Theo Thole and the graphical methods

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December 20, 2002

Abstract

Graphical methods for angular momentum coupling were almost unknown in solid state physics before Theo Thole used them with so much success. Many people are now drawing funny little lines in their notebooks and articles. This is a personal recollection of some aspects of what could be called Theo's problem solving method.

Keywords: Graphical methods, Angular momentum

1 Introduction

Although this paper was written by two persons, the authors will designate themselves as "I". This unusual procedure is due to the fact that only one of us has known Theo Thole, and expressions such as "one of the authors" are clearly too clumsy. The present article would like to be a contribution to the understanding of Theo's approach to physical problems.

During one of his stays in Orsay, he explained to me that what he much enjoyed in his work was to take a real problem, such as an experimental spectrum, to travel through a completely abstract world, apparently disconnected from terrestrial reality, then to go down to a half-hearthly space (the computer) to finally answer the physical question by reproducing (and understanding) the spectrum. As other great physicists (e.g. E.P. Wigner), he was filled with wonder at the unreasonable connections between nature and formal mathematical constructions.

His use of group theory is famous, but his work with graphical methods is also exemplary of this aspect. He started from a spectroscopic technique, he drew a few graphs, he programmed

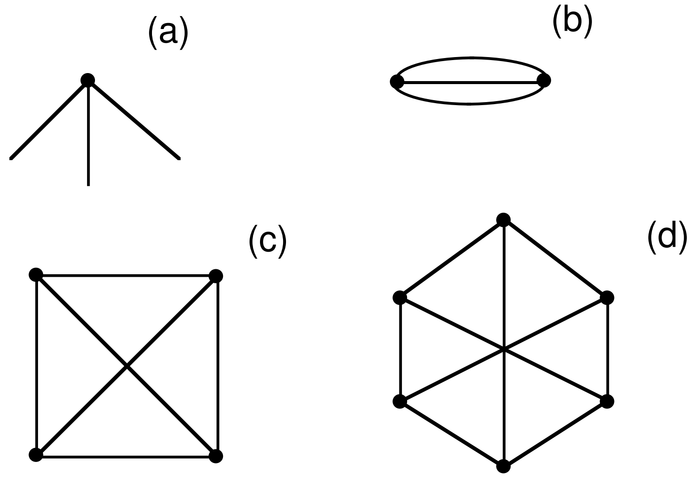

Figure 1: Angular momentum graphs: (a) 3-jm, (b) 3-j (θ graph), (c) 6-j (K_4 graph), (d) 9-j ($K_{3,3}$ graph)

them and explained experimental results. His wonder was that these strange drawings had something to do with x-rays, magnets, picoamps and ultra-high vacuum chambers.

In September 1991, Theo (exceptionally) took part in a conference in Aussois. He advised me to play with graphical methods. After months of work, I could start calculating some matrix elements and I had photocopied many papers on the subject. When he was at LURE in February 1993, Theo looked at some of them and was very excited by two articles. One was pure mathematics, without any reference whatsoever to angular momenta, and the other was the description of a computer program to reduce angular momentum graphs to sums of products of 6-j symbols.

Then, I started collecting papers on these two subjects, without knowing exactly how Theo wanted to use them. The present paper is a summary of this collection.

2 Angular momentum graphs

An angular momentum graph represents a sum of products of Wigner 3-j symbols (also called 3-jm symbols). They build $3n$-j symbols, where $3n$ is the number of edges (i.e. the number of angular momenta entering the graph). The basic symbol is the Wigner 3-jm symbol (Fig.1.a), which is the brick but not really a $3n$-j symbol because it has open edges. The real 3-j symbol (Fig.1b) represents the triangle condition. The 6-j symbol (Fig.1c) and the 9-j symbol (Fig.1d) are often used. They are sums of products of respectively four and six Wigner 3-jm symbols. The 6-j symbols appear, for instance, when three angular momenta are coupled in different orders.

Although there are early examples of angular momentum graphs [1], the basic theorems and the first applications were discovered by three Lithuanian physicists between 1957 and 1960, Levinsonas, Vanagas and Jucys, and summarized in Ref.[2]. It is not possible to give here a reasonable account of the graphical methods in angular momentum theory. Excellent presentations of these methods can be found in books [3, 4] and review articles [5, 6].

Before Theo's contribution, angular momentum graphical methods were almost exclusively restricted to atomic spectroscopy [4, 7, 8]. Even in this field, graphs were seldom used (Cowan

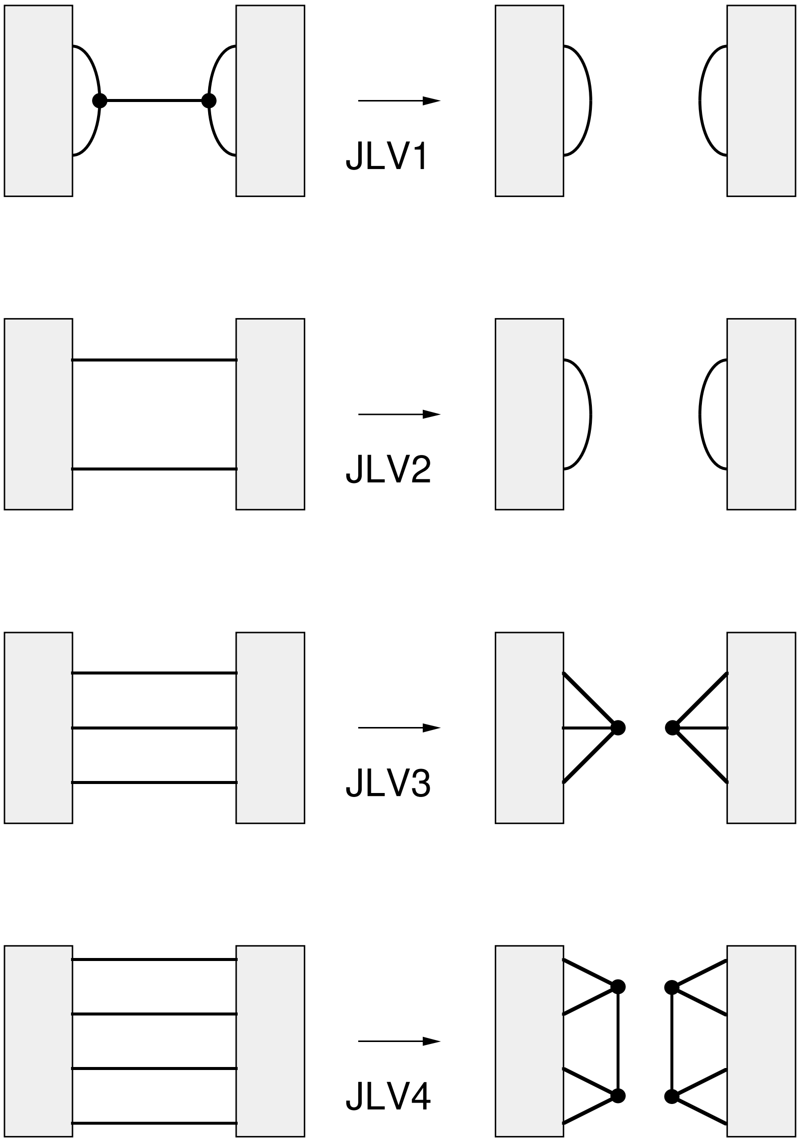

Figure 2: Cutting rules of Jucys, Levinsonas and Vanagas. The grey boxes represent the rest of the graph.

describes them in only two pages of his book [9]).

For the rest of the discussion, we need only to know the cutting rules of Jucys, Levinsonas and Vanagas. These rules JLV1, JLV2, JLV3 and JLV4 are used to cut lines between graphs (see Fig.2). The cutting rules JLV2, JLV3, JLV4, and beyond, can be derived from JLV1 and the orthogonality of Clebsch-Gordan coefficients (this is left as an exercise to the reader). We now switch to the mathematical results. For mathematicians, general angular momentum graphs are called connected cubic multigraphs with dangling edges.

3 Cubic graphs

The first operation which is done on an angular momentum graph is the closure of the dangling edges, and the removing of multiple edges. What is left is a connected cubic graph, that is a graph for which each vertex has three edges. A cubic graph has $3n$ edges (a $3n$-j symbol) and $2n$ vertices. Cubic graphs have attracted mathematicians for many years because of their beautiful properties. For instance, the 4-colour problem is equivalent to the question whether it is possible to colour the edges of a planar cubic graph with three colours so that the edges incident to any vertex have three different colours.

3.1 Definition

We must start with a few definitions. A graph G is disconnected if it can be drawn as two graphs G_1 and G_2 without an edge between G_1 and G_2. A graph is connected if it is not disconnected. A set of k edges splitting a graph G into two smaller graphs is called a k-cut of G: if you cut these edges, the graph becomes disconnected. A graph is k-connected if it has no k'-cut with $k' < k$. If a cubic graph has a 1-cut, it can be simplified by JLV1 along the 1-cut. If it has a 2-cut, it can be simplified by JLV2 along the 2-cut. Once all the 1- and 2-cuts have been exhausted, the remaining graphs are 3-connected. Now the general definition cannot be pushed further, because each set of edges incident to a vertex is a 3-cut. To go further, mathematicians have invented another notion: a graph is cyclically k-edge connected if it cannot be drawn as two graphs G_1 and G_2 with at most $k - 1$ edges between G_1 and G_2 such that G_1 and G_2 contain cycles. In other words, a cyclically k-edge connected graph cannot be cut across less than k edges into two non-trivial graphs (what we call a trivial graph is a tree). A graph is planar when it can be drawn on a plane without crossing edges.

A 3-connected graph is cyclically 3-edge connected. If it is not cyclically 4-edge connected, it can be drawn as two non trivial subgraphs linked by three edges. These three edges are cut by JLV3. The decomposition of a general angular momentum graph, using JLV1, JLV2 and JLV3 can be proved to be unique [10, 11], and the resulting graphs are 6-js, 9-js and cyclically 4-edge connected cubic graphs [10, 11] (they are called irreducible graphs in the physical literature). Moreover, Fouquet and Thuillier proved that, if a graph can be decomposed into 6-js and 9-js (and no larger graphs) then the original graph can be drawn on a surface (possibly non orientable) of genus n, where n is the number of 9-js in the decomposition [11]. In other words, a graph that can be decomposed into 6-js is a planar graph, a graph that can be decomposed into 6-js and one (two) 9-js can be written without crossing lines on a torus (doughnut), and so on.

The cyclically 4-edge connected graphs can be further simplified using JLV4, but the decomposition is no longer unique, and physical insight must now guide the choice of the right cut. Cyclically 4-edge connected graphs are important in physics because it is where you start to think, the previous steps being automatic.

Any cyclically 4-edge connected cubic graph can be obtained from the 9-j graph by repeatedly joining the midpoint of two non-adjacent lines [2, 12].

3.2 Enumeration

The enumeration of connected cubic graphs was carried out in Refs. [2, 13, 14, 15, 16]. There is one 6-j (this graph is called K_4 in the mathematical literature), two 9-j (only one of them cannot be decomposed by JLV3, it is the usual 9-j coefficient, called $K_{3,3}$ in mathematics), there are five 12-j, two of them are cyclically 4-edge connected (in the mathematical literature, they are called the cube Q_3 and the twisted cube Q'_3, see Fig.3). There are 19 15-j symbols,

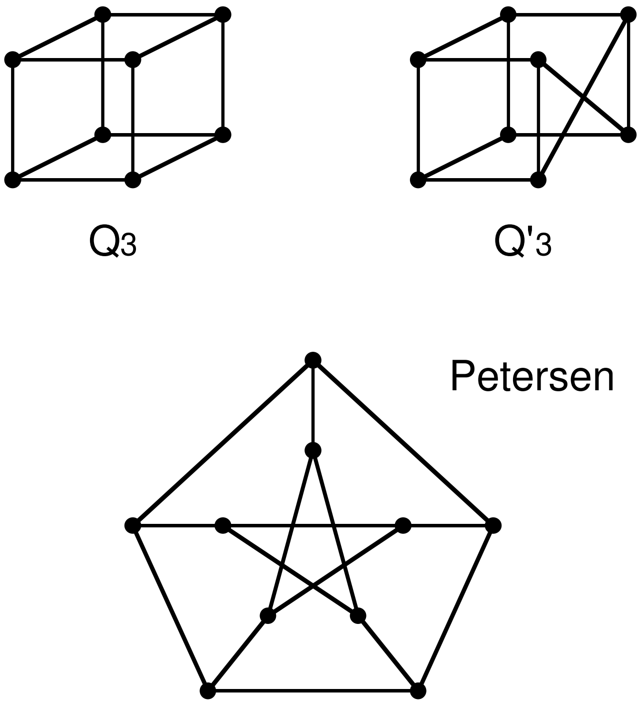

Figure 3: The cyclically 4-edge connected 12-j graphs: the cube (Q_3) and the twisted cube (Q'_3). The smallest cyclically 5-edge connected graph is a 15-j graph: the Petersen graph.

Table 1. Enumeration of angular momentum graphs

k	6-j	9-j	12-j	15-j	18-j	21-j	24-j	27-j	30-j	33-j	36-j	39-j
	1	2	5	19	85	509	4060	41301	510489	7319447	117940535	2094480864
1	0	0	0	1	4	29	186	1435	12671	131820	1590900	21940512
2	0	0	1	4	24	139	1046	9398	101668	1278335	18248616	290147706
3	-	1	2	9	39	257	2221	24368	317326	4714012	77803419	1405452231
4	0	-	2	4	16	75	560	5660	73236	1107206	18724996	346300839
5	0	0	0	1	2	8	46	435	5556	87693	1565058	30458890
6	0	0	0	0	0	1	1	5	32	381	7545	180683
7	0	0	0	0	0	0	0	0	0	0	1	3

but only five of them are cyclically 4-edge connected. One of them is the Petersen graph, the smallest cyclically 5-edge connected graph (see Fig.3).

Since no extended enumeration of cyclically k-edge connected graphs was available in the literature, we have generated the $3n$-j symbols up to n=13 using the program `minibaum3` [17] and have computed their connectivities. Table 1 summarizes the results. The first row is the total number of connected $3n$-j graphs. When k is one, two or three, the number is the number of strictly k-connected graphs, when k is four to seven, the number is the number of strictly cyclically k-edge connected graphs (strictly means that they are not cyclically $k+1$-edge connected). Up to 21-j, this table agrees with the results Rumšas and Jucys obtained in 1965 [13]. However, for the number of irreducible 24-j symbols, they give 576 instead of 560+46+1=607. The dashes concern the 6-j and 9-j symbols, which are not cyclically 4-edge connected but are irreducible (they cannot be simplified by JLV1, JLV2 and JLV3). This table shows that most graphs are decomposable.

An enumeration of labelled cyclically 4-edge connected cubic graphs was done in Ref.[10]. They are much more numerous than the usual (non-labelled) cyclically 4-edge connected cubic graphs, since the number of ways of labelling a graph G is $(2n)!/a(G)$, where $a(G)$ is the number of automorphisms of G (the number of permutations of the vertices of G which leave G unchanged). The enumeration of automorphisms of cubic graphs was done in Ref.[18] where it was shown that the number of automorphisms divides $3n2^n$ for a $3n$-j symbol. Isomorphisms between graphs and automorphisms of a graph can be calculated with the program `nauty` [19]. Algorithms that have a better asymptotical worst case appearance were proposed in Refs.[20, 21] but never implemented. Wormald [10] gives an asymptotic formula for the number of cyclically 4-edge connected graphs. Better results are obtained by dividing the number of labelled cyclically 4-edge connected graphs by $(2n)!$.

3.3 Classification

Many works were carried out on the classification of cubic graphs, and on the non-removable edges in cyclically k-edge-connected cubic graphs [22, 23, 24, 25, 26, 27]. These works are important because the non-removable edges are precisely the edges that must be cut to simplify the angular momentum diagrams most economically. The smallest cubic graphs without cycles of size $k-1$ or less are called cubic k-cages. For all known cases cubic, k-cages are cyclically k-edge connected. Therefore, the k-cages are also the smallest cyclically k-edge connected cubic graphs.

Cages have been calculated for different k (see Refs. [28, 29]). These symbols seem to be too complicated to be useful, but such a $3n$-j symbol can be met when comparing general electron couplings (not shell by shell) for atoms with n electrons. Therefore, the corresponding element is given to show the relevance of the symbols.

- $k = 3$ This is K_4, the 6-j symbol (He).
- $k = 4$ This is $K_{3,3}$, the 9-j symbol (Li).
- $k = 5$ This is the Petersen graph, Fig.3, a special 15-j symbol to which a whole book is dedicated [30], because of its wonderful properties (B).
- $k = 6$ This is a 21-j symbol called the Heawood graph (N) (Fig.4).
- $k = 7$ This is a 36-j symbol called the McGee graph (Mg).
- $k = 8$ This is a 45-j symbol called the Levi graph or the Tutte-Coxeter graph (P).
- $k = 9$ This is a 87-j symbol. For $k = 9$, the k-cage is not unique. There are 18 non-isomorphic cubic cages for $k = 9$, the Biggs-Hoare graph, the Evans graph and the McKay graphs (Cu).
- $k = 10$ This is a 105-j symbol. There are three non-isomorphic graphs, the O'Keefe-Wong graphs (Br).
- $k = 11$ This is a 168-j symbol. One is known, the Balaban graph, but might be not unique (Ba).
- $k = 12$ This is a unique 189-j symbol: the generalized hexagon (Eu).

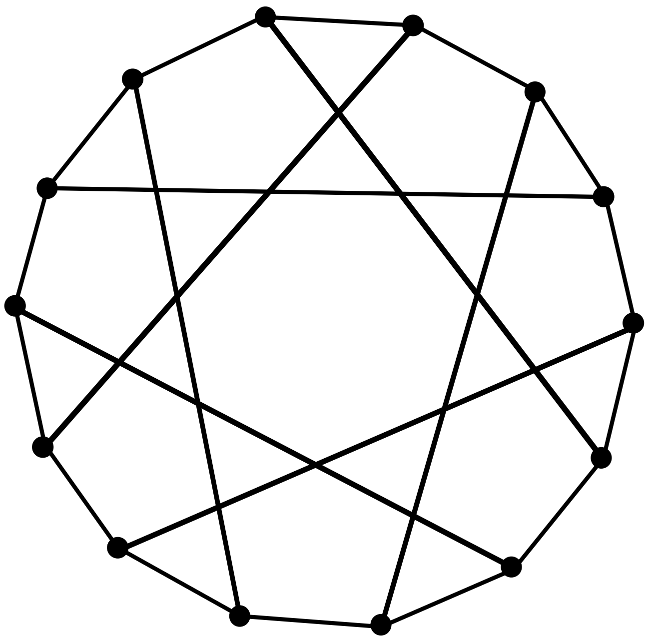

Figure 4: The smallest cyclically 6-edge-connected graph is a 21-j symbol: the Heawood graph.

- $k = 13$ From k=13, the number of edges of the cages is unknown. It is known that the 13-cage is at least a 303-j symbol (this was established after 2.3 years of cpu time). We reach now the element Md, and leave the range of common matter.

Some "minimal" cyclically 5-edge connected graphs were classified in Ref.[31]. Cyclically k-edge connected cubic graphs have other strange properties. For instance, any five edges of a cyclically 5-edge connected cubic graph lie on a cycle [32]. As a matter of fact, almost all cubic graphs are hamiltonian [33] (there is a cycle through all vertices that never uses any vertex more than once). For instance the smallest non-hamiltonian 3-connected cubic planar graphs are 57-j symbols [34]. Hamiltonian cycles do not seem to be very important in physics, except that they allow for a nice drawing of the graph, where all vertices are on an external ring. This is not possible for the non-hamiltonian Petersen graph, as can be seen in Fig.20.6 of Ref.[2], where the Petersen graph is called 15-j coefficient of the fifth kind, and drawn with a vertex in the middle of the graph. Besides, the Petersen graph is the only non-hamitonian cyclically 4-edge connected $3n$-j symbol for $n \leq 8$ and there are only two non-hamiltonian irreducible 27-j symbols.

4 Computer reduction of graphs

The second feature of Theo's method was the actual writing of computer programs. Therefore, he was very interested in the algorithms that were proposed to simplify angular momentum graphs [35, 36, 37]. Among these three references, the one by Bordarier looked most interesting. I went with Valérie Briois to the Aimé Cotton laboratory, in Orsay, where Bordarier defended his thesis. Nobody knew what happened to Bordarier's program but we obtained a copy of his PhD thesis where we learnt that his program made wonderful things. It took any angular momentum graph and could simplify it by cutting it most economically (so that the resulting sum of products of $6\text{-}j$ symbols is over a minimum number of additional angular momenta introduced by JLV4). Then the program could convert the resulting graph into an analytical formula, keeping track of all the nasty phase factors. We finally succeeded in reaching Bordarier in a national computer centre in Montpellier. He told us that large parts of his program were written in assembly language to make it faster and that the machine was thrown away a long time ago, so that no trace of the program remains. He was also very surprised to learn that his program was still interesting 23 years after it was written.

Theo took Bordarier's thesis to Groningen, although it was in French (Theo told me quite often that he could speak excellent French, but I never heard him uttering a word of it). Theo probably intended to write a program carrying out an automatic simplification of angular momentum graphs. I do not know whether he realized this.

From the mathematical side, some programs have been written to study cubic graphs [38, 17], but none of them was used to simplify angular momentum graphs. Further information on cubic graphs can be obtained from the web page of Gordon Royle [39].

5 Conclusion

In early 1994, I worked hard with angular momentum diagrams to calculate sum rules for resonant scattering spectroscopy. In February, Theo came to LURE, and I showed him proudly my many pages of calculations. He looked vaguely at the first page and said "Oh, you get an exchange energy." I was flabbergasted. How could he do within one second what took me weeks? He went even further than I, since I had not realized that my result was an exchange energy. To relieve me of my state of shock, Theo drew a few graphs on the blackboard, which summarized all my calculations. This was a combination of diagrams and second quantization, as described by Carra at this conference and that Theo was further studying in the book by Stedman [40].

This article described only one part of Theo's method. Once, he explained to us the rest of it: "When something looks too difficult, you just have to work very hard and you can do it". But he was the only one to achieve this.

6 Acknowledgements

My first thanks go to Theo Thole who taught me so much, with his philosophical sense of humor. I contacted many people to gather information on cubic graphs. We gratefully aknowledge the help of Henri Thuillier and Jean-Luc Fouquet, William McCuaig, Margaret Morton and Marston Conder, Andreas Weber, Eugene Luks and Christoph Hoffman. I am grateful to Yves Bordarier for many comments on his PhD thesis.

References

[1] R.J. Ord-Smith. The symmetry relations of the $12\text{-}j$ symbol. *Phys. Rev.*, 94(5):1227–8, 1954.

[2] A.P. Jucys, I.B. Levinsonas, and V.V. Vanagas. *Mathematical Apparatus of the Theory of Angular Momentum*. Israel Program for Scientific Translations, Jerusalem, 1962.

[3] D.M. Brink and G.K. Satchler. *Angular Momentum*. Oxford University Press, London, second edition, 1968.

[4] I. Lindgren and J. Morrison. *Atomic Many-Body Theory*. Springer-Verlag, Berlin, 1982.

[5] J.S. Briggs. Evaluation of matrix elements from a graphical representation of the angular integral. *Rev. Mod. Phys.*, 43(2):189–230, 1971.

[6] P.G.H. Sandars. Graphical methods in angular momentum theory. In M. Chrétien and E. Lipworth, editors, *Lectures in Theoretical Physics, Brandeis University Summer Institute*, volume 1, pages 171–216, New York, 1969. Gordon and Breach.

[7] A. Matulis and A.A. Bandzaitis. On a perturbation expansion of the matrix element of the atomic transition operator (in Russian). *Lietuvos Fizikos Rinkinys*, 5(4):453–62, 1965.

[8] J. Oreg, W.H. Goldstein, A. Bar-Shalom, and M. Klapisch. Configuration average of general n-body symmetrical tensor operator. *J. Comput. Phys.*, 91:460–77, 1990.

[9] R.D. Cowan. *The Theory of Atomic Structure and Spectra*. University of California Press, Berkeley, 1981.

[10] N.C. Wormald. Enumeration of cyclically 4-connected cubic graphs. *J. Graph Theory*, 9:563–73, 1985.

[11] J.-L. Fouquet and H. Thuillier. Decomposition of 3-connected cubic graphs. *Discrete Math.*, 114:181–98, 1993.

[12] N.C. Wormald. Classifying k-connected cubic graphs. In A.F. Horadam and W.D. Wallis, editors, *Combinatorial Mathematics IV*, volume 748 of *Lecture Notes in Mathematics*, pages 199–206, Berlin, 1979. Springer-Verlag.

[13] P.D. Rumšas and A.P. Jucys. $24j$-coefficients (in Russian). *Lietuvos Fizikos Rinkinys*, 5(2):197–214, 1965.

[14] A.T. Balaban, R. Vancea, I. Motoc, and S. Holban. FORTRAN IV program for computing the numbers of general cubic graphs on p vertices. *J. Chem. Inf. Comput. Sci.*, 26:72–6, 1986.

[15] Chengxue Zhang and Yuansheng Yang. Counting of regular graphs (in Chinese). *J. Dalian Univ. Techn.*, 29(4):389–98, 1989.

[16] R.W. Robinson and N.C. Wormald. Numbers of cubic graphs. *J. Graph Theory*, 7:463–67, 1983.

[17] G. Brinkmann. Fast generation of cubic graphs. *J. Graph Theory*, 23(2):139–149, 1996.

[18] N.C. Wormald. On the number of automorphisms of a regular graph. *Proc. Amer. Math. Soc*, 76(2):345–8, 1979.

[19] B.D. McKay. `nauty` users' guide (version 1.5), Technical Report TR-CS-90-02, Computer Science Dept., Australian National University (1990). The program is available from the author at http://cs.anu.edu.au/$\sim$bdm.

[20] Z. Galil, C.M. Hoffmann, E.M. Luks, C.P. Schnorr, and A. Weber. An $O(n^3 \log n)$ deterministic and an $O(n^3)$ Las Vegas isomorphism test for trivalent graphs. *J. Assoc. Comput. Mach.*, 34(3):513–31, 1987.

[21] A. Weber. *Isomorphieprobleme für trivalente Graphen (in German).* PhD thesis, University of Frankfurt, 1982.

[22] H. Thuillier. *Contribution à l'étude des graphes cubiques et des graphes gracieux (in French).* PhD thesis, University of Paris, Orsay, 1987.

[23] W.D. McCuaig. *Edge reductions in cyclically k-connected cubic graphs.* PhD thesis, University of Waterloo, 1987.

[24] L.D. Andersen, H. Fleischner, and B. Jackson. Removable edges in cyclically 4-edge-connected cubic graphs. *Graphs and Combinatorics*, 4:1–21, 1988.

[25] J.-L. Fouquet and H. Thuillier. k-minimal 3-connected cubic graphs. *Ars Combinatoria*, 26:149–90, 1988.

[26] J.-L. Fouquet and H. Thuillier. Non removable edges in 3-connected cubic graphs. *Graphs and Combinatorics*, 7:119–141, 1991.

[27] W.D. McCuaig. Edge reduction in cyclically k-connected cubic graphs. *J. Combin. Theory Series B*, 56:16–44, 1992.

[28] G. Brinkmann, B.D. McKay, and C. Saager. The smallest cubic graphs of girth nine. *Combinatorics, Probability and Computing*, 4:317–329, 1996.

[29] D. Ashlock and D. Schweizer. Graphical construction of cubic cages. *Congressus Numerantium*, 112:213–21, 1995.

[30] D.A. Holton and J. Sheehan. *The Petersen Graph.* Cambridge University Press, Cambridge, 1993.

[31] R.E.L. Aldred, D.A. Holton, and B. Jackson. Uniform cyclic edge connectivity in cubic graphs. *Combinatorica*, 11(2):81–96, 1991.

[32] R.E.L. Aldred and D.A. Holton. Cycles through fived edges in 3-connected cubic graphs. *Graphs and Combinatorics*, 3:299–311, 1987.

[33] R.W. Robinson and N.C. Wormald. Almost all cubic graphs are hamiltonian. *Random Structures and Algorithms*, 3(2):117–25, 1992.

[34] D.A. Holton and B.D. McKay. The smallest non-hamiltonian 3-connected cubic planar graphs have 38 vertices. *J. Combin. Theory Series B*, 45:304–19, 1988.

[35] P.D. Rumšas, A.A. Bandzaitis, and A.P. Jucys. On the expansion of $3nj$-coefficients (in Russian). *Lietuvos Fizikos Rinkinys*, 5(2):197–214, 1965.

[36] Y. Bordarier. *Contribution à l'emploi de méthodes graphiques en spectroscopie atomique (in French).* PhD thesis, University of Paris, Orsay, 1970.

[37] D.J. Newman and J. Wallis. Reduction of angular momentum expressions by matrix arithmetic. *J. Phys. A: Math. Gen.*, 9(12):2021–33, 1976.

[38] N.C. Wormald. Generating random regular graphs. *J. Algorithms*, 5:247–80, 1984.

[39] Combinatorial Catalogues, Department of Computer Science, University of Western Australia, http://www.cs.uwa.edu.au:80/$\sim$gordon.

[40] G.E. Stedman. *Diagram techniques in group theory*. Cambridge University Press, Cambridge, 1990.