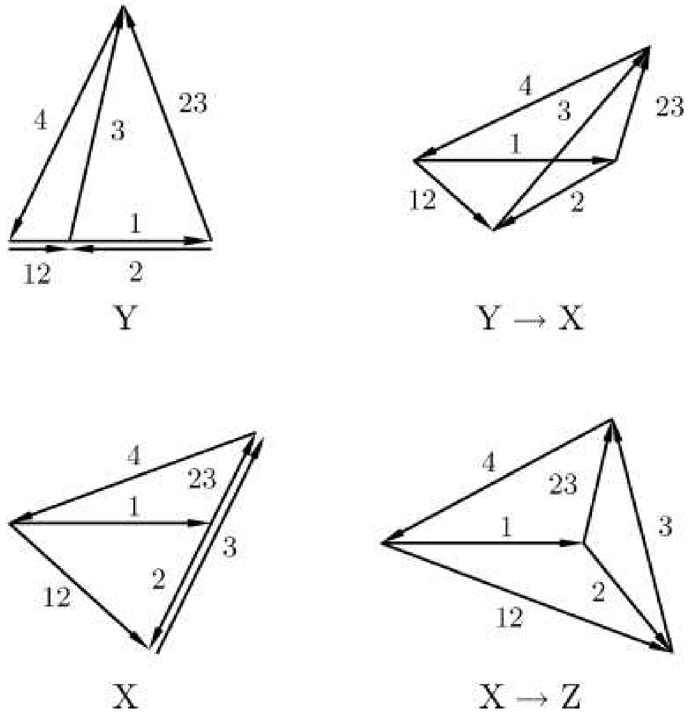
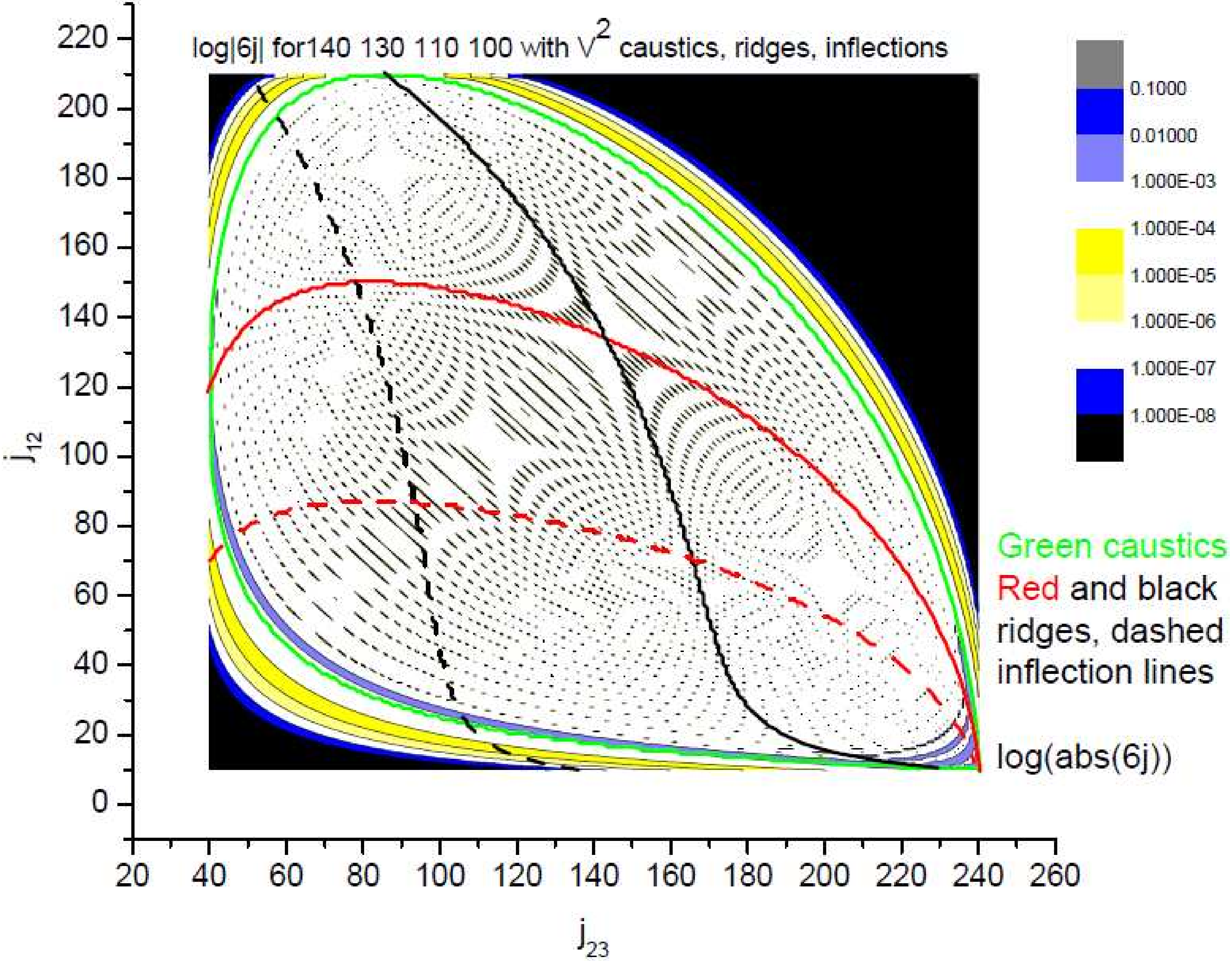
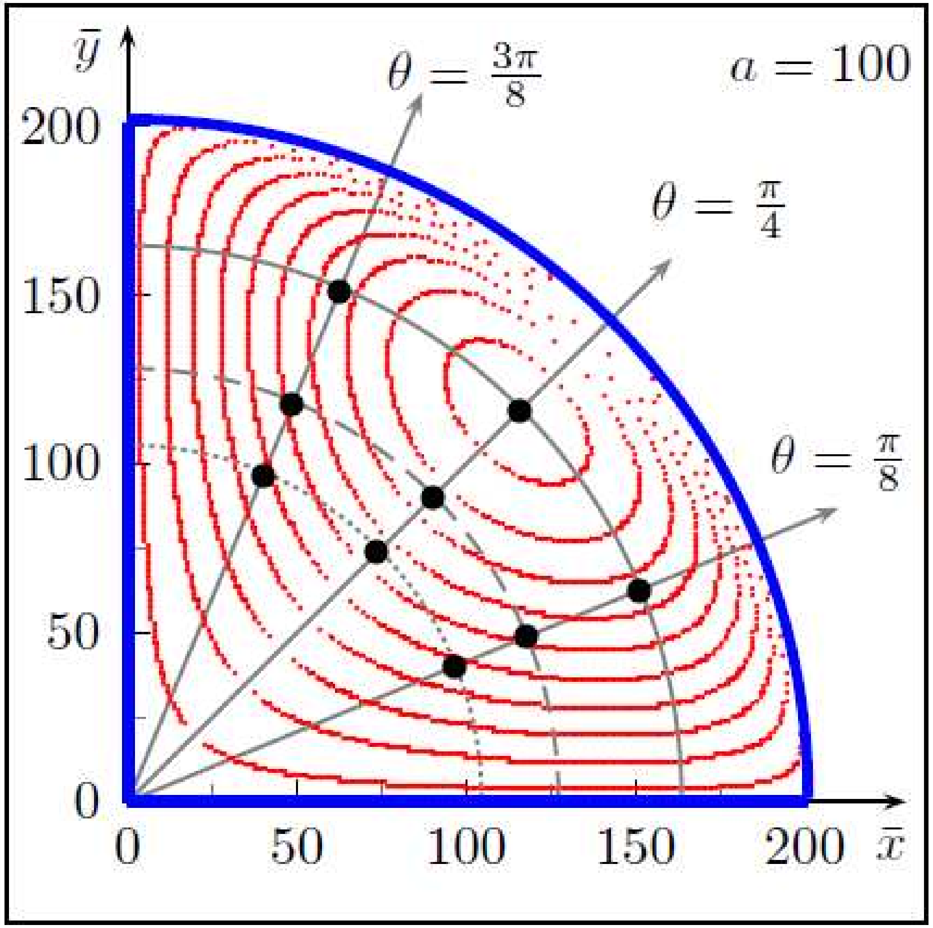
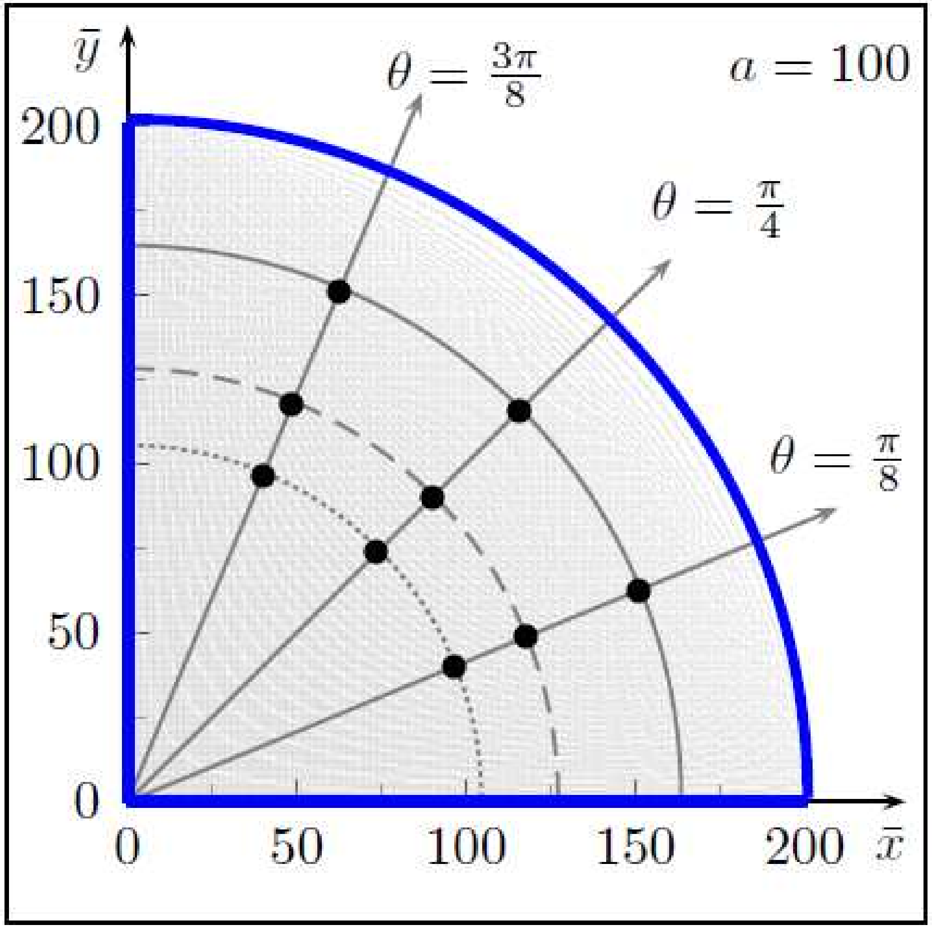


Figure 4. A sequence of four flat tetrahedra, moving around the caustic line of Figure 3 in a counterclockwise direction from point Y. The parameters are the same as in Figure 3. The numbers 1, 2, etc., refer to vectors $\mathbf{J}_1$, $\mathbf{J}_2$, etc.


log|6j| for140 130 110 100 with V^2 caustics, ridges, inflections
j_{12}
220
200
180
160
140
120
100
80
60
40
20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
j_{23}
0.1000
0.01000
1.000E-03
1.000E-04
1.000E-05
1.000E-06
1.000E-07
1.000E-08
Green caustics
Red and black ridges, dashed inflection lines
log(abs(6j))


$\bar{y}$
$\theta = \frac{3\pi}{8}$
$a = 100$
$\theta = \frac{\pi}{4}$
$\theta = \frac{\pi}{8}$
200
150
100
50
0
0
50
100
150
200
$\bar{x}$


$\bar{y}$
$\theta = \frac{3\pi}{8}$
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200
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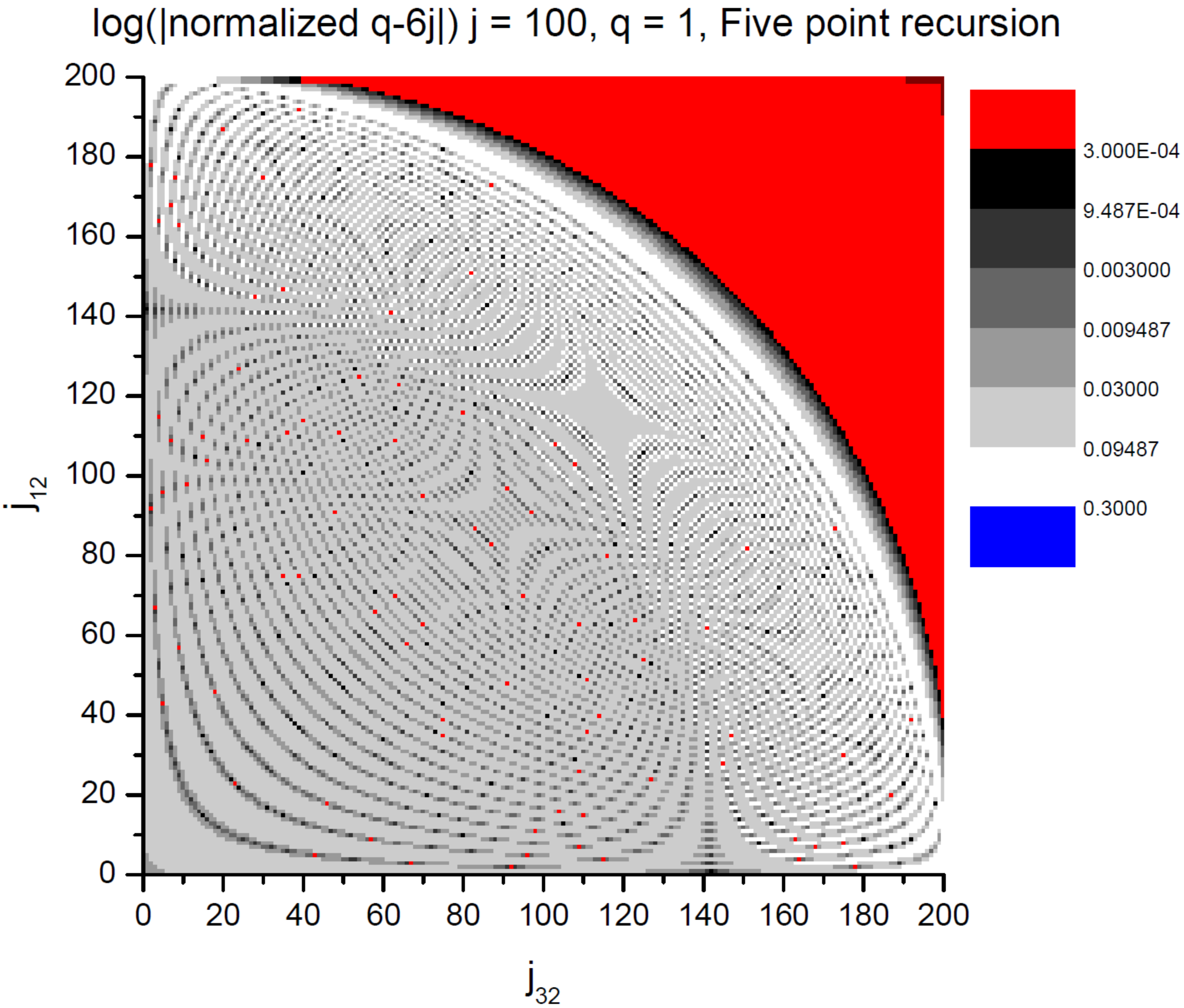
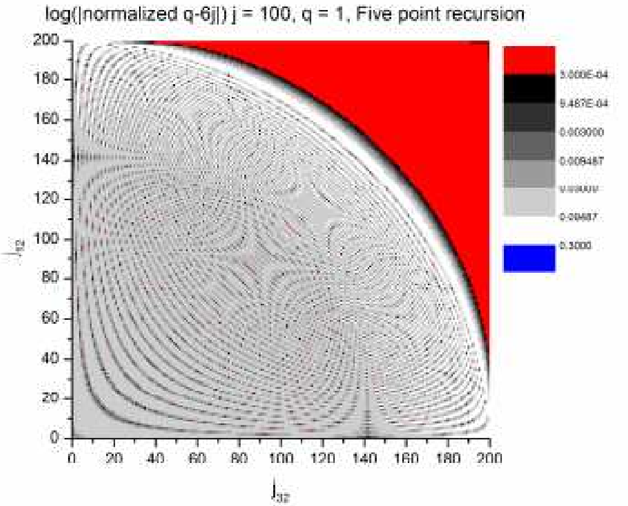
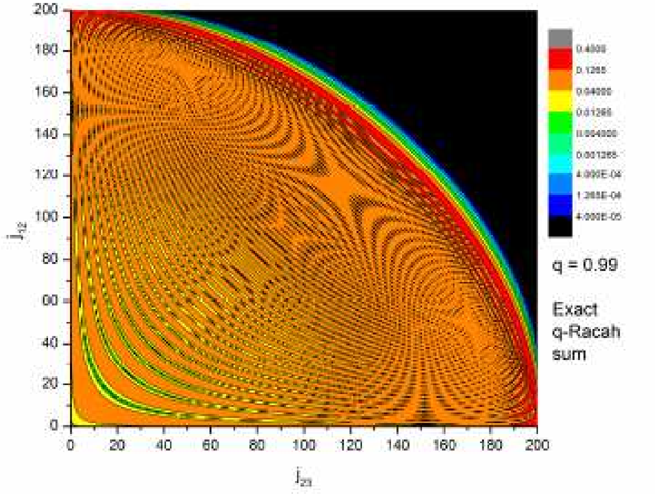
150
200
$\bar{x}$


log(|normalized q-6j|) j = 100, q = 1, Five point recursion
j_12
j_32
0
20
40
60
80
100
120
140
160
180
200
3.000E-04
9.487E-04
0.003000
0.009487
0.03000
0.09487
0.3000

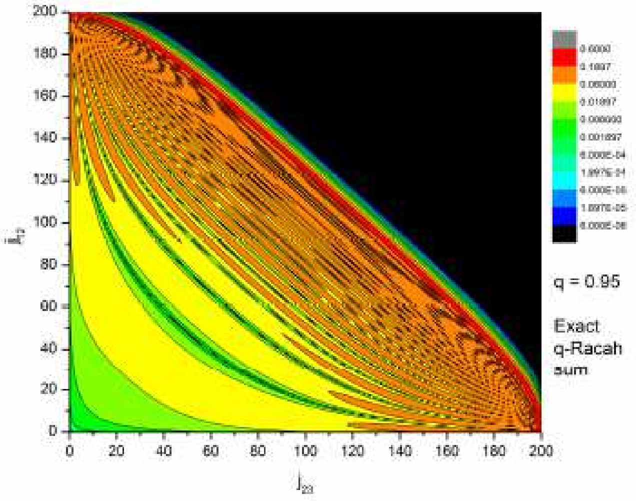
$$\begin{Bmatrix} 100 & 100 & j_{12} \\ 100 & 100 & j_{23} \end{Bmatrix}_q$$



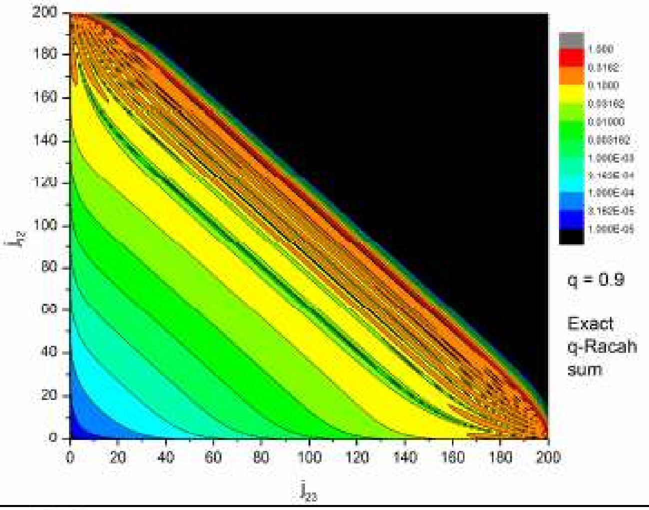
$q = 1$



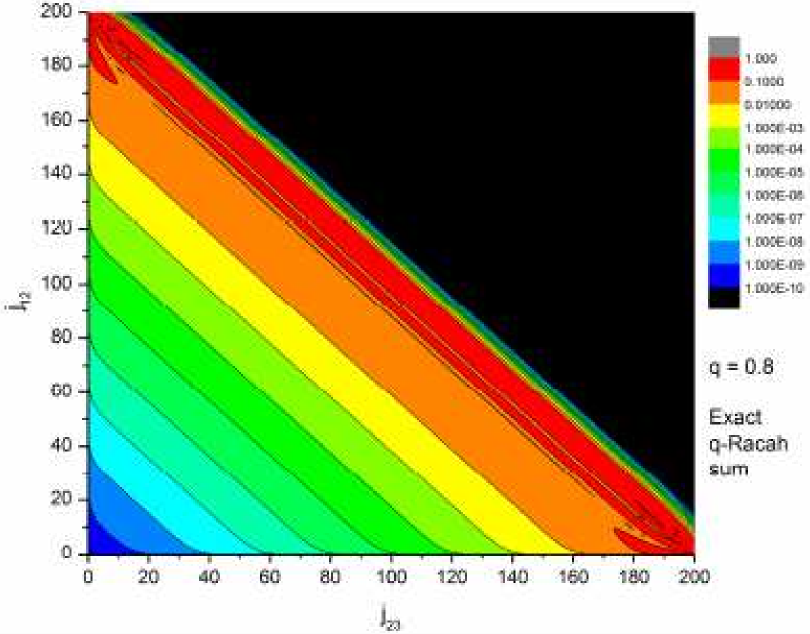
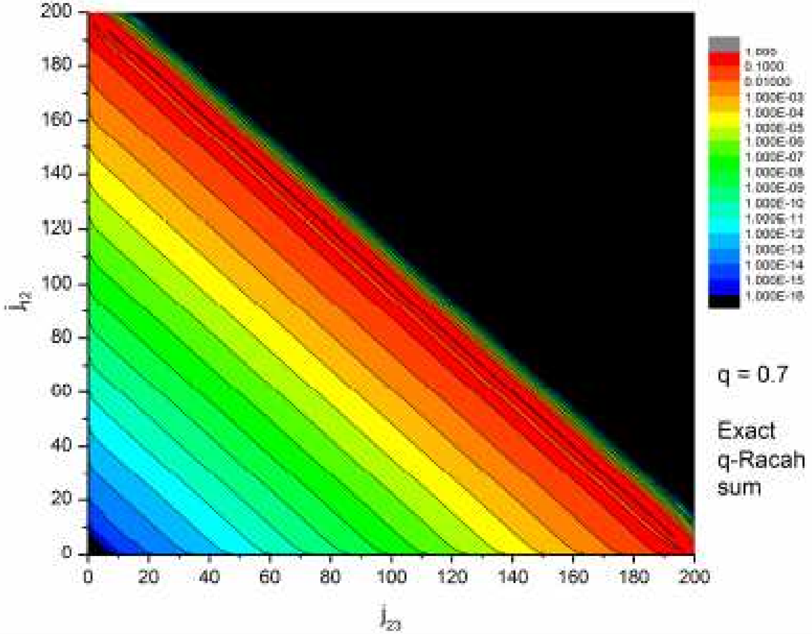
$q = 0.99$



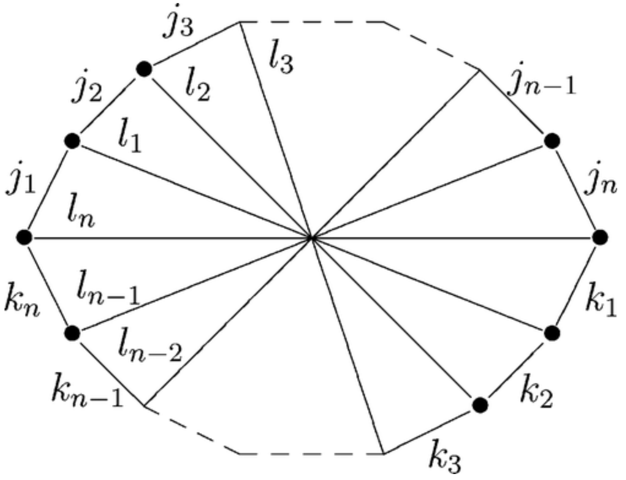
$q = 0.95$



$q = 0.9$

200 180 160 140 120 100 80 60 40 20 0 j_{12} 0 20 40 60 80 100 120 140 160 180 200 j_{23} 1.000 0.1000 0.01000 1.000E-03 1.000E-04 1.000E-05 1.000E-06 1.000E-07 1.000E-08 1.000E-09 1.000E-10 q = 0.8 Exact q-Racah sum	200 180 160 140 120 100 80 60 40 20 0 j_{12} 0 20 40 60 80 100 120 140 160 180 200 j_{23} 1.000 0.1000 0.01000 1.000E-03 1.000E-04 1.000E-05 1.000E-06 1.000E-07 1.000E-08 1.000E-09 1.000E-10 1.000E-11 1.000E-12 1.000E-13 1.000E-14 1.000E-15 1.000E-16 q = 0.7 Exact q-Racah sum
$q = 0.8$	$q = 0.7$

15106 *J. Phys. Chem. A* **2009,** *113,* 15106–15117



3*nj* Morphogenesis and Semiclassical Disentangling[†]

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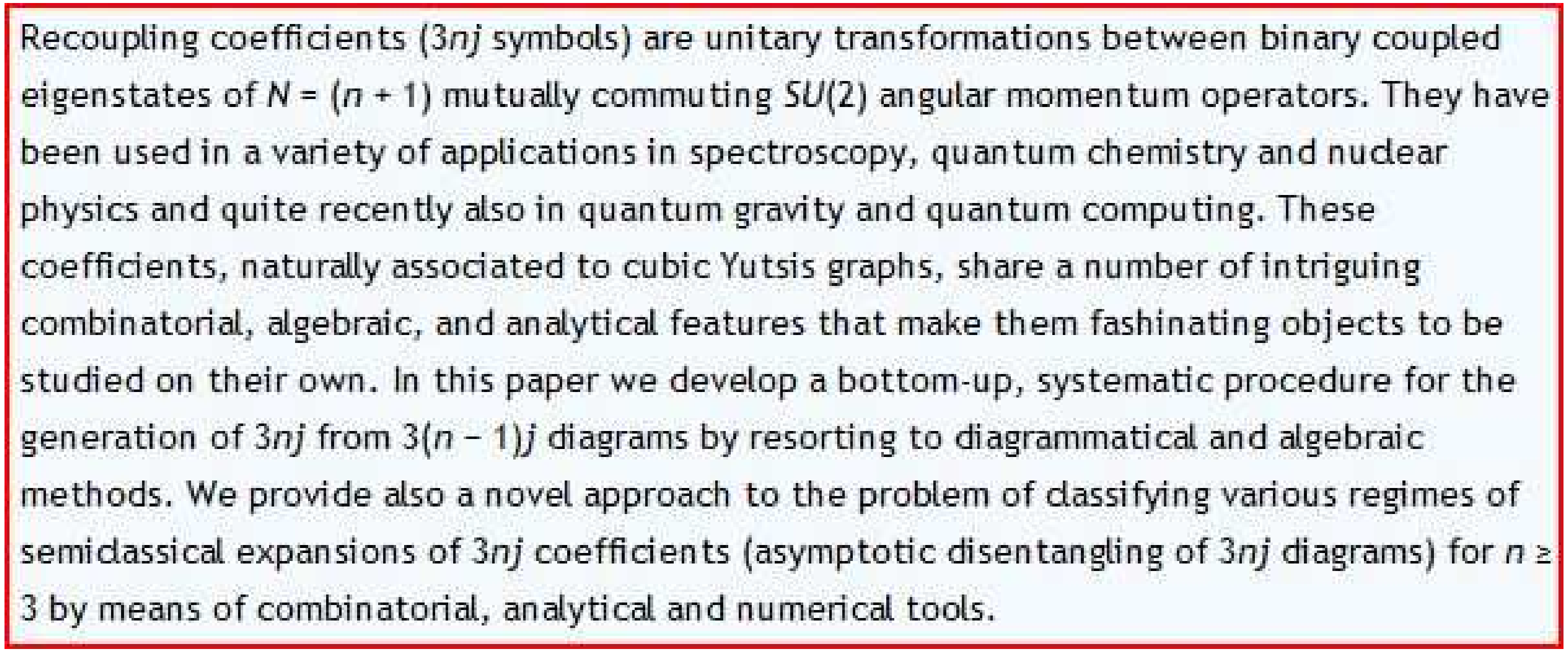
Recoupling coefficients (3*nj* symbols) are unitary transformations between binary coupled eigenstates of $N = (n + 1)$ mutually commuting $SU(2)$ angular momentum operators. They have been used in a variety of applications in spectroscopy, quantum chemistry and nuclear physics and quite recently also in quantum gravity and quantum computing. These coefficients, naturally associated to cubic Yutsis graphs, share a number of intriguing combinatorial, algebraic, and analytical features that make them fashinating objects to be studied on their own. In this paper we develop a bottom-up, systematic procedure for the generation of 3*nj* from $3(n - 1)j$ diagrams by resorting to diagrammatical and algebraic methods. We provide also a novel approach to the problem of classifying various regimes of semiclassical expansions of 3*nj* coefficients (asymptotic disentangling of 3*nj* diagrams) for $n \geq 3$ by means of combinatorial, analytical and numerical tools.

Semiclassical disentangling of spin-networks: exact computation and large angular momentum asymptotics of 3nj-symbols

The venerable ***3nj*-symbols** of quantum angular momentum theory, originated in applications to molecular, atomic, nuclear and particle physics, crucial to many fields of science, play a role for example as **spin networks** in approaches to quantum gravity, as simulators in quantum computing, as discrete polynomials in computational science. The *3nj* symbols for n>2 and the related spin networks are built as specific sums of products of *6j* symbols. The focus of this presentation is on the ***9j* symbol**, well known in its role as the matrix element of the transformation between *LS* and *jj* coupling schemes, but exhibiting features prototypical of more complex spin networks. Although closed form expressions are well known, modern applications require efficient computational procedures for **large values of the entries** .so far based on recurrence schemes, but we demonstrate that direct summations of the defining series can now be efficiently performed without overflow and losses of precision using multiple precision arithmetics. This allows us to experiment numerically on the simplest spin networks, and to check **asymptotic formulas.**

For the *9j* symbols, the first nontrivially “**entangled**” spin network, we give the basics of asymptotic approximations when some of the entries are large--the **semiclassical** limit ,gathering insight on how spin networks in such a limit effectively “disentangle”, witnessing the transition from quantum mechanics, accompanied by phenomena such as loss of coherence and localization.. Important are those studies which aim at understanding what happens when all entries become large, so preserving the beautiful underlying symmetry of these fundamental objects of the geometry of the quantum world. The basic paper is that by Ponzano and Regge (1968), Neville (1972) and Schulten and Gordon (1975). For *3j* symbols, and for a general perspective, see our work (JPA, 2007). Here we study the behaviour when only some of the entries are large. Relevant formulas are well established for n=2, extremely useful in spectroscopic applications . Large angular momenta correspond to the case of **discrete functions becoming continuous** in the limit, so inverting the point of view, yielding discrete analogs of functions of continuous variable, exploited in our **hyperquantization algorithm**.

In the limit of six large entries, our formula leads to the product of two ***d*** matrix elements. illustrating " **disentangling**" of the network: the *9j* arises as sum of products of 6j,but in the limit, the sum disappears. This semiclassical disentangling may apply also to *3nj* where *n* >3.This conjecture, certainly valid in many cases is to be proven for general spin networks. We can discuss this disentangling from many viewpoints (**classical locality, wavefuction separability, decoherence**) of relevance in quantum gravity, discrete mathematics, quantum computing. In quantum mechanics separability of a d-dimensional problem means expressing a wavefunction as a product of wavefunctions of smaller problems, otherwise you have to include coupling by expanding on a linear combination. Non-separability leads to interference, non-locality, etc.

Computation of mathematical special functions and angular momentum 3*nj*-symbols

We have also checked the formulas numerically, establishing quantitatively their accuracy for approximations, or in the reverse their possible use to build up multidimensional discrete basis sets in applied quantum mechanics and signal processing.

R. Anderson and we calculate the ***3nj* symbols** and Wigner ***d* functions** by directly summing the defining series using multiprecision arithmetic (MPFUN905),which allows convenient calculation of **hypergeometric** functions, of small and large argument by their series definition, without the necessity of using recurence relations, integral and rational representations, or asymptotic approximations.