Quantum and semiclassical spin networks: from atomic and molecular physics to quantum computing and gravity

Vincenzo Aquilanti[†], Ana Carla P. Bitencourt[†],
Cristiane da S. Ferreira[†],
Annalisa Marzuoli[‡] and Mirco Ragni[†(1)]

January 9, 2009

[†]Dipartimento di Chimica, Università di Perugia, via Elce di Sotto 8, 06123 Perugia (Italy)
[‡]Dipartimento di Fisica Nucleare e Teorica, Università degli Studi di Pavia and Istituto Nazionale di Fisica Nucleare, Sezione di Pavia, via A. Bassi 6, 27100 Pavia (Italy)

Abstract

The mathematical apparatus of quantum–mechanical angular momentum (re)coupling, developed originally to describe spectroscopic phenomena in atomic, molecular, optical and nuclear physics, is embedded in modern algebraic settings which emphasize the underlying combinatorial aspects. $SU(2)$ recoupling theory, involving Wigner's $3nj$ symbols, as well as the related problems of their calculations, general properties, asymptotic limits for large entries, plays nowadays a prominent role also in quantum gravity and quantum computing applications. We refer to the ingredients of this theory –and of its extension to other Lie and quantum group– by using the collective term of 'spin networks'.

Recent progress is recorded about the already established connections with the mathematical theory of discrete orthogonal polynomials (the so–called Askey Scheme), providing powerful tools based on asymptotic expansions, which correspond on the physical side to various levels of semi–classical limits. These results are useful not only

in theoretical molecular physics but also in motivating algorithms for the computationally demanding problems of molecular dynamics and chemical reaction theory, where large angular momenta are typically involved. As for quantum chemistry, applications of these techniques include selection and classification of complete orthogonal basis sets in atomic and molecular problems, either in configuration space (Sturmian orbitals) or in momentum space. In this paper we list and discuss some aspects of these developments –such as for instance the hyperquantization algorithm– as well as a few applications to quantum gravity and topology, thus providing evidence of a unifying background structure.

1 Introduction

The (re)coupling theory of many $SU(2)$ angular momenta –the Racah-Wigner tensor algebra– is the most exhaustive framework in dealing with interacting many–angular momenta quantum systems that can be modeled by means of conservative polylocal two–body interactions [1]. The essential features of this algebra can be encoded, for each fixed number $N = (n+1)$ of angular momentum variables, into a combinatorial object, the *spin network graph*. Vertices are associated with finite–dimensional, binary coupled Hilbert spaces while edges correspond to either phase or Racah transforms (implemented by $6j$ symbols) acting on states in such a way that the quantum transition amplitude between any pair of vertices is provided by a suitable $3nj$ symbol.

One of the goals of this paper is to promote this combinatorial setting to (families of) *computational quantum graphs* (Sec.2), to be thought of as a sort of 'abacus' encoding diagrammatical rules encountered in quantum collision theory [2] or, more in general, as computational spaces of simulators able to support quantum algorithms for computational problems arising in mathematics and theoretical physics [3]. Progress in the semiclassical limits is accounted for in Sec. 3. A few examples are then briefly addressed, emphasis being placed on those semiclassical versions of the construction, which turn out to play a crucial role in many different contexts, ranging from molecular physics (Sec. 4) and quantum computing and discrete quantum gravity models (Sec. 5). An outlook to applications and a list of perspectives for future work are collected in the concluding Sec. 6.

2 $SU(2)$ recoupling schemes as spin network graphs

Important ingredients of modern theoretical physics and chemistry are intimately linked to the mathematical theory of classical (as opposed to q–deformed) orthogonal polynomials, in particular of hypergeometric families. The recently proposed formalization of the latter within the Askey and Nikiforov schemes [4, 5] places Racah polynomials –and their q–deformed analogs [6]– at the top of a hierarchy from which all the most relevant families are obtained as particular cases or via suitable limiting procedures. Although the study of such morphology may be considered as an exercise in special function theory, relationships among families, addition formulas, linearization formulas and sum rules look like obscure manipulations of abstract quantities unless a coherent interpretation arising from physical applications could be disclosed. Physical applications, on the other hand, can lead to new insights into previously unnoticed properties and relationships.

Dealing with the quantum theory of angular momentum, Racah found a finite sum expression for the basic 'recoupling' coefficients or $6j$ symbols, representing matrix elements for the orthogonal basis transformation between two alternative binary coupling schemes of three angular momenta. Extensive developments of graphical techniques, initiated by the Yutsis school [7], allow one to deal efficiently with recouplings of $(n+1)$ angular momenta, involving the so–called $3nj$ symbols (see the handbook [8] and the review [1] (Topic 12) also for a complete list of references).

An introduction and some nomenclature are exhibited in [2], where the 'spin networks', as well as the underlying 'moves', are shown to be closely related to the tree–like graphical representation of hyperspherical coordinates and harmonics, as originally suggested in Ref. [9].

Explicit formulas and basic relationships among recoupling coefficients and harmonic superpositions (or *transplant* coefficients) and Racah polynomials can be found in [10] and in references therein. The close relationship of both vector recoupling coefficients and superposition matrix elements between alternative hyperspherical harmonics with orthogonal polynomials of a discrete variable made it possible to develop a common classification scheme, from which a number of relations and properties can be derived [2]. The important case of S^3 harmonics, discussed in [11] from the viewpoint of hydrogenoid orbitals in momentum space, is reviewed in [12], where further applications for quantum chemistry are outlined.

The underlying mathematical background of the developments discussed in [2], involves objects like the $3nj$ symbols of angular momentum theory (and their next of kin, the superposition coefficients) which are candidates for further study as

orthogonal polynomials of $(n-1)$ discrete variables.

The basic features of spin network graphs are illustrated in Fig. 1 for the significant case of binary coupling schemes of four angular momenta and their recoupling represented by a Wigner $9j$ coefficient. We refer to [2] for more details on their use as 'abacus', namely as graphical devices for practical calculations. For the construction of the abacus a proper look in terms of 'presentation' of discrete groups shows that the basic tools are the three operations corresponding to the presentation of the icosahedral group [13, 14]. From a geometrical viewpoint, the abacus essentially mixes (according to a well–known presentation of the icosahedral symmetries) pentagonal and hexagonal cycles, whose deep origin can be traced in abstract algebraic theories[15].

3 Semiclassical spin networks

According to Bohr correspondence principle, classical concepts become increasingly valid in regimes where all (or just a few) quantum numbers are 'large' (as will be illustrated in Sec. 4, such regimes are quite commonly encountered in every–day analysis of atomic and molecular dynamical processes).

In handling with angular momenta variables measured in units of $\hbar$, the classical limit $\hbar \to 0$ implies in particular that, for finite angular momenta, the j–quantum numbers are much larger than one.

In the case in which all the six angular momenta are large, the Racah $6j$ symbol admits a well defined *asymptotic limit*, whose absolute square (probability) corresponds to the *classical limit* of the associated physical observables. Following [16, 17, 18] and [1] (Topic 9) (where a self contained treatment of various asymptotics of angular momentum functions is given, together with the list of original references), recall that the square of the symbol has the limiting value given by the Wigner formula

$$\left\{ \begin{array}{ccc} a & b & d \\ c & f & e \end{array} \right\}^2 \sim \frac{1}{12\pi\, V} \tag{1}$$

where V is the Euclidean volume of the tetrahedron formed by the six angular momentum 'vectors'.

A major breakthrough in semiclassical analysis is provided by the Ponzano–Regge asymptotic formula for the $6j$ symbol [16]

$$\left\{ \begin{array}{ccc} a & b & d \\ c & f & e \end{array} \right\} \sim \frac{1}{\sqrt{24\pi V}} \exp\left\{ i \left(\sum_{r=1}^{6} \ell_r\, \theta_r + \frac{\pi}{4} \right) \right\} , \tag{2}$$

where the limit is taken for all entries $\gg 1$ (recall that $\hbar = 1$) and $\ell_r \equiv j_r + 1/2$ with $\{j_r\} = \{a, b, c, d, e, f\}$. V is now the Euclidean volume of the tetrahedron

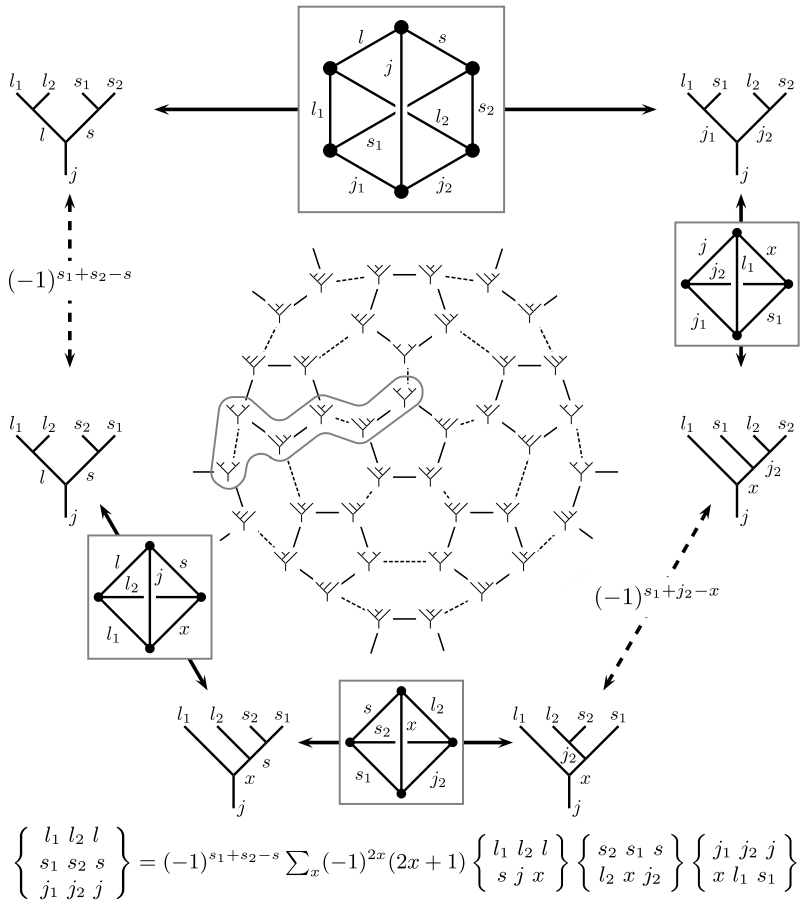

Figure 1: Spin networks are illustrated here for the case of two quantum systems, 1 and 2, each endowed with both spin and orbital angular momentum, giving a state with total angular momentum j (coupling described by spin–orbit terms in the Hamiltonian). The two alternative ways of pairing s_1, s_2, l_1, l_2, traditionally referred to as ls and jj couplings, are encoded in the top left and right 'binary trees'. Their recoupling –achieved by joining edges with identical labels– leads to the 3–valent, not planar graph (of the Yutsis–type, as referred to in the literature). The associated recoupling matrix elements give the $9j$ symbol, represented by the 3×3 array on the left–hand side of the formula. In the center a portion of what we call an 'abacus', namely an aid in obtaining the procedure for getting the decomposition illustrated in the rest of the external region of the figure: the three complete graphs on 4 vertices are associated with suitably labelled $6j$ symbols, while dotted arrows correspond to phase changes. The structure of the spin network graph displays continuous and dashed lines as well as typical pentagonal and hexagonal cycles (providing an overall 'fullerene'-like pattern), associated with the Biedenharn–Elliott and Racah identities, respectively.

with edges of lengths $\{\ell_r\}$, calculated by using the Cayley determinant (note the shift $j \to j + 1/2$ with respect to the variables employed in calculating the volume in (1)) and finally θ_r is the angle between the outer normals to the faces which share the edge ℓ_r.

The probability amplitude (2) has the form of a semiclassical wave function since the factor $1/\sqrt{24\pi V}$ is slowly varying with respect to the spin variables, while the exponential is a rapidly oscillating dynamical phase (such behavior complies with the fact that the square of this asymptotic expression reproduces Wigner's result (1)). Moreover, according to Feynman path sum interpretation of quantum mechanics, the argument of the exponential represents a classical action, and indeed it can be read as $\sum p\,\dot{q}$ for pairs (p, q) of canonical variables (angular momenta and conjugate angles). A mathematically sophisticated analysis of Ponzano–Regge result can be found in [19], where recent developments in the study of the asymptotics of $3j$ and $6j$ symbols are also reviewed.

An interesting issue –arising in connection with the interpretation of spin networks as computational quantum graphs– concerns the phenomenon of *disentanglement*. One of the main features of states belonging to the binary coupled Hilbert spaces, whose 'recoupling' gives the $6j$ Racah coefficient, is to represent effectively 'entangled' quantum states (namely states that cannot be reduced to a product of states containing quantum numbers of the individual components). Then the Racah transform (implemented by means of a $6j$ symbol, see the lefthand side of (2)), being a quantum transition amplitude, takes care of the fact that the operators $\mathbf{J}_d^2$ and $\mathbf{J}_e^2$, whose eigenvalues are $d(d+1)$ and $e(e+1)$ respectively, do not belong to the same set of mutually commuting operators and thus cannot be measured simultaneously. On the other hand, when reaching the semiclassical limit as can be seen from the righthand side of (2), the six entries of the $6j$ symbol appear to be on the same footing, a feature that can be viewed as a 'disentanglement' of the underlying 'semiclassical' spin networks. Work is in progess for what concerns the $9j$ symbol [20].

4 Molecular Physics

4.1 Atomic collisions and molecular spectroscopy

A presentation of angular momentum theory from the viewpoint of these applications, is given by Zare [21]. The theory developed about thirty years ago in [22] dealt with five alternative representations for the quantum-mechanical close-coupling formulation [22, 23, 24] of the motion along the internuclear distance of a vibrating diatomic molecule or colliding atoms having internal (spin and/or electronic) angular momenta. This unified frame transformation approaches of atomic

collision theory and concepts of molecular spectroscopy, is originally due to Hund. The physical picture and the relevant nomenclature are reviewed in Ref [25], see also [26]. Explicitly [27], starting from a sum rule equivalent to the Biedenharn–Elliott relation, (a pentagonal closed path on the abacus of Fig. 1) we obtain the definition of a $6j$ symbol as a sum of four $3j$ symbols by taking a proper limit, since one angular momentum is much larger than the others[25].

The coupling schemes of four angular momenta are illustrated in Ref.[25] as the basic ingredients underlying the classification of the five Hund cases and the relationships among representations. It was shown that the transition from one coupling scheme to another is performed by an orthogonal transformation whose matrix elements can be written in terms of 6j symbols. In the pentagonal arrangement of five alternative coupling schemes for four angular momenta (represented by the tree-like graphs at the vertices) [27], connections (the sides of the pentagon) are realized by orthogonal matrices and are related to $6j$ symbols. This was the archetype for the abacus in Fig. 1. Recent extensions of this approach have shown that in a general theory of interacting open shell atoms, $3nj$ symbols up to $n = 6$ occur [28].

4.2 Reaction dynamics: Hyperquantization

An important message that we have learned from work reviewed in Sec. 4.1 is the view that a continuous variable limit is obtained at high angular momenta from the discrete structure typical of quantum mechanics. The opposite viewpoint can be considered as well, namely the semiclassical limit may describe a continuous structure, and quantum angular momentum algebra provides discretization.

The search for both alternative reference frames and angular momentum coupling schemes has been a major challenge in quantum mechanics since its origin, and tranformations among them are represented by vector–coupling and recoupling coefficients, respectively. The relevant equations can then be formulated in terms of quantum numbers, which approximately correspond to constants of motion of the systems under study. Fundamental advances have been achieved over the years within this framework: in the last Fifties Jacob and Wick introduced the helicity formalism, widely used for the theoretical treatment of a variety of collisional problems; extending Hund's introduction of alternative coupling schemes for a diatomic molecule carrying electronic, spin, and rotational angular momenta (See Sec. 4.1). These developments fit into the frame transformation theory pioneered by Fano and coworkers in the Seventies.

Indeed, for general anisotropic interaction, discretization procedures can be introduced by exploiting Racah algebra, which fosters the introduction of alternative coupling schemes labeled by 'artificial' quantum numbers. This method

has been shown to provide an elegant and powerful tool for the solution of the reactive scattering Schröndinger equation and, at present, a considerable number of methods have been developed in this spirit, among which the 'hyperquantization' algorithm, outlined in greater detail in a number of references [29, 27, 30]. The technique relies on the hyperspherical coordinate approach when used for few-body processes, including rearrangement. For instance, in a reactive triatomic process, the reaction coordinate is represented by the hyperradius, which is a measure of the total inertia of the system, and an adiabatic representation of the total eigenfunction with respect to this coordinate is adopted. In such a way, a quantization problem on the surface of the a hypersphere (in this case the sphere in a 6–dimensional Euclidean space) must be solved for fixed values of the hyperradius. Then coupled–channel equations are integrated applying a standard propagation procedure. The success of this approach is strictly dependent on the accuracy and the effectiveness of the method used to solve the fixed hyperradius problem. The computation of the adiabatic eigenvalues containing detailed information on the structure, rotations, and internal modes parametrically in the hyperrradius is typically very demanding. The hyperquantization algorithm exploits the peculiar properties of the discrete analogues of hyperspherical harmonics, *i.e.* generalized $3j$ symbols or Hahn polynomials, orthogonal on a grid of points that span the interaction region [31]. The computationally advantageous aspect of this algorithm, besides the elegance of unifying under the language of angular momentum theory the dynamical treatment of a reaction, is the structure of the Hamiltonian matrix: its kinetic part is simple, universal, highly symmetric, and sparse, while the potential displays the diagonal form characteristic of the stereodirected representations of the previous section. The hyperquantization algorithm, when implemented for reactive scattering calculations [27], allows considerable savings in memory requirements for storage and in computing time for the building up and diagonalization of large basis sets, exploiting the sparseness and the symmetry properties of the Hamiltonian matrix.

5 Quantum gravity and quantum computing

5.1 Discretized quantum gravity in dimension 3

There exists an intriguing physical interpretation of the Ponzano–Regge asymptotics (2) once we recognize that the expression in the exponential represents the classical Regge action [32] –namely the discretized version of Einstein–Hilbert action of General Relativity – for the tetrahedron associated with the $6j$ symbol in the semiclassical limit.

In Fig. 1 the tetrahedral symmetry of each $6j$ symbol is encoded into the

corresponding 4–vertex graph, where the six entries of the symbol are associated with edges and its four triads with faces of a tetrahedron embedded in Euclidean 3–space (see *e.g.* [8] for more details on the symmetries and the geometrical properties of this symbol).

In Regge's approach to General Relativity, the edge lengths of a 'triangulated spacetime' are taken as discrete counterparts of the metric tensor appearing in the usual action for gravity and angular variables (deficit angles) are related to the scalar curvature obtained from the Riemann tensor. Technically speaking, a Regge spacetime is a piecewise linear (PL) manifold of dimension D dissected into simplices, namely triangles in $D = 2$, tetrahedra in $D = 3$, 4-simplices in $D = 4$ and so on. 'Regge Calculus' became in the early 80's the starting point for a novel approach to quantization of General Relativity known as simplicial quantum gravity (see [33] and references therein). The quantization procedure most commonly adopted is the Euclidean path sum approach, namely the discretized version Feynman path integral describing D–dimensional geometries undergoing 'quantum fluctuations'. According to this prescription, the asymptotic functional (2) –to be understood here as the semiclassical limit of a sum over truly 'quantum' fluctuations – turns out to be associated with the simplest 3–dimensional 'spacetime', the Euclidean tetrahedron. The construction of the so–called Ponzano–Regge 'state sum' representing the quantum partition function of simplicial 3–gravity will not be discussed further (see *e.g.* [3] Sec. 5, for an account).

Several years after Ponzano–Regge paper, a regularized version of their state sum –based on representation theory of a 'quantum' deformation of the group $SU(2)$– was proposed in [34] and shown to be a well–defined (finite) topological invariant for closed 3–manifolds. Since then there has been a renewed interest also in the asymptotics (2) both in connection with the study of 3–manifold geometry (and higher–dimensional generalizations [35]) and in addressing 'loop quantum gravity' models, see *e.g.* [36] and references therein.

5.2 Quantum automata and topological invariants

In the past few years there has been a tumultuous activity aimed at introducing novel conceptual schemes for quantum computing. The model of quantum simulator proposed in [37, 3] and further discussed in [38, 39] relies on the recoupling theory of $SU(2)$ angular momenta and can be viewed as a generalization to arbitrary values of the spin variables of the usual quantum–circuit model based on 'qubits' and Boolean gates [40]. The basic ingredient of such general scheme for universal quantum computing are indeed encoded into spin network computational graphs of the type depicted in the central portion of Fig. 1). Such pictorial representation makes it clear that the computational space of the simulator complies

with the architecture of (families of) 'automata'[1]. According with this kind of interpretation, a computational process on the spin network can be associated with a *directed path*, namely an ordered sequence of vertices and edges starting from an initial quantum state, say $|s>_{in}$, and ending in some set of final states $\{|s>_{fin}\}$.

In a series of papers [41, 42, 43, 44, 45] families of automata arising from the q–deformed analog of the spin network simulator have been implemented in order to deal with classes of computationally–hard problems in geometric topology (topological invariants associated with knots and with closed 3–dimensional manifolds)[2].

From the point of view of classical complexity theory, computing such invariants is 'hard', namely could be achieved by a classical computer only by resorting to an exponential amount of resources. A computational process which requires an amount of resources that grows at most polynomially with the size of the computational problem is referred to as 'efficient' (*cfr.* [45] and references therein for an account of algorithmic questions involving braid group and topological invariants ok knots).

In [41, 42], efficient (*i.e.* running in polynomial time) quantum algorithms for approximating, within an arbitrarily small range, $SU(2)_q$–colored polynomial invariants of knots have been explicitly worked out. In [44] such algorithms have been generalized to deal with 3–manifold invariants, while in [43] connections among quantized geometries, topological quantum field theory and quantum computing are discussed in detail.

6 Extensions and applications

Besides q–deformation, for alternative extensions of spin networks see [46], where 'ternary trees' are introduced to represent graphically the basic features of 'elliptic' coordinate sets on S^2 and S^3 (S^d denotes the standard d–sphere embedded in the $(d+1)$–dimensional Euclidean space) and of the corresponding harmonics. Interestingly, moving continuously along the edges of the abacus of Fig. 1 can be associated to the variation of the modulus of elliptic functions [47, 48, 49].

In Sec. 4.2, we have outlined how the concepts of reference frame transformations and of alternative angular momentum coupling schemes in quantum mechan-

[1] An automaton in computer science is a graph whose nodes encode 'internal states' while a link between two nodes represents an admissibile 'transition' between the corresponding states.

[2] A topological invariant is a quantity –typically a number or a polynomial– that depends only on the global topology of the geometrical object and not on its local metric properties.

ics lead to different representations of the quantum scattering matrix and provide a powerful guide for the analysis of atomic and molecular collisions. In particular, we have exemplified atomic and molecular elastic and inelastic collisions, but extensions to reactive scattering are most interesting and extensive applications have been worked out. Dynamical calculations for the system He+H_2^+ [50, 51] and for the benchmark reaction F+H_2 [52, 53] have been performed, also including fine–structure and isotopic effects on reactivity.

Also, a new class of entrance and exit channel indices in the scattering matrix has been worked out. Through the hyperspherical coordinate formulation referred to in Sec. 4.2, the hyperrradial problem is essentially equivalent to that of scattering from anisotropic potentials, and such a "stereodirected representation" of the scattering matrix can be used to derive information about the stereodynamincs of an atom–diatom reaction. A quantity that can be reconducted to properties measured in beam experiments on oriented molecules is the reaction probabilitiy as a function of the *steric quantum number* (see *e.g.* [26]).

Since present quantum–mechanical calculations are becoming feasible for reactive encounters on realistic potential energy surfaces (the hyperquatization algorithm provides an efficient machinery in this direction), stereodynamical properties exploiting the stereodirected representation have been reported, specifically for the reaction of HF with Li [54, 55] and of F with H_2 [56].

Further perspectives concerning the extension of angular momentum theory to hyperspaces and the use of modern advances in the theory of orthogonal polynomials of a discrete variable have been reviewed [57]. Among applications, it is worth mentioning the possibility of representing polarization parameters by 'discrete' multipole moments [58, 59] and potential energy surfaces by orthogonal discrete basis sets [60].

The study of asymptotic expansions of $3nj$ symbols for $n > 2$, as well as of different types of asymptotics (in which only a few variables are large, while the other ones are kept 'quantized') represents a major challenge not only in the framework of the formal theory of hypergeometric polynomials and related hierarchies [4], but also in view of applications to specific physical problems arising in connections with all the topics discussed in the previous Sections 4 and 5. A key example is the crucial occurrence of $9j$ symbols in the many center problem in quantum chemistry, either in Sturmian orbital or in momentum space approaches [61, 62].

Finally, for what concerns the issues discussed in Sec. 5, further algorithmic problems regarding (spin network–type) quantum geometry, topological quantum field theories in dimension 3 and associated 2–dimensional lattice models (as well as relations among them) are currently addressed [63].

7 Acknowledgments

Thanks are due to Robert Littlejohn [Berkeley, California], RogerAnderson [Santa Cruz, California] and Mario Rasetti [Turin, Italy]. Doctoral fellowships to ACPB by Capes, Brazil, and to CSF by Alban, EU, is gratefully acknowledged. Support by Italian Agencies ASI and MIUR are also acknowledged.

References

[1] L. C. Biedenharn and J. D. Louck. *The Racah–Wigner Algebra in Quantum Theory*. Encyclopedia of Mathematics and its Applications Vol 9, G–C. Rota Ed. Addison–Wesley Publ. Co. Reading MA 1981.

[2] V. Aquilanti and C. Coletti. 3nj-symbols and harmonic superposition coefficients: an icosahedral abacus. *Chem. Phys. Lett.*, 344:601–611, 2001.

[3] A. Marzuoli and M. Rasetti. Computing spin networks. *Ann. Phys.*, 318:345–407, 2005.

[4] R. Koekoek and R. Swarttouw. The askey-scheme of hypergeometric orthogonal polynomials and its q-analogue. Technical report, TU Delft, The Netherlands, 1998. Anonymous ftpsite:ftp.twi.tudelft.nl, directory:/pub/publications/tech-reports.

[5] A. F. Nikiforov, S. K. Suslov, and V. B. Uvarov. *Classical Orthogonal Polynomials of a Discrete Variable*. Springer-Verlag, Berlin, 1991.

[6] L. C. Biedenharn and M. A. Lohe. *Quantum Group Symmetry and q-Tensor Algebras*. World Scientific, Singapore, 1995.

[7] A. P. Yutsis, I. B. Levinson, and V. V. Vanagas. *Mathematical Apparatus of the Theory of Angular Momentum*. Israel Program for Scientific Translation, Jerusalem, 1962.

[8] D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii. *Quantum Theory of Angular Momentum*. World Scientific, Singapore, 1988.

[9] N. Vilenkin, G. Kuznetsov, and Y. Smorodinskii. *Sov. J. Nucl. Phys*, 2:645, 1966.

[10] V Aquilanti, S. Cavalli, and C. Coletti. Angular and hyperangular momentum recoupling, harmonic superposition and racah polynomials. a recursive algorithm. *Chem Phys. Lett.*, 344:587–600, 2001.

[11] V. Aquilanti, S. Cavalli, and C. Coletti. Hyperspherical symmetry of hydrogenic orbitals and recoupling coefficients among alternative bases. *Phys. Rev. Lett.*, 80:3209–3212, 1998.

[12] V. Aquilanti, S. Cavalli, C. Coletti, Daniela Di Domenico, and G. Grossi. Hyperspherical harmonics as sturmian orbitals in momentum space: a systematic approach to the few-body coulomb problem. *Int. Rev. Phys. Chem.*, 20:673–709, 2001.

[13] H. S. M. Coxeter and W. O. J. Moser. *Generators and Relations for Discrete Groups*. Springer, Berlin, 1965.

[14] M. Rasetti and T. Regge. *Rivista Del Nuovo Cimento*, 4:1–34, 1981.

[15] S. Majid. *Int. J. Mod. Phys. A*, 5:1, 1990.

[16] G. Ponzano and T. Regge. *Semiclassical Limit of Racah coefficients*. in F. Bloch et al (Eds.), Spectroscopic and Group Theoretical Methods in Physics; North–Holland, Amsterdam, 1968.

[17] K. Schulten and R. G. Gordon. Exact recursive evaluation of 3j- and 6j–coefficients for quantum–mechanical coupling of angular momenta. *J. Math. Phys.*, 16:1961–1970, 1975.

[18] K. Schulten and R. G. Gordon. Semiclassical approximations to 3j and 6j–coefficients for quantum–mechanical coupling of angular momenta. *J. Math. Phys.*, 16:1971–1988, 1975.

[19] V. Aquilanti, H. M. Haggard, R.G. Littlejohn, and L. Yu. Semiclassical analysis of wigner 3j-symbol. *J. Phys. A*, 40:5637–5674, 2007.

[20] R. W. Anderson, V. Aquilanti, and C. da Silva Ferreira. *in preparation*.

[21] R. N. Zare. *Angular Momentum*. John Wiley and Sons, 1988.

[22] V. Aquilanti and G. Grossi. Angular momentum coupling schemes in the quantum mechanical treatment of p-state atom collisions. *J. Chem. Phys.*, 73:1165–1172, 1980.

[23] V. Aquilanti, P. Casavecchia, A. Laganà, and G. Grossi. Decoupling approximations in the quantum mechanical treatment of p-state atom collisions. *J. Chem. Phys.*, 73:1173–1180, 1980.

[24] V. Aquilanti, G. Grossi, and A. Laganà. Approximate selection rules for intramultiplet and depolarization cross sections in atomic collisions. *Nuovo Cimento B*, 63:7–14, 1981.

[25] V. Aquilanti, S. Cavalli, and G. Grossi. Hund's cases for rotating diatomic molecules and for atomic collisions: angular momentum coupling schemes and orbital alignment. *Z. Phys. D.*, 36:215–219, 1996.

[26] V. Aquilanti, S. Cavalli, and A. Volpi. Angular momentum coupling schemes for molecular collisions: the stereodirected representation. *Phys. Essays*, 13:412–420, 2000.

[27] V. Aquilanti, S. Cavalli, D. De Fazio, A. Volpi, A. Aguilar, X. Giménez, and J. Maria Lucas. Hyperquantization algorithm: II. implementation for the F+H_2 reaction dynamics including open-shell and spin-orbit interaction. *J. Chem. Phys.*, 109:3805–3818, 1998.

[28] R. V. Krems, G. C. Groenenboom, and A. Dalgarno. *J. Phys. Chem. A*, 108:8941–8948, 2004.

[29] V. Aquilanti, S. Cavalli, and D. De Fazio. Hyperquantization algorithm: I. theory for triatomic systems. *J. Chem. Phys.*, 109:3792–3804, 1998.

[30] V. Aquilanti, S. Cavalli, A. Volpi, and D. De Fazio. The a+bc reaction by the hyperquantization algorithm: the symmetric hyperspherical parametrization for j>0. *Adv. Quant. Chem.*, 39:103–121, 2001.

[31] V. Aquilanti, S. Cavalli, and D. De Fazio. Angular and hyperangular momentum coupling coefficients as hahn polynomials. *J. Phys. Chem.*, 99:15694–15698, 1995.

[32] T. Regge. General relativity without coordinates. *Nuovo Cimento*, 19:558–571, 1961.

[33] R. M. Williams. Regge calculus: a bibliography and brief review. *Class. Quantum Grav.*, 9:1409–1422, 1992.

[34] V. Turaev and O. Ya. Viro. State sum invariants of 3–manifolds and quantum–6j symbols. *Topology*, 31:865–902, 1992.

[35] G. Carbone, M. Carfora, and A. Marzuoli. Hierarchies of invariant spin models. *Nucl. Phys. B*, 595:654–688, 2001.

[36] C. Rovelli. *Quantum Gravity*. Cambridge University Press, Cambridge, 2007.

[37] A. Marzuoli and M. Rasetti. Spin network quantum simulator. *Phys. Lett. A*, 306:79–87, 2002.

[38] A. Marzuoli and M. Rasetti. Spin network setting of topological quantum computation. *Int. J. Quant. Inf.*, 3:65–72, 2005.

[39] A. Marzuoli and M. Rasetti. Coupling of angular momenta: an insight into analogic/discrete and local/global models of computation. *Nat. Computing*, 6:151–168, 2007.

[40] M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, 2000.

[41] S. Garnerone, A. Marzuoli, and M. Rasetti. Quantum computation of universal link invariants. *Open Sys. & Infor. Dyn.*, 13:373–382, 2006.

[42] S. Garnerone, A. Marzuoli, and M. Rasetti. Quantum automata, braid group and link polynomials. *Quant. Inform. Comp.*, 7:479–503, 2007.

[43] S. Garnerone, A. Marzuoli, and M. Rasetti. Quantum geometry and quantum algorithms. *J. Phys. A: Math. Theor.*, 40:3047–3066, 2007.

[44] S. Garnerone, A. Marzuoli, and M. Rasetti. Efficient quantum processing of 3–manifold topological invariants. *arXiv: quant-ph/0703037*.

[45] S. Garnerone, A. Marzuoli, and M. Rasetti. Quantum knitting. *Laser Phys.*, 11:1582–1594, 2006.

[46] V. Aquilanti, S. Cavalli, and G. Grossi. Hyperspherical coordinates for molecular dynamics by the method of trees and the mapping of potential energy surfaces for triatomic systems. *J. Chem. Phys.*, 86:1362–1375, 1986.

[47] V. Aquilanti, A. Caligiana, and S. Cavalli. Hydrogenic elliptic orbitals, coulomb sturmian sets. recoupling coefficients among alternative bases. *Int. J. Quant. Chem.*, 92:99–117, 2003.

[48] V. Aquilanti, A. Caligiana, S. Cavalli, and C. Coletti. Hydrogenic orbitals in momentum space and hyperspherical harmonics. elliptic sturmian basis sets. *Int. J. Quant. Chem.*, 92:212–228, 2003.

[49] V. Aquilanti and S. Tonzani. Three-body problem in quantum mechanics: Hyperspherical elliptic coordinates and harmonic basis sets. *J. Chem. Phys.*, 120(9):4066–4073, 2004.

[50] P. Palmieri, C. Puzzarini, V. Aquilanti, G. Capecchi, S. Cavalli, D. De Fazio, A. Aguilar, X. Giménez, and J. M. Lucas. Ab initio dynamics of the He + $H_2^+ \rightarrow HeH^+ + H$ reaction: a new potential energy surfaces and quantum mechanical cross sections. *Mol. Phys.*, 98:1835–1849, 2000.

[51] V. Aquilanti, G. Capecchi, S. Cavalli, D. De Fazio, P. Palmieri, C. Puzzarini, A. Aguilar, X. Giménez, and J. M. Lucas. The He + H_2^+ reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronounced resonance pattern. *Chem. Phys. Lett.*, 318:619–628, 2000.

[52] V. Aquilanti, S. Cavalli, D. De Fazio, A. Volpi, A. Aguilar, X. Giménez, and J. M. Lucas. Probabilities for the F + $H_2 \rightarrow$ HF + H reaction by the hyperquantization algorithm: Alternative sequential diagonalization schemes. *Phys. Chem. Chem. Phys.*, 1:1091–1098, 1999.

[53] V. Aquilanti, S. Cavalli, D. De Fazio, A. Volpi, A. Aguilar, X. Giménez, and J.M. Lucas. Exact reaction dynamics by the hyperquantization algorithm: integral and differential cross section for F + H_2, including long-range and spin-orbit effects. *Phys. Chem. Chem. Phys.*, 4:401–415, 2002.

[54] J. M. Alvariño, V. Aquilanti, S. Cavalli, S. Crocchianti, A. Laganà, and T. Martinez. Exact quantum stereodynamics: The steric effect for the Li + HF → LiF + H reaction. *J. Chem. Phys.*, 107:3339–3340, 1997.

[55] J. M. Alvariño, V. Aquilanti, S. Cavalli, S. Crocchianti, A. Laganà, and T. Martinez. 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.

[56] J. Aldegunde, J. M. Alvariño, D. De Fazio, S. Cavalli, G. Grossi, and V. Aquilanti. Quantum stereodynamics of the F + H_2 → HF + H reaction by the stereodirected s-matrix approach. *Chem. Phys.*, 304:251–259, 2004.

[57] V. Aquilanti and G. Capecchi. Harmonic analysis and discrete polynomials. from semiclassical angular momentum theory to the hyperquantization algorithm. *Theor. Chem. Accounts*, 104:183–188, 2000.

[58] V. Aquilanti, D. Ascenzi, D. Cappelletti, R. Fedeli, and F. Pirani. Molecular beam scattering of nitrogen molecules in supersonic seeded beams: a probe of rotational alignment. *J. Phys. Chem. A.*, 101:7648–7656, 1997.

[59] R. W. Anderson and V. Aquilanti. The discrete representation correspondence between quantum and classical spatial distributions of angular momentum vectors. *J. Chem. Phys.*, 124:214104 (9 pages), 2006.

[60] V. Aquilanti, G. Capecchi, S. Cavalli, C. Adamo, and V. Barone. Representation of potential energy surfaces by discrete polynomials: proton transfer in malonaldehyde. *Phys. Chem. Chem. Phys.*, 2:4095–4103, 2000.

[61] V. Aquilanti and A. Caligiana. Sturmian approach to one-electron many-center systems: integrals and iteration schemes. *Chem. Phys. Lett.*, 366:157–164, 2002.

[62] James Avery and John Avery. *Generalized Sturmians and Atomic Spectra*. World Scientific, Singapore, 2006.

[63] Z. Kàdàr, Annalisa Marzuoli, and M. Rasetti. Braiding and entanglement in spin networks: a combinatorial description of topological phases. *Int. J. Quantum Inf.*, 2008 (in press).