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Simplification of the spectral analysis of the volume operator in loop quantum gravity

J Brunnemann and T Thiemann

Perimeter Institute for Theoretical Physics and University of Waterloo Waterloo, Ontario, Canada

E-mail: jbrunnemann@perimeterinstitute.ca and tthiemann@perimeterinstitute.ca

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Abstract
The volume operator plays a crucial role in the definition of the quantum dynamics of loop quantum gravity (LQG). Efficient calculations for dynamical problems of LQG can therefore be performed only if one has sufficient control over the volume spectrum. While closed formulae for the matrix elements are currently available in the literature, these are complicated polynomials in $6j$ symbols which in turn are given in terms of Racah's formula which is too complicated in order to perform even numerical calculations for the semiclassically important regime of large spins. Hence, so far not even numerically the spectrum could be accessed. In this paper, we demonstrate that by means of the Elliot–Biedenharn identity one can get rid of all the $6j$ symbols for any valence of the gauge-invariant vertex, thus immensely reducing the computational effort. We use the resulting compact formula to study numerically the spectrum of the gauge-invariant 4-vertex. The techniques derived in this paper could also be of use for the analysis of spin–spin interaction Hamiltonians of many-particle problems in atomic and nuclear physics.

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1. Introduction

The volume operator [1, 2] plays a pivotal role in the definition of the quantum dynamics [4–6] of loop quantum gravity (LQG) [3]. Since the success of LQG depends on whether the quantum dynamics reproduces classical general relativity (GR) coupled to quantum matter in the semiclassical regime it is of upmost importance to know as much as possible about the spectrum of the volume operator.

The volume operator has been studied to some extent in the literature [7–10] and it is well known that its spectrum is entirely discrete. However, so far only a closed formula for its matrix elements has been found. Unfortunately, not only is the formula for the matrix elements a complicated polynomial in $6j$ symbols involving extended sums over intertwiners, in addition the $6j$ symbols themselves are not easy to compute. Namely, the only known closed expression for the $6j$ symbols is Racah's famous formula which in turn involves fractions of factorials of large numbers and sums whose range depends in a complicated way on the entries of the $6j$ symbol. Accordingly, even powerful computer program such as *Mathematica* or *Maple* run very fast out of memory even for moderate values of the spin labels on the edges adjacent to the vertex in question. For instance, the current authors were not able to go beyond $j = 3$ when numerically computing the eigenvalues for a gauge invariant, 4-valent vertex, just using the matrix element formulae available in the literature. Thus, in order to make progress, analytical work is mandatory.

In this paper, which is based on the diploma thesis [11], we simplify the matrix element formula as given in [10] tremendously: using an identity due to Elliot and Biedenharn we are able to get rid of all the sums over intertwiners and all the $6j$ symbols in the final formula, no matter how large the valence of the vertex is. The closed expression we obtain is a harmless polynomial of simple roots of fractional expressions in the spins and intertwiners, without factorials, that label the spin network functions in question. We reproduce the closed expression for the gauge-invariant 4-vertex which has been discovered first by de Pietri [8].

This formula should be of interest for a wide range of applications. First of all, it opens access to the numerical analysis of dynamical questions in canonical LQG. In particular, there is now work in progress aiming at extending the spectacular results of [12] from the cosmological minisuperspace truncation to the full theory. Possible first applications are alluded to in the conclusion. Next, the techniques presented here could be of use for numerical investigations of convergence issues of spin foam models; see e.g. [13] and references therein. Furthermore, our methods reveal that the time has come to put LQG calculations on a supercomputer. Finally, it is conceivable that our formalism is of some use in the physics of many-particle spin–spin interactions as, e.g., in atomic or nuclear physics.

The present paper is organized as follows. In section 2, we review the definition of the volume operator as derived in [2] and the closed expression for its matrix elements established in [10]. Knowledge of LQG [1] is not at all necessary for the purpose of this paper, which can be read also as a paper on the spectral analysis of a specific interaction Hamiltonian for a large spin system.

The main result of this paper is contained in section 3 where we derive the simplification of the matrix elements. At the danger of boring the reader we display all the intermediate steps. We do this because we feel that without these steps the proof, which in part is a complicated book-keeping problem, cannot be understood. The compact final formula is (45).

In section 4, we use our formalism in order to study the gauge-invariant 4-vertex. The simplification of the matrix element formula now enables us to diagonalize the volume operator in a couple of hours for spin occupations of up to a $2j_{\max} \approx 10^2$. More efficient programming and compiler-based programming languages such as *Lisp* should be able to go significantly higher. Among the 'spectroscopy experiments' we performed are the investigation of the computational effort, the possible existence of a volume gap (smallest non-zero eigenvalue), the spectral density distribution and the relative number of degenerate (zero volume) configurations. Among the surprises, we find numerical evidence for a universal density distribution in terms of properly rescaled quantities valid at large spin. Next, there is numerical evidence for the existence of a volume gap at least for the 4-valent vertex. Finally, it seems that the eigenvalues form distinguishable series just like for the hydrogen atom, which provides a numerical criterion for the question, which part of the spectrum remains unaffected when removing the finite size 'cut-off' $j_{\max}$.

In section 5, we summarize our results and in the appendices we provide combinatorial and analytical background information which hopefully make the paper self-contained.

2. Revision of known results

This section summarizes the definition of the volume operator of LQG and reviews the matrix element formula proved in [10]. Readers not familiar with LQG can view the volume operator as a specific spin–spin interaction Hamiltonian for a many-particle system. After some introductory remarks for the benefit of the reader with an LQG background, we will switch to a corresponding angular momentum description immediately which makes knowledge of LQG unnecessary for the purposes of this paper.

In LQG, typical states are cylindrical functions f_γ which are labelled by graphs γ. The graph itself can be thought of as a collection $E(\gamma)$ of its oriented edges e which intersect in their endpoints which we call the vertices of γ. The set of vertices will be denoted by $V(\gamma)$. The cylindrical functions f_γ depend on $SU(2)$ matrices h_e which have the physical interpretation of holonomies of an $SU(2)$-connection along the edges $e \in E(\gamma)$.

In [1, 2], the operator describing the volume of a spatial region R, namely the volume operator $\hat{V}(R)_\gamma$ acting on the cylindrical functions over a graph γ, was derived as

$$\hat{V}(R)_\gamma = \int_R \mathrm{d}^3 p \sqrt{\widehat{\det(q)(p)_\gamma}} = \int_R \mathrm{d}^3 p \hat{V}(p)_\gamma \tag{1}$$

where

$$\hat{V}(p)_\gamma = \ell_P^3 \sum_{v \in V(\gamma)} \delta^3(p,v) \hat{V}_{v,\gamma} \tag{2}$$

$$\hat{V}_{v,\gamma} = \sqrt{\left| \frac{\mathrm{i}}{3! \cdot 8} \sum_{\substack{e_I, e_J, e_K \in E(\gamma) \\ e_I \cap e_J \cap e_K = v}} \epsilon(e_I, e_J, e_K) q_{IJK} \right|} \tag{3}$$

$$q_{IJK} = \epsilon_{ijk} X_I^i X_J^j X_K^k. \tag{4}$$

The sum has to be taken over all vertices $v \in V(\gamma)$ of the graph γ and at each vertex v over all possible triples (e_I, e_J, e_K) of edges of the graph γ adjacent to v. Here, $\epsilon(e_I, e_J, e_K)$ is the sign of the cross product of the three tangent vectors of the edges (e_I, e_J, e_K) at the vertex v and we have assumed without loss of generality that all edges are outgoing from v.

X_I^i are the right invariant vector fields on $SU(2)$ acting on the holonomy entries of the cylindrical functions. They satisfy the commutation relation $\left[X_I^i, X_J^j\right] = -2\delta_{IJ}\epsilon^{ijk} X_I^k$. The self-adjoint right invariant vector fields $Y_J^j := \frac{\mathrm{i}}{2} X_J^j$ fulfilling $\left[Y_I^i, Y_J^j\right] = \mathrm{i}\delta_{IJ}\epsilon^{ijk} Y_I^k$ are equivalent to the action of angular momentum operators J_I^i. It is this algebraic property which we use in order to derive the spectral properties of the volume operator: it turns out that the Hilbert space of LQG reduces on cylindrical functions over a graph γ to that of an abstract spin system familiar from the theory of angular momentum in quantum mechanics. There are as many degrees of freedom as there are edges in γ and furthermore we can diagonalize all $\hat{V}_{v,\gamma}$ simultaneously as they are obviously mutually commuting. Hence, in what follows familiarity with LQG is not at all necessary; abstractly, we are just dealing with an interaction Hamiltonian in a many-particle spin system.

We can therefore replace

$$q_{IJK} = \left(\frac{2}{\mathrm{i}}\right)^3 \epsilon_{ijk} J_I^i J_J^j J_K^k. \tag{5}$$

Using furthermore the antisymmetry of ϵ_{ijk} and the fact that $\left[J_I^i, J_J^j\right] = 0$ whenever $I \neq J$, we can restrict the summation in (3) to $I < J < K$ if we simultaneously write a factor 3! in front of the sum. The result is

$$\hat{V}_{v,\gamma} = \sqrt{\left|\sum_{I<J<K} \epsilon(e_I, e_J, e_K)\epsilon_{ijk} J_I^i J_J^j J_K^k\right|}. \tag{6}$$

Now the following identity holds:

$$\epsilon_{ijk} J_I^i J_J^j J_K^k = \frac{\mathrm{i}}{4}[(J_{IJ})^2, (J_{JK})^2] \tag{7}$$

where $J_{IJ} = J_I + J_J$. This relation can be derived by writing down every commutator as $[(J_{IJ})^2, (J_{JK})^2] = \sum_{i,j=1}^{3} \left[\left(J_I^i + J_J^i\right)^2, \left(J_J^j + J_K^j\right)^2\right]$, using the identity $[a, bc] = [a, b]c + b[a, c]$ for the commutator, using the angular momentum commutation relations (A.1) and the fact that $\left[J_I^i, J_J^j\right] = 0$ whenever $I \neq J$.

We may summarize

$$\hat{V}_{v,\gamma} = \sqrt{\left|Z \cdot \sum_{I<J<K} \epsilon(e_I, e_J, e_K)\hat{q}_{IJK}\right|} \tag{8}$$

where $\hat{q}_{IJK} := [(J_{IJ})^2, (J_{JK})^2]$ and $Z = \frac{\mathrm{i}}{4}$.

Unless announced differently we will study the operator

$$\hat{q}_{IJK} := [(J_{IJ})^2, (J_{JK})^2] \tag{9}$$

in the following.

2.1. Matrix elements in terms of 3nj-symbols

Now we can apply the recoupling theory of n angular momenta to represent $\hat{q}_{IJK}$ in a recoupling scheme basis using the definitions (A.1)–(A.3) given in the appendix.

We will do this with respect to the standard basis (A.2), where we can now easily restrict our calculations to gauge-invariant spin network states, by demanding the total angular momentum j and the total magnetic quantum number M to vanish, that means we will take into account only recoupling schemes, coupling the outgoing spins at the vertex v to resulting angular momentum 0.

In terms of the recoupling schemes these states are given by

$$|\vec{g}(IJ)\vec{j}\,j = 0 M = 0\rangle := |\vec{g}(IJ)\rangle \tag{10}$$

where we introduced an abbreviation, since the quantum numbers $\vec{j}\,j = 0M = 0$ are the same for every gauge-invariant spin network state with respect to one vertex v.

We will now represent $\hat{q}_{IJK} := [(J_{IJ})^2, (J_{JK})^2]$ in the standard-recoupling scheme basis of definition (A.2) where $|\vec{a}\rangle := |\vec{a}(12)\rangle$, $|\vec{a}'\rangle := |\vec{a}'(12)\rangle$.

The point is that by construction a recoupling scheme basis $|\vec{g}(IJ)\rangle$ diagonalizes the operator $(G_2)^2 = (J_{IJ})^2 = (J_I + J_J)^2$ that is

$$(G_2)^2|\vec{g}(IJ)\rangle = g_2(IJ)(g_2(IJ) + 1)|\vec{g}(IJ)\rangle. \tag{11}$$

Furthermore, every recoupling scheme $|\vec{g}(IJ)\rangle$ can be expanded in terms of the standard basis via its expansion coefficients, the $3nj$-symbols given by definition (A.3) in the appendix. So, it is possible to express

$$\begin{aligned}
\langle\vec{a}|\hat{q}_{IJK}|\vec{a}'\rangle &= \langle\vec{a}|[(J_{IJ})^2, (J_{JK})^2]|\vec{a}'\rangle \\
&= \langle\vec{a}|(J_{IJ})^2(J_{JK})^2]|\vec{a}'\rangle - \langle\vec{a}|(J_{JK})^2(J_{IJ})^2|\vec{a}'\rangle \\
&= \sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)[\langle\vec{a}|\vec{g}(IJ)\rangle\langle\vec{g}_{IJ}|J_{JK}^2|\vec{a}'\rangle - \langle\vec{a}|J_{JK}^2|\vec{g}_{IJ}\rangle\langle\vec{g}(IJ)|\vec{a}'\rangle] \\
&= \sum_{\vec{g}(IJ),\vec{g}(JK),\vec{g}''(12)} g_2(IJ)(g_2(IJ)+1)g_2(JK)(g_2(JK)+1)\langle\vec{g}(IJ)|\vec{g}''\rangle\langle\vec{g}(JK)|\vec{g}''\rangle \\
&\quad\times [\langle\vec{g}(IJ)|\vec{a}\rangle\langle\vec{g}(JK)|\vec{a}'\rangle - \langle\vec{a}(JK)|\vec{g}\rangle\langle\vec{g}(IJ)|\vec{a}'\rangle] \\
&= \sum_{\vec{g}''(12)} \Bigg[\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle\vec{g}(IJ)|\vec{g}''\rangle\langle\vec{g}(IJ)|\vec{a}\rangle \\
&\quad\times \sum_{\vec{g}(JK)} g_2(JK)(g_2(JK)+1)\langle\vec{g}(JK)|\vec{g}''\rangle\langle\vec{g}(JK)|\vec{a}'\rangle\Bigg] - [\vec{a} \Longleftrightarrow \vec{a}']
\end{aligned} \tag{12}$$

which is again an antisymmetric matrix possessing purely imaginary eigenvalues (we could alternatively consider the Hermitian version by multiplying all matrix elements by the imaginary unit i). Here, we have inserted suitable recoupling schemes $|\vec{g}(IJ)\rangle$, $|\vec{g}(JK)\rangle$ diagonalizing $(J_{IJ})^2$ and $(J_{JK})^2$ and their expansion in terms of the standard basis $|\vec{g}(12)\rangle$ by using the completeness of the recoupling schemes $|\vec{g}(IJ)\rangle$ for arbitrary $I \neq J$:[1]

$$\mathbb{1} = \sum_{\vec{g}(IJ)} |\vec{g}(IJ)\rangle\langle\vec{g}(IJ)|. \tag{13}$$

So we have as a first step expressed the matrix elements of $\hat{q}_{IJK}$ in terms of $3nj$-symbols.

2.2. Closed expression for the $3nj$-symbols

The $3nj$-symbols occurring in (12) can be expressed in terms of the individual recouplings implicit in their definition.

2.2.1. Preparations. In [10] the two following lemmas are derived:

Lemma 2.1 (contraction on identical coupling order)**.**

$$\begin{aligned}
\langle\vec{g}(IJ)|\vec{g}'\rangle &= \langle g_2(j_I,j_J), g_3(g_2,j_1),\ldots,g_{I+1}(g_I,j_{I-1}), g_{I+2}(g_{I+1},j_{I+1}),\ldots,g_J(g_{J-1},j_{J-1})| \\
&\quad\times |g_2''(j_1,j_2), g_3''(g_2'',j_3),\ldots,g_{I+1}''(g_I'',j_{I-1}), \\
&\quad\times g_{I+2}''(g_{I+1}'',j_{I+1}),\ldots,g_J''(g_{J-1}'',j_J)\rangle\delta_{g_J,g_J''}\cdots\delta_{g_{n-1},g_{n-1}''}.
\end{aligned}$$

Lemma 2.2 (interchange of coupling order)**.**

$$\begin{aligned}
&\langle g_2'(j_1,j_2),\ldots,g_K'(g_{K-1}',j_K), g_{K+1}'(g_K',j_{K+1}), g_{K+2}'(g_{K+1}',j_{K+2})| \\
&\qquad\times |g_2(j_1,j_2),\ldots,g_K(g_{K-1},j_K), g_{K+1}(g_K,j_{K+2}), g_{K+2}(g_{K+1},j_{K+1})\rangle \\
&\quad= \langle g_{K+1}'(g_K,j_{K+1}), g_{K+2}'(g_{K+1}',j_{K+2})|g_{K+1}(g_K,j_{K+2}), \\
&\qquad\times g_{K+2}(g_{K+1},j_{K+1})\rangle\delta_{g_2'g_2}\delta_{g_3'g_3}\cdots\delta_{g_K'g_K}\cdot\delta_{g_{K+2}'g_{K+2}}.
\end{aligned}$$

[1] The summation has to be extended over all possible intermediate recoupling steps $g_2,\ldots,g_{n-1}$ that is $|j_r - j_q| \leqslant g_k(j_q,j_r) \leqslant j_q + j_r$ allowed by theorem A.1 given in the appendix.

2.2.2. Closed expression for the $3nj$*-symbols.* Now we can reduce out the $3nj$-symbol. In what follows we will not explicitly write down the δ-expressions occurring by using lemmas 2.1 and 2.2, but keep them in mind.

Collecting all the terms mentioned in [10], one obtains the following equation for the $3nj$-symbols:

$$
\begin{aligned}
\langle\vec{g}(IJ)|\vec{g}'(12)\rangle = &\sum_{h_2(j_I,j_1)} \langle g_2(j_I,j_J), g_3(g_2,j_1)|h_2(j_I,j_1), g_3(h_2,j_J)\rangle \\
&\times \sum_{h_3(h_2,j_2)} \langle g_3(h_2,j_J), g_4(g_3,j_2)|h_3(h_2,j_2), g_4(h_3,j_J)\rangle \\
&\vdots \quad \vdots \qquad\qquad \vdots \\
&\times \sum_{h_{I-1}(h_{I-2},j_{I-2})} \langle g_{I-1}(h_{I-2},j_J), g_I(g_{I-1},j_{I-2})|h_{I-1}(h_{I-2},j_{I_2}), g_I(h_{I-1},j_J)\rangle \\
&\times \langle g_I(h_{I-1},j_J), g_{I+1}(g_I,j_{I-1})|g'_I(h_{I-1},j_{I-1}), g_{I+1}(g'_I,j_J)\rangle \\
&\times \langle g_{I+1}(g'_I,j_J), g_{I+2}(g_{I+1},j_{I+1})|g'_{I+1}(g'_I,j_{I+1}), g_{I+2}(g'_{I+1},j_J)\rangle \\
&\times \langle g_{I+2}(g'_{I+1},j_J), g_{I+3}(g_{I+2},j_{I+2})|g'_{I+2}(g'_{I+1},j_{I+2}), g_{I+3}(g'_{I+2},j_J)\rangle \\
&\vdots \qquad\qquad\qquad\qquad \vdots \\
&\times \langle g_{J-1}(g'_{J-2},j_J), g_J(g_{J-1},j_{J-1})|g'_{J-1}(g'_{J-2},j_{J-1}), g_J(g'_{J-1},j_J)\rangle \\
&\times \langle h_2(j_I,j_1), h_3(h_2,j_2)|g'_2(j_1,j_2), h_3(g'_2,j_I)\rangle \\
&\times \langle h_3(g'_2,j_I), h_4(h_3,j_3)|g'_3(g'_2,j_3), h_4(g'_3,j_I)\rangle \\
&\times \langle h_4(g'_3,j_I), h_5(h_4,j_4)|g'_4(g'_3,j_4), h_5(g'_4,j_I)\rangle \\
&\vdots \qquad\qquad \vdots \\
&\times \langle h_{I-1}(g'_{I-2},j_I), g'_I(h_{I-1},j_{I-1})|g'_{I-1}(g'_{I-2},j_{I-1}), g'_I(g'_{I-1},j_I)\rangle. \qquad (14)
\end{aligned}
$$

3. Simplification of the matrix elements

3.1. $3nj$*-symbols expressed in terms of* $6j$*-symbols*

It is now obvious that we can express (14) via the $6j$-symbols defined as in (B.1):

$$
\begin{aligned}
&\langle j_{12}(j_1,j_2), j(j_{12},j_3)|j_{23}(j_2,j_3), j(j_1,j_{23})\rangle \\
&\quad = [(2j_{12}+1)(2j_{23}+1)]^{\frac{1}{2}}(-1)^{j_1+j_2+j_3+j}\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23}\end{Bmatrix}. \qquad (15)
\end{aligned}
$$

Here, we have used the fact that $j_1+j_2+j_3+j$ is integer. Now the definition of the $6j$-symbol in terms of Clebsh–Gordon coefficients (CGC) come into play. Because of the properties of the CGC we can change the order of coupling in every recoupling scheme in (14) taking care of the minus signs we create:

$$
\begin{aligned}
&\langle j_{12}(j_1,j_2), j(j_{12},j_3)|j_{23}(j_2,j_3), j(j_1,j_{23})\rangle \\
&\quad = (-1)^{j_{12}-j_1-j_2}\langle j_{12}(j_2,j_1), j(j_{12},j_3)|j_{23}(j_2,j_3), j(j_1,j_{23})\rangle \\
&\quad = (-1)^{j_{12}-j_1-j_2}(-1)^{j_{23}-j_2-j_3}\langle j_{12}(j_2,j_1), j(j_{12},j_3)|j_{23}(j_3,j_2), j(j_1,j_{23})\rangle \\
&\quad = (-1)^{j_{12}-j_1-j_2}(-1)^{j_{23}-j_2-j_3}(-1)^{j-j_{12}-j_3} \\
&\qquad \times \langle j_{12}(j_2,j_1), j(j_3,j_{12})|j_{23}(j_3,j_2), j(j_1,j_{23})\rangle \\
&\quad = (-1)^{j_{12}-j_1-j_2}(-1)^{j_{23}-j_2-j_3}(-1)^{j-j_{12}-j_3}(-1)^{j-j_1-j_{23}} \\
&\qquad \times \langle j_{12}(j_2,j_1), j(j_3,j_{12})|j_{23}(j_3,j_2), j(j_{23},j_1)\rangle.
\end{aligned}
$$

In this way, we are able to change the coupling order in (14) to get the order required for a translation into the $6j$-symbols. With these preparations, we are now able to express (14) in terms of $6j$-symbols:

$$
\begin{aligned}
&\langle \vec{g}(IJ)|\vec{g}'(12)\rangle \\
&= \sum_{h_2} (-1)^{-j_I-j_J+g_2}(-1)^{h_2+j_J-g_3}(-1)^{j_I+j_J+j_1+g_3}\sqrt{(2g_2+1)(2h_2+1)}\begin{Bmatrix} j_J & j_I & g_2 \\ j_1 & g_3 & h_2 \end{Bmatrix} \\
&\times \sum_{h_3} (-1)^{-j_J-h_2+g_3}(-1)^{h_3+j_J-g_4}(-1)^{j_J+h_2+j_2+g_4}\sqrt{(2g_3+1)(2h_3+1)}\begin{Bmatrix} j_J & h_2 & g_3 \\ j_2 & g_4 & h_3 \end{Bmatrix} \\
&\vdots \quad \vdots \qquad\qquad \vdots \qquad\qquad\qquad \vdots \\
&\vdots \quad \vdots \qquad\qquad \vdots \qquad\qquad\qquad \vdots \\
&\times \sum_{h_{I-1}} (-1)^{-j_J-h_{I-2}+g_{I-1}}(-1)^{h_{I-1}+j_J-g_I}(-1)^{j_J+h_{I-2}+j_{I-2}+g_I}\sqrt{(2g_{I-1}+1)(2h_{I-1}+1)} \\
&\qquad\qquad \times \begin{Bmatrix} j_J & h_{I-2} & g_{I-1} \\ j_{I-2} & g_I & h_{I-1} \end{Bmatrix} \\
&\times (-1)^{-j_J-h_{I-1}+g_I}(-1)^{j_J+g'_I-g_{I+1}}(-1)^{j_J+h_{I-1}+j_{I-1}+g_{I+1}}\sqrt{(2g_I+1)(2g'_I+1)} \\
&\qquad\qquad \times \begin{Bmatrix} j_J & h_{I-1} & g_I \\ j_{I-1} & g_{I+1} & g'_I \end{Bmatrix} \\
&\times (-1)^{-j_J-g'_I+g_{I+1}}(-1)^{j_J+g'_{I+1}-g_{I+2}}(-1)^{j_J+g'_I+j_{I+1}+g_{I+2}}\sqrt{(2g_{I+1}+1)(2g'_{I+1}+1)} \\
&\qquad\qquad \times \begin{Bmatrix} j_J & g'_I & g_{I+1} \\ j_{I+1} & g_{I+2} & g'_{I+1} \end{Bmatrix} \\
&\times (-1)^{-j_J-g'_{I+1}+g_{I+2}}(-1)^{j_J+g'_{I+2}-g_{I+3}}(-1)^{j_J+g'_{I+1}+j_{I+2}+g_{I+3}}\sqrt{(2g_{I+2}+1)(2g'_{I+2}+1)} \\
&\qquad\qquad \times \begin{Bmatrix} j_J & g'_{I+1} & g_{I+2} \\ j_{I+2} & g_{I+3} & g'_{I+2} \end{Bmatrix} \\
&\vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
&\vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
&\times (-1)^{-j_J-g'_{J-2}+g_{J-1}}(-1)^{j_J+g'_{J-1}-g_J}(-1)^{j_J+g'_{J-2}+j_{J-1}+g_J}\sqrt{(2g_{J-1}+1)(2g'_{J-1}+1)} \\
&\qquad\qquad \times \begin{Bmatrix} j_J & g'_{J-2} & g_{J-1} \\ j_{J-1} & g_J & g'_{J-1} \end{Bmatrix} \\
&\times (-1)^{j_I+g'_2-h_3}(-1)^{j_I+j_1+j_2+h_3}\sqrt{(2h_2+1)(2g'_2+1)}\begin{Bmatrix} j_I & j_1 & h_2 \\ j_2 & h_3 & g'_2 \end{Bmatrix} \\
&\times (-1)^{-g'_2-j_I+h_3}(-1)^{j_I+g'_3-h_4}(-1)^{j_I+g'_2+j_3+h_4}\sqrt{(2h_3+1)(2g'_3+1)}\begin{Bmatrix} j_I & g'_2 & h_3 \\ j_3 & h_4 & g'_3 \end{Bmatrix} \\
&\times (-1)^{-g'_3-j_I+h_4}(-1)^{j_I+g'_4-h_5}(-1)^{j_I+g'_3+j_4+h_5}\sqrt{(2h_4+1)(2g'_4+1)}\begin{Bmatrix} j_I & g'_3 & h_4 \\ j_4 & h_5 & g'_4 \end{Bmatrix} \\
&\vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
&\vdots \qquad\qquad \vdots \qquad\qquad \vdots
\end{aligned}
$$

$$\times (-1)^{-g'_{I-2}-j_I+h_{I-1}} (-1)^{j_I+g'_{I-1}-g_I} (-1)^{j_I+g'_{I-2}+j_{I-1}+g'_I} \sqrt{(2h_{I-1}+1)(2g'_{I-1}+1)}$$
$$\times \begin{Bmatrix} j_I & g'_{I-2} & h_{I-1} \\ j_{I-1} & g'_I & g'_{I-1} \end{Bmatrix}. \tag{16}$$

This is the complete expression of (14) with all the exponents written in detail which are caused by the reordering of the coupling schemes while bringing them into a form suitable for (B.1). We want to emphasize that we have the freedom to invert the signs in each of the exponents of (16) when convenient for our calculation.

3.2. The matrix elements in terms of 6j-symbols

Taking a closer look at (12), a basic structure contained in the matrix elements of the volume operator appears:

$$\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle \vec{g}(IJ)|\vec{g}''(12)\rangle\langle \vec{g}(IJ)|\vec{a}(12)\rangle. \tag{17}$$

Using (16) we now express the $3nj$-symbols occurring in (17) via $6j$-symbols. For $\langle \vec{g}(IJ)|\vec{g}''(12)\rangle$ we use $h_2, \ldots, h_{I-1}$ as intermediate summation variables and for its (-1)-exponents the sign convention we chose in (16). For $\langle \vec{g}(IJ)|\vec{a}(12)\rangle$ we use $k_2, \ldots, k_{I-1}$ as intermediate summation variables and for its (-1)-exponents the negative of every exponent in (16), since every exponent is an integer number. Writing down carefully all these expressions most of the exponents can be cancelled.

The result of this is (using the abbreviation $A(x, y) = \sqrt{(2x+1)(2y+1)}$)

$$\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle \vec{g}(IJ)|\vec{g}''(12)\rangle\langle \vec{g}(IJ)|\vec{a}(12)\rangle = \sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)$$
$$\times \sum_{h_2} (-1)^{h_2} A(g_2, h_2) \begin{Bmatrix} j_J & j_I & g_2 \\ j_1 & g_3 & h_2 \end{Bmatrix} \sum_{k_2} (-1)^{-k_2} A(g_2, k_2) \begin{Bmatrix} j_J & j_I & g_2 \\ j_1 & g_3 & k_2 \end{Bmatrix}$$
$$\times \sum_{h_3} (-1)^{h_3} A(g_3, h_3) \begin{Bmatrix} j_J & h_2 & g_3 \\ j_2 & g_4 & h_3 \end{Bmatrix} \sum_{k_3} (-1)^{-k_3} A(g_3, k_3) \begin{Bmatrix} j_J & k_2 & g_3 \\ j_2 & g_4 & k_3 \end{Bmatrix}$$
$$\vdots \quad \vdots \qquad \vdots \quad \vdots \qquad \vdots$$
$$\vdots \quad \vdots \qquad \vdots \quad \vdots \qquad \vdots$$
$$\times \sum_{h_{I-1}} (-1)^{h_{I-1}} A(g_{I-1}, h_{I-1}) \begin{Bmatrix} j_J & h_{I-2} & g_{I-1} \\ j_{I-2} & g_I & h_{I-1} \end{Bmatrix} \sum_{k_{I-1}} (-1)^{-k_{I-1}} A(g_{I-1}, k_{I-1})$$
$$\times \begin{Bmatrix} j_J & k_{I-2} & g_{I-1} \\ j_{I-2} & g_I & k_{I-1} \end{Bmatrix}$$
$$\times (-1)^{g''_I} A(g_I, g''_I) \begin{Bmatrix} j_J & h_{I-1} & g_I \\ j_{I-1} & g_{I+1} & g''_I \end{Bmatrix} (-1)^{-a_I} A(g_I, a_I) \begin{Bmatrix} j_J & k_{I-1} & g_I \\ j_{I-1} & g_{I+1} & a_I \end{Bmatrix}$$
$$\times (-1)^{g''_{I+1}} A(g_{I+1}, g''_{I+1}) \begin{Bmatrix} j_J & g''_I & g_{I+1} \\ j_{I+1} & g_{I+2} & g''_{I+1} \end{Bmatrix} (-1)^{-a_{I+1}} A(g_{I+1}, a_{I+1}) \begin{Bmatrix} j_J & a_I & g_{I+1} \\ j_{I+1} & g_{I+2} & a_{I+1} \end{Bmatrix}$$
$$\times (-1)^{g''_{I+2}} A(g_{I+2}, g''_{I+2}) \begin{Bmatrix} j_J & g''_{I+1} & g_{I+2} \\ j_{I+2} & g_{I+3} & g''_{I+2} \end{Bmatrix} (-1)^{-a_{I+2}} A(g_{I+2}, a_{I+2}) \begin{Bmatrix} j_J & a_{I+1} & g_{I+2} \\ j_{I+2} & g_{I+3} & a_{I+2} \end{Bmatrix}$$

$$
\begin{aligned}
&\vdots \qquad\qquad\qquad\qquad \vdots \qquad\qquad\qquad\qquad \vdots\\
&\vdots \qquad\qquad\qquad\qquad \vdots \qquad\qquad\qquad\qquad \vdots\\
&\times (-1)^{g''_{J-1}} A(g_{J-1}, g''_{J-1}) \begin{Bmatrix} j_J & g''_{J-2} & g_{J-1} \\ j_{J-1} & g_J & g''_{J-1} \end{Bmatrix} (-1)^{-a_{J-1}} A(g_{J-1}, a_{J-1}) \\
&\qquad\qquad \times \begin{Bmatrix} j_J & a_{J-2} & g_{J-1} \\ j_{J-1} & g_J & a_{J-1} \end{Bmatrix} \\
&\times (-1)^{g''_2} A(h_2, g''_2) \begin{Bmatrix} j_I & j_1 & h_2 \\ j_2 & h_3 & g''_2 \end{Bmatrix} (-1)^{-a_2} A(k_2, a_2) \begin{Bmatrix} j_I & j_1 & k_2 \\ j_2 & k_3 & a_2 \end{Bmatrix} \\
&\times (-1)^{h_3+g''_3} A(h_3, g''_3) \begin{Bmatrix} j_I & g''_2 & h_3 \\ j_3 & h_4 & g''_3 \end{Bmatrix} (-1)^{-k_3-a_3} A(k_3, a_3) \begin{Bmatrix} j_I & a_2 & k_3 \\ j_3 & k_4 & a_3 \end{Bmatrix} \\
&\times (-1)^{h_4+g''_4} A(h_4, g''_4) \begin{Bmatrix} j_I & g''_3 & h_4 \\ j_4 & h_5 & g''_4 \end{Bmatrix} (-1)^{-k_4-a_4} A(k_4, a_4) \begin{Bmatrix} j_I & a_3 & k_4 \\ j_4 & k_5 & a_4 \end{Bmatrix} \\
&\vdots \qquad\qquad\qquad\qquad \vdots \qquad\qquad\qquad\qquad \vdots\\
&\vdots \qquad\qquad\qquad\qquad \vdots \qquad\qquad\qquad\qquad \vdots\\
&\times (-1)^{h_{I-1}+g''_{I-1}} A(h_{I-1}, 2g'_{I-1}) \begin{Bmatrix} j_I & g''_{I-2} & h_{I-1} \\ j_{I-1} & g''_I & g'_{I-1} \end{Bmatrix} (-1)^{-k_{I-1}-a_{I-1}} A(k_{I-1}, a_{I-1}) \\
&\qquad\qquad \times \begin{Bmatrix} j_I & a_{I-2} & k_{I-1} \\ j_{I-1} & a_I & a_{I-1} \end{Bmatrix}.
\end{aligned}
\tag{18}
$$

Up to now we have only made a translation between different notation. The reason for doing such an amount of writing will become clear soon: using identities between the $6j$-symbols it is possible to derive a much shorter closed expression for the matrix elements by evaluating step by step all the summations in (18).

3.3. A useful identity

Before we can start the evaluation we want to derive an identity which will be essential. We want to evaluate the following sum:

$$
F(j_{12}, j'_{12}) := \sum_{j_{23}} (2j_{23}+1) j_{23}(j_{23}+1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j'_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix}.
\tag{19}
$$

There exist numerous closed expressions for $6j$-symbols, whose entries have special relations. They are much more manageable than the general expression given in appendix B.2 (Racah formula). One of them reads as ([14], p 130)

$$
\begin{Bmatrix} a & b & c \\ 1 & c & b \end{Bmatrix} = (-1)^{a+b+c+1} \frac{2[b(b+1)+c(c+1)-a(a+1)]}{[2b(2b+1)(2b+2)2c(2c+1)(2c+2)]^{\frac{1}{2}}}.
\tag{20}
$$

Using the shorthand $X(b, c) = 2b(2b+1)(2b+2)2c(2c+1)(2c+2)$ and the fact that $a+b+c$ is integer, we can rewrite the equation to obtain

$$
a(a+1) = (-1)^{a+b+c} \begin{Bmatrix} a & b & c \\ 1 & c & b \end{Bmatrix} X(b, c)^{\frac{1}{2}} + [(b+1)+c(c+1)].
\tag{21}
$$

Putting $a = j_{23}$ and inserting (21) into (19), one finds for $F(j_{12}, j'_{12})$ for any b, c

$$F(j_{12}, j'_{12}) = \frac{1}{2}(-1)^{b+c} X(b,c)^{\frac{1}{2}}$$
$$\times \overbrace{\sum_{j_{23}} (-1)^{j_{23}}(2j_{23}+1) \begin{Bmatrix} j_{23} & b & c \\ 1 & c & b \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j'_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix}}^{I}$$
$$+ \frac{b(b+1)+c(c+1)}{(2j_{12}+1)} \underbrace{\sum_{j_{23}} (2j_{12}+1)(2j_{23}+1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j'_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix}}_{\delta_{j_{12} j'_{12}}} \quad (22)$$

where we have used the orthogonality relation (B.6) for the $6j$-symbols. Let us take a closer look at the three $6j$-symbols of I on the right-hand side of (22). We now apply some permutations to the rows and columns of the first $6j$-symbol within I which leave this $6j$-symbol invariant, see (B.4), (B.5). After that we have for I

$$I = \sum_{j_{23}} (-1)^{j_{23}}(2j_{23}+1) \begin{Bmatrix} b & b & 1 \\ c & c & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j'_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix}.$$

Now we fix $b = j_1, c = j_4$ and can evaluate

$$I = \sum_{j_{23}} (-1)^{j_{23}}(2j_{23}+1) \begin{Bmatrix} j_1 & j_1 & 1 \\ j_4 & j_4 & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j'_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix}$$
$$= (-1)^{-(j_{12}+j_1+j_1+j_3+j_2+1+j_4+j'_{12}+j_4)} \begin{Bmatrix} j_{12} & j_1 & j_2 \\ j_1 & j'_{12} & 1 \end{Bmatrix} \begin{Bmatrix} 1 & j_{12} & j'_{12} \\ j_3 & j_4 & j_4 \end{Bmatrix}$$

Here, we have used the Elliot–Biedenharn identity (B.8). Inserting this back into (22) yields

$$F(j_{12}, j'_{12}) = \frac{1}{2}(-1)^{j_1+j_4}(-1)^{-(j_{12}+j_1+j_1+j_3+j_2+1+j_4+j'_{12}+j_4)} X(j_1,j_4)^{\frac{1}{2}}$$
$$\times \begin{Bmatrix} j_{12} & j_1 & j_2 \\ j_1 & j'_{12} & 1 \end{Bmatrix} \begin{Bmatrix} 1 & j_{12} & j'_{12} \\ j_3 & j_4 & j_4 \end{Bmatrix} + \frac{j_1(j_1+1)+j_4(j_4+1)}{(2j_{12}+1)} \delta_{j_{12} j'_{12}}.$$

Using that, by definition of the $6j$-symbols (B.1), $(j_{12}+j_1+j_2)$ and $(j_3+1+j_4+j'_{12})$ are integer numbers, we can invert their common sign in the exponent of (-1). After summing up all the terms in the exponents and performing some permutations on the arguments of the $6j$-symbols according to (B.4), (B.5) we obtain the final result for $F(j_{12}, j'_{12})$:

$$F(j_{12}, j'_{12}) := \sum_{j_{23}} (2j_{23}+1) j_{23}(j_{23}+1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j'_{12} \\ j_3 & j_4 & j_{23} \end{Bmatrix}$$
$$= \frac{1}{2}(-1)^{j_1+j_2+j_3+j_4+j_{12}+j'_{12}+1} X(j_1,j_4)^{\frac{1}{2}} \begin{Bmatrix} j_2 & j_1 & j_{12} \\ 1 & j'_{12} & j_1 \end{Bmatrix} \begin{Bmatrix} j_3 & j_4 & j_{12} \\ 1 & j'_{12} & j_4 \end{Bmatrix}$$
$$+ \frac{j_1(j_1+1)+j_4(j_4+1)}{(2j_{12}+1)} \delta_{j_{12} j'_{12}} \quad (23)$$

with $X(j_1, j_4) = 2j_1(2j_1+1)(2j_1+2)2j_4(2j_4+1)(2j_4+2)$.

Remark. By the integer/positivity requirements of the factorials occurring in the definition of the $6j$-symbols of (23), see (B.2), we can read off restrictions for j_{12}, j'_{12}, namely, the selection rules

$$j'_{12} = \begin{cases} j_{12} - 1 \\ j_{12} \\ j_{12} + 1. \end{cases}$$

3.4. Precalculation

After these preparations we can now go *in medias res*: we will carry out all the summations in (18). Step by step we will only write down (with reordered prefactors) the terms containing the actual summation variable, suppressing all the other terms and sums in (18).

We start with the summation over $\vec{g}(IJ)$ (using again the shorthand $A(x, y) = \sqrt{(2x+1)(2y+1)}$ and the fact that $A(g_2, h_2) \cdot A(g_2, k_2) = A(h_2, k_2) \cdot (2g_2+1)$. Additionally, we will frequently use the integer conditions (B.2)):

- Summation over g_2:

$$A(h_2,k_2)(-1)^{h_2-k_2}\sum_{g_2} g_2(g_2+1)(2g_2+1)\begin{Bmatrix} j_J & j_I & g_2\\ j_1 & g_3 & h_2\end{Bmatrix}\begin{Bmatrix} j_J & j_I & g_2\\ j_1 & g_3 & k_2\end{Bmatrix}$$

$$\overset{(B.4),(B.5)}{=} A(h_2,k_2)(-1)^{h_2-k_2}\sum_{g_2} g_2(g_2+1)(2g_2+1)\begin{Bmatrix} j_I & j_1 & h_2\\ g_3 & j_J & g_2\end{Bmatrix}\begin{Bmatrix} j_I & j_1 & k_2\\ g_3 & j_J & g_2\end{Bmatrix}$$

$$\overset{(25)}{=} A(h_2,k_2)(-1)^{h_2-k_2}\Bigg[\frac{1}{2}(-1)^{\overbrace{j_I+j_1+h_2}^{\text{integer}}+g_3+j_J+1+k_2}X(j_I,j_J)^{\frac{1}{2}}$$
$$\times\begin{Bmatrix} j_1 & j_I & h_2\\ 1 & k_2 & j_I\end{Bmatrix}\begin{Bmatrix} g_3 & j_J & h_2\\ 1 & k_2 & j_J\end{Bmatrix}+\frac{j_I(j_I+1)+j_J(j_J+1)}{2h_2+1}\delta_{h_2k_2}\Bigg]$$

$$=\underbrace{A(h_2,k_2)\frac{1}{2}(-1)^{-j_I-j_1+j_J+1}X(j_I,j_J)^{\frac{1}{2}}\begin{Bmatrix} j_1 & j_I & h_2\\ 1 & k_2 & j_I\end{Bmatrix}}_{M_2}(-1)^{g_3}\begin{Bmatrix} g_3 & j_J & h_2\\ 1 & k_2 & j_J\end{Bmatrix}$$
$$+\underbrace{[j_I(j_I+1)+j_J(j_J+1)]}_{N}\delta_{h_2k_2}.$$

- Summation over g_3:

$$A(h_3,k_3)(-1)^{h_3-k_3}\sum_{g_3}\left[M_2(-1)^{g_3}\begin{Bmatrix} g_3 & j_J & h_2\\ 1 & k_2 & j_J\end{Bmatrix}+N\delta_{h_2k_2}\right](2g_3+1)\begin{Bmatrix} j_J & h_2 & g_3\\ j_2 & g_4 & h_3\end{Bmatrix}$$
$$\times\begin{Bmatrix} j_J & k_2 & g_3\\ j_2 & g_4 & k_3\end{Bmatrix}=A(h_3,k_3)(-1)^{h_3-k_3}\Bigg\{M_2\sum_{g_3}(-1)^{g_3}(2g_3+1)$$
$$\times\begin{Bmatrix} g_3 & j_J & h_2\\ 1 & k_2 & j_J\end{Bmatrix}\begin{Bmatrix} j_J & h_2 & g_3\\ j_2 & g_4 & h_3\end{Bmatrix}\begin{Bmatrix} j_J & k_2 & g_3\\ j_2 & g_4 & k_3\end{Bmatrix}$$
$$+N\delta_{h_2k_2}\sum_{g_3}(2g_3+1)\begin{Bmatrix} j_J & h_2 & g_3\\ j_2 & g_4 & h_3\end{Bmatrix}\begin{Bmatrix} j_J & k_2 & g_3\\ j_2 & g_4 & k_3\end{Bmatrix}\Bigg\}$$

$$\overset{(B.4),(B.5)}{=} A(h_3,k_3)(-1)^{h_3-k_3}\Bigg\{M_2\sum_{g_3}(-1)^{g_3}(2g_3+1)\begin{Bmatrix} j_J & j_J & 1\\ h_2 & k_2 & g_3\end{Bmatrix}\begin{Bmatrix} j_J & h_3 & g_4\\ j_2 & g_3 & h_2\end{Bmatrix}$$
$$\times\begin{Bmatrix} j_J & g_4 & k_3\\ j_2 & k_2 & g_3\end{Bmatrix}+\frac{N}{(2k_3+1)}\delta_{h_2k_2}\sum_{g_3}(2k_3+1)(2g_3+1)\begin{Bmatrix} j_J & g_4 & h_3\\ j_2 & h_2 & g_3\end{Bmatrix}$$
$$\times\begin{Bmatrix} j_J & g_4 & k_3\\ j_2 & h_2 & g_3\end{Bmatrix}\begin{Bmatrix} 1 & h_3 & k_3\\ j_2 & k_2 & h_2\end{Bmatrix}+\frac{N}{(2k_3+1)}\delta_{h_2k_2}\delta_{h_3k_3}\Bigg\}$$

$$\stackrel{(B.2),(B.4),(B.5)}{=} M_2 \underbrace{A(h_3,k_3)(-1)^{-j_2+h_2+k_2+1}\begin{Bmatrix} j_2 & h_2 & h_3 \\ 1 & k_3 & k_2 \end{Bmatrix}}_{M_3}(-1)^{g_4} \times \begin{Bmatrix} g_4 & j_J & h_3 \\ 1 & k_3 & j_J \end{Bmatrix} + N\delta_{h_2k_2}\delta_{h_3k_3}.$$

Note. That is in principle the same term with the same index order as we got from the summation over g_2.

- Generally, we have for the summation over g_i for $4 \leqslant i \leqslant I$:

$$A(h_i,k_i)(-1)^{h_i-k_i}\sum_{g_i}\left\{\left[M_2\cdots M_{i-1}(-1)^{g_i}\begin{Bmatrix} g_i & j_J & h_{i-1} \\ 1 & k_{i-1} & j_J \end{Bmatrix} + N\delta_{h_2k_2}\cdots\delta_{h_{i-1}k_{i-1}}\right]\right.$$
$$\left.\times(2g_i+1)\begin{Bmatrix} j_J & h_{i-1} & g_i \\ j_{i-1} & g_{i+1} & h_i \end{Bmatrix}\begin{Bmatrix} j_J & k_{i-1} & g_i \\ j_{i-1} & g_{i+1} & k_i \end{Bmatrix}\right\}$$
$$= A(h_i,k_i)(-1)^{h_i-k_i}\left\{M_2\cdots M_{i-1}\sum_{g_i}(-1)^{g_i}(2g_i+1)\begin{Bmatrix} g_i & j_J & h_{i-1} \\ 1 & k_{i-1} & j_J \end{Bmatrix}\right.$$
$$\times\begin{Bmatrix} j_J & h_{i-1} & g_i \\ j_{i-1} & g_{i+1} & h_i \end{Bmatrix}\begin{Bmatrix} j_J & k_{i-1} & g_i \\ j_{i-1} & g_{i+1} & k_i \end{Bmatrix}$$
$$\left.+N\delta_{h_2k_2}\cdots\delta_{h_{i-1}k_{i-1}}\sum_{g_i}(2g_i+1)\begin{Bmatrix} j_J & h_{i-1} & g_i \\ j_{i-1} & g_{i+1} & h_i \end{Bmatrix}\begin{Bmatrix} j_J & k_{i-1} & g_i \\ j_{i-1} & g_{i+1} & k_i \end{Bmatrix}\right\}$$
$$\stackrel{(B.4),(B.5)}{=} A(h_i,k_i)(-1)^{h_i-k_i}\left\{M_2\cdots M_{i-1}\sum_{g_i}(-1)^{g_i}(2g_i+1)\begin{Bmatrix} j_J & j_J & 1 \\ h_{i-1} & k_{i-1} & g_i \end{Bmatrix}\right.$$
$$\times\begin{Bmatrix} j_J & h_i & g_{i+1} \\ j_{i-1} & g_i & h_{i-1} \end{Bmatrix}\begin{Bmatrix} j_J & g_{i+1} & k_i \\ j_{i-1} & k_{i-1} & g_i \end{Bmatrix} + \frac{N}{(2k_i+1)}\delta_{h_2k_2}\cdots\delta_{h_{i-1}k_{i-1}}$$
$$\left.\times\sum_{g_i}(2k_i+1)(2g_i+1)\begin{Bmatrix} j_J & h_i & g_{i+1} \\ j_{i-1} & g_i & h_{i-1} \end{Bmatrix}\begin{Bmatrix} j_J & g_{i+1} & k_i \\ j_{i-1} & k_{i-1} & g_i \end{Bmatrix}\right\}$$
$$\stackrel{(B.4),(B.5)}{=} A(h_i,k_i)(-1)^{h_i-k_i}\left\{M_2\cdots M_{i-1}(-1)^{-(h_i+j_J+j_{i-1}+\overbrace{j_J+g_{i+1}+1+k_i}^{\text{integer}}+\overbrace{h_{i-1}+k_{i-1}}^{\text{integer}})}\right.$$
$$\left.\times\begin{Bmatrix} h_i & j_J & g_{i+1} \\ j_J & k_i & 1 \end{Bmatrix}\begin{Bmatrix} 1 & h_i & k_i \\ j_{i-1} & k_{i-1} & h_{i-1} \end{Bmatrix} + N\delta_{h_2k_2}\cdots\delta_{h_{i-1}k_{i-1}}\delta_{h_ik_i}\right\}$$
$$\stackrel{(B.2),(B.4)(B.5)}{=} M_2\cdots M_{i-1}\underbrace{A(h_i,k_i)(-1)^{-j_{i-1}+h_{i-1}+k_{i-1}+1}\begin{Bmatrix} j_{i-1} & h_{i-1} & h_i \\ 1 & k_i & k_{i-1} \end{Bmatrix}}_{M_i}(-1)^{g_{i+1}}$$
$$\times\begin{Bmatrix} g_{i+1} & j_J & h_i \\ 1 & k_i & j_J \end{Bmatrix} + N\delta_{h_2k_2}\cdots\delta_{h_{i-1}k_{i-1}}\delta_{h_ik_i}.$$

- For the summation over g_{I+1}, we have the same terms as above with a slight difference in one index (underlined):

$$
\begin{aligned}
&A(h_{I+1},k_{I+1})(-1)^{h_{I+1}-k_{I+1}}\sum_{g_{I+1}}\left\{\left[M_2\cdots M_I(-1)^{g_{I+1}}\begin{Bmatrix} g_{I+1} & j_J & h_I\\ 1 & k_I & j_J\end{Bmatrix}+N\delta_{h_2k_2}\cdots\delta_{h_Ik_I}\right]\right.\\
&\qquad\left.\times(2g_{I+1}+1)\begin{Bmatrix} j_J & h_I & g_{I+1}\\ \underline{j_{I+1}} & g_{I+2} & h_{I+1}\end{Bmatrix}\begin{Bmatrix} j_J & k_I & g_{I+1}\\ \underline{j_{I+1}} & g_{I+2} & k_{I+1}\end{Bmatrix}\right\}\\
&\quad= M_2\cdots M_I\underbrace{A(h_{I+1},k_{I+1})(-1)^{-j_{I+1}+h_I+k_I+1}\begin{Bmatrix} j_{I+1} & h_I & h_{I+1}\\ 1 & k_{I+1} & k_I\end{Bmatrix}}_{\tilde M_{I+1}}(-1)^{g_{I+2}}\\
&\qquad\times\begin{Bmatrix} g_{I+2} & j_J & h_{I+1}\\ 1 & k_{I+1} & j_J\end{Bmatrix}+N\delta_{h_2k_2}\cdots\delta_{h_Ik_I}\delta_{h_{I+1}k_{I+1}}.
\end{aligned}
$$

- Summation over g_i for $I+2\leqslant i\leqslant J-1$:

$$
\begin{aligned}
&A(h_i,k_i)(-1)^{h_i-k_i}\sum_{g_i}\left\{\left[M_2\cdots M_I\tilde M_{I+1}\cdots\tilde M_{i-1}(-1)^{g_i}\begin{Bmatrix} g_i & j_J & h_{i-1}\\ 1 & k_{i-1} & j_J\end{Bmatrix}\right.\right.\\
&\qquad\left.\left.+N\delta_{h_2k_2}\cdots\delta_{h_{i-1}k_{i-1}}\right](2g_i+1)\begin{Bmatrix} j_J & h_{i-1} & g_i\\ \underline{j_i} & g_{i+1} & h_i\end{Bmatrix}\begin{Bmatrix} j_J & k_{i-1} & g_i\\ \underline{j_i} & g_{i+1} & k_i\end{Bmatrix}\right\}\\
&\quad= M_2\cdots M_I\tilde M_{I+1}\cdots\tilde M_{i-1}\underbrace{A(h_i,k_i)(-1)^{-j_i+h_{i-1}+k_{i-1}+1}\begin{Bmatrix} j_{i-1} & h_{i-1} & h_i\\ 1 & k_i & k_{i-1}\end{Bmatrix}}_{\tilde M_i}\\
&\qquad\times(-1)^{g_{i+1}}\begin{Bmatrix} g_{i+1} & j_J & h_i\\ 1 & k_i & j_J\end{Bmatrix}+N\delta_{h_2k_2}\cdots\delta_{h_{i-1}k_{i-1}}\delta_{h_ik_i}.
\end{aligned}
$$

Here, we keep the following notation in mind:

$$
\begin{array}{lll}
h_1 = j_I & k_1 = j_I & J\leqslant i\leqslant N: g_i = g_i'' = a_i\\
h_2 = h_2(j_I, j_1) & k_2 = k_2(j_I, j_1) & \\
h_3 = h_3(h_2, j_2) & k_3 = k_3(k_2, j_2) & \\
\vdots & \vdots & \\
h_{I-1} = h_{I-1}(h_{I-2}, j_{I-2}) & k_{I-1} = k_{I-1}(k_{I-2}, j_{I-2}) & \\
h_I = g_I'' & k_I = a_I & \\
h_{I+1} = g_{I+1}'' & k_{I+1} = a_{I+1} & \\
\vdots & \vdots & \\
h_{J-1} = g_{J-1}'' & k_{J-1} = a_{J-1}. &
\end{array}
\tag{24}
$$

We have now carried out completely the summation over $\vec g(IJ)$ in (18). After this we write down the remaining terms of this summation and the terms of (18) which have not taken part in the summation yet. So, we end up with (do not get confused about the notation $A(x,y)=\sqrt{(2x+1)(2y+1)}$ where A, A_i are abbreviations from certain terms)

$$
\sum_{\vec g(IJ)} g_2(g_2+1)\langle\vec g(IJ)|\vec g''\rangle\langle\vec g(IJ)|\vec a\rangle
$$

$$
=\sum_{\substack{h_2,\ldots,h_{I-1}\\ k_2,\ldots,k_{I-1}}}\left[\overbrace{\prod_{n=2}^{I}M_n\prod_{m=I+1}^{J-1}\tilde M_m\times(-1)^{a_J}\begin{Bmatrix} a_J & j_J & g_{J-1}''\\ 1 & a_{J-1} & j_J\end{Bmatrix}}^{\text{part I}}+\overbrace{N\prod_{n=2}^{J-1}\delta_{h_nk_n}}^{\text{part II}}\right]\times\text{remaining terms}
$$

$$
= \sum_{\substack{h_2,\ldots,h_{I-1}\\ k_2,\ldots,k_{I-1}}} \Bigg[\frac{1}{2}(-1)^{j_J - j_I - \sum_{n=1}^{I-1} j_n - \sum_{m=I+1}^{J-1} j_m} X(j_I, j_J)^{\frac{1}{2}} \overbrace{(-1)^{+1} A(h_2,k_2) \begin{Bmatrix} j_1 & j_I & h_2 \\ 1 & k_2 & j_I \end{Bmatrix}}^{A}
$$

$$
\times \prod_{n=3}^{I} \overbrace{A(h_n,k_n)(-1)^{h_{n-1}+k_{n-1}+1} \begin{Bmatrix} j_{n-1} & h_{n-1} & h_n \\ 1 & k_n & k_{n-1} \end{Bmatrix}}^{A_1 \leftrightarrow n=3, A_2 \leftrightarrow n=4, A_3 \leftrightarrow n=5, \ldots, A_{I-2} \leftrightarrow n=I}
$$

$$
\times \prod_{n=I+1}^{J-1} A(g''_n, a_n)(-1)^{g''_{n-1}+a_{n-1}+1} \begin{Bmatrix} j_n & g''_{n-1} & g''_n \\ 1 & a_n & a_{n-1} \end{Bmatrix}
$$

$$
\times (-1)^{a_J} \begin{Bmatrix} a_J & j_J & g''_{J-1} \\ 1 & a_{J-1} & j_J \end{Bmatrix} + [j_I(j_I+1) + j_J(j_J+1)] \prod_{n=2}^{J-1} \delta_{h_n k_n} \Bigg]
$$

$$
\times \underbrace{(-1)^{g''_2} A(h_2, g''_2) \begin{Bmatrix} j_I & j_1 & h_2 \\ j_2 & h_3 & g''_2 \end{Bmatrix}}_{B_1} \quad \underbrace{(-1)^{-a_2} A(k_2, a_2) \begin{Bmatrix} j_I & j_1 & k_2 \\ j_2 & k_3 & a_2 \end{Bmatrix}}_{C_1}
$$

$$
\times \underbrace{(-1)^{h_3-k_3+g''_3} A(h_3, g''_3) \begin{Bmatrix} j_I & g''_2 & h_3 \\ j_3 & h_4 & g''_3 \end{Bmatrix}}_{B_2} \quad \underbrace{(-1)^{-a_3} A(k_3, a_3) \begin{Bmatrix} j_I & a_2 & k_3 \\ j_3 & k_4 & a_3 \end{Bmatrix}}_{C_2}
$$

$$
\times \underbrace{(-1)^{h_4-k_4+g''_4} A(h_4, g''_4) \begin{Bmatrix} j_I & g''_3 & h_4 \\ j_4 & h_5 & g''_4 \end{Bmatrix}}_{B_3} \quad \underbrace{(-1)^{-a_4} A(k_4, a_4) \begin{Bmatrix} j_I & a_3 & k_4 \\ j_4 & k_5 & a_4 \end{Bmatrix}}_{C_3}
$$

$$
\vdots \qquad\qquad \vdots \qquad\qquad \vdots
$$

$$
\times \underbrace{(-1)^{h_{I-1}-k_{I-1}+g''_{I-1}} A(h_{I-1}, 2g'_{I-1}) \begin{Bmatrix} j_I & g''_{I-2} & h_{I-1} \\ j_{I-1} & g''_I & g'_{I-1} \end{Bmatrix}}_{B_{I-2}}
$$

$$
\times \underbrace{(-1)^{-a_{I-1}} A(k_{I-1}, a_{I-1}) \begin{Bmatrix} j_I & a_{I-2} & k_{I-1} \\ j_{I-1} & a_I & a_{I-1} \end{Bmatrix}}_{C_{I-2}}. \tag{25}
$$

After noting this intermediate result, we finally have to execute the remaining summations of (25), namely the summations over $h_2, \ldots, h_{I-1}$ and $k_2, \ldots, k_{I-1}$ (leaving out the signs $(-1)^{g''_i - a_i}$, since they will be cancelled, as we will see, due to the occurrence of $\delta_{g''_i a_i}$-terms in the following calculations).

First, we do this summation for *part I of* (25):

- First step:
  summation over h_2:

$$
\sum_{h_2} \overbrace{(-1)^{+1} A(h_2,k_2) \begin{Bmatrix} j_1 & j_I & h_2 \\ 1 & k_2 & j_I \end{Bmatrix}}^{A} \overbrace{(-1)^{h_2+k_2+1} A(h_3,k_3) \begin{Bmatrix} j_2 & h_2 & h_3 \\ 1 & k_3 & k_2 \end{Bmatrix}}^{A_1}
$$

$$\times \overbrace{A(h_2, g_2'')\begin{Bmatrix} j_I & j_1 & h_2 \\ j_2 & h_3 & g_2'' \end{Bmatrix}}^{B_1}$$

$$\overset{(B.4),(B.4)}{=} (-1)^{k_2} A(k_2, g_2'') A(h_3, k_3)$$

$$\times \underbrace{\sum_{h_2} (-1)^{h_2}(2h_2+1) \begin{Bmatrix} j_1 & k_2 & j_I \\ 1 & j_I & h_2 \end{Bmatrix} \begin{Bmatrix} k_2 & k_3 & j_2 \\ h_3 & h_2 & 1 \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & g_2'' \\ h_3 & j_I & h_2 \end{Bmatrix}}$$

$$\overset{(B.8)}{=} (-1)^{-(\overbrace{k_3+j_I+1+g_2''}^{\text{integer}}+k_2+j_1+h_3+j_2)} \begin{Bmatrix} k_3 & k_2 & j_2 \\ j_1 & g_2'' & j_I \end{Bmatrix} \begin{Bmatrix} j_I & k_3 & g_2'' \\ h_3 & j_I & 1 \end{Bmatrix}$$

$$\overset{(B.2)}{=} (-1)^{k_3+j_I+1+g_2''-k_2-j_1-h_3-j_2-j_I} \begin{Bmatrix} k_3 & k_2 & j_2 \\ j_1 & g_2'' & j_I \end{Bmatrix} \begin{Bmatrix} j_I & k_3 & g_2'' \\ h_3 & j_I & 1 \end{Bmatrix}$$

$$= \underbrace{(-1)^{g_2''+1+k_3-j_1-j_2-h_3} A(h_3, k_3) \begin{Bmatrix} j_I & k_3 & g_2'' \\ h_3 & j_I & 1 \end{Bmatrix}}_{D_1} \underbrace{A(k_2, g_2'') \begin{Bmatrix} k_3 & k_2 & j_2 \\ j_1 & g_2'' & j_I \end{Bmatrix}}_{E_1}; \tag{26}$$

summation over k_2:

$$\sum_{k_2} \overbrace{A(k_2, g_2'') \begin{Bmatrix} k_3 & k_2 & j_2 \\ j_1 & g_2'' & j_I \end{Bmatrix}}^{E_1} \overbrace{A(k_2, a_2) \begin{Bmatrix} j_I & j_1 & k_2 \\ j_2 & k_3 & a_2 \end{Bmatrix}}^{C_1}$$

$$\overset{(B.4),(B.5)}{=} \frac{A(a_2, g_2'')}{(2a_2+1)} \underbrace{\sum_{k_2} (2k_2+1)(2a_2+1) \begin{Bmatrix} j_1 & j_2 & g_2'' \\ k_3 & j_I & k_2 \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & a_2 \\ k_3 & j_I & k_2 \end{Bmatrix}}_{\overset{(B.6)}{=} \delta_{g_2'' a_2}} = \delta_{g_2'' a_2}. \tag{27}$$

- Second step:
  summation over h_3:

$$\sum_{h_3} \overbrace{(-1)^{g_2''+1+k_3-j_1-j_2-h_3} A(h_3, k_3) \begin{Bmatrix} j_I & k_3 & g_2'' \\ h_3 & j_I & 1 \end{Bmatrix}}^{D_1} \overbrace{(-1)^{h_3+k_3+1} A(h_4, k_4) \begin{Bmatrix} j_3 & h_3 & h_4 \\ 1 & k_4 & k_3 \end{Bmatrix}}^{A_2}$$

$$\times \overbrace{(-1)^{h_3-k_3} A(h_3, g_3'') \begin{Bmatrix} j_I & g_2'' & h_3 \\ j_3 & h_4 & g_3'' \end{Bmatrix}}^{B_2}$$

$$= (-1)^{g_2''-j_1-j_2+k_3} A(k_3, g_3'') A(h_4, k_4)$$

$$\times \underbrace{\sum_{h_3} (-1)^{h_3}(2h_3+1) \begin{Bmatrix} j_I & k_3 & g_2'' \\ h_3 & j_I & 1 \end{Bmatrix} \begin{Bmatrix} j_3 & h_3 & h_4 \\ 1 & k_4 & k_3 \end{Bmatrix} \begin{Bmatrix} j_I & g_2'' & h_3 \\ j_3 & h_4 & g_3'' \end{Bmatrix}}$$

$$\overset{(B.4),(B.5)}{=} \sum_{h_3} (-1)^{h_3}(2h_3+1) \begin{Bmatrix} g_2'' & k_3 & j_I \\ 1 & j_I & h_3 \end{Bmatrix} \begin{Bmatrix} k_3 & k_4 & j_3 \\ h_4 & h_3 & 1 \end{Bmatrix} \begin{Bmatrix} g_2'' & j_3 & g_3'' \\ h_4 & j_I & h_3 \end{Bmatrix}$$

$$\overset{(B.8)}{=} (-1)^{-(\overbrace{k_4+j_I+1+g_3''}^{\text{integer}}+k_3+g_2''+h_4+j_I)} \begin{Bmatrix} k_4 & k_3 & j_3 \\ g_2'' & g_3'' & j_I \end{Bmatrix} \begin{Bmatrix} j_I & k_4 & g_3'' \\ h_4 & j_I & 1 \end{Bmatrix}$$

$$\overset{(B.2)}{=} (-1)^{k_4+j_I+1+g_3''-k_3-g_2''-h_4-j_3-j_I} \begin{Bmatrix} k_4 & k_3 & j_3 \\ g_2'' & g_3'' & j_I \end{Bmatrix} \begin{Bmatrix} j_I & k_4 & g_3'' \\ h_4 & j_I & 1 \end{Bmatrix}$$

$$= \underbrace{(-1)^{g_3''+1+k_4-j_1-j_2-j_3-h_4} A(h_4,k_4) \begin{Bmatrix} j_I & k_4 & g_3'' \\ h_4 & j_I & 1 \end{Bmatrix}}_{D_2} \underbrace{A(k_3,g_3'') \begin{Bmatrix} k_4 & k_3 & j_3 \\ g_2'' & g_3'' & j_I \end{Bmatrix}}_{E_2}; \tag{28}$$

summation over k_3:

$$\sum_{k_3} \overbrace{A(k_3,g_3'') \begin{Bmatrix} k_4 & k_3 & j_3 \\ g_2'' & g_3'' & j_I \end{Bmatrix}}^{E_2} \overbrace{A(k_3,a_3) \begin{Bmatrix} j_I & a_2 & k_3 \\ j_3 & k_4 & a_3 \end{Bmatrix}}^{C_2}$$
$$\overset{(29),(B.4),(B.5)}{=} \frac{A(a_3,g_3'')}{(2a_3+1)} \underbrace{\sum_{k_3} (2k_3+1)(2a_3+1) \begin{Bmatrix} a_2 & j_3 & g_3'' \\ k_4 & j_I & k_3 \end{Bmatrix} \begin{Bmatrix} a_2 & j_3 & a_3 \\ k_4 & j_I & k_3 \end{Bmatrix}}_{\overset{(B.6)}{=}\delta_{g_3'' a_3}} = \delta_{g_3'' a_3}. \tag{29}$$

- Third step:
summation over h_4:

$$\sum_{h_4} \overbrace{(-1)^{g_3''+1+k_4-j_1-j_2-j_3-h_4} A(h_4,k_4) \begin{Bmatrix} j_I & k_4 & g_3'' \\ h_4 & j_I & 1 \end{Bmatrix}}^{D_2} \overbrace{(-1)^{h_4+k_4+1} A(h_5,k_5) \begin{Bmatrix} j_4 & h_4 & h_5 \\ 1 & k_5 & k_4 \end{Bmatrix}}^{A_3}$$
$$\times \overbrace{(-1)^{h_4-k_4} A(h_4,g_4'') \begin{Bmatrix} j_I & g_3'' & h_4 \\ j_4 & h_5 & g_4'' \end{Bmatrix}}^{B_3}$$
$$= (-1)^{g_3''-j_1-j_2-j_3+k_4} A(k_4,g_4'') A(h_5,k_5)$$
$$\times \underbrace{\sum_{h_4} (-1)^{h_4}(2h_4+1) \begin{Bmatrix} j_I & k_4 & g_3'' \\ h_4 & j_I & 1 \end{Bmatrix} \begin{Bmatrix} j_4 & h_4 & h_5 \\ 1 & k_5 & k_4 \end{Bmatrix} \begin{Bmatrix} j_I & g_3'' & h_4 \\ j_4 & h_5 & g_4'' \end{Bmatrix}}$$
$$\overset{(B.4),(B.5)}{=} \sum_{h_4} (-1)^{h_4}(2h_4+1) \begin{Bmatrix} g_3'' & k_4 & j_I \\ 1 & j_I & h_4 \end{Bmatrix} \begin{Bmatrix} k_4 & k_5 & j_4 \\ h_5 & h_4 & 1 \end{Bmatrix} \begin{Bmatrix} g_3'' & j_4 & g_4'' \\ h_5 & j_I & h_4 \end{Bmatrix}$$
$$\overset{(B.8)}{=} (-1)^{-(\overbrace{k_5+j_I+1+g_4''}^{\text{integer}}+k_4+g_3''+h_5+j_4+j_I)} \begin{Bmatrix} k_5 & k_4 & j_4 \\ g_3'' & g_4'' & j_I \end{Bmatrix} \begin{Bmatrix} j_I & k_5 & g_4'' \\ h_5 & j_I & 1 \end{Bmatrix}$$
$$\overset{(B.2)}{=} (-1)^{k_5+j_I+1+g_4''-k_4-g_3''-h_5-j_4-j_I} \begin{Bmatrix} k_5 & k_4 & j_4 \\ g_3'' & g_4'' & j_I \end{Bmatrix} \begin{Bmatrix} j_I & k_5 & g_4'' \\ h_5 & j_I & 1 \end{Bmatrix}$$
$$= \underbrace{(-1)^{g_4''+1+k_5-j_1-j_2-j_3-j_4-h_5} A(h_5,k_5) \begin{Bmatrix} j_I & k_5 & g_4'' \\ h_5 & j_I & 1 \end{Bmatrix}}_{D_3} \underbrace{A(k_4,g_4'') \begin{Bmatrix} k_5 & k_4 & j_4 \\ g_3'' & g_4'' & j_I \end{Bmatrix}}_{E_3}; \tag{30}$$

summation over k_4:

$$\sum_{k_4} \overbrace{A(k_4,g_4'') \begin{Bmatrix} k_5 & k_4 & j_4 \\ g_3'' & g_4'' & j_I \end{Bmatrix}}^{E_3} \overbrace{A(k_4,a_4) \begin{Bmatrix} j_I & a_3 & k_4 \\ j_4 & k_5 & a_4 \end{Bmatrix}}^{C_3}$$
$$\overset{(31),(B.4),(B.5)}{=} \frac{A(a_4,g_4'')}{(2a_4+1)} \underbrace{\sum_{k_4} (2k_4+1)(2a_4+1) \begin{Bmatrix} a_3 & j_4 & g_4'' \\ k_5 & j_I & k_4 \end{Bmatrix} \begin{Bmatrix} a_3 & j_4 & a_4 \\ k_5 & j_I & k_4 \end{Bmatrix}}_{\overset{(B.6)}{=}\delta_{g_4'' a_4}} = \delta_{g_4'' a_4}. \tag{31}$$

In this way, we successively carry out all the summations until the last step:

- Last step:
  summation over h_{I-1}:

$$
\begin{aligned}
&\sum_{h_{I-1}} \overbrace{(-1)^{g''_{I-1}+1+k_{I-1}-\sum_{n=1}^{I-2} j_n - h_{I-1}} A(h_{I-1},k_{I-1}) \begin{Bmatrix} j_I & k_{I-1} & g''_{I-2} \\ h_{I-1} & j_I & 1 \end{Bmatrix}}^{D_{I-3}} \\
&\times \overbrace{(-1)^{h_{I-1}+k_{I-1}+1} A(h_I,k_I) \begin{Bmatrix} j_{I-1} & h_{I-1} & h_I \\ 1 & k_I & k_{I-1} \end{Bmatrix}}^{A_{I-2}} \\
&\times \overbrace{(-1)^{h_{I-1}-k_{I-1}} A(h_{I-1},g''_{I-1}) \begin{Bmatrix} j_I & g''_{I-2} & h_{I-1} \\ j_{I-1} & g''_I & g''_{I-1} \end{Bmatrix}}^{B_{I-2}} \\
&= (-1)^{g''_{I-2}-\sum_{n=1}^{I-2} j_n + k_{I-1}} A(k_{I-1},g''_{I-1}) A(h_I,k_I) \\
&\times \underbrace{\sum_{h_{I-1}} (-1)^{h_{I-1}} (2h_{I-1}+1) \begin{Bmatrix} j_I & k_{I-1} & g''_{I-2} \\ h_{I-1} & j_I & 1 \end{Bmatrix} \begin{Bmatrix} j_{I-1} & h_{I-1} & h_I \\ 1 & k_I & k_{I-1} \end{Bmatrix} \begin{Bmatrix} j_I & g''_{I-2} & h_{I-1} \\ j_{I-1} & g''_I & g''_{I-1} \end{Bmatrix}} \\
&\overset{(B.4),(B.5)}{=} \sum_{h_{I-1}} (-1)^{h_{I-1}} (2h_{I-1}+1) \begin{Bmatrix} g''_{I-2} & k_{I-1} & j_I \\ 1 & j_I & h_{I-1} \end{Bmatrix} \begin{Bmatrix} k_{I-1} & k_I & j_{I-1} \\ h_I & h_{I-1} & 1 \end{Bmatrix} \\
&\qquad \times \begin{Bmatrix} g''_{I-2} & j_{I-1} & g''_{I-1} \\ h_I & j_I & h_{I-1} \end{Bmatrix} \\
&\overset{(B.8)}{=} (-1)^{-(\overbrace{k_I+j_I+1+g''_{I-1}}^{\text{integer}}+k_{I-1}+g''_{I-2}+h_I+j_{I-1}+j_I)} \begin{Bmatrix} k_I & k_{I-1} & j_{I-1} \\ g''_{I-2} & g''_{I-1} & j_I \end{Bmatrix} \begin{Bmatrix} j_I & k_I & g''_{I-1} \\ h_I & j_I & 1 \end{Bmatrix} \\
&\overset{(B.2)}{=} (-1)^{k_I+j_I+1+g''_{I-1}-k_{I-1}-g''_{I-2}-h_I-j_{I-1}-j_I} \begin{Bmatrix} k_I & k_{I-1} & j_{I-1} \\ g''_{I-2} & g''_{I-1} & j_I \end{Bmatrix} \begin{Bmatrix} j_I & k_I & g''_{I-1} \\ h_I & j_I & 1 \end{Bmatrix} \\
&= \underbrace{(-1)^{g''_{I-1}+1+k_I \sum_{n=1}^{I-1} j_n - h_I} A(h_I,k_I) \begin{Bmatrix} j_I & k_I & g''_{I-1} \\ h_I & j_I & 1 \end{Bmatrix}}_{D_{I-2}} \underbrace{A(k_{I-1},g''_{I-1}) \begin{Bmatrix} k_I & k_{I-1} & j_{I-1} \\ g''_{I-2} & g''_{I-1} & j_I \end{Bmatrix}}_{E_{I-2}};
\end{aligned}
\tag{32}
$$

summation over k_{I-1}:

$$
\begin{aligned}
&\sum_{k_{I-1}} \overbrace{A(k_{I-1},g''_{I-1}) \begin{Bmatrix} k_I & k_{I-1} & j_{I-1} \\ g''_{I-2} & g''_{I-1} & j_I \end{Bmatrix}}^{E_{I-2}} \overbrace{A(k_{I-1},a_{I-1}) \begin{Bmatrix} j_I & a_{I-2} & k_{I-1} \\ j_{I-1} & k_I & a_{I-1} \end{Bmatrix}}^{C_{I-2}} \\
&\overset{(B.4),(B.5)}{=} \frac{A(a_{I-1},g''_{I-1})}{(2a_{I-1}+1)} \\
&\qquad \times \underbrace{\sum_{k_{I-1}} (2k_{I-1}+1)(2a_{I-1}+1) \begin{Bmatrix} a_{I-2} & j_{I-1} & g''_{I-1} \\ a_I & j_I & k_{I-1} \end{Bmatrix} \begin{Bmatrix} a_{I-2} & j_{I-1} & a_{I-1} \\ a_I & j_I & k_{I-1} \end{Bmatrix}}_{\overset{(B.6)}{=} \delta_{g''_{I-1} a_{I-1}}} \\
&= \delta_{g''_{I-1} a_{I-1}}.
\end{aligned}
\tag{33}
$$

Here, we have used that $g''_{I-2} = a_{I-2}$ resulting from the summation over k_{I-2} and additionally the fact that $a_I = k_I$ from (24).

At the end of the *part I* summation over $h_2, \ldots, h_{I-1}, k_2, \ldots, k_{I-1}$, we can now summarize the remaining terms of (25) resulting in the term D_{I-2} from the summation over h_{I-1} in (32).

With $g''_{I-1} = a_{I-1}$ from (33), $h_I = g''_I, k_I = a_I$ from (24), we obtain the drastically simplified formula:

$$\sum_{\substack{h_2,\ldots,h_{I-1}\\k_2,\ldots,k_{I-1}}} \left[\prod_{n=2}^{I} M_n \prod_{m=I+1}^{J-1} \tilde{M}_m \times (-1)^{a_J} \begin{Bmatrix} a_J & j_J & g''_{J-1} \\ 1 & a_{J-1} & j_J \end{Bmatrix}\right] \times \text{remaining terms}$$
$$= (-1)^{a_{I-1}+1}(-1)^{a_I - g''_I}(-1)^{-\sum_{n=1}^{I-1} j_n} A(g''_I, a_I) \begin{Bmatrix} j_I & a_I & a_{I-1} \\ g''_I & j_I & 1 \end{Bmatrix}$$
$$\times \prod_{m=I+1}^{J-1} \tilde{M}_m \times (-1)^{a_J} \begin{Bmatrix} a_J & j_J & g''_{J-1} \\ 1 & a_{J-1} & j_J \end{Bmatrix}. \qquad (34)$$

Now the summation for *part II* in (25) is the last task in order to complete our calculation: let us write down this expression (again suppressing the $(-1)^{g''_i - a_i}$ signs) with the product $\prod_{n=2}^{J-1} \delta_{h_n k_n}$ evaluated (this cancels the summation over k_2 and all the exponents in $(-1)^{h_i - k_i}$):

$$\sum_{\substack{h_2,\ldots,h_{I-1}\\k_2,\ldots,k_{I-1}}} \left[N \prod_{n=2}^{J-1} \delta_{h_n k_n}\right] \times \text{remaining terms}$$
$$= [j_I(j_I+1) + j_J(j_J+1)] \sum_{h_2,\ldots,h_{I-1}} \times \underbrace{A(h_2, g''_2) \begin{Bmatrix} j_I & j_1 & h_2 \\ j_2 & h_3 & g''_2 \end{Bmatrix}}_{B_1} \underbrace{A(h_2, a_2) \begin{Bmatrix} j_I & j_1 & h_2 \\ j_2 & k_3 & a_2 \end{Bmatrix}}_{C_1}$$
$$\times \underbrace{A(h_3, g''_3) \begin{Bmatrix} j_I & g''_2 & h_3 \\ j_3 & h_4 & g''_3 \end{Bmatrix}}_{B_2} \underbrace{A(h_3, a_3) \begin{Bmatrix} j_I & a_2 & h_3 \\ j_3 & k_4 & a_3 \end{Bmatrix}}_{C_2}$$
$$\times \underbrace{A(h_4, g''_4) \begin{Bmatrix} j_I & g''_3 & h_4 \\ j_4 & h_5 & g''_4 \end{Bmatrix}}_{B_3} \underbrace{A(h_4, a_4) \begin{Bmatrix} j_I & a_3 & h_4 \\ j_4 & k_5 & a_4 \end{Bmatrix}}_{C_3}$$
$$\vdots \qquad \vdots \qquad \vdots$$
$$\times \underbrace{A(h_{I-1}, 2g'_{I-1}) \begin{Bmatrix} j_I & g''_{I-2} & h_{I-1} \\ j_{I-1} & g''_I & g'_{I-1} \end{Bmatrix}}_{B_{I-2}} \underbrace{A(h_{I-1}, a_{I-1}) \begin{Bmatrix} j_I & a_{I-2} & h_{I-1} \\ j_{I-1} & a_I & a_{I-1} \end{Bmatrix}}_{C_{I-2}}. \qquad (35)$$

Looking at (35) we can see that every summation gives rise to an orthogonality relation between the $6j$-symbols as follows.

Every sum in (35) has the following form (again using the conventions in (24)):

$$\sum_{h_n} A(h_n, g''_n) \begin{Bmatrix} j_I & g''_{n-1} & h_n \\ j_n & h_{n+1} & g''_n \end{Bmatrix} A(h_n, a_n) \begin{Bmatrix} j_I & a_{n-1} & h_n \\ j_n & h_{n+1} & a_n \end{Bmatrix}$$
$$= \frac{A(g''_i, a_i)}{(2a_i+1)} \sum_{h_n} (2h_i+1)(2a_i+1) \begin{Bmatrix} j_I & g''_{n-1} & h_n \\ j_n & h_{n+1} & g''_n \end{Bmatrix} \begin{Bmatrix} j_I & a_{n-1} & h_n \\ j_n & h_{n+1} & a_n \end{Bmatrix} \stackrel{\text{(B.6)}}{=} \delta_{g''_i a_i}. \qquad (36)$$

One has to start with the summation over h_2. This gives $\delta_{g''_2 a_2}$.

Secondly, the summation over h_3 is carried out by using the result $\delta_{g''_2 a_2}$ from the summation before. In this way, one can step by step sum over all h_i up to h_{I-1}.

The final result for *part II* in (25) is

$$\sum_{\substack{h_2,\ldots,h_{I-1}\\k_2,\ldots,k_{I-1}}} \left[N\prod_{n=2}^{J-1}\delta_{h_n k_n}\right] \times \text{ remaining terms} = [j_I(j_I+1)+j_J(j_J+1)]\prod_{n=2}^{J-1}\delta_{g''_n a_n}. \tag{37}$$

Now we have solved the problem posed in (19) and can write down the remarkably simplified expression by using the results of (34), (37). Note that we have inserted δ-expressions coming from lemma 2.1.

$$\begin{aligned}
&\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle\vec{g}(IJ)|\vec{g}''(12)\rangle\langle\vec{g}(IJ)|\vec{a}(12)\rangle\\
&\quad=\frac{1}{2}(-1)^{j_J-j_I-\sum_{n=1}^{I-1}j_n-\sum_{m=I+1}^{J-1}j_m}X(j_I,j_J)^{\frac{1}{2}}\\
&\qquad\times(-1)^{a_{I-1}}(-1)^{a_I-g''_I}(-1)^{-\sum_{n=1}^{I-1}j_n}(-1)^{+1}\sqrt{(2g''_I+1)(2a_I+1)}\begin{Bmatrix}a_{I-1} & a_I & j_I\\ 1 & j_I & g''_I\end{Bmatrix}\\
&\qquad\times\prod_{n=I+1}^{J-1}\sqrt{(2g''_n)(2a_n+1)}(-1)^{g''_{n-1}+a_{n-1}+1}\begin{Bmatrix}j_n & g''_{n-1} & g''_n\\ 1 & a_n & a_{n-1}\end{Bmatrix}\\
&\qquad\times(-1)^{a_J}\begin{Bmatrix}a_J & j_J & g''_{J-1}\\ 1 & a_{J-1} & j_J\end{Bmatrix}\prod_{n=2}^{I-1}\delta_{g''_n a_n}\prod_{n=J}^{N}\delta_{g''_n a_n}\\
&\qquad+[j_I(j_I+1)+j_J(j_J+1)]\prod_{n=2}^{N}\delta_{g''_n a_n}.
\end{aligned}\tag{38}$$

For configurations (I, J) one has to take all terms of (38), which are in suitable limits, e.g. if $J = I + 1$ then the product $\prod_{n=I+1}^{J-1}\cdots$ is not to be taken into account. Note that for special configurations $I < J$ certain terms drop out, e.g. if $J = I + 1$ then $\prod_{n=I+1}^{J-1}$ is not taken into account.

Let us for clarity explicitly discuss four special cases of the edge-labelling I, J, namely ($I = 1$, J arbitrary), ($I = 1$, $J = 2$), ($I = 2$, J arbitrary) and ($I = 2$, $J = 3$).

We will display for every case the parts remaining from (18)

Note that again $A(x, y) = \sqrt{(2x + 1)(2y + 1)}$ and the conventions of (24) are kept in mind:

3.4.1. $I = 1$, J arbitrary

$$\begin{aligned}
&\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle\vec{g}(IJ)|\vec{g}''(12)\rangle\langle\vec{g}(IJ)|\vec{a}(12)\rangle\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\\
&\times(-1)^{g''_{I+1}}A(g_{I+1},g''_{I+1})\begin{Bmatrix}j_J & g''_I & g_{I+1}\\ j_{I+1} & g_{I+2} & g''_{I+1}\end{Bmatrix}(-1)^{-a_{I+1}}A(g_{I+1},a_{I+1})\begin{Bmatrix}j_J & a_I & g_{I+1}\\ j_{I+1} & g_{I+2} & a_{I+1}\end{Bmatrix}\\
&\times(-1)^{g''_{I+2}}A(g_{I+2},g''_{I+2})\begin{Bmatrix}j_J & g''_{I+1} & g_{I+2}\\ j_{I+2} & g_{I+3} & g''_{I+2}\end{Bmatrix}(-1)^{-a_{I+2}}A(g_{I+2},a_{I+2})\begin{Bmatrix}j_J & a_{I+1} & g_{I+2}\\ j_{I+2} & g_{I+3} & a_{I+2}\end{Bmatrix}\\
&\vdots\qquad\qquad\qquad\vdots\qquad\qquad\qquad\qquad\qquad\vdots\\
&\vdots\qquad\qquad\qquad\vdots\qquad\qquad\qquad\qquad\qquad\vdots
\end{aligned}$$

$$\times\ (-1)^{g''_{J-1}} A(g_{J-1}, g''_{J-1}) \begin{Bmatrix} j_J & g''_{J-2} & g_{J-1} \\ j_{J-1} & g_J & g''_{J-1} \end{Bmatrix} (-1)^{-a_{J-1}} A(g_{J-1}, a_{J-1})$$

$$\times \begin{Bmatrix} j_J & a_{J-2} & g_{J-1} \\ j_{J-1} & g_J & a_{J-1} \end{Bmatrix}$$

$$= \frac{1}{2}(-1)^{J_J + j_1 - \sum_{n=2}^{J-1} j_n} X(j_1, j_J)^{\frac{1}{2}} \prod_{n=2}^{J-1} A(g''_n, a_n)(-1)^{g''_{n-1}+a_{n-1}+1} \begin{Bmatrix} j_n & g''_{n-1} & g_n \\ 1 & a_n & a_{n-1} \end{Bmatrix}$$

$$\times\ (-1)^{a_J} \begin{Bmatrix} j_J & a_{J-2} & g_{J-1} \\ j_{J-1} & g_J & a_{J-1} \end{Bmatrix} \prod_{n=J}^{N} \delta_{g''_n a_n} + [j_1(j_1+1) + j_J(j_J+1)] \prod_{n=2}^{N} \delta_{g''_n a_n}. \tag{39}$$

3.4.2. $I = 1, J = 2$

$$\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle \vec{g}(IJ)|\vec{g}''(12)\rangle\langle \vec{g}(IJ)|\vec{a}(12)\rangle = a_2(a_2+1)\prod_{n=2}^{N} \delta g''_n a_n. \tag{40}$$

3.4.3. $I = 2$, *J arbitrary*

$$\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle \vec{g}(IJ)|\vec{g}''(12)\rangle\langle \vec{g}(IJ)|\vec{a}(12)\rangle = \sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)$$

$$\times (-1)^{g''_I} A(g_I, g''_I) \begin{Bmatrix} j_J & h_{I-1} & g_I \\ j_{I-1} & g_{I+1} & g''_I \end{Bmatrix} (-1)^{-a_I} A(g_I, a_I) \begin{Bmatrix} j_J & k_{I-1} & g_I \\ j_{I-1} & g_{I+1} & a_I \end{Bmatrix}$$

$$\times (-1)^{g''_{I+1}} A(g_{I+1}, g''_{I+1}) \begin{Bmatrix} j_J & g''_I & g_{I+1} \\ j_{I+1} & g_{I+2} & g''_{I+1} \end{Bmatrix} (-1)^{-a_{I+1}} A(g_{I+1}, a_{I+1}) \begin{Bmatrix} j_J & a_I & g_{I+1} \\ j_{I+1} & g_{I+2} & a_{I+1} \end{Bmatrix}$$

$$\times (-1)^{g''_{I+2}} A(g_{I+2}, g''_{I+2}) \begin{Bmatrix} j_J & g''_{I+1} & g_{I+2} \\ j_{I+2} & g_{I+3} & g''_{I+2} \end{Bmatrix} (-1)^{-a_{I+2}} A(g_{I+2}, a_{I+2}) \begin{Bmatrix} j_J & a_{I+1} & g_{I+2} \\ j_{I+2} & g_{I+3} & a_{I+2} \end{Bmatrix}$$

$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$

$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$

$$\times (-1)^{g''_{J-1}} A(g_{J-1}, g''_{J-1}) \begin{Bmatrix} j_J & g''_{J-2} & g_{J-1} \\ j_{J-1} & g_J & g''_{J-1} \end{Bmatrix} (-1)^{-a_{J-1}} A(g_{J-1}, a_{J-1})$$

$$\times \begin{Bmatrix} j_J & a_{J-2} & g_{J-1} \\ j_{J-1} & g_J & a_{J-1} \end{Bmatrix}$$

$$= \frac{1}{2}(-1)^{J_J - j_2 - j_1 + 1 - \sum_{n=3}^{J-1} j_n} X(j_2, j_J)^{\frac{1}{2}} A(a_2, g''_2) \begin{Bmatrix} j_1 & j_2 & g''_2 \\ 1 & a_2 & j_2 \end{Bmatrix}$$

$$\times \prod_{n=3}^{J-1} A(g''_n, a_n)(-1)^{g''_{n-1}+a_{n-1}+1} \begin{Bmatrix} j_n & g''_{n-1} & g_n \\ 1 & a_n & a_{n-1} \end{Bmatrix}$$

$$\times (-1)^{a_J} \begin{Bmatrix} j_J & a_{J-2} & g_{J-1} \\ j_{J-1} & g_J & a_{J-1} \end{Bmatrix} \prod_{n=J}^{N} \delta_{g''_n a_n} + [j_2(j_2+1) + j_J(j_J+1)] \prod_{n=2}^{N} \delta_{g''_n a_n}. \tag{41}$$

3.4.4. $I = 2, J = 3$

$$\sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle \vec{g}(IJ)|\vec{g}''(12)\rangle\langle \vec{g}(IJ)|\vec{a}(12)\rangle = \sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)$$
$$\times (-1)^{g_I''} A(g_I, g_I'') \begin{Bmatrix} j_J & h_{I-1} & g_I \\ j_{I-1} & g_{I+1} & g_I'' \end{Bmatrix} (-1)^{-a_I} A(g_I, a_I) \begin{Bmatrix} j_J & k_{I-1} & g_I \\ j_{I-1} & g_{I+1} & a_I \end{Bmatrix}$$
$$= \frac{1}{2}(-1)^{j_3-j_2-j_1} X(j_2, j_J)^{\frac{1}{2}} A(a_2, g_2'') \begin{Bmatrix} j_1 & j_2 & g_2'' \\ 1 & a_2 & j_2 \end{Bmatrix} (-1)^{a_3} \begin{Bmatrix} g_3 & j_3 & g_2'' \\ 1 & a_2 & j_3 \end{Bmatrix}$$
$$+ [j_2(j_2+1) + j_3(j_3+1)] \prod_{n=2}^{N} \delta_{g_n'' a_n}. \qquad (42)$$

3.5. Explicit formula for the matrix elements

After having finished the precalculations in the last section, we are now in the position to evaluate the whole matrix element in (12) by using (38).

We have now (again we abbreviate $A(x, y) = \sqrt{(2x+1)(2y+1)}$)

$$\langle \vec{a}(12)|\hat{q}_{IJK}|\vec{a}'(12)\rangle = \sum_{\vec{g}''(12)} \sum_{\vec{g}(IJ)} g_2(IJ)(g_2(IJ)+1)\langle \vec{g}(IJ)|\vec{g}''(12)\rangle\langle \vec{g}(IJ)|\vec{a}(12)\rangle$$
$$\times \sum_{\vec{g}(JK)} g_2(JK)(g_2(JK)+1)\langle \vec{g}(JK)|\vec{g}''(12)\rangle\langle \vec{g}(JK)|\vec{a}(12)\rangle$$
$$- [\vec{a}(12) \Longleftrightarrow \vec{a}'(12)]$$
$$\overset{(40)}{=} \sum_{\vec{g}''(12)} \Bigg[\Bigg[\frac{1}{2}(-1)^{j_J - j_I - \sum_{n=1}^{I-1} j_n - \sum_{m=I+1}^{J-1} j_m} (-1)^{a_{I-1}} (-1)^{a_I - g_I''} (-1)^{-\sum_{n=1}^{I-1} j_n} (-1)^{+1}$$
$$\times X(j_I, j_J)^{\frac{1}{2}} A(g_I'', a_I) \begin{Bmatrix} a_{I-1} & a_I & j_I \\ 1 & j_I & g_I'' \end{Bmatrix} \prod_{n=I+1}^{J-1} A(g'', a_n)(-1)^{g_{n-1}''+a_{n-1}+1}$$
$$\times \begin{Bmatrix} j_n & g_{n-1}'' & g_n'' \\ 1 & a_n & a_{n-1} \end{Bmatrix} (-1)^{a_J} \begin{Bmatrix} a_J & j_J & g_{J-1}'' \\ 1 & a_{J-1} & j_J \end{Bmatrix} \prod_{n=2}^{I-1} \delta_{g_n'' a_n} \prod_{n=J}^{N} \delta_{g_n'' a_n} \Bigg]$$
$$+ \Bigg[[j_I(j_I+1) + j_J(j_J+1)] \prod_{n=2}^{N} \delta_{g_n'' a_n}\Bigg]\Bigg]$$
$$\times \Bigg[\Bigg[\frac{1}{2}(-1)^{j_K - j_J - \sum_{n=1}^{J-1} j_n - \sum_{m=J+1}^{K-1} j_m} (-1)^{a_{J-1}} (-1)^{a_I' - g_I''} (-1)^{-\sum_{n=1}^{J-1} j_n} (-1)^{+1}$$
$$\times X(j_J, j_K)^{\frac{1}{2}} A(g_J'', a_J') \begin{Bmatrix} a_{J-1}' & a_J' & j_J \\ 1 & j_J & g_J'' \end{Bmatrix}$$
$$\times \prod_{n=J+1}^{K-1} A(g'', a_n')(-1)^{g_{n-1}''+a_{n-1}'+1} \begin{Bmatrix} j_n & g_{n-1}'' & g_n'' \\ 1 & a_n' & a_{n-1}' \end{Bmatrix}$$
$$\times (-1)^{a_K'} \begin{Bmatrix} a_K' & j_K & g_{K-1}'' \\ 1 & a_{K-1}' & j_K \end{Bmatrix} \prod_{n=2}^{J-1} \delta_{g_n'' a_n'} \prod_{n=K}^{N} \delta_{g_n'' a_n'} \Bigg]$$
$$+ \Bigg[[j_J(j_J+1) + j_K(j_K+1)] \prod_{n=2}^{N} \delta_{g_n'' a_n'}\Bigg]\Bigg] - [\vec{a}(12) \Longleftrightarrow \vec{a}'(12)]$$

$$
\begin{aligned}
&= \Bigg[\Bigg[\frac{1}{2}(-1)^{j_J-j_I-\sum_{n=1}^{I-1}j_n-\sum_{m=I+1}^{J-1}j_m}(-1)^{a_{I-1}}(-1)^{a_I-a'_I}(-1)^{-\sum_{n=1}^{I-1}j_n}(-1)^{+1}\\
&\times X(j_I,j_J)^{\frac{1}{2}}A(a'_I,a_I)\begin{Bmatrix} a_{I-1} & a_I & j_I\\ 1 & j_I & a'_I\end{Bmatrix}\\
&\times\prod_{n=I+1}^{J-1}A(a'_n,a_n)(-1)^{a'_{n-1}+a_{n-1}+1}\begin{Bmatrix} j_n & a'_{n-1} & a'_n\\ 1 & a_n & a_{n-1}\end{Bmatrix}(-1)^{a_J}\begin{Bmatrix} a_J & j_J & a'_{J-1}\\ 1 & a_{J-1} & j_J\end{Bmatrix}\Bigg]\\
&\times\Bigg[\frac{1}{2}(-1)^{j_K-j_J-\sum_{n=1}^{J-1}j_n-\sum_{m=J+1}^{K-1}j_m}(-1)^{a_{J-1}}(-1)^{a'_I-a_I}(-1)^{-\sum_{n=1}^{J-1}j_n}(-1)^{+1}\\
&\times X(j_J,j_K)^{\frac{1}{2}}A(a'_J,a'_J)\begin{Bmatrix} a'_{J-1} & a'_J & j_J\\ 1 & j_J & a'_J\end{Bmatrix}\\
&\times\prod_{n=J+1}^{K-1}A(a_n,a'_n)(-1)^{a_{n-1}+a'_{n-1}+1}\begin{Bmatrix} j_n & a_{n-1} & a_n\\ 1 & a'_n & a'_{n-1}\end{Bmatrix}\\
&\times(-1)^{a'_K}\begin{Bmatrix} a'_K & j_K & a_{K-1}\\ 1 & a'_{K-1} & j_K\end{Bmatrix}\Bigg]\Bigg]\prod_{n=2}^{I-1}\delta_{a_na'_n}\prod_{n=K}^{N}\delta_{a_na'_n}\\
&+\Bigg[\Bigg[\frac{1}{2}(-1)^{j_J-j_I-\sum_{n=1}^{I-1}j_n-\sum_{m=I+1}^{J-1}j_m}(-1)^{a_{I-1}}(-1)^{a_I-a'_I}(-1)^{-\sum_{n=1}^{I-1}j_n}(-1)^{+1}\\
&\times X(j_I,j_J)^{\frac{1}{2}}A(a'_I,a_I)\begin{Bmatrix} a_{I-1} & a_I & j_I\\ 1 & j_I & a'_I\end{Bmatrix}\\
&\times\prod_{n=I+1}^{J-1}A(a'_n,a_n)(-1)^{a'_{n-1}+a_{n-1}+1}\begin{Bmatrix} j_n & a'_{n-1} & a'_n\\ 1 & a_n & a_{n-1}\end{Bmatrix}\\
&\times(-1)^{a_J}\begin{Bmatrix} a_J & j_J & a'_{J-1}\\ 1 & a_{J-1} & j_J\end{Bmatrix}\Bigg][j_J(j_J+1)+j_K(j_K+1)]\Bigg]\prod_{n=2}^{I-1}\delta_{a_na'_n}\prod_{n=J}^{N}\delta_{a_na'_n}\\
&+\Bigg[\Bigg[\frac{1}{2}(-1)^{j_K-j_J-\sum_{n=1}^{J-1}j_n-\sum_{m=J+1}^{K-1}j_m}(-1)^{a_{J-1}}(-1)^{a'_J-a_J}(-1)^{-\sum_{n=1}^{J-1}j_n}(-1)^{+1}\\
&\times X(j_J,j_K)^{\frac{1}{2}}A(a_J,a'_J)\begin{Bmatrix} a'_{J-1} & a'_J & j_J\\ 1 & j_J & a_J\end{Bmatrix}\\
&\times\prod_{n=J+1}^{K-1}A(a_n,a'_n)(-1)^{a_{n-1}+a'_{n-1}+1}\begin{Bmatrix} j_n & a_{n-1} & a_n\\ 1 & a'_n & a'_{n-1}\end{Bmatrix}\\
&\times(-1)^{a'_K}\begin{Bmatrix} a'_K & j_K & a_{K-1}\\ 1 & a'_{K-1} & j_K\end{Bmatrix}\Bigg][j_I(j_I+1)+j_J(j_J+1)]\Bigg]\prod_{n=2}^{J-1}\delta_{a_na'_n}\prod_{n=K}^{N}\delta_{a_na'_n}\\
&+[[j_J(j_J+1)+j_K(j_K+1)][j_I(j_I+1)+j_J(j_J+1)]]\prod_{n=2}^{N}\delta_{a_na'_n}\\
&-[\vec{a}(12)\Longleftrightarrow\vec{a}'(12)].
\end{aligned}
\tag{43}
$$

Here, we have in the last step carried out the summation over $\vec{g}''_{12}$ by evaluating all the δ-expressions. Finally, we take a closer look at the symmetry properties which the four terms of the sum in (43) have with respect to the interchange $[\vec{a}(12) \Longleftrightarrow \vec{a}'(12)]$, that is the simultaneous replacement $a_n \to a'_n, a'_n \to a_n$ for all $n = 1, \ldots, N$:

- *Fourth term.* Due to the product of $\delta_{a_n a'_n}$-expressions this term is obviously symmetric under $[\vec{a}(12) \Longleftrightarrow \vec{a}'(12)]$.
- *Third term.* The symmetry is not obvious, we will show it part by part:
  (1) In the (-1)-exponents $a_{J-1} = a'_{J-1}, a'_K = a_K$ by the δ-expressions at the end of the term.
  (2) The term $(-1)^{a'_J - a_J}$ is not changed by interchanging $a'_J \leftrightarrow a_J$, since $a'_J - a_J$ is an integer number and therefore the first formula of (B.3) holds. The integer statement is verified by the fact that $\vec{a}_{12}, \vec{a}'_{12}$ are *standard recoupling schemes*, defined as in (A.2). Therefore, they recouple all $j_1, \ldots, j_N$ successively together according to theorem (A.1). Since $\vec{a}_{12}, \vec{a}'_{12}$ contain temporarily recoupled angular momenta, namely $a_k = a_k(a_{k-1}, j_K), a'_k = a'_k(a'_{k-1}, j_k)$ for which $|a_{k-1} - j_k| \leqslant a_k \leqslant a_{k-1} + j_k, |a'_{k-1} - j_k| \leqslant a'_k \leqslant a'_{k-1} + j_k$, the integer or half-integer property of each component a_k, a'_K is only caused by the order the involved spins $j_1, \ldots, j_N$ are coupled together. Since this order is the same in $\vec{a}_{12}, \vec{a}'_{12}$, the components a_k, a'_K are simultaneously (for every $k = 1, \ldots, N$) either half-integer or integer and therefore every sum or difference $a_k \pm a'_k$ is integer.
  (3) The same statement as in (1) holds for a'_{J-1}, a'_K as the entries in the upper-left corner of the two $6j$-symbols before and after the product in the middle of them.
  (4) In the product of the $6j$-symbols the exponent of (-1) contains only a sum $a_{n-1} + a'_{n-1}$ and is therefore symmetric.
  (5) All prefactors $A(a_k, a'_k), k = J, \ldots, K-1$, are symmetric too.
  (6) Finally, all $6j$-symbols in the third term turn out to be symmetric, if we recall that they are invariant under an interchange of their last two columns (B.4) followed by an interchange of the upper and lower arguments of their last two columns (B.5).
- *Second term.* The symmetry is again not obvious, so we will show it part by part:
  (1) In the (-1)-exponents $a_{I-1} = a'_{I-1}, a'_J = a_J$ by the δ-expressions at the end of the term.
  (2) The term $(-1)^{a_I - a'_I}$ is again not changed by interchanging $a_I \leftrightarrow a'_I$, by the same integer statement as under point (2) in the third term discussion.
  (3) The same statement as in (1) holds for a_{I-1}, a_J as the entries in the upper-left corner of the two $6j$-symbols before and after the product in the middle of them.
  (4) In the product of the $6j$-symbols, the exponent of the (-1) contains only a sum $a'_{n-1} + a_{n-1}$ and is therefore symmetric.
  (5) All prefactors $A(a'_k, a_k), k = I, \ldots, J-1$, are symmetric too.
  (6) Finally (again) all $6j$-symbols in the third term turn out to be symmetric, if we recall that they are invariant under an interchange of their last two columns (B.4) followed by an interchange of the upper and lower arguments of their last two columns (B.5).
- *First term.* This term is *not* symmetric under $[\vec{a}(12) \Longleftrightarrow \vec{a}'(12)]$. Arguments similar to the ones we gave in the previous points now let us conclude that:
  (1) The prefactors $(-1)^{a_J}, (-1)^{a'_{J-1}}$ are not symmetric with respect to the interchange of $a_J \to a'_J, a'_{J-1} \to a_{J-1}$.
  (2) The two $6j$-symbols containing a_J, a'_{J-1} in the upper-left corner are not symmetric either.

The analysis has revealed that the last three terms in the sum of (43) are symmetric in $\vec{a}(12)$ and $\vec{a}'(12)$, hence after an antisymmetrization with respect to the interchange of $\vec{a}(12)$ and $\vec{a}'(12)$ only the first term in (43) survives.

Summarizing, we get by explicitly writing down all the terms occurring through the antisymmetrization:

$$
\begin{aligned}
\langle\vec{a}(12)|\hat{q}_{IJK}|\vec{a}'(12)\rangle = \Bigg[\Bigg[& \frac{1}{2}(-1)^{j_J - j_I - \sum_{n=1}^{I-1} j_n - \sum_{m=I+1}^{J-1} j_m}(-1)^{a_{I-1}}(-1)^{a_I - a'_I}(-1)^{-\sum_{n=1}^{I-1} j_n}(-1)^{+1} \\
& \times X(j_I, j_J)^{\frac{1}{2}} A(a'_I, a_I)\begin{Bmatrix} a_{I-1} & a_I & j_I \\ 1 & j_I & a'_I \end{Bmatrix} \prod_{n=I+1}^{J-1} A(a'_n, a_n)(-1)^{a'_{n-1}+a_{n-1}+1} \\
& \times \begin{Bmatrix} j_n & a'_{n-1} & a'_n \\ 1 & a_n & a_{n-1} \end{Bmatrix} \underline{(-1)^{a_J}\begin{Bmatrix} a_J & j_J & a'_{J-1} \\ 1 & a_{J-1} & j_J \end{Bmatrix}}\Bigg] \\
& \times \Bigg[\frac{1}{2}(-1)^{j_K - j_J - \sum_{n=1}^{J-1} j_n - \sum_{m=J+1}^{K-1} j_m}\underline{(-1)^{a'_{J-1}}}(-1)^{a'_I - a_I}(-1)^{-\sum_{n=1}^{J-1} j_n}(-1)^{+1} \\
& \times X(j_J, j_K)^{\frac{1}{2}} A(a'_J, a_J)\underline{\begin{Bmatrix} a'_{J-1} & a'_J & j_J \\ 1 & j_J & a'_J \end{Bmatrix}} \prod_{n=J+1}^{K-1} A(a_n, a'_n)(-1)^{a_{n-1}+a'_{n-1}+1} \\
& \times \begin{Bmatrix} j_n & a_{n-1} & a_n \\ 1 & a'_n & a'_{n-1} \end{Bmatrix} (-1)^{a'_K}\begin{Bmatrix} a'_K & j_K & a_{K-1} \\ 1 & a'_{K-1} & j_K \end{Bmatrix}\Bigg]\Bigg] \prod_{n=2}^{I-1}\delta_{a_n a'_n}\prod_{n=K}^{N}\delta_{a_n a'_n} \\
- \Bigg[\Bigg[& \frac{1}{2}(-1)^{j_J - j_I - \sum_{n=1}^{I-1} j_n - \sum_{m=I+1}^{J-1} j_m}(-1)^{a'_{I-1}}(-1)^{a'_I - a_I}(-1)^{-\sum_{n=1}^{I-1} j_n}(-1)^{+1} \\
& \times X(j_I, j_J)^{\frac{1}{2}} A(a_I, a'_I)\begin{Bmatrix} a'_{I-1} & a'_I & j_I \\ 1 & j_I & a_I \end{Bmatrix} \prod_{n=I+1}^{J-1} A(a_n, a'_n)(-1)^{a_{n-1}+a'_{n-1}+1} \\
& \times \begin{Bmatrix} j_n & a_{n-1} & a_n \\ 1 & a'_n & a'_{n-1} \end{Bmatrix} \underline{(-1)^{a_J}\begin{Bmatrix} a'_J & j_J & a_{J-1} \\ 1 & a'_{J-1} & j_J \end{Bmatrix}}\Bigg] \\
& \times \Bigg[\frac{1}{2}(-1)^{j_K - j_J - \sum_{n=1}^{J-1} j_n - \sum_{m=J+1}^{K-1} j_m}\underline{(-1)^{a_{J-1}}}(-1)^{a'_I - a_I}(-1)^{-\sum_{n=1}^{J-1} j_n}(-1)^{+1} \\
& \times X(j_J, j_K)^{\frac{1}{2}} A(a_J, a'_J)\underline{\begin{Bmatrix} a_{J-1} & a_J & j_J \\ 1 & j_J & a'_J \end{Bmatrix}} \prod_{n=J+1}^{K-1} A(a'_n, a_n)(-1)^{a'_{n-1}+a_{n-1}+1} \\
& \times \begin{Bmatrix} j_n & a'_{n-1} & a'_n \\ 1 & a_n & a_{n-1} \end{Bmatrix} (-1)^{a_K}\begin{Bmatrix} a_K & j_K & a'_{K-1} \\ 1 & a_{K-1} & j_K \end{Bmatrix}\Bigg]\Bigg] \prod_{n=2}^{I-1}\delta_{a_n a'_n}\prod_{n=K}^{N}\delta_{a_n a'_n}.
\end{aligned}
\tag{44}
$$

Here, we have underlined the terms, which are different with respect to the antisymmetrization (recall that $(-1)^{a_I - a'_I} = (-1)^{-(a_I - a'_I)} = (-1)^{a'_I - a_I}$), because the exponent is an integer number. All the other terms are symmetric under the interchange $\vec{a}(12) \Longleftrightarrow \vec{a}'(12)$, again because of the symmetry properties (B.4), (B.5) and the symmetrization by the δ-expressions.

Before we write down the final result we can simplify the exponents in (44):

$$
\begin{aligned}
& (-1)^{-\sum_{n=1}^{I-1} j_n - \sum_{m=I+1}^{J-1} j_m}(-1)^{-\sum_{n=1}^{I-1} j_n}(-1)^{-\sum_{n=1}^{J-1} j_n - \sum_{m=J+1}^{K-1} j_m}(-1)^{-\sum_{n=1}^{J-1} j_n} \\
&\qquad = (-1)^{-2\sum_{n=1}^{I-1} j_n}(-1)^{-\sum_{n=I+1}^{J-1} j_n}(-1)^{-2\sum_{n=1}^{J-1}}(-1)^{-\sum_{n=J+1}^{K-1} j_n} \\
&\qquad = (-1)^{-\sum_{n=I+1}^{J-1} j_n}(-1)^{-2\sum_{n=I}^{J-1} j_n}(-1)^{-\sum_{n=J+1}^{K-1} j_n}
\end{aligned}
$$

$$= (-1)^{2j_I - 3\sum_{n=I+1}^{J-1} j_n - \sum_{n=J+1}^{K-1} j_n}$$
$$= (-1)^{2j_I + \sum_{n=I+1}^{J-1} j_n - \sum_{n=J+1}^{K-1} j_n}.$$

Now we are able to give a closed expression of the matrix elements of $\hat{q}_{IJK}$ in terms of standard-recoupling scheme basis (12). In order to avoid confusion we assume that $I > 1$, $J > I + 1$; the remaining cases will be discussed below.

Theorem.

$$\begin{aligned}
\langle \vec{a}|\hat{q}_{IJK}|\vec{a}'\rangle = \frac{1}{4}(-1)^{j_K+j_I+a_{I-1}+a_K}(-1)^{a_I-a'_I}(-1)^{\sum_{n=I+1}^{J-1} j_n}(-1)^{-\sum_{p=J+1}^{K-1} j_p} \\
\times X(j_I, j_J)^{\frac{1}{2}} X(j_J, j_K)^{\frac{1}{2}} \sqrt{(2a_I+1)(2a'_I+1)}\sqrt{(2a_J+1)(2a'_J+1)} \\
\times \begin{Bmatrix} a_{I-1} & j_I & a_I \\ 1 & a'_I & j_I \end{Bmatrix} \left[\prod_{n=I+1}^{J-1} \sqrt{(2a'_n+1)(2a_n+1)}(-1)^{a'_{n-1}+a_{n-1}+1}\right. \\
\left.\times \begin{Bmatrix} j_n & a'_{n-1} & a'_n \\ 1 & a_n & a_{n-1} \end{Bmatrix}\right] \left[\prod_{n=J+1}^{K-1} \sqrt{(2a'_n+1)(2a_n+1)}(-1)^{a'_{n-1}+a_{n-1}+1}\right. \\
\left.\times \begin{Bmatrix} j_n & a'_{n-1} & a'_n \\ 1 & a_n & a_{n-1} \end{Bmatrix}\right] \begin{Bmatrix} a_K & j_K & a_{K-1} \\ 1 & a'_{K-1} & j_K \end{Bmatrix} \\
\times \left[(-1)^{a'_J+a'_{J-1}} \begin{Bmatrix} a_J & j_J & a'_{J-1} \\ 1 & a_{J-1} & j_J \end{Bmatrix} \begin{Bmatrix} a'_{J-1} & j_J & a'_J \\ 1 & a_J & j_J \end{Bmatrix} - (-1)^{a_J+a_{J-1}}\right. \\
\left.\times \begin{Bmatrix} a'_J & j_J & a'_{J-1} \\ 1 & a_{J-1} & j_J \end{Bmatrix} \begin{Bmatrix} a_{J-1} & j_J & a'_J \\ 1 & a_J & j_J \end{Bmatrix}\right] \prod_{n=2}^{I-1} \delta_{a_n a'_n} \prod_{n=K}^{N} \delta_{a_n a'_n}
\end{aligned} \tag{45}$$

with $X(j_1, j_2) = 2j_1(2j_1+1)(2j_1+2)2j_2(2j_2+1)(2j_2+2)$. *Note that all* $6j$*-symbols still appearing are just abbreviations for the following simple expressions in which summations or products (factorials) no longer need to be carried out as compared to (B.2), e.g. (using* $s = a + b + c$*),*

$$\begin{Bmatrix} a & b & c \\ 1 & c & b \end{Bmatrix} = (-1)^{s+1} \frac{2[b(b+1)c(c+1) - a(a+1)]}{[2b(2b+1)(2b+2)2c(2c+1)(2c+2)]^{\frac{1}{2}}} \tag{46}$$

$$\begin{Bmatrix} a & b & c \\ 1 & c-1 & b \end{Bmatrix} = (-1)^{s} \left[\frac{2(s+1)(s-2a)(s-2b)(s-2c+1)}{2b(2b+1)(2b+2)(2c-1)2c(2c+1)}\right]^{\frac{1}{2}} \tag{47}$$

$$\begin{Bmatrix} a & b & c \\ 1 & c-1 & b-1 \end{Bmatrix} = (-1)^{s} \left[\frac{s(s+1)(s-2a-1)(s-2a)}{(2b-1)2b(2b+1)(2c-1)2c(2c+1)}\right]^{\frac{1}{2}} \tag{48}$$

$$\begin{Bmatrix} a & b & c \\ 1 & c-1 & b+1 \end{Bmatrix} = (-1)^{s} \left[\frac{(s-2b-1)(s-2b)(s-2c+1)(s-2c+2)}{(2b+1)(2b+2)(2b+3)(2c-1)2c(2c+1)}\right]^{\frac{1}{2}}. \tag{49}$$

Remark (gauge invariance)**.** Recall that a vertex is said to be gauge invariant if the angular momenta coming from the edges $e_1, \ldots, e_N$ meeting in the vertex v are coupled to a resulting angular momentum $j = g_N = 0$. Using the notation from (A.5), this means

$$J := \sum_{i=1}^{N} J_i =: G_N = G_{N-1} + J_N \stackrel{!}{=} 0. \tag{50}$$

This implies

$$G_{N-1} = G_{N-2} + J_{N-1} \stackrel{!}{=} -J_N \tag{51}$$

$$\rightsquigarrow G_{N-2} = G_{N-3} + J_{N-2} = -J_N - J_{N-1}. \tag{52}$$

But that gives $g_{N-1} = j_N$ and a certain restriction on which values g_{N-2} can take due to the Clebsh–Gordon theorem A.1:

$$\max\left(|j_{N-2} - g_{N-3}|, |j_N - j_{N-1}|\right) \leqslant g_{N-2} \leqslant \min\left(j_{N-2} + g_{N-3}, j_N + j_{N-1}\right). \tag{53}$$

This relation will become useful when we consider gauge invariance later.

As promised we now display the remaining cases of (45) explicitly. They are obtained, if some of the special cases (39)–(42) are involved.

3.5.1. $I = 1, J, K$ arbitrary

$$\begin{aligned}\langle\vec{a}|\hat{q}_{1JK}|\vec{a}'\rangle = {}& \frac{1}{4}(-1)^{j_K - j_1 + a_K + 1}(-1)^{\sum_{n=2}^{J-1} j_n}(-1)^{-\sum_{p=J+1}^{K-1} j_p} X(j_1, j_J)^{\frac{1}{2}} \\ & \times X(j_J, j_K)^{\frac{1}{2}}\sqrt{(2a_J + 1)(2a'_J + 1)} \\ & \times \left[\prod_{n=2}^{J-1}\sqrt{(2a'_n + 1)(2a_n + 1)}(-1)^{a'_{n-1} + a_{n-1} + 1}\begin{Bmatrix} j_n & a'_{n-1} & a'_n \\ 1 & a_n & a_{n-1}\end{Bmatrix}\right] \\ & \times \left[\prod_{n=J+1}^{K-1}\sqrt{(2a'_n + 1)(2a_n + 1)}(-1)^{a'_{n-1} + a_{n-1} + 1}\begin{Bmatrix} j_n & a'_{n-1} & a'_n \\ 1 & a_n & a_{n-1}\end{Bmatrix}\right] \\ & \times \begin{Bmatrix} a_K & j_K & a_{K-1} \\ 1 & a'_{K-1} & j_K\end{Bmatrix}\left[(-1)^{a'_J + a'_{J-1}}\begin{Bmatrix} a_J & j_J & a'_{J-1} \\ 1 & a_{J-1} & j_J\end{Bmatrix}\begin{Bmatrix} a'_{J-1} & j_J & a'_J \\ 1 & a_J & j_J\end{Bmatrix}\right. \\ & \left. - (-1)^{a_J + a_{J-1}}\begin{Bmatrix} a'_J & j_J & a'_{J-1} \\ 1 & a_{J-1} & j_J\end{Bmatrix}\begin{Bmatrix} a_{J-1} & j_J & a'_J \\ 1 & a_J & j_J\end{Bmatrix}\right]\prod_{n=K}^{N}\delta_{a_n a'_n}.\end{aligned} \tag{54}$$

3.5.2. $I = 1, J = 2, K$ arbitrary

$$\begin{aligned}\langle\vec{a}|\hat{q}_{12K}|\vec{a}'\rangle = {}& \frac{1}{4}(-1)^{j_K - j_1 - j_2 + a_K + 1}(-1)^{\sum_{n=2}^{J-1} j_n}(-1)^{-\sum_{p=J+1}^{K-1} j_p} \\ & \times X(j_2, j_K)^{\frac{1}{2}}\sqrt{(2a_2 + 1)(2a'_2 + 1)}\begin{Bmatrix} j_1 & j_2 & a_2 \\ 1 & a'_2 & j_2\end{Bmatrix} \\ & \times \left[\prod_{n=3}^{K-1}\sqrt{(2a'_n + 1)(2a_n + 1)}(-1)^{a'_{n-1} + a_{n-1} + 1}\begin{Bmatrix} j_n & a'_{n-1} & a'_n \\ 1 & a_n & a_{n-1}\end{Bmatrix}\right] \\ & \times \begin{Bmatrix} a_K & j_K & a_{K-1} \\ 1 & a'_{K-1} & j_K\end{Bmatrix}[a_2(a_2 + 1) - a'_2(a'_2 + 1)]\prod_{n=K}^{N}\delta_{a_n a'_n}.\end{aligned} \tag{55}$$

3.5.3. $I = 1, J = 2, K = 3$. This case is actually the easiest. We will use it in the next section. Therefore, we will write down the calculation explicitly. We start with (40), (42) to obtain

$$\langle\vec{a}|\hat{q}_{123}|\vec{a}'\rangle = a_2(a_2+1)\prod_{n=2}^{N}\delta_{g''_n a_n}\Bigg[\frac{1}{2}(-1)^{j_2-j_1+j_3}X(j_2,j_3)^{\frac{1}{2}}\sqrt{(2g''_2+1)(2a'_2+1)}\begin{Bmatrix} j_1 & j_2 & g''_2 \\ 1 & a'_2 & j_2 \end{Bmatrix}$$
$$\times(-1)^{a_3}\begin{Bmatrix} a_3 & j_3 & g''_2 \\ 1 & a'_2 & j_3 \end{Bmatrix}\prod_{n=3}^{N}\delta_{a_n a'_n} + [j_2(j_2+1)+j_3(j_3+1)]\prod_{n=2}^{N}\delta_{a_n a'_n}\Bigg]$$
$$-(\vec{a}\longleftrightarrow\vec{a}') = (a_2(a_2+1) - a'_2(a'_2+1))$$
$$\times\Bigg[\frac{1}{2}(-1)^{j_2-j_1+j_3}X(j_2,j_3)^{\frac{1}{2}}\sqrt{(2a'_2+1)(2a_2+1)}\begin{Bmatrix} j_1 & j_2 & a_2 \\ 1 & a'_2 & j_2 \end{Bmatrix}$$
$$\times(-1)^{a_3}\begin{Bmatrix} a_3 & j_3 & a_2 \\ 1 & a'_2 & j_3 \end{Bmatrix}\Bigg]\prod_{n=3}^{N}\delta_{a_n a'_n}. \tag{56}$$

Now the conditions for the arguments in the definition of the $6j$-symbols (B.2) give certain relations for a_2, a'_2 occurring in (56), namely,

$$a'_2 = \begin{cases} a_2 - 1 \\ a_2 \\ a_2 + 1. \end{cases}$$

We can choose either the first or the third case to obtain a non-vanishing matrix element. We choose $a'_2 = a_2 - 1$ (the other choice would give us a sign, due to the antisymmetry of $\hat{q}$). So, we continue (considering only the nontrivial information a_2, a'_2 contained in the recoupling schemes $\vec{a}, \vec{a}'$):

$$\langle a_2|\hat{q}_{123}|a_2-1\rangle = (a_2(a_2+1) - (a_2-1)a_2)$$
$$\times\Bigg[\frac{1}{2}(-1)^{j_2-j_1+j_3}x(j_2,j_3)^{\frac{1}{2}}\sqrt{(2(a_2-1)+1)(2a_2+1)}\begin{Bmatrix} j_1 & j_2 & a_2 \\ 1 & a_2-1 & j_2 \end{Bmatrix}$$
$$\times(-1)^{a_3}\begin{Bmatrix} a_3 & j_3 & a_2 \\ 1 & a_2-1 & j_3 \end{Bmatrix}\Bigg]. \tag{57}$$

Now we can rewrite the second $6j$-symbol in (57) by using the identity[2]

$$\begin{Bmatrix} a & b & c \\ 1 & c-1 & b \end{Bmatrix} = \sqrt{\frac{2a(2a+1)(2a+2)}{2b(2b+1)(2b+2)}}\begin{Bmatrix} b & a & c \\ 1 & c-1 & a \end{Bmatrix}$$

$$\langle a_2|\hat{q}_{123}|a_2-1\rangle = 2a_2\frac{1}{2}(-1)^{j_2-j_1+j_3}X(j_2,j_3)^{\frac{1}{2}}\sqrt{(2a_2-1)(2a_2+1)}\begin{Bmatrix} j_1 & j_2 & a_2 \\ 1 & a_2-1 & j_2 \end{Bmatrix}$$
$$\times(-1)^{a_3}\sqrt{\frac{2a_3(2a_3+1)(2a_3+2)}{2j_3(2j_3+1)(2j_3+2)}}\begin{Bmatrix} j_3 & a_3 & a_2 \\ 1 & a_2-1 & a_3 \end{Bmatrix}. \tag{58}$$

At the last step we once more use (47) to express all $6j$-symbols in (58) explicitly. Furthermore, we use the fact that $j_3 + a_2 + a_3$ is an integer number and therefore $(-1)^{2(j_3+a_2+a_3)} = 1$ (one can see this by applying the integer conditions (B.2) to the second $6j$-symbol in (58)). Additionally, recall the shortcut introduced earlier: $X(j_2, j_3) = 2j_2(2j_2+1)(2j_2+2)2j_3(2j_3+1)(2j_3+2)$. After carefully expanding all the terms and cancelling all identical terms in the numerator and

[2] This follows directly from (47).

the denominator, the explicit result is

$$\langle a_2|\hat{q}_{123}|a_2-1\rangle = \frac{1}{\sqrt{(2a_2-1)(2a_2+1)}}[(j_1+j_2+a_2+1)(-j_1+j_2+a_2)(j_1-j_2+a_2) \times (j_1+j_2-a_2+1)(j_3+a_3+a_2+1)(-j_3+a_3+a_2)(j_3-a_3+a_2) \times (j_3+a_3-a_2+1)]^{\frac{1}{2}} = -\langle a_2-1|\hat{q}_{123}|a_2\rangle. \quad (59)$$

The analytical result for this special case coincides with the result already obtained by graphical methods in [8], if one considers the gauge-invariant 4-vertex (see the next section!) by putting $a_2 \to j_{12}$ and $a_3 \to j_4$ (as a consequence of applying the definition of the standard-recoupling schemes (definition A.2) to a 4-vertex).

3.5.4. Comparison: computational effort. At the end of this section, we want to compare the computational effort one has to invest for calculating the matrix element (12) using the full definition in terms of $6j$-symbols (18) or the derived formula (45) instead. We will give here only a rough estimate, since for the full definition (19) the calculation can hardly be done for all possible combinations of arguments.

Consider an N-valent monochromatic vertex[3] v with N outgoing edges $e_1,\ldots,e_N$, each carrying the spin $j_1=\cdots=j_N=j_{\max}$. Assume, we had to calculate the matrix element (12) for a certain combination of the triple $I<J<K$, namely $I\approx(J-I)\approx(K-J):=L\sim\frac{N}{3}\gg 1$.

Let us first discuss the full definition using (12) with (18) inserted.

Consider first the definition (B.2) of the $6j$-symbols: we will only pay attention to the w-coefficient, since the number of Δ-coefficients is constant. By the requirement for the summation variable $n(\max[j_1+j_2+j_{12}, j_1+j+j_{23}, j_3+j_2+j_{23}, j_3+j+j_{12}] \leqslant n \leqslant \min[j_1+j_2+j_3+j, j_2+j_{12}+j+j_{23}, j_{12}+j_1+j_{23}+j_3])$, we can (if we put $j_1=j_2=j_3=j=j_{\max}, j_{23}=j_{12}=2j$) extract $0\leqslant n\leqslant 4j$. That is, we have approximately $4j_{\max}$ summations and therefore $7\cdot 4j_{\max}$ factorials to calculate for every $6j$-symbol.

Now look at the definition of the $3nj$-symbol in terms of $6j$-symbols (16): we have approximately $2I=2L$ $6j$-symbols, due to summation over the intermediate recoupling steps h_k and additionally $J-I=L$ $6j$-symbols not involved in that summation, a constant number which we can drop. Now in the worst case, $0\leqslant h_1\leqslant 2j_{\max}, j_{\max}\leqslant h_2\leqslant 2j_{\max}+j_{\max},\ldots,(I-1)j_{\max}\leqslant h_{I-1}\leqslant(I+1)j_{\max}$. Therefore, each h_k $(2\leqslant k\leqslant(I-1))$ can take $2j_{\max}$ different values and we have thus about $(2j_{\max})^I$ possible combinations for h_k. So we had to calculate all $2I(2j_{\max})^I=2L(2j_{\max})^L$ $6j$-symbols.

Every term in the sum (12) contains a product of four $3nj$-symbols. Now the summation over $\vec{g}(IJ), \vec{g}(JK), \vec{g}''(12)$ again gives (under the assumption that each intermediate angular momentum $g(IJ)_k, g(JK)_k, g(12)''_k$ can take $2j_{\max}$ different values, but only $(J-I)\approx(K-J):=L$ intermediate steps of each summation contribute to calculations, due to the δ-terms in (14)), for each matrix element approximately $(2\cdot 2j_{\max})^{3L}3nj$-symbols to calculate. Summarizing these three steps we end up with a computational effort of approximately

$$7\cdot 4j_{\max}\cdot 2L(2j_{\max})^L\cdot(2\cdot 2j_{\max})^{3L}\sim(j_{\max})^{4L}\sim(j_{\max})^{\frac{4}{3}N}$$

calculations of *factorials* occurring in (B.2).

It is much easier to discuss the effort one has in the case of using the derived equation (45). We have only a product of special $6j$-symbols containing *no summation and factorials at all*.

[3] Of course this special case is not that expensive, because it is the most symmetric case. But it illustrates the estimates for the general case with different spins.

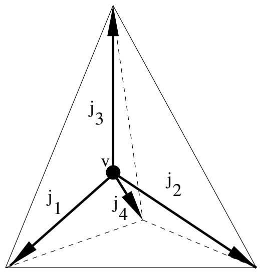

Figure 1. The configuration at the 4-vertex: four outgoing edges each carrying a representation of $SU(2)$ with a weight according to j_1, j_2, j_3, j_4.

So, one only has to carry out the product consisting of only $K - I = 2L \sim \frac{2}{3}N$ factors, *independent* of $j_{\max}$.

Be aware that this estimate given is only rough, one could introduce the symmetry properties (B.4), (B.5) and additionally keep in memory previously calculated $6j$- or $3nj$-symbols to save calculation time. Nevertheless, the computational effort for the calculation of the matrix element (12) depends on $j_{\max}$ if one uses the original formulae (12) with (18). This is no longer the case if one uses (45). It is clear that if one wants to numerically compute all the matrix elements then one cannot get very much over $j_{\max} = 2$ with (12).

3.5.5. Conclusion. We have shown in the last section that it is possible to explicitly evaluate the matrix elements of the volume operator in (12). Here, by 'explicitly' we mean that there are no more $6j$-symbols in the final expression. The derived formula is a simple algebraic function of the spin quantum numbers, no factorials appear any longer and no conditional summations, implicit in Racah's formula for the $6j$-symbol, have to be carried out anymore. Thus, the computational effort in order to evaluate the matrix elements has decreased by a huge order of magnitude, which grows with growing maximal spin $j_{\max}$. This simplification has been achieved by the discovery of a nontrivial fact, namely, that the highly involved formula (12) or (18) is like a telescopic sum of the form $\sum_{n=1}^{N}(a_n - a_{n-1}) = a_N - a_0$ once one takes the orthogonality relations of the $6j$-symbols and the Elliot–Biedenharn identity into account.

A first observation is that the matrices defined by (45) show a banded structure, that is a rich selection rule structure. Non-vanishing entries are only on certain parallels to the main diagonal, because of the restrictions of the presence of an entry 1 in every $6j$-symbol contained in (45).

4. Gauge-invariant 4-vertex

In this section we will examine in more detail the gauge-invariant 4-vertex, that is the configuration of edges as shown in figure 1.

We have four edges $e_1, \ldots, e_4$ outgoing at the vertex v carrying the spins $j_1, \ldots, j_4$ and the corresponding representations of $SU(2)$, $\pi_{j_1}, \ldots, \pi_{j_4}$.

The square $\hat{Q}_v = \hat{V}_v^2$ of the volume operator represented in terms of the standard-recoupling scheme basis was (note that in what follows we will stick to the squared version of the volume operator, therefore of all eigenvalues we write down, the square root has to be taken in order to obtain the spectral behaviour of the volume operator itself)

$$\hat{Q}_v := Z \cdot \sum_{I<J<K} \epsilon(I,J,K)[(J_{IJ})^2, (J_{JK})^2]$$
$$= Z \cdot \sum_{I<J<K} \epsilon(I,J,K)\hat{q}_{IJK}. \qquad (60)$$

Since we have four edges the summation in (60) has to be extended over the combinations $(I < J < K) = (1,2,3), (1,2,4), (1,3,4), (2,3,4)$.

The point is now that due to gauge invariance the four angular momenta $j_1, \ldots, j_4$ should couple to a resulting zero-angular momentum $j = 0$ at the vertex v. For this reason the angular momentum operators $J_1, \ldots, J_4$ hold due to (53)

$$J_1 + J_2 + J_3 + J_4 = 0 \qquad (61)$$

which implies

$$J_4 = -(J_1 + J_2 + J_3). \qquad (62)$$

It follows that

$$\begin{aligned}\hat{q}_{124} &= -(\hat{q}_{121} + \hat{q}_{122} + \hat{q}_{123}) = -\hat{q}_{123}\\ \hat{q}_{134} &= -(\hat{q}_{131} + \hat{q}_{132} + \hat{q}_{133}) = -\hat{q}_{132}\\ \hat{q}_{234} &= -(\hat{q}_{231} + \hat{q}_{232} + \hat{q}_{233}) = -\hat{q}_{231}.\end{aligned} \qquad (63)$$

Here, we have used the fact that $\hat{q}_{IJJ} + \hat{q}_{IJI} = 0\ \forall I, J$.[4]

Thus, (60) reduces to

$$\sum_{I<J<K} \epsilon(I,J,K)\hat{q}_{IJK} = \epsilon(1,2,3)\hat{q}_{123} + \epsilon(1,2,4)\hat{q}_{124} + \epsilon(1,3,4)\hat{q}_{134} + \epsilon(2,3,4)\hat{q}_{234}$$
$$= [\epsilon(1,2,3) - \epsilon(1,2,4) + \epsilon(1,3,4) - \epsilon(2,3,4)]\hat{q}_{123}$$
$$= 2 \cdot \hat{q}_{123} \qquad (64)$$

where we have used in the last line the configuration of the four edges outgoing from v described above to obtain the orientation (± 1) of every triple of tangent vectors corresponding to three distinct edges (note that for different orientations of $e_1, \ldots, e_4$ just the prefactor 2 changes). This brings us precisely into the situation of the last example in the previous section. We can now explicitly write down the matrix elements of $\hat{Q}_v$ represented in a basis of standard gauge-invariant recoupling schemes $|\vec{a}(12)j = 0 M = 0\rangle = |a_2\rangle$, $|\vec{a}'(12)j = 0 M = 0\rangle = |a'_2\rangle$. For simplicity, we relabel $a_2 \to j_{12}, a_3 = a'_3 \to j_4, a'_2 \to j'_{12}, a_3 = a'_3 \to j_4$.

Now the non-vanishing matrix elements in (59) are

$$\langle j_{12}|\hat{q}_{123}|j_{12} - 1\rangle = \frac{1}{\sqrt{(2j_{12}-1)(2j_{12}+1)}}[(j_1 + j_2 + j_{12} + 1)(-j_1 + j_2 + j_{12})(j_1 - j_2 + j_{12})$$
$$\times (j_1 + j_2 - j_{12} + 1)(j_3 + j_4 + j_{12} + 1)(-j_3 + j_4 + j_{12})(j_3 - j_4 + j_{12})$$
$$\times (j_3 + j_4 - j_{12} + 1)]^{\frac{1}{2}} = -\langle j_{12} - 1|\hat{q}_{123}|j_{12}\rangle. \qquad (65)$$

By (55) we get certain restrictions for the values that j_{12} may take[5]:

$$\max(|j_1 - j_2|, |j_3 - j_4|) \leqslant j_{12} \leqslant \min(j_1 + j_2, j_3 + j_4). \qquad (66)$$

Therefore, the dimension n of the matrix-representation A of $\hat{q}_{123}$ in the standard basis is given by

$$n := \dim A = \min(j_1 + j_2, j_3 + j_4) - \max(|j_1 - j_2|, |j_3 - j_4|) + 1$$
$$= j_{12}^{\max} - j_{12}^{\min} + 1. \qquad (67)$$

[4] To see this, just take the definition $\hat{q}_{IJK} = [(J_{IJ})^2, (J_{JK})^2]$ and expand the resulting commutators. Alternatively, use the antisymmetry of $\hat{q}_{IJJ} \sim \epsilon_{ijk} J_I^j J_J^j J_J^k$ to see that $\hat{q}_{IJJ} + \hat{q}_{IJI} = \hat{q}_{IJJ} - \hat{q}_{JII} = 0$.

[5] We may label w.l.o.g. edges in such a way that $0 < j_1 \leqslant j_2 \leqslant j_3 \leqslant j_4 \leqslant (j_1 + j_2 + j_3)$ and $j_1 + j_2 + j_3 + j_4 =$ integral.

We find for the matrix A (labelling the rows by j_{12} and the columns by j'_{12}, where the first row/column equals $j_{12} = j'_{12} = j_{12}^{\min}$ increasing down to the last row/column with $j_{12} = j'_{12} = j_{12}^{\max}$ and using the abbreviation for the matrix element $a_k := \mathrm{i} \cdot \langle j_{12}^{\min} + k | \hat{q}_{123} | j_{12}^{\min} + k - 1 \rangle$ (where i is the imaginary unit[6]), $k = 1, \ldots, n-1$ and $a_0 = a_n = 0$ [7])

$$A = \begin{pmatrix} 0 & -a_1 & 0 & \cdots & \cdots & 0 \\ a_1 & 0 & -a_2 & & & \vdots \\ 0 & a_2 & 0 & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & -a_{n-1} \\ 0 & \cdots & \cdots & \cdots & a_{n-1} & 0 \end{pmatrix}. \tag{68}$$

That is, the matrix A possesses a banded matrix structure which is called a *Jacobi* matrix. Note that a_k are purely imaginary, because A is Hermitian and its eigenvalues are real. We will discuss the spectral theory of A by analytical and numerical methods. Note the following advantages of the gauge-invariant case over the gauge variant:

- The dimension of A scales only linearly with the spins outgoing at the vertex v (this advantage will be useful for the numerical studies).
- There is no sum over matrices left any longer, as would be the case for the gauge-variant 4-vertex.
- Due to the formulation in a recoupling scheme basis we have automatically implemented gauge invariance.

4.1. Analytical investigations

4.1.1. Eigenvalues. As pointed out before, all eigenvalues λ of A are real and come in pairs $\pm\lambda$. The special case of zero eigenvalues will be discussed below. One can find upper bounds for the eigenvalues by applying the theorem of *Geršgorin* (see [26], p 465).

Theorem 4.1 (Geršgorin)**.**
Every characteristic root λ of an $(n \times n)$-matrix A lies in at least one of the discs

$$|a_{ii} - \lambda| \leqslant \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}| \qquad i = 1, \ldots, n.$$

That is, every eigenvalue lies in a disc centred at the diagonal element a_{ii} with radius of the sum of moduli of the off-diagonal elements a_{ij}, $i \neq j$ of the ith row or column (called the ith row or column sum). In the case of the gauge-invariant 4-vertex this theorem simplifies due to the banded matrix structure of (68) and the fact that $a_{ii} = 0$ to

$$|\lambda| \leqslant \sum_{j \neq i} |a_{ij}| = |a_{ii-1}| + a_{ii+1}. \tag{69}$$

We will give an upper and a lower bound for the eigenvalue spectrum in terms of the leading polynomial order of the largest angular momentum $j_{\max} = \max(j_1, \ldots, j_4)$.

[6] This only changes the spectrum of A from being antisymmetric to Hermitian and therefore rotates its spectrum from purely imaginary to purely real.
[7] Just insert $j_{12} = j_{12}^{\min}$ or $j_{12} = j_{12}^{\min} + n = j_{12}^{\max}$ into the matrix element (65).

By inspection of (68) one can see that the row sum introduced in theorem 4.1 is dependent on the modulus of each of the matrix elements $a_i(j_{12}) := \langle j_{12}|\hat{q}_{123}|j_{12}-1\rangle$, $i = 1,\ldots,n-1$. This observation will be useful for obtaining an upper bound for the modulus of the eigenvalues of A. On the other hand we could also use theorem 4.1 for giving a lower bound of the eigenvalues if we could guarantee the existence of the inverse A^{-1} that is the absence of the eigenvalue 0, which will be discussed explicitly in appendix C. Then the upper bound of the eigenvalues of A^{-1} would give us a lower bound of the non-zero eigenvalues of A. However, due to the general formula for the matrix element of the inverse matrix

$$(A^{-1})_{ij} = \frac{\det M_{ij}}{\det A} \tag{70}$$

(where M_{ij} denotes the sub-determinant of A with row i and column j deleted) all the entries of A^{-1} will be of the order $\frac{1}{a_i(j_{12})}$. We can therefore try to find the extrema of the matrix element (65) in terms of the spins $j_1,\ldots,j_4$ by partial differentiation[8]. Note that we have the freedom to choose $j_1 \leqslant j_2 \leqslant j_3 \leqslant j_4 = j_{\max}$, since the matrix element (65) is symmetric under permutations of $j_1,\ldots,j_4$:

$$\begin{aligned}
\frac{\partial a(j_{12})}{\partial j_1} &\stackrel{!}{=} 0 \Leftrightarrow j_1^{(0)} = -\frac{1}{2} + \frac{1}{2}\sqrt{1+4j_{12}^2+4j_2+4j_2^2}\\
\frac{\partial a(j_{12})}{\partial j_2} &\stackrel{!}{=} 0 \Leftrightarrow j_2^{(0)} = -\frac{1}{2} + \frac{1}{2}\sqrt{1+4j_{12}^2+4j_1+4j_1^2}\\
\frac{\partial a(j_{12})}{\partial j_3} &\stackrel{!}{=} 0 \Leftrightarrow j_3^{(0)} = -\frac{1}{2} + \frac{1}{2}\sqrt{1+4j_{12}^2+4j_4+4j_4^2}\\
\frac{\partial a(j_{12})}{\partial j_4} &\stackrel{!}{=} 0 \Leftrightarrow j_4^{(0)} = -\frac{1}{2} + \frac{1}{2}\sqrt{1+4j_{12}^2+4j_3+4j_3^2}.
\end{aligned} \tag{71}$$

If we want all relations of (71) to be fulfilled at the same time with strictly positive values of $j_1,\ldots,j_4$ then we have to demand

$$j_1 \stackrel{!}{=} j_2 := m \qquad \text{and} \qquad j_3 \stackrel{!}{=} j_4 := j_{\max}. \tag{72}$$

Therefore, (67) reads due to the ordering $j_1 \leqslant j_2 \leqslant j_3 \leqslant j_4 = j_{\max}$ as

$$0 \leqslant j_{12} \leqslant 2m. \tag{73}$$

And the matrix element (65) simplifies to

$$a(j_{12}) = \frac{j_{12}^2}{\sqrt{4j_{12}^2-1}}\big[\big[(2a+1)^2 - j_{12}^2\big]\big[(2j_{\max}+1)^2 - j_{12}^2\big]\big]^{\frac{1}{2}}. \tag{74}$$

(i) *Largest eigenvalue*

By inspection of (74) we can maximize the order of $j_{\max}$ contained in the matrix element by putting

$$m \sim j_{\max} \rightsquigarrow a(j_{12}) \sim j_{\max}^3. \tag{75}$$

The result is an upper bound on the growth of the maximum eigenvalues of the matrix A

[8] We will list here only those solutions which allow positive values for $j_1,\ldots,j_4$ and mutually different j_1, j_2, j_3, j_4!

with the maximum angular momentum $j_{\max}$:[9]

$$|\lambda_{\max}(j_{\max})| \sim j_{\max}^3 \Rightarrow |V_{\max}(j_{\max})| \sim j_{\max}^{\frac{3}{2}}. \tag{76}$$

(ii) *Smallest non-zero eigenvalue*
By assuming the existence of the inverse A^{-1} with a sparse population of entries of the order $\frac{1}{a_k}$, one can minimize the order of $j_{\max}$ contained in the matrix element (that is maximizing the matrix elements of A^{-1}) by putting

$$m \sim 1 \ll j_{\max} \rightsquigarrow a(j_{12}) \sim j_{\max}. \tag{77}$$

The result is an upper bound on the growth of the maximum eigenvalues of the matrix A^{-1} with the maximum angular momentum $j_{\max}$ and therefore for the smallest non-zero eigenvalue of A:[10]

$$|\lambda_{\min}(j_{\max})| \sim j_{\max} \Rightarrow |V_{\min}(j_{\max})| \sim j_{\max}^{\frac{1}{2}}. \tag{78}$$

These are first estimates, we will come back to this, when we discuss the numerical investigations, since the theorem 4.1 and our approximations tell us nothing about the numerical coefficients in front of the leading powers of $j_{\max}$. Nevertheless, this estimate will give us a certain criterion for completeness of numerically calculated eigenvalues: since the smallest eigenvalue $\lambda_{\min}$ grows with $j_{\max}$ we can at a certain value of $j_{\max}$ be sure of having calculated the complete volume spectrum for all $V \leqslant V_{\min}$ as we shall see in the numerical section below.

4.1.2. Eigenvectors for $\lambda = 0$. Posing the eigenvalue problem $A\Psi = \lambda\Psi$ for the matrix A, we obtain a three term recursion relation that every eigenvector Ψ of A has to fulfil:

$$\begin{aligned} &a_{k-1}\Psi_{k-1} - a_k\Psi_{k+1} = \lambda\Psi_k \qquad \text{with} \quad a_0 = a_n = 0, \\ &\lambda \in \mathbb{R}, \quad a_k (0 < k < n) \text{ purely imaginary.} \end{aligned} \tag{79}$$

We can now check, whether the eigenvalue $\lambda = 0$ belongs to the spectrum. This decouples the recursion relation (79) to give

$$a_{k-1}\Psi_{k-1} - a_k\Psi_{k+1} = 0. \tag{80}$$

Now for consistency of (80)

$$\begin{aligned} &k = n : a_{n-1}\Psi_{n-1} = 0 \qquad \text{and therefore} \quad \Psi_{n-1} = \Psi_{n-3} = \cdots = 0 \\ &k = 1 : -a_1\Psi_2 = 0 \qquad \text{and therefore} \quad \Psi_2 = \Psi_4 = \cdots = 0. \end{aligned} \tag{81}$$

But this means that the matrix A can only have an eigenvector $\Psi \neq 0$ if the dimension n of A is odd, because if n would be even, then all components of Ψ would be forced to vanish by (81).

That means we will only obtain $\lambda = 0$ as a eigenvalue in configurations with odd dimension of A. We can now construct explicitly the eigenvector Ψ for odd n: first we choose $\Psi_1 = x$ with $x = \text{const} \in \mathbb{C}$. Then from

$$\frac{a_{k-1}}{a_k} = \frac{\Psi_{k+1}}{\Psi_{k-1}} \tag{82}$$

[9] This result coincides with that already obtained in [24]. Note that the number of terms in each row/column sum is equal to 2 due to the special structure (68) of the matrix A and therefore independent of $j_{\max}$.

[10] Note that one should really use $(A^{-1})_{ij}$ which can be a complicated polynomial in A_{ij}. This is indeed the case as shown in appendix C and therefore the result presented here is at best a rough estimate.

we find the general expression

$$\Psi_{2r+1} = x \cdot \frac{\prod_{s=1}^{r} a_{2s-1}}{\prod_{s=1}^{r} a_{2s}} \qquad \text{where } r = 1, 2, \ldots, \frac{n-1}{2} \qquad n = \dim A \qquad x = \Psi_1. \tag{83}$$

Since as were chosen to be purely imaginary, all odd components $\Psi_3, \ldots, \Psi_n$ of Ψ are real, all even components $\Psi_2, \ldots, \Psi_{n-1}$ are identical to zero, because of (81). Finally we can fix $\Psi_1 = x$ to be (up to the sign of $x = \Psi_1$)

$$x = \Psi_1 = \pm \left[1 + \sum_{r=1}^{\frac{n-1}{2}} \left| \frac{\prod_{s=1}^{r} a_{2s-1}}{\prod_{s=1}^{r} a_{2s}} \right|^2 \right]^{-\frac{1}{2}}. \tag{84}$$

Summarizing, the eigenvalue $\lambda = 0$ only occurs in the spectra of matrices A, possessing an odd dimension n, as a single eigenvalue (since its eigenspace is only one dimensional due to the uniqueness of construction of the eigenvector Ψ up to a constant rescaling). Hence, we have shown that A is singular iff n is odd and in that case $\lambda = 0$ has multiplicity 1.

4.1.3. Monochromatic 4-vertex ($j_1 = j_2 = j_3 = j_4 = j$). Observing this special case, the matrix elements in (65) simplify dramatically to

$$\langle j_{12} | \hat{q}_{123} | j_{12} - 1 \rangle = \frac{1}{\sqrt{4(j_{12})^2 - 1}} (j_{12})^2 [n^2 - (j_{12})^2] \tag{85}$$

where $0 \leqslant j_{12} \leqslant 2j$ and $\dim A = n = 2j + 1$.

4.2. Numerical investigations

In this section, we will describe numerical calculations done for the gauge-invariant 4-vertex. We will (after describing the set-up) sketch the computational effort first. Secondly we will give a conjecture about the volume gap, that is the smallest non-vanishing eigenvalue as a result of the calculations. As a third step, we will take a look on the accuracy of the upper bound given by theorem 4.1. Finally, we will present some spectral estimates.

4.2.1. General set-up. We calculated for the gauge-invariant 4-vertex the spectra of all possible edge-spin configurations j_1, j_2, j_3, j_4 up to a maximal spin of $j_{\max} = 50$ using the mathematical software *Maple* 7. Since the matrix element (65) is symmetric with respect to interchange of js, we calculated the spectra of all $\hat{Q}_v(j_1, j_2, j_2, j_3)$ for

$$0 < j_1 \leqslant j_2 \leqslant j_3 \leqslant j_4 \leqslant \min(j_1 + j_2 + j_3, j_{\max}) \quad \text{and} \quad j_1 + j_2 + j_3 + j_4 \text{ integral}. \tag{86}$$

Thus we compute less than $\frac{1}{4!}$ configurations, without losing any information. The conditions on the right-hand side of (86) ensure that we exclude all trivial configurations, since if $j_1 + j_2 + j_3 < j_4$ or $j_1 + j_2 + j_3 + j_4$ is not integral it would be impossible to recouple them to resulting zero-angular momentum, being the definition for gauge invariance. If one spin is identical to zero, then the obtained configuration would also be trivial, since it would then effectively describe a gauge-invariant 3-vertex, which vanishes identically, hence we also impose $j_1 \cdot j_2 \cdot j_3 \cdot j_4 > 0$.

The possible values for the intermediate recoupled j_{12} are then due to (66) and the order of the angular momenta introduced above (since we have sorted the $j_1, \ldots, j_4$ by their modulus and each $j \geqslant 0$, we can leave out the modulus notation in (66) by writing j s in certain order):

$$\max(j_2 - j_1, j_4 - j_3) \leqslant j_{12} \leqslant \min(j_1 + j_2, j_3 + j_4) = j_1 + j_2. \tag{87}$$

The dimension of the matrix A of such a configuration is then according to (67) given by

$$\dim A = \dim(j_1, j_2, j_3, j_4) = j_1 + j_2 - \max(j_2 - j_1, j_4 - j_3) + 1. \tag{88}$$

For every configuration then the matrix elements according to (65) are calculated and inserted into a numerical matrix. This matrix is then numerically diagonalized, its eigenvalues are sorted ascending and from this spectrum all eigenvalues $\geqslant 0$ are taken. These data are then written into a file linewise, each line starting with the values of $j_1, \ldots, j_4$ and the total number of saved eigenvalues followed by the sorted list of the eigenvalues itself. Of course, we have to keep in mind the multiplicity 2 of every saved eigenvalue >0. Additionally, we have to pay attention to the ordering procedure we applied on $j_1, \ldots, j_4$ whenever we work with the number of eigenvalues, since we have suppressed certain multiplicities. The following table gives the resulting multiplicity factors by which eigenvalue numbers resulting from corresponding spin configurations should be multiplied[11]:

	All spins different	One pair equal	Two pairs equal	Three spins equal	All spins equal
No ordering	$\frac{4!}{1!} = 24$	$\frac{4!}{2!} = 12$	$\frac{4!}{2!\cdot 2!} = 6$	$\frac{4!}{3!} = 4$	$\frac{4!}{4!} = 1$

4.2.2. Computational effort. According to the above set-up we would expect the following.

- *Number of configurations*
  First of all we choose integer spins for simplicity, that is $j_J \to a_J = 2 \cdot j_J$ and assume all as to be different (we therefore neglect configurations containing equal spins which are dominated by those with different spins). We choose one of the four integer spins to be maximal and constant, say $a_K = a_{\max} := \max\,(a_L)$, $L = 1, \ldots, 4$, and then by condition (86) we have $a_K \leqslant \min\left(\sum_{L \neq K} a_L, a_{\max}\right)$. Therefore, $a_{\max} \leqslant \sum_{L \neq K} a_L$. Labelling the three remaining a_L by a_1, a_2, a_3 we get from that $a_3 \geqslant a_{\max} - a_2 - a_1$. But this is only a question of counting the number N of points of a three-dimensional cubic lattice fulfilling the last condition which is given by

$$N(a_{\max}) = \sum_{a_1=1}^{a_{\max}} \sum_{a_2=1}^{a_{\max}} \sum_{a_3=1}^{a_{\max}} 1 - \sum_{a_1=1}^{a_{\max}-2} \sum_{a_2=1}^{a_{\max}-a_1} \sum_{a_3=1}^{a_{\max}-a_1-a_2} 1. \tag{89}$$

  Finally, we add $\sum_{a_{\max}=1}^{c_{\max}} N(a_{\max})$. The result is the total number of calculations $N(c_{\max})$. Due to the integer condition in (86), which becomes an even-number condition in as, we have to divide that number by 2 and to multiply it by 4, since we have chosen one of the four integer spins to maximal arbitrarily. If we finally plug in $c_{\max} = 2 \cdot j_{\max}$, we get for the number of configurations $N\left(j_{\max} \geqslant \frac{3}{2}\right)$ with all spins different (figure 2)

$$N(j_{\max}) = \frac{20}{3} \cdot j_{\max}^4 + 12 \cdot j_{\max}^3 + \frac{7}{3} \cdot j_{\max}^2 - 5 \cdot j_{\max} + 2. \tag{90}$$

  This can be compared to the numerically fitted curve of the number of configurations N_{num}:

$$N_{\text{num}}(j_{\max}) = 6.67 \cdot j_{\max}^4 + 13.33 \cdot j_{\max}^3 + 11.42 \cdot j_{\max}^2 - 8.30 \cdot j_{\max} + 2.22. \tag{91}$$

[11] In general we have $N!$ possibilities to arrange a list of N elements, but having M identical elements, each of them with multiplicity $K_1, K_2, \ldots, K_M$ in that list, we can only have $\frac{N!}{K_1! \cdot K_2! \cdots K_M!}$ different arrangements of the elements of that list.

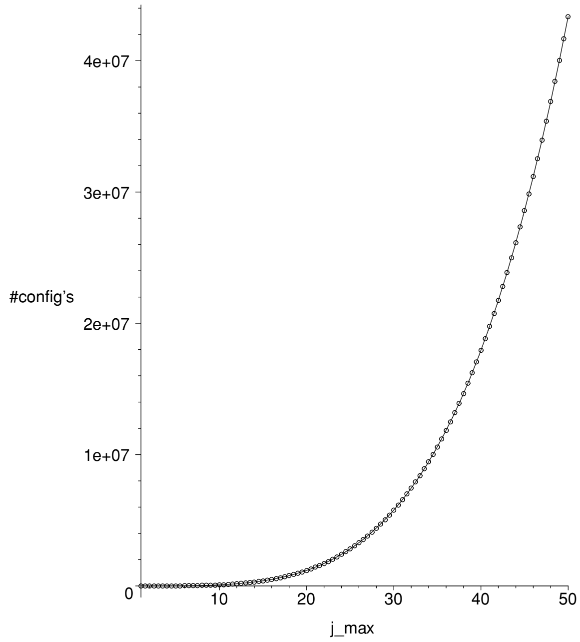

Figure 2. Number of configurations $N(j_{\max})$.

- *Number of eigenvalues*
  To calculate the expected number of eigenvalues $E(j_{\max})$ (figure 3) we have to sum over the dimensions of the individual representation matrix of the volume operator which is given by

$$\dim = \min(j_1 + j_2, j_3 + j_4) - \max(|j_2 - j_1|, |j_4 - j_3|). \tag{92}$$

  One would expect that $E(j_{\max}) \sim j_{\max}^5$. From the numerical calculation we get for the total number of eigenvalues (including 0-eigenvalues and multiplicities)

$$E(j_{\max}) = 2.67 \cdot j_{\max}^5 + 10.00 \cdot j_{\max}^4 + 15.52 \cdot j_{\max}^3 + 7.92 \cdot j_{\max}^2 + 27.90 \cdot j_{\max} - 77.23. \tag{93}$$

4.2.3. First impressions. We drove the calculations up to a value of $j_{\max} = 50$.[12] Our primary goal is to obtain some hints on a possibly analytical eigenvalue distribution function for large $j_{\max}$.

Therefore, as a start we scanned through all the configurations saved in a file and computed an eigenvalue density by distributing the possible eigenvalues λ into discrete intervals of width $\Delta\lambda = 0.5$ where λ belongs to the interval $I_n = \text{round}\left(\frac{\lambda}{\Delta\lambda} + 0.5\right) = [\lambda_n - \Delta\lambda, \lambda_n]$ where $\lambda_n = n \cdot \Delta\lambda, n = 1, 2, \ldots$.

For this we take the square root of the calculated eigenvalues, since we computed the spectrum of the square of the eigenvalues of $\hat{V}_v$, and the interval width $\Delta\lambda$ does not scale linearly if we would first sort in the eigenvalues of $\hat{Q}_v$ and then took the square root. Furthermore, we drop the prefactor Z in what follows.

[12] This maximal value is limited to the capacities of the mathematical software *Maple* 7 on the computer used (Intel XEON machine with two 1.7 GHz processors). Future calculations will go much further, since *Maple* 7 is only an interpreter programming language.

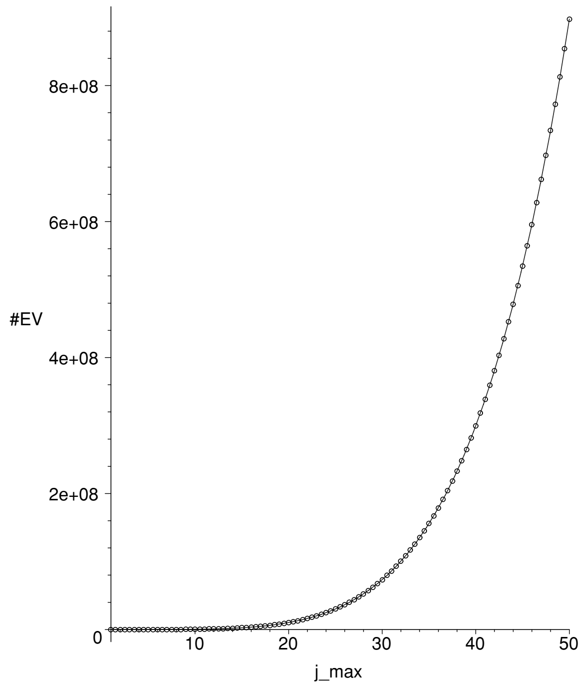

Figure 3. Number of eigenvalues obtained independent of $j_{\max}$.

Then we plot the logarithm +1 of the total number of eigenvalues >0 (including their multiplicity) according to the multiplicity tabular given before in a certain interval I_n against $2 \cdot j_{\max}$ and the volume eigenvalues denoted by $2 \cdot V$ (the form of the axes labels with prefactors 2 as well as the +1 in the logarithm are only for technical reasons). The result is given in figure 4.

The diagram suggests that for each interval I_n only configurations up to $j_{\max}^{(n)}$ matter. Configurations with $j_{\max} > j_{\max}^{(n)}$ do not increase the number of eigenvalues in the interval I_n. Therefore, we are led to the idea that it would be interesting to look separately at configurations with fixed $j_{\max}$ instead of counting all eigenvalues belonging to an interval coming from all configurations with $j_4 \leqslant j_{\max}$.

Additionally, it would be good to know the effect that our cut-off $j_{\max} = 50$ has on the calculated eigenvalue spectrum. This is done in what follows.

4.2.4. Lower bound for the spectrum. For this purpose we will split the matrices to be calculated[13] into the sets of matrices indexed by configurations with fixed $j_4 = j = j_{\max}$. We then inspect the ordered spectra of every set and try to find some regularity in the spin configurations j_1, j_2, j_3, j_4 producing the eigenvalues.

As we have calculated all configurations up to $j_{\max} = 50$ we have 100 sets of matrices S_j where each set is labelled by $j = \frac{1}{2}, 1, \ldots, j_{\max} - \frac{1}{2}, j_{\max}$.

In each set, we consider the first 100 positive eigenvalues ordered by values. Additionally to every eigenvalue we denote the spin configuration of the matrix giving rise to it and the

[13] Due to our set-up.

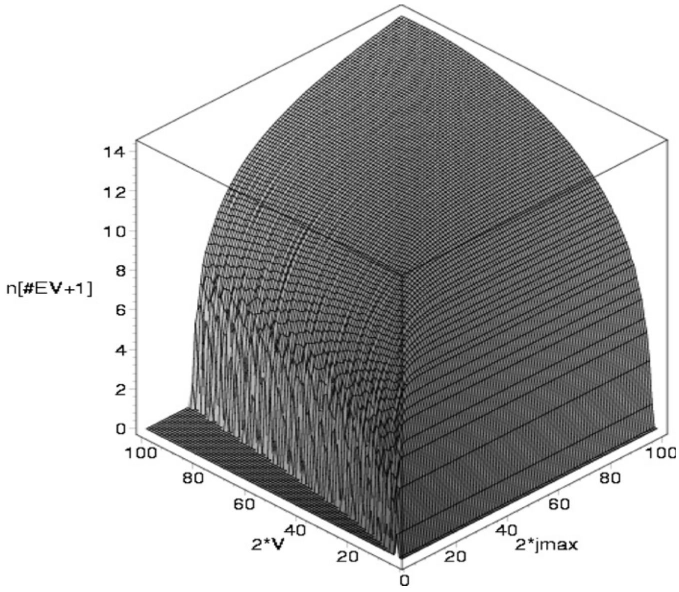

Figure 4. The logarithm of the number of eigenvalues in the intervals $I_n = [\lambda_n - \Delta\lambda, \lambda_N]$ $\lambda_n = n \cdot \Delta\lambda$ as a function of $j_{\max}$.

position k the eigenvalue takes in the ordered list of eigenvalues of this set S_j. Thus, achieved datasets are written into a file.

Hence, we create a function

$$\lambda : (j, k) \longrightarrow \lambda_k(j) \tag{94}$$

where $\lambda_k(j)$ is the kth eigenvalue in S_j.

It turns out that the map $(j, k) \longrightarrow \lambda_k(j)$ indeed displays a regularity, that is, the eigenvalues seem to produce series being separated from each other. Every series can be associated with a certain position in the ordered spectrum of a matrix set S_j with given $j_4 = j \leqslant j_{\max}$. The positions are taken from a minimal j on, as series k will not have contributions from S_j with too low j. It turns out that the lowest eigenvalues of each matrix set S_j are precisely the lowest eigenvalues of the low-dimensional matrices with low spin configurations $j_1 \leqslant j_2 \leqslant j_3 \leqslant j \leqslant (j_1 + j_2 + j_3)$.

Remarkably each of these matrices has rank smaller than 9 (that is, the nontrivial part of the characteristic polynomial can be reduced to a polynomial of degree less than or equal to 4), hence we can find analytic expressions for these lowest eigenvalues.

We will give here a table containing the first 12 series of eigenvalues. In the second column, we write down the smallest j from which (by inspection of the data) the noted order k is reached. Additionally, we note the spin configuration. The eigenvalues given are always the smallest ones $\neq 0$ of the according matrix giving rise to $\lambda_k(j)$ with the given spin configuration.

Surprisingly, the first smallest eigenvalues are not equally distributed between even and odd configurations (the latter possessing 0-eigenvalues), but mainly contributed by the even configurations (we give in the second table the first odd configurations). Note again that these eigenvalues of $\hat{Q}_v$ are the square of the eigenvalues of $\hat{V}_v$ and that each eigenvalue has a multiplicity according to the multiplicity table given above.

Even configurations

k	Valid $j \geqslant$	j_1	j_2	j_3	j_4	$\lambda_k(j)$	c_k
1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	j	j	$2\sqrt{j(j+1)}$	2
2	2	$\frac{1}{2}$	1	$j-\frac{1}{2}$	j	$2\sqrt{(j+1)(2j-1)}$	$2\sqrt{2}$
3	3	$\frac{3}{2}$	$\frac{3}{2}$	j	j	$2\sqrt{17j^2+17j-21-\sqrt{208j^4+416j^3-344j^2-552j+441}}$	$2\sqrt{17-\sqrt{208}}$
4	$\frac{13}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$j-1$	j	$2\sqrt{3}\sqrt{(j+1)(j-1)}$	$2\sqrt{3}$
5	4	$\frac{1}{2}$	2	$j-\frac{3}{2}$	j	$2\sqrt{2}\sqrt{(j+1)(2j-3)}$	4
6	$\frac{7}{2}$	1	1	$j-1$	j	$4\sqrt{j(j+1)}$	4
7	20	$\frac{1}{2}$	$\frac{3}{2}$	j	j	$2\sqrt{(2j+3)(2j-1)}$	4
8	$\frac{11}{2}$	$\frac{3}{2}$	2	$j-\frac{1}{2}$	j	$\sqrt{108j^2+54j-216-6\sqrt{228j^4+228j^3-903j^2-480j+1152}}$	$\sqrt{108-6\sqrt{228}}$
9	$\frac{65}{2}$	$\frac{5}{2}$	$\frac{5}{2}$	j	j	Too long but analytical expression	
10	10	$\frac{1}{2}$	$\frac{5}{2}$	$j-2$	j	$2\sqrt{5}\sqrt{(j+1)(j-2)}$	$2\sqrt{5}$
11	11	$\frac{1}{2}$	3	$j-\frac{5}{2}$	j	$2\sqrt{3}\sqrt{(j+1)(2j-5)}$	$2\sqrt{6}$
12	18	1	$\frac{3}{2}$	$j-\frac{3}{2}$	j	$2\sqrt{3}\sqrt{(j+1)(2j-3)}$	$2\sqrt{6}$

Odd configurations

k	j_1	j_2	j_3	j_4	$\lambda_k(j)$
24	1	$\frac{3}{2}$	$j-\frac{1}{2}$	j	$2\sqrt{14j^2+7j-16}$
61	2	2	j	j	$2\sqrt{52j^2+52j-114-18\sqrt{4j^4+8j^3-16j^2-20j+33}}$

All of these expressions have, to leading order, the form

$$\lim_{j\to\infty}\frac{\lambda_k(j)}{j}=c_k \tag{95}$$

where c_k increases with k. Thus, for sufficiently large j the series $j \longrightarrow \lambda_k(j)$ are approximate lines of different inclinations.

As an illustration we will give a plot of the first eight eigenvalue series, that is, we plot for each j the first eight eigenvalues of the associated matrix series S_j. Then we connect the first, second, third, and so on, eigenvalues with a line (figure 5). Here, it becomes obvious that for small j not all series are present, that is $\lambda_k(j)$ is ill defined below the threshold j given in the table for each k.

Thus, we are given a certain numerical criterion to decide which part of the spectrum of the volume operator for the 4-vertex is already entirely calculated for a given cut-off $j_{\max}$: given an eigenvalue λ^2, draw a horizontal line in figure 5 and find the intersection with the first eigenvalue series that is $k=1$: $\exists j$ with $\lambda_1(j)^2=\lambda^2$. The value $j(\lambda)$ at which this happens gives the maximal value $j_{\max}(\lambda)$ which we have to consider in order to find configurations giving rise to eigenvalues $\leqslant \lambda$, because all eigenvalues produced by $j > j(\lambda)$ are larger than λ because numerically $\lambda_k(j) > \lambda_1(j)\ \forall\ k > 1$.

According to the table above $\lambda_1(j)^2 = 2\sqrt{j(j+1)} \overset{!}{=} \lambda^2$ and therefore $j(\lambda) = -\frac{1}{2}+\sqrt{\frac{1}{2}+\frac{\lambda^4}{4}}$. Thus, for $j_{\max}=50$ we can trust to have computed the complete spectrum only for $\lambda \leqslant \lambda_{\max}(j_{\max}) = \sqrt{2}\sqrt[4]{j_{\max}(j_{\max}+1)}$, i.e., $\lambda_{\max}=1.4\sqrt{50}\approx 10$.

4.2.5. Upper bound for the spectrum. By observation of the numerical matrices in S_j it turns out that the maximal eigenvalues $\lambda_{\max^{(j)}} = \left(V_{\max}^{(j)}\right)^2$ of configurations with fixed $j_4 = j$ are

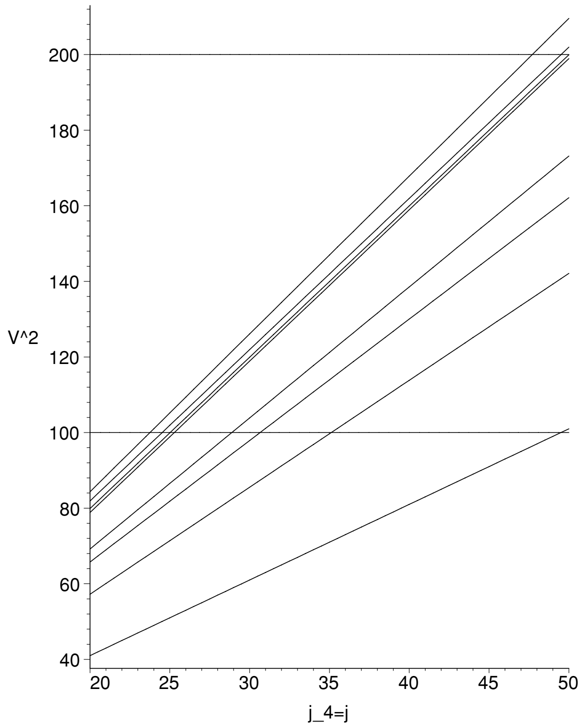

Figure 5. The evolution of the first positive eight eigenvalues $\lambda_k(j) := V^2, k = 1, \ldots, 8$ of $\hat{Q}_v$ independent of $j_4 = j$. Note that each line represents eigenvalues with multiplicity given by the table in section 1.

contributed by matrices of the monochromatic vertex, that is $j_1 = j_2 = j_3 = j_4 = j$ as we expected from our estimates (76). We already wrote the matrix elements of this special case in (85) $(0 \leqslant j_{12} \leqslant 2j)$:

$$\frac{1}{\mathrm{i}} a_k(k = j_{12}) := \langle j_{12}|\hat{q}_{123}|j_{12} - 1\rangle = \frac{1}{\sqrt{4(j_{12})^2 - 1}}(j_{12})^2[(2j + 1)^2 - (j_{12})^2]. \tag{96}$$

Now theorem 4.1 provides us with upper bounds for the moduli of eigenvalues of a matrix in terms of its row or column sums. It is natural to ask now how the biggest eigenvalue $\lambda^{(j)}_{\max}$ and the maximal row or column sum of the monochromatic matrix A of type (68) fit together. It is clear from the structure of A that the inequality given in theorem 4.1 for the biggest eigenvalue reads

$$\left|\lambda^{(j)}_{\max}\right| \leqslant \max[|a_k| + |a_{k+1}|] =: L_{\max} \qquad k = 1, \ldots, n - 2.$$

Therefore, we look for the maximal matrix element of A defined by (96) by differentiating the given expression with respect to j_{12} and find the value $j_{12}^{\max}$ of j_{12} maximizing the matrix element. There are several extrema, but the desired one turns out to be

$$j_{12}^{\max} = \frac{1}{6}\sqrt{24j^2 + 24j + 12 + 6\sqrt{16j^4 + 32j^3 + 8j^2 - 8j - 2}} \tag{97}$$

where *for large j*

$$j_{12}^{\max} \stackrel{j\to\infty}{\longrightarrow} \frac{2}{\sqrt{3}}. \tag{98}$$

Since j_{12} can only take positive integer values, we then choose the maximal row sum which is given by

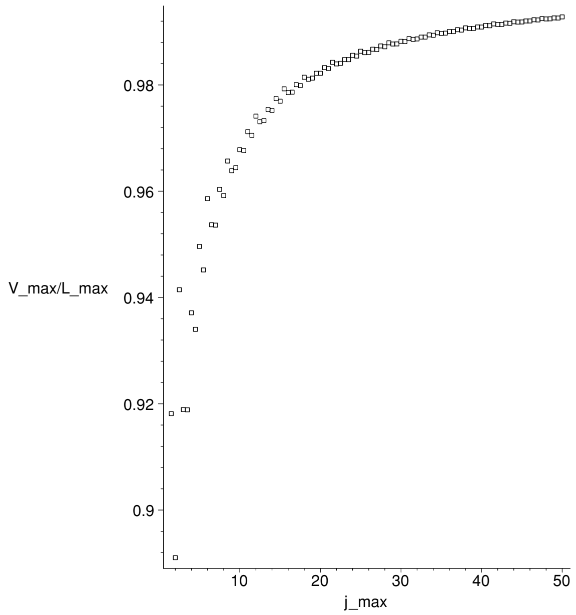

Figure 6. The quotient $\lambda_{\max}^{(j)}/L_{\max}$ as a function of j.

$$L_{\max} = \left|a_{\text{round}(j_{12}^{\max})}\right| + \left|a_{\text{round}(j_{12}^{\max})-1}\right|.$$

Plotting the quotient $\lambda_{\max}^{(j)}\big/L_{\max}$ as a function of $j = j_{\max}$ we find that this ratio converges to 1 as j increases as shown in figure 6.

Therefore, we have numerical evidence for the following large j behaviour of the biggest eigenvalue in a matrix set S_j:

$$\lambda_{\max}^{(j)} \stackrel{j\to\infty}{\longrightarrow} L_{\max}(j) \approx 2\left|a_{j_{12}^{\max}}\left(j_{12}^{\max} = \tfrac{1}{\sqrt{3}}j\right)\right| \approx \sqrt{3}\tfrac{11}{9}j^3. \tag{99}$$

Here, we have inserted $j_{12}^{\max}$ in equation (96) for the matrix elements to obtain $a_{j_{12}^{\max}}$ and approximated the maximal row sum $L_{\max}$ by $2\cdot\left|a_{j_{12}^{\max}}\right|$. Finally, we keep only the leading order of j in the expression and arrive at the result (99). This coincides with the result obtained in [24].

4.2.6. Spectral density. We now turn to a first investigation of how to get a reliable numerical estimate for the spectral density.

Let us first briefly discuss the behaviour of the 0-eigenvalues. We have proven that they only occur as a single member of the spectra of matrices with odd dimension. Therefore, counting the number of odd configurations is equal to counting the number of 0-eigenvalues. Since the total number of configurations grows with $j_{\max}^4$ we also fit the total number of 0-eigenvalues with a fourth-order polynomial, whose coefficient in leading order should approximately be half the coefficient we found when we fitted the total number of configurations, since we expect odd and even configurations to be nearly equally distributed (under restriction of (86)) (figure 7).

The fitted polynomial is found to be

$$\#\text{0-eigenvalues}(j_{\max}) = 3.33\cdot j_{\max}^4 + 10.00\cdot j_{\max}^3 + 10.66\cdot j_{\max}^2 - 7.10\cdot j_{\max} - 0.85.$$

Indeed, the coefficient 3.33 of $j_{\max}^4$ is half the coefficient obtained for the total number of configurations before. The difference of the other coefficients seems to be caused by the

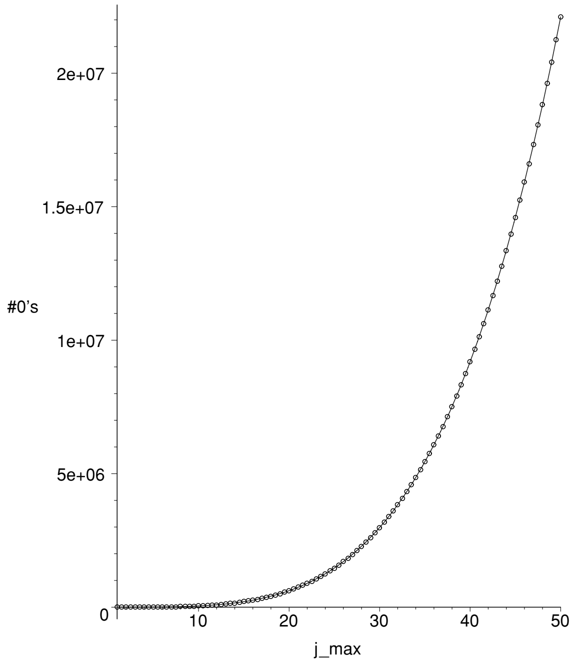

Figure 7. The total number of 0-eigenvalues contained in all configurations allowed by (86) depending on $j_{\rm max}$.

restrictions given in (86). In what follows we will omit the number of 0-eigenvalues, since their behaviour does not contribute to the spectrum of non-zero eigenvalues. Note that their relative number as compared to the total number of all eigenvalues is of the order of $j_{\rm max}^{-1}$.

Let us first recall how we define an eigenvalue density. We will take the square roots of the eigenvalues > 0 of $\hat{Q}_v$ obtained in the numerical computation and split the real axis labelling the eigenvalues V of $\hat{V}$ into identical intervals of the length ΔV. Then, each eigenvalue $V = n \cdot \Delta V$ $(n = 1, 2, \ldots)$ is assigned to an interval-number I_n defined by $I_n = \mathrm{round}\big(\frac{V}{\Delta V} + 0.5\big)$. In the third step, we add up all eigenvalues belonging to the same interval I_n to get the number of eigenvalues in the interval $[V - \Delta V, V]$.

Now we define the interval density N_I of eigenvalues in the interval I for fixed $j_4 = j$ by

$$N_I(j) := \frac{\#\ \mathrm{eigenvalues}(I)}{\Delta V}. \tag{100}$$

Since we want to have a normalized density ρ

$$\int_{V_{\rm min}}^{V_{\rm max}} \rho_I \,\mathrm{d}V \stackrel{!}{=} 1,$$

we divide the interval densities N_I by the number of eigenvalues different from 0 to get the final definition of the eigenvalue density:

$$\rho_I(j) := \frac{\#\ \mathrm{eigenvalues}(I)}{\Delta V \cdot (\#\ \mathrm{total\ eigenvalues} - \#\ 0\ \mathrm{eigenvalues})}. \tag{101}$$

These densities are then represented by a point at $V = n \cdot \Delta V$ for each interval I_n. These points are joined then (they can be fitted by polynomials for instance) to display the desired normalized eigenvalue density ρ. This gives us, for instance for $j_4 = j = 50$, the plot as shown in figure 8 for a fit with a fourth-order polynomial in the eigenvalues V $(\Delta V = 0.5)$.

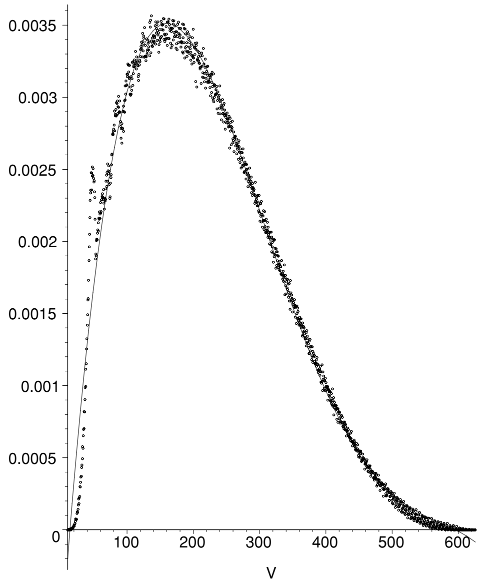

Figure 8. The eigenvalue density for $j_4 = 50$ (points) fitted by a fourth-order polynomial (solid line).

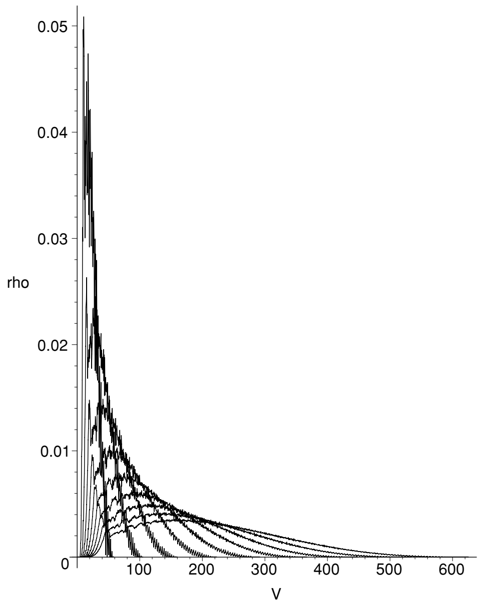

Figure 9. The eigenvalue densities for $j_4 = 10, 15, \ldots, 50$ (just look at the biggest eigenvalues in order to identify which curve belongs to which j). The points representing the eigenvalue density are joined by lines.

This can be done for every matrix set S_j with fixed $j = j_4$. Remarkably it seems to be true that the eigenvalue densities in figure 9 are fitted quite well by fourth-order polynomials (figure 10). But it is even more surprising that if we rescale the obtained densities, by putting their width $W := V_{\max}(j) - V_{\min}(j) \to 1$ and their height $H(j) := \max(\rho_I(j)) \to 1$ (where

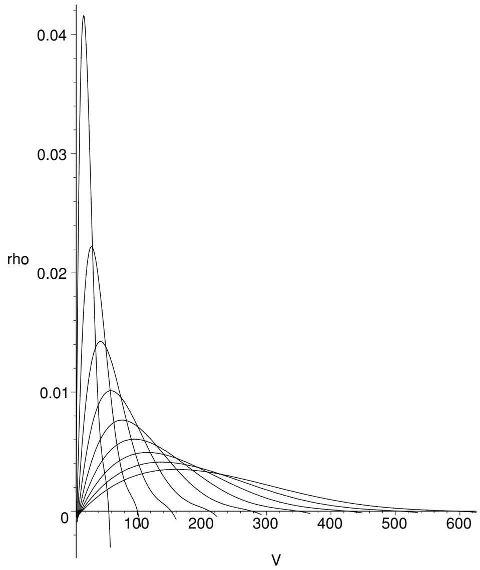

Figure 10. A fit of the spectra described in figure 9 by polynomials of fourth order.

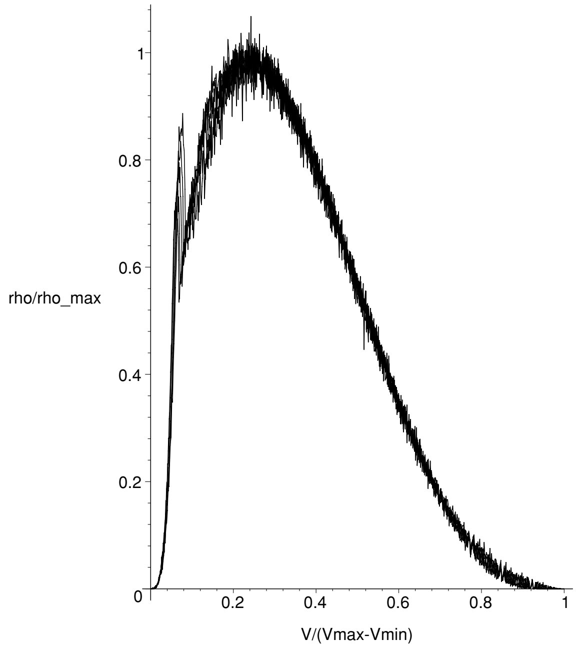

Figure 11. The eigenvalue densities for $j_4 = 30, 35, \ldots, 50$ in a 'fully normalized' rescaling, that is, $V \to \frac{V-V_{\min}}{V_{\min}-V_{\max}}$, $\rho_I \to \frac{\rho_I}{\max(\rho_I)}$.

$\max(\rho_I(j))$ is taken from the fit curves) and plotting the resulting rescaled distributions for different values of $j_4 = j$ into the interval [0, 1] as given in figures 11 and 12, the distribution seems to possess a similar shape.

Hence, the normalized distributions seem to be *independent of* j, that is, universal. This discussion suggests to try to define a limit distribution. By taking into account the behaviour

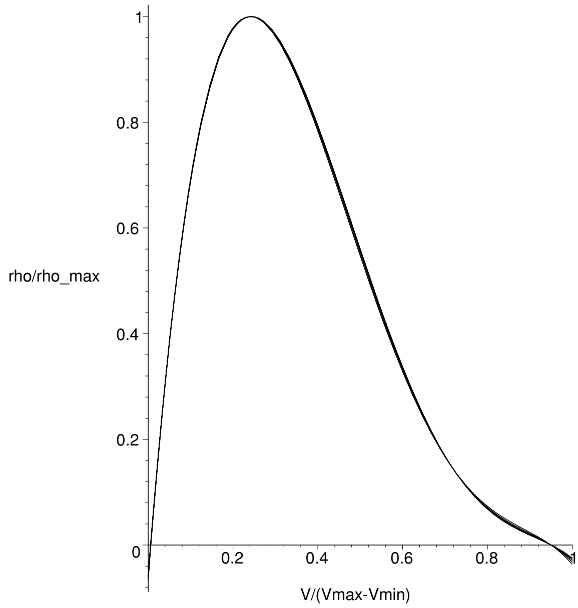

Figure 12. The fit curves of the spectra in 'fully normalized' rescaling.

of the ratio of the distance between the beginning of the distributions $V_{\min}(j)$ to the value $V(H(j))$ at which the maximum $H(j)$ of the distribution is situated and the total length of the distribution $V_{\max}(j) - V_{\min}(j)$,

$$\Delta(j) := \frac{V(H(j)) - V_{\min}(j)}{V_{\max}(j) - V_{\min}(j)}.$$

The ratio $\Delta(j)$ should tend to a constant value for $j = j_4 \to \infty$ in the presence of a limit common shape of all distributions. Moreover, we want to find out the quality of the fits taken by calculating the average squared difference between the fitted curves and the real spectra given by (all quantities at given j)

$$\chi^2 := \frac{1}{\max(\rho_I)(V_{\max} - V_{\min})} \sum_{I(V_{\min})}^{I(V_{\max})} \left(\rho_I - \rho_I^{(\text{fitted})}\right)^2.$$

These quantities seem to behave in a way which is convenient for us (see figures 13 and 14).

That is, the fit quality improves as j is growing and it seems possible that the ratio $\Delta(j)$ indeed has a certain limit of ≈0.25.

4.2.7. Density of the eigenvalues of the volume operator—discussion. Despite the interesting properties and the occurrence of some systematics in the spectral density in the matrix sets, we were unable up to this point to give an estimate of the density of eigenvalues of the whole volume operator so far.

The problem is first that the fourth-order polynomials were chosen only for the reason that they contain the lowest number of parameters (5) that the achieved spectra can be satisfactorily fitted by. There is more computational work to be done to ensure the presence of a limiting eigenvalue distribution. If this turned out to be the case, then we have to look for certain points, the parameters of the fitted curves of the eigenvalue distribution are fixed by.

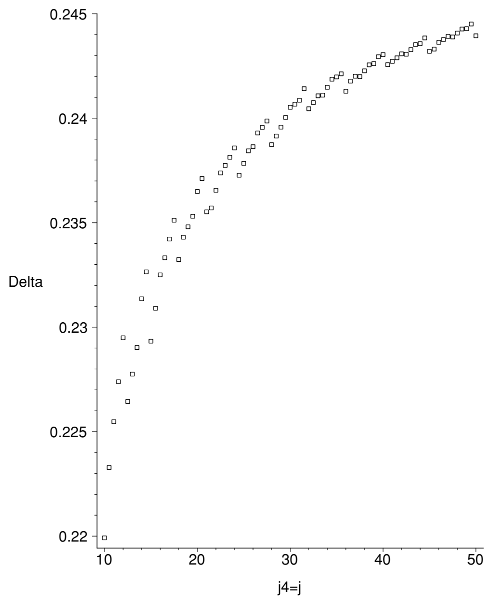

Figure 13. The ratio $\Delta(j)$ dependent on $j_4 = j$.

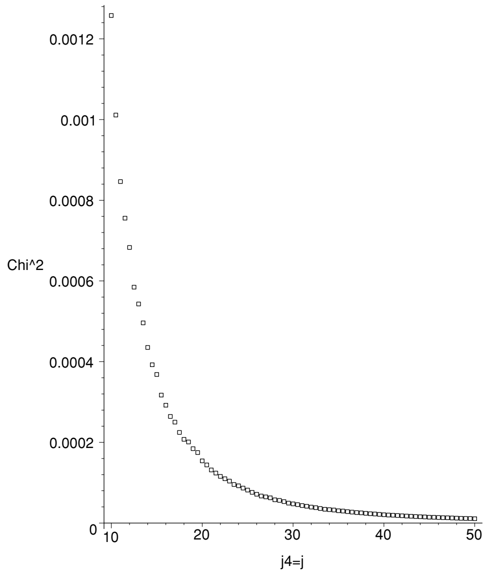

Figure 14. The sum of the squared distances between points of the eigenvalue densities and the fitted curves, χ^2 (defined as above), independent of $j_4 = j$.

What we know (at least our computations up to now encourage us to think that we know) are four parameters: the maximum volume $V_{\max} \sim j_{\max}^{\frac{3}{2}}$, the minimal volume $V_{\min} \sim j_{\max}^{\frac{1}{2}}$, the maximum of the distribution, situated (see figure 13) at $\sim 0.25 \cdot V_{\max}$ and we know the total number $E^{(j_4=j_{\max})}$ of eigenvalues which can be obtained from the total number of eigenvalues $E^{(\mathrm{tot})}$ for each $j_{\max}$ by considering $E^{(j_4=j_{\max})} = E^{(\mathrm{tot})}(j_{\max}) - E^{(\mathrm{tot})}\left(j_{\max} - \frac{1}{2}\right)$. Then we could

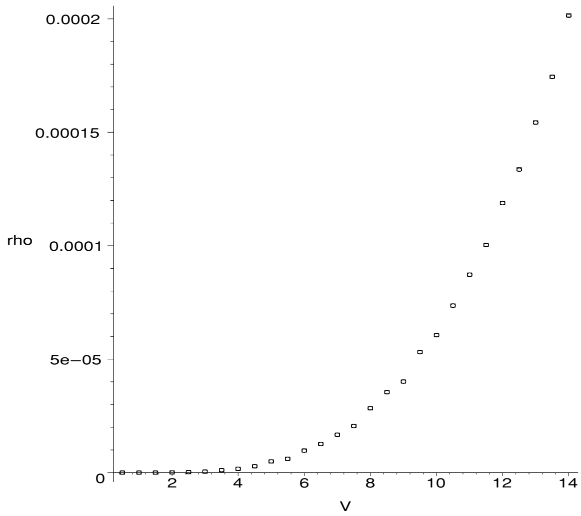

Figure 15. The eigenvalue density of the total volume operator (circles) and the extended eigenvalue density (boxes) for $j_{\max} = 50$ on a 4-valent vertex.

compute the eigenvalue density in an interval $[V_1, V_2]$ by a superposition of all configurations with $V_{\min} < V_2$ and $V_{\max} > V_1$.

The second problem is then to give a fit function for the total density of eigenvalues for all configurations. There is one conjecture, based on a similar behaviour for the spectrum of the area operator (which is easier to handle), that this eigenvalue density should behave as

$$\rho(V) = \alpha\, \mathrm{e}^{\beta V^{\gamma}}.$$

We have tried to fit the part of the spectrum we have fully calculated ($V \leqslant V_{\max}(j_{\max} = 50)$) by this formula. But it seemed to be impossible to give certain values to the three parameters, especially to γ. Maybe the calculated part of the spectrum is still to small, i.e. not sufficient for statistics or one must also consider higher valent vertices. Of course, the conjecture could also be wrong. So, it is left as an open task to fix the density of eigenvalues.

Let us conclude by displaying here the complete calculated part of the eigenvalue density of the volume operator for $j_{\max} = 50$, according to our numerical criterion, that we can rely on for given $j_{\max}$ on the part of the spectrum with $V \leqslant \sqrt{2\sqrt{j_{\max}(j_{\max}+1)}}$. That is for $j_{\max} = 50$ (as we calculated) we have obtained the full spectrum up to $V \approx 10$.

By inspection of figure 5 we can extend this part up to $V \approx \sqrt{200} \sim 14$ if we draw a horizontal line in figure 5 at a given $10 \leqslant V \leqslant 14$ and count the eigenvalue series situated below that line. If we assume that these series grow linearly with growing $j_{\max}$, as we expect, and there do not occur additional eigenvalue series at higher $j_{\max}$ then we can simply extend the curves $j \longrightarrow \lambda_k(j)$ linearly for $k = 1, \ldots, 8$ and can thereby estimate (approximately) the additional contributions not yet calculated explicitly for $V^2 \leqslant 200$, that is, for the $k = 7$ eigenvalue series.

Therefore, we display the original spectrum (circles) and the extended spectrum (boxes) normalized with respect to the total number of non-zero eigenvalues of the original spectrum (we have chosen again an interval width $\Delta V = 0.5$, the eigenvalue density is defined as in (101)) in figure 15.

5. Summary and outlook

In this paper, we have analysed the spectral properties of the volume operator defined in loop quantum gravity.

We discussed the matrix representation of the volume operator with respect to gauge-invariant spin network functions and were able to derive a drastically simplified formula for the matrix elements of the volume operator with respect to the latter.

It turned out that there exist certain selection rules for the matrix elements and all the matrices are *i*-times an antisymmetric matrix with the structure of a Jacobi matrix, meaning that non-vanishing matrix elements are only situated on certain off-diagonals.

We were able to determine the kernel, that is, the eigenstates for the eigenvalue 0, of the volume operator with respect to the gauge-invariant 4-vertex analytically as given in (83), (84). We have done numerical investigations for the gauge-invariant 4-vertex. Our numerical investigations support the analytical estimate that there exists a smallest eigenvalue V_{min} dependent on the maximal spin j_{max} via $V_{\mathrm{min}} \sim (j_{\mathrm{max}})^{\frac{1}{2}}$ and a maximal eigenvalue $V_{\mathrm{max}} \sim (j_{\mathrm{max}})^{\frac{3}{2}}$. Therefore we were able to find certain numerical indicators for the completeness of a numerically computed part of the spectrum. Moreover, we found that the geometrical intuition is reflected in the spectrum: at given j_{max}, the lowest non-zero eigenvalues come from rather 'distorted', almost flat tetrahedra with large spin on some edges and low spin on the others. On the other hand, the largest eigenvalues come from regular tetrahedra with large spin on all edges.

For future analysis one should extend the numerical calculations for the gauge-invariant 4-vertex and higher *n*-valent vertices to verify and possibly extend (for higher valence vertices) the regularities of the spectra obtained (for the gauge-invariant 4-vertex) for single matrix sets S_j with $j_4 = j$ at higher spins. In particular, it would be interesting to see whether there exists a volume gap as $n \longrightarrow \infty$. This, however, requires more computing power and better programming than we have used in this paper.

The formula derived for the matrix elements with respect to a gauge-invariant *n*-valent vertex can be used to analyse the whole spectrum of the volume operator numerically and analytically. Further simplifications are conceivable.

Note again that the restriction to 4-valued vertices and $j_{\mathrm{max}} \leqslant 50$ was only due to the computational capacity of the used mathematical software *Maple 7* and computer. By using a compiler-based programming language and optimized numerical matrix-diagonalizing routines we expect to be able to go much beyond the above computational limits.

Due to the results presented in this paper it seems to the authors that there are good chances for getting sufficient control about the spectral behaviour of the volume operator in the future, especially when it comes to dynamical questions in LQG.

As a first qualitative application in that respect, note the following: We have shown analytically that the volume operator of full LQG has zero eigenvalues at arbitrarily large j_{max} and that their number grows as j_{max}^4 as compared to the total number of eigenvalues which grows as j_{max}^5, at least for the gauge-invariant 4-vertex which should be the most interesting case from a triangulation point of view. Moreover, the volume gap increases as $j_{\mathrm{max}}^{1/2}$. It follows that the full spectrum contains many 'flat directions' or 'valleys' of zero volume and the walls of the valleys presumably get steeper as we increase j_{max}. Therefore we might find arbitrarily large eigenvalues as close as we want to zero eigenvalues and hence the 'derivative' (rather: difference) of the spectrum around zero volume which enters the Hamiltonian constraint through the curvature operator, while well defined as shown in [4, 5], could be unbounded from above. Therefore, the full spectrum could not share an important property of the spectrum in the cosmological truncation of LQG [12] where the derivative of the spectrum at zero volume is bounded from above. As this property has been somewhat important in [12], some of the results of [12] might have to be revisited in the full theory. The challenge would be to show that the curvature expectation value remains bounded when the system is prepared in a semiclassical state for LQG, see, e.g. [35] and references therein. First evidence for this and further analysis will be presented soon in [36] thus reaffirming the spectacular results of [12] in the full theory.

Acknowledgments

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Appendix A. Basics of recoupling theory

A.1. Angular momentum in quantum mechanics

For the angular momentum operator $\vec{J} = (J_1, J_2, J_3)$ (where each component has to be seen as an operator) we have the following commutation relations:

$$[J_i, J_j] = \mathrm{i} \cdot \epsilon_{ijk} J_k \qquad [J^2, J_j] = 0 \tag{A.1}$$

with $J^2 = \vec{J}^2 = J_1^2 + J_2^2 + J_3^2$.

Additionally, we can define

$$J_+ = J_1 + \mathrm{i}J_2 \qquad J_- = J_1 - \mathrm{i}J_2 \tag{A.2}$$

with (using (A.1))

$$[J^2, J_\pm] = 0 \qquad [J_3, J_+] = J_+ \qquad [J^2, J_-] = -J_- \qquad [J_+, J_-] = 2J_3. \tag{A.3}$$

Since every angular momentum state is completely determined[14] by its total angular momentum quantum number j (where $J^2 = j(j+1)$) and one component say J_3 (where $J_3 = -j, -j+1, \ldots, j-1, j$), we then associate for certain j a $(2j+1)$-dimensional[15] Hilbert space $\mathcal{H}$ equipped with an orthonormal basis $|jm\rangle$, $m = J_3$, where

$$\langle jm|jm'\rangle = \delta_{mm'}. \tag{A.4}$$

$|jm\rangle$ simultaneously diagonalize the two operators of the squared angular momentum J^2 and the magnetic quantum number J_3 [14]:

$$J^2|jm\rangle = j(j+1)|jm\rangle \qquad J_3|jm\rangle = m|jm\rangle. \tag{A.5}$$

That is, $|jm\rangle$ is a maximal set of simultaneous eigenvectors of J^2 and J_3.

On these eigenvectors, the other operators act as

$$J_+|jm\rangle = \sqrt{j(j+1) - m(m+1)}|jm+1\rangle \qquad J_-|jm\rangle = \sqrt{j(j+1) - m(m-1)}|jm-1\rangle. \tag{A.6}$$

A.2. Fundamental recoupling

Equipped with a small part of representation theory we can easily understand what happens if we couple several angular momenta. For that we first repeat the well-known theorem of Clebsh and Gordan on tensor products of representations of $SU(2)$:

[14] In the sense that we have a maximal set of simultaneously measurable observables.

[15] For fixed j there are $2j+1$ values which J_3 can take.

Theorem A.1 (Clebsh and Gordan)**.** *Having two irreducible representations π_{j_1}, π_{j_2} of $SU(2)$ with weights j_1, j_2 their tensor product space splits into a direct sum of irreducible representations $\pi_{j_{12}}$ with $|j_1 - j_2| \leqslant j_{12} \leqslant j_1 + j_2$ such that*

$$\pi_{j_1} \otimes \pi_{j_2} = \pi_{j_1+j_2} \oplus \pi_{j_1+j_2-1} \oplus \cdots \oplus \pi_{|j_1-j_2+1|} \oplus \pi_{|j_1-j_2|}.$$

Equivalently, we can write for the resulting representation space $\mathcal{H}^{(D)} = \mathcal{H}^{(D_1)} \otimes \mathcal{H}^{(D_2)}$ (where $D_1 = 2j_1 + 1$, $D_2 = 2j_2 + 1$, $D = D_1 \cdot D_2$ denote the dimensions of the Hilbert spaces):

$$\mathcal{H}^{(D)} = \mathcal{H}^{(D_1)} \otimes \mathcal{H}^{(D_2)} = \bigoplus_{j_{12}=|j_1-j_2|}^{j_1+j_2} \mathcal{H}^{(2j_{12}+1)}. \tag{A.7}$$

Or in other words, if we couple two angular momenta j_1, j_2 we can get resulting angular momenta j_{12} varying in the range $|j_1 - j_2| \leqslant j_{12} \leqslant j_1 + j_2$.

The tensor product space of two representations of $SU(2)$ decomposes into a direct sum of representation spaces, that is, one space for every possible value of recoupling j_{12} with the according dimension $2j_{12} + 1$.

A.3. Recoupling of two angular momenta

According to (A.7), we can expand for each value of j_{12} the elements $|j_1 j_2; j_{12}(j_1, j_2)M\rangle \in \mathcal{H}^{(2j_{12}+1)}$ called 'coupled states' into the tensor basis $|j_1 m_1\rangle \otimes |j_2 m_2\rangle$ of $\mathcal{H}^{(D)}$:

$$|j_1 j_2; j_{12}(j_1, j_2), M\rangle = \sum_{m_1+m_2=M} \underbrace{\langle j_1 m_1; j_2 m_2 | j_1 j_2; j_{12}(j_1, j_2), M\rangle}_{C_{m_1 m_2}} |j_1 m_1\rangle \otimes |j_2 m_2\rangle. \tag{A.8}$$

Here, $C_{m_1 m_2} \in \mathbb{R}$ denotes the expansion coefficients, the so-called Clebsh–Gordan coefficients. On the right-hand side $|j_1 m_1; j_2 m_2\rangle = |j_1 m_1\rangle \otimes |j_2 m_2\rangle$.

If we change the order of coupling then $C_{m_1 m_2}$ changes its sign:

$$\begin{aligned}\langle j_1 m_1; j_2 m_2 | j_{12}(j_1, j_2) M = m_1 + m_2\rangle &= (-1)^{j_{12}-j_1-j_2} \langle j_2 m_2; j_1 m_1 | j_{12}(j_2, j_1) M = m_1 + m_2\rangle \\ &= (-1)^{-j_{12}+j_1+j_2} \langle j_2 m_2; j_1 m_1 | j_{12}(j_2, j_1) M = m_1 + m_2\rangle.\end{aligned}$$

As $\mp j_{12} \pm (j_1 + j_2)$ is an integer number we are allowed to switch the signs in the exponent of the factor (-1). The coupled states again form an orthonormal basis:

$$\langle j_1 j_2; j_{12}(j_1, j_2), M | j_1 j_2; j_{12}(j_1, j_2), M\rangle \stackrel{!}{=} 1 \tag{A.9}$$

$$\langle j_1 j_2; \widetilde{j_{12}}(j_1, j_2), \widetilde{M} | j_1 j_2; j_{12}(j_1, j_2), M\rangle \stackrel{!}{=} \delta_{\widetilde{j_{12}}, j_{12}} \delta_{\widetilde{M} M}. \tag{A.10}$$

In (A.10), $\delta_{\widetilde{j_{12}}, j_{12}}$ comes from the orthogonality of $\mathcal{H}^{(2j_{12}+1)}$ in (A.7), $\delta_{\widetilde{M} M}$ is caused by the othogonality of the single $|j_1 m_1\rangle, |j_2 m_2\rangle$ (A.4)—since always $M = m_1 + m_2$.

Normalization of the recoupled states (A.9) implies, according to (A.4),

$$\sum_{m_1+m_2=M} |\langle j_1 j_2; j_{12}(j_1, j_2), M | j_1 j_2; j_{12}(j_1, j_2), M\rangle|^2 = \sum_{m_1+m_2=M} |C_{m_1 m_2}|^2 = 1. \tag{A.11}$$

Furthermore, the *Clebsh–Gordan coefficients are all real*, which is not obvious, but a result of two conventions one usually requires [14]

(1) $|j_1 j_2; j_{12}(j_1, j_2) = j_1 + j_2 M = j_1 + j_2\rangle = |j_1 m_1 = j_1\rangle \otimes |j_2 m_2 = j_2\rangle$.
(2) All matrix elements of $J_3^{(D_1)}$, which are nondiagonal in $|j_1 j_2; j_{12}(j_1, j_2) M\rangle$ are real and nonnegative.

The maximal set of simultaneously diagonalizable (that is commuting) $2 \cdot 2$ operators (A.5) of the single Hilbert spaces $\mathcal{H}^{(D_1)}$, $\mathcal{H}^{(D_2)}$ is then in $\mathcal{H}^{(D)}$ replaced[16] by four operators: total angular momentum $(J^{(D)})^2$, total projection quantum number $J_3^{(D)}$, single total angular momenta $(J^{(D_1)})^2$, $(J^{(D_2)})^2$:

$$(J^{(D)})^2 = (J^{(D_1)} + J^{(D_2)})^2 \qquad J_3^{(D)} = J_3^{(D_1)} + J_3^{(D_2)} \qquad (J^{(D_1)})^2 \qquad (J^{(D_2)})^2, \tag{A.12}$$

which are simultaneously diagonal in the new basis manifested through

$$\begin{aligned}
(J^{(D)})^2|j_1 j_2; j_{12}(j_1, j_2), M\rangle &= j_{12}(j_{12}+1)|j_1 j_2; j_{12}(j_1, j_2), M\rangle \\
J_3^{(D)}|j_1 j_2; j_{12}(j_1, j_2), M\rangle &= M|j_1 j_2; j_{12}(j_1, j_2), M\rangle \\
(J^{(D_1)})^2|j_1 j_2; j_{12}(j_1, j_2), M\rangle &= j_1(j_1+1)|j_1 j_2; j_{12}(j_1, j_2), M\rangle \\
(J^{(D_2)})^2|j_1 j_2; j_{12}(j_1, j_2), M\rangle &= j_2(j_2+1)|j_1 j_2; j_{12}(j_1, j_2), M\rangle.
\end{aligned} \tag{A.13}$$

A.4. Recoupling of three angular momenta—6j-symbols

In this way, we can expand the recoupling of three angular momenta in terms of CGC:

$$\begin{aligned}
|j_{12}(j_1, j_2), j(j_{12}, j_3)\rangle &= |j_{12}(j_1, j_2) j_3; j(j_{12}, j_3) M = m_1 + m_2 + m_3\rangle \\
&= \sum_{m_{12} m_3} \langle j_{12} m_{12}; j_3 m_3 | j_{12} j_3; j m_{12} + m_3\rangle \cdot |j_{12} m_{12}\rangle |j_3 m_3\rangle \\
&= \sum_{m_{12} m_3} \langle j_{12} m_{12}; j_3 m_3 | j_{12} j_3; j m_{12} + m_3\rangle \cdot \\
&\quad \sum_{m_1 m_2} \langle j_1 m_1; j_2 m_2 | j_1 j_2; j_{12} m_{12} = m_1 + m_2\rangle \cdot |j_1 m_1\rangle |j_2 m_2\rangle |j_3 m_3\rangle \\
&= \sum_{m_1 m_2} \langle j_{12} m_1 + m_2; j_3 M - m_1 - m_2 | j_{12} j_3; j M\rangle \cdot \\
&\quad \times \langle j_1 m_1; j_2 m_2 | j_1 j_2; j_{12} m_1 + m_2\rangle \cdot |j_1 m_1\rangle |j_2 m_2\rangle |j_3 M - m_1 - m_2\rangle.
\end{aligned} \tag{A.14}$$

As we can see, as we couple angular momenta successively, the order of coupling plays an important role. Different orders of coupling will lead to different phases of the wavefunctions (see (A.9)). Concerning this, it would be nice to have a transformation connecting different ways of recoupling. This transformation between two different ways of coupling three angular momenta j_1, j_2, j_3 to a resulting j defines the $6j$-symbols; see appendix B.

A.5. Recoupling of n angular momenta—3nj-symbols

As mentioned before the case of successive coupling of three angular momenta to a resulting j can be generalized. For this purpose, let us first comment on the generalization principle before we go into detailed definitions.

Theorem A.1 can be applied to a tensor product of n representations $\pi_{j_1} \otimes \pi_{j_2} \otimes \cdots \otimes \pi_{j_n}$ by reducing step by step every pair of representations. This procedure has to be carried out until all tensor products are reduced out. One then ends up with a direct sum of representations each of them having a weight corresponding to an allowed value of the total angular momentum the n single angular momenta $j_1, j_2, \ldots, j_n$ can couple to.

[16] We are a bit 'sloppy' in using this notation. To be correct, we would have to write

$(J^{(D)})^2 = (J^{(D_1)} \otimes \mathbb{1}_{\mathcal{H}^{(D_2)}} + \mathbb{1}_{\mathcal{H}^{(D_1)}} \otimes J^{(D_2)})^2 \qquad J_3^{(D)} = J_3^{(D_1)} \otimes \mathbb{1}_{\mathcal{H}^{(D_2)}} + \mathbb{1}_{\mathcal{H}^{(D_1)}} \otimes J_3^{(D_2)}$ and

$(J^{(D_1)})^2 = (J^{(D_1)})^2 \otimes \mathbb{1}_{\mathcal{H}^{(D_2)}} \qquad (J^{(D_2)})^2 = \mathbb{1}_{\mathcal{H}^{(D_1)}} \otimes (J^{(D_2)})^2$.

But there is an arbitrariness in how one couples the n angular momenta together, that is, the order by which $\pi_{j_1} \otimes \pi_{j_2} \otimes \cdots \otimes \pi_{j_n}$ is reduced out (by applying A.1) matters.

Let us now have a system of n angular momenta. First, we fix a labelling of these momenta such that we have $j_1, j_2, \ldots, j_n$. Again the first choice would be a tensor basis $|\vec{j}\vec{m}\rangle$ of all single angular momentum states $|j_k m_k\rangle$, $k = 1, \ldots, n$ defined by

$$|\vec{j}\vec{m}\rangle = |(j_1, j_2, \ldots, j_n)(m_1, m_2, \ldots, m_n)\rangle := \bigotimes_{k=1}^{n} |j_k m_k\rangle \tag{A.15}$$

with the maximal set of $2n$ commuting operators $(J_I)^2, J_I^3$ $(I = 1, \ldots, n)$.

Now we proceed as in section A.3 finding the commuting operators according to (A.13), that is, a basis in which the total angular momentum $(J_{\text{tot}})^2 = (J)^2 = (J_1 + J_2 + \cdots + J_n)^2$ is diagonal (quantum number j) together with the total magnetic quantum number $J^3_{\text{tot}} = J^3 = J_1^3 + J_2^3 + \cdots + J_n^3$ (quantum number M).

As $(J)^2$ and J^3 are two operators, we need $2(n-1)$ more quantum numbers of operators commuting with each other and with $(J)^2$ and J^3 to have again a maximal set. We choose therefore the n operators $(J_I)^2, I = 1, \ldots, n$ of total single angular momentum (quantum numbers $(j_1, \ldots, j_n) := \vec{j}$). So, we are left with the task of finding additional $n-2$ operators commuting with the remaining ones. For this purpose, we define

Definition A.1 (recoupling scheme).
A recoupling scheme $|\vec{g}(IJ)\vec{j}jm\rangle$ *is an orthonormal basis, diagonalizing besides* $(J)^2, J^3, (J_I)^2$ $(I = 1, \ldots, n)$ *the squares of the additional* $n-2$ *operators* $G_2, G_3, \ldots, G_{n-1}$ *defined as*[17]
$G_1 := J_I$, $G_2 := G_1 + J_J$, $G_3 := G_2 + J_1$, $G_4 := G_3 + J_2, \ldots$, $G_I := G_{I-1} + J_{I-2}$, $G_{I+1} := G_I + J_{I-1}$, $G_{I+2} := G_{I+1} + J_{I+1}$, $G_{I+3} := G_{I+2} + J_{I+2}, \ldots$, $G_J := G_{J-1} + J_{J-1}$, $G_{J+1} := G_J + J_{J+1}$, $G_{J+2} := G_{J+1} + J_{J+2}, \ldots$, $G_{n-1} := G_{n-2} + J_{n-1}$.
The vector $\vec{g}(IJ) := (g_2(j_I, j_J), g_3(g_2, j_1), \ldots, g_{I+1}(g_I, j_{I-1}), g_{I+2}(g_{I+1}, j_{I+1}), \ldots, g_J(g_{j-1}, j_{j-1}), g_{j+1}(g_J, j_{j+1}), \ldots, g_{n-1}(g_{n-2}, j_{n-1}))$ *carries as quantum numbers the* $n-2$ *eigenvalues of the operators* $(G_2)^2, \ldots, (G_{n-1})^2$.

So, we recouple first the angular momenta labelled by I, J where $I < J$ and secondly all the other angular momenta successively (all labels are with respect to the a fixed label set), by taking into account the allowed values for each recoupling according to theorem A.1.

Let us define furthermore the so-called standard recoupling scheme or standard basis:

Definition A.2 (standard basis). *A recoupling scheme based on the pair* $(I, J) = (1, 2)$ *with*

$$G_K = \sum_{L=1}^{K} J_L$$

is called standard basis.

Using definition A.1 with the commutation relations (A.1) and the fact that single angular momentum operators acting on different single angular momentum Hilbert spaces commute[18], one can easily check that for every recoupling scheme

(i) G_Is fulfil the angular momentum algebra (A.1).
(ii) $(J)^2, (J_I)^2, (G_K)^2, J^3$ commute with each other $\forall\, I, K = 1, \ldots, n$.

[17] Note that formally $G_n := G_{n-1} + J_n = J_{\text{total}}$.
[18] That is $[J_I^i, J_J^j] = 0$ whenever $I \neq J$.

Note that it is sufficient to prove these two points in the standard basis $\vec{g}(12)$, because every other basis $\vec{g}(IJ)$ is related to it by simply relabelling the n angular momenta.

We have thus succeeded in giving an alternative description of an n angular momenta system by all possible occurring intermediate recoupling stages G_I instead of using the individual magnetic quantum numbers.

Obviously, every orthonormal basis spanned by a recoupling scheme $|\vec{g}(IJ)\vec{j}jm\rangle$ is singled out by the labelling, namely, the index pair (IJ) and therefore not identical, as we have already seen in the case of the *two* angular momentum problem. So, we are in need of a transformation connecting the different bases, that is, expressing one basis, e.g. belonging to the pair (IJ), in terms of another basis, e.g. belonging to the pair (KL), respectively. This leads to the following:

Definition A.3 (3*nj*-symbol)**.** *The generalized expansion coefficients of a recoupling scheme in terms of the standard-recoupling scheme are called* $3nj$*-symbols:*

$$|\vec{g}(IJ)\vec{j}jm\rangle = \sum_{\text{all } \vec{g}'(12)} \underbrace{\langle \vec{g}'(12)\vec{j}jm|\vec{g}(IJ)\vec{j}jm\rangle}_{3nj\text{-symbol}} |\vec{g}'(12)\vec{j}jm\rangle.$$

The summation has to be extended over all possible values of the intermediate recouplings $\vec{g}'(12) = (g_2'(j_1, j_2), g_3'(g_2', j_3), \ldots, g_{n-1}'(g_{n-2}', j_{n-1})$*, that is all values of each component* g_k' *allowed by theorem A.1.*

In calculations we will suppress the quantum numbers $\vec{j}, j, m$, since they are identical all the time, and write $\langle \vec{g}(IJ)|\vec{g}'(12)\rangle$. Note, additionally, the following properties of the $3nj$-symbols:

(i) They are real, due to the possibility of expressing them as Clebsh–Gordan coefficients:

$$\langle \vec{g}(IJ)|\vec{g}'(12)\rangle = \langle \vec{g}'(12)|\vec{g}(IJ)\rangle.$$

(ii) They are rotationally invariant, i.e. independent of the magnetic quantum numbers m_k occurring in (A.15).

Appendix A. Properties of the 6j-symbols

In this section, we will give an overview on the $6j$-symbols because they are the basic structure we will use in our recoupling calculations, every coupling of n angular momenta can be decomposed into them. For further details we refer to [14, 15].

B.1. Definition

The $6j$-symbol is defined as ([14] p 92)

$$\begin{aligned}
\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} &:= [(2j_{12}+1)(2j_{23}+1)]^{-\frac{1}{2}}(-1)^{j_1+j_2+j_3+j} \\
&\quad \times \langle j_{12}(j_1, j_2), j(j_{12}, j_3)|j_{23}(j_2, j_3), j(j_1, j_{23})\rangle \\
&= [(2j_{12}+1)(2j_{23}+1)]^{-\frac{1}{2}}(-1)^{j_1+j_2+j_3+j} \sum_{m_1 m_2} \langle j_1 m_1; j_2 m_2 | j_1 j_2 j_{12} m_1 + m_2\rangle \\
&\quad \times \langle j_{12} m_1 + m_2; j_3 m - m_1 - m_2 | j_{12} j_3 j m\rangle \\
&\quad \times \langle j_2 m_2; j_3 m - m_1 - m_2 | j_2 j_3 j_{23} m - m_1\rangle \\
&\quad \times \langle j_1 m_1; j_{23} m - m_1 | j_1 j_{23} j m\rangle. \qquad \text{(B.1)}
\end{aligned}$$

The terms under the summation are called Clebsh–Gordon coefficients.

B.2. Explicit evaluation of the 6j-symbols

A general formula for the numerical value of the $6j$-symbols has been derived by Racah ([19], [14], p 99)

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} = \Delta(j_1, j_2, j_{12})\Delta(j_1, j, j_{23})\Delta(j_3, j_2, j_{23})\Delta(j_3, j, , j_{12}) w \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix},$$

$$\times\ \Delta(a, b, c) = \sqrt{\frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!}} w \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix}$$

$$= \sum_n (-1)^n (n+1)![(n-j_1-j_2-j_{12})!(n-j_1-j-j_{23})!$$
$$\times\ (n-j_3-j_2-j_{23})!(n-j_3-j-j_{12})!]^{-1}[(j_1+j_2+j_3+j-n)!$$
$$\times\ (j_2+j_{12}+j+j_{23}-n)!(j_{12}+j_1+j_{23}+j_3-n)!]^{-1}. \tag{B.2}$$

The sum has to be extended over all positive integer values of n such that no factorial in the denominator has a negative argument. That is,

$$\max[j_1+j_2+j_{12}, j_1+j+j_{23}, j_3+j_2+j_{23}, j_3+j+j_{12}] \leqslant n$$
$$\leqslant \min[j_1+j_2+j_3+j, j_2+j_{12}+j+j_{23}, j_{12}+j_1+j_{23}+j_3].$$

Remark. From (B.2) we are provided with some additional requirements the arguments of the $6j$-symbols have to fulfil. Certain sums or differences of them have to be integer to be proper ($\equiv$integer) arguments for the factorials:

from $\Delta(a, b, c)$ one gets

- a, b, c have to fulfil the triangle inequalities: $(a+b-c) \geqslant 0, (a-b+c) \geqslant 0, (-a+b+c) \geqslant 0$,
- $(\pm a \pm b \pm c)$ has to be an integer number;

from the w-coefficient one gets

- $j_1+j_2+j_3+j, j_2+j_{12}+j+j_{23}, j_{12}+j_1+j_{23}+j_3$ are integer numbers.

The following (trivial but important) relations are frequently used in calculations involving $6j$-symbols:

$$\begin{aligned} &(-1)^z = (-1)^{-z} && \forall\, z \in \mathbb{Z} \\ &(-1)^{2z} = 1 && \forall\, z \in \mathbb{Z} \\ &(-1)^{3k} = (-1)^{-k} && \forall\, k = \frac{z}{2} \quad \text{with} \quad z \in \mathbb{Z}. \end{aligned} \tag{B.3}$$

B.3. Symmetry properties

The $6j$-symbols are invariant

- under any permutation of the columns:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_2 & j_3 & j_1 \\ j_5 & j_6 & j_4 \end{Bmatrix} = \begin{Bmatrix} j_3 & j_1 & j_2 \\ j_6 & j_4 & j_5 \end{Bmatrix}$$
$$= \begin{Bmatrix} j_2 & j_1 & j_3 \\ j_5 & j_4 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_3 & j_2 \\ j_4 & j_6 & j_5 \end{Bmatrix} = \begin{Bmatrix} j_3 & j_2 & j_1 \\ j_6 & j_5 & j_4 \end{Bmatrix}; \tag{B.4}$$

- under interchange of the upper and lower arguments of two columns at the same time, for example,

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_5 & j_6 \\ j_4 & j_2 & j_3 \end{Bmatrix}. \tag{B.5}$$

B.4. Orthogonality and sum rules

Orthogonality relations

$$\sum_{j_{23}} (2j_{12}+1)(2j'_{12}+1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j'_{12} \\ j_3 & j & j_{23} \end{Bmatrix} = \delta_{j_{12} j'_{12}}. \tag{B.6}$$

Composition relation

$$\sum_{j_{23}} (-1)^{j_{23}+j_{31}+j_{12}} (2j_{23}+1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} \begin{Bmatrix} j_2 & j_3 & j_{23} \\ j_1 & j & j_{31} \end{Bmatrix} = \begin{Bmatrix} j_3 & j_1 & j_{31} \\ j_2 & j & j_{12} \end{Bmatrix}. \tag{B.7}$$

Sum rule of Elliot and Biedenharn

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_{123} & j_{23} \end{Bmatrix} \begin{Bmatrix} j_{23} & j_1 & j_{123} \\ j_4 & j & j_{14} \end{Bmatrix} = (-1)^{j_1+j_2+j_3+j_4+j_{12}+j_{23}+j_{14}+j_{123}+j} \sum_{j_{124}} (-1)^{j_{124}} (2j_{124}+1)$$
$$\times \begin{Bmatrix} j_3 & j_2 & j_{23} \\ j_{14} & j & j_{124} \end{Bmatrix} \begin{Bmatrix} j_2 & j_1 & j_{12} \\ j_4 & j_{124} & j_{14} \end{Bmatrix} \begin{Bmatrix} j_3 & j_{12} & j_{123} \\ j_4 & j & j_{124} \end{Bmatrix}. \tag{B.8}$$

Appendix C. Comment on the smallest non-vanishing eigenvalue

In this section, we will briefly summarize what can be done to obtain a lower bound of the spectrum of the matrices occurring when expressing the volume operator on a recoupling scheme basis at the gauge invariant 4-vertex. This is mainly done to illustrate the remarkable symmetries in that case. The idea is to obtain a lower bound of the non-zero eigenvalues by applying theorem 4.1, on the inverse matrix, giving an upper bound for its eigenvalues and therefore a lower bound for the non-zero volume spectrum.

The general form for the gauge-invariant 4-vertex was obtained in (68)

$$A = \begin{pmatrix} 0 & -a_1 & 0 & \cdots & \cdots & 0 \\ a_1 & 0 & -a_2 & & & \vdots \\ 0 & a_2 & 0 & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & -a_{n-1} \\ 0 & \cdots & \cdots & \cdots & a_{n-1} & 0 \end{pmatrix}. \tag{C.1}$$

We have explicitly discussed the 0-eigenvalues contained in the spectrum of A in section 4.1.2. We know that only in the odd-dimensional case the matrix A is singular, containing one 0-eigenvalue with the according eigenvector

$${}^{(n)}\Psi := x \cdot \left[1, 0, \frac{a_1}{a_2}, 0, \frac{a_1 a_3}{a_2 a_4}, 0, \ldots, \frac{a_1 a_3 \cdots a_{n-2}}{a_2 a_4 \cdots a_{n-1}}\right] \tag{C.2}$$

where $n := \dim A$ and x is an arbitrary scaling factor. We will denote the kth element of ${}^{(n)}\Psi$ by ${}^{(n)}\Psi_k$. For technical reasons, we will set $x = \frac{y}{{}^{(n)}\Psi_n}$ in the following to obtain

$$^{(n)}\Xi := y \cdot \left[\frac{a_2 a_4 \cdots a_{n-1}}{a_1 a_3 \cdots a_{n-2}}, 0, \ldots, \frac{a_2 a_4}{a_1 a_3}, 0, \frac{a_2}{a_1}, 0, 1\right]. \tag{C.3}$$

C.1. Even dimension n of A

Since A is regular in that case we can invert it to find

$$A^{-1} = \begin{pmatrix} 0 & \frac{\Xi_{n-1}}{a_1} & 0 & \frac{\Xi_{n-3}}{a_3} & 0 & \frac{\Xi_{n-5}}{a_5} & 0 & \cdots & \cdots & \frac{\Xi_1}{a_{n-1}} \\ -\frac{\Xi_{n-1}}{a_1} & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 0 & \frac{\Xi_{n-1}}{a_3} & 0 & \frac{\Xi_{n-3}}{a_5} & 0 & \cdots & \cdots & \frac{\Xi_3}{a_{n-1}} \\ -\frac{\Xi_{n-3}}{a_3} & 0 & -\frac{\Xi_{n-1}}{a_3} & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\Xi_{n-1}}{a_5} & 0 & \cdots & \cdots & \frac{\Xi_5}{a_{n-1}} \\ -\frac{\Xi_{n-5}}{a_5} & 0 & -\frac{\Xi_{n-3}}{a_5} & 0 & -\frac{\Xi_{n-1}}{a_5} & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ddots & & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \ddots & 0 & \frac{\Xi_{n-1}}{a_{n-1}} \\ -\frac{\Xi_1}{a_{n-1}} & 0 & -\frac{\Xi_3}{a_{n-1}} & 0 & -\frac{\Xi_5}{a_{n-1}} & 0 & \cdots & \cdots & -\frac{\Xi_{n-1}}{a_{n-1}} & 0 \end{pmatrix} \tag{C.4}$$

where we have used the components $^{(n-1)}\Xi_k := \Xi_k$ of the 0-eigenvector $^{(n-1)}\Xi$ of the $(n-1)$ odd-dimensional case with scaling factor $y = 1$.

C.2. Odd dimension of A

Since A is not regular we have to project out its nullspace $^{(n)}\Xi$ first (with arbitrary prefactor y). This can be done by applying a similarity transformation W on A to obtain $R := W^{-1}AW$:

$$W = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & \cdots & 0 & \Xi_1 \\ 0 & 1 & 0 & 0 & \cdots & \cdots & 0 & \Xi_2 \\ 0 & 0 & 1 & 0 & & & \vdots & \vdots \\ 0 & 0 & 0 & 1 & & & \vdots & \vdots \\ \vdots & & & & \ddots & & \vdots & \vdots \\ \vdots & & & & & & 1 & \Xi_{n-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & \Xi_n \end{pmatrix}$$

$$W^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & \cdots & 0 & -\frac{\Xi_1}{\Xi_n} \\ 0 & 1 & 0 & 0 & \cdots & \cdots & 0 & -\frac{\Xi_2}{\Xi_n} \\ 0 & 0 & 1 & 0 & & & \vdots & \vdots \\ 0 & 0 & 0 & 1 & & & \vdots & \vdots \\ \vdots & & & & \ddots & & \vdots & \vdots \\ \vdots & & & & & & 1 & -\frac{\Xi_{n-1}}{\Xi_n} \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & \frac{1}{\Xi_n} \end{pmatrix}. \tag{C.5}$$

Now one can check that (all even components of ${}^{(n)}\Xi$ vanish, again $y = 1$)

$$R := W^{-1}AW = \left(\begin{array}{cccccccc|c} 0 & -a_1 & 0 & 0 & \cdots & \cdots & & -\frac{\Xi_1}{\Xi_n}a_{n-1} & 0 \\ a_1 & 0 & -a_2 & 0 & \cdots & \cdots & & 0 & 0 \\ 0 & a_2 & 0 & -a_3 & \cdots & \cdots & & -\frac{\Xi_3}{\Xi_n}a_{n-1} & 0 \\ 0 & 0 & a_3 & 0 & \ddots & & & \vdots & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & & \vdots & \vdots \\ \vdots & & & & \ddots & \ddots & & -a_{n-2} - \frac{\Xi_{n-1}}{\Xi_n}a_{n-1} & 0 \\ \vdots & & & & & & a_{n-2} & 0 & 0 \\ \hline 0 & \cdots & \cdots & \cdots & \cdots & 0 & & \frac{a_{n-1}}{\Xi_n} & 0 \end{array}\right). \tag{C.6}$$

To discuss the non-zero spectrum of A it is sufficient to discuss the now regular submatrix $\tilde{R}$ being the submatrix of R with the nth row and column deleted. One obtains

$$\tilde{R}^{-1} = \begin{pmatrix} 0 & \frac{\Xi_{n-1}}{a_1} & 0 & \frac{\Xi_{n-3}}{a_3} & 0 & \frac{\Xi_{n-5}}{a_5} & 0 & \cdots & \cdots & \frac{\Xi_1}{a_{n-1}} \\ M_{21} & 0 & M_{23} & 0 & M_{25} & 0 & M_{27} & \cdots & M_{2n-1} & 0 \\ 0 & 0 & 0 & \frac{\Xi_{n-1}}{a_3} & 0 & \frac{\Xi_{n-3}}{a_5} & 0 & \cdots & \cdots & \frac{\Xi_3}{a_{n-1}} \\ M_{41} & 0 & M_{43} & 0 & M_{45} & 0 & M_{47} & \cdots & M_{4n-1} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\Xi_{n-1}}{a_5} & 0 & \cdots & \cdots & \frac{\Xi_5}{a_{n-1}} \\ M_{61} & 0 & M_{63} & 0 & M_{65} & 0 & M_{67} & \cdots & M_{6n-1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \ddots & & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \ddots & 0 & \frac{\Xi_{n-1}}{a_{n-1}} \\ M_{n-11} & 0 & M_{n-13} & 0 & M_{n-15} & 0 & \cdots & \cdots & M_{n-1n-2} & 0 \end{pmatrix}. \tag{C.7}$$

Here, $M_{ij} = \frac{\det \tilde{R}_{(ij)}}{\det \tilde{R}}$ and $\tilde{R}_{(ij)}$ is a shortcut for the submatrix of $\tilde{R}$ one obtains by deleting row i and column j. Basically this is the definition for the matrix element of the inverse matrix. Since, unfortunately, M_{ij} are hard to control (but of order $\frac{1}{a}$) we are unable to give an explicit upper bound for the spectrum of $\tilde{R}^{-1}$ and therefore a lower bound on the spectrum of A according to theorem 4.1. It is remarkable, however, that half of the structure of (C.4) is being reproduced by the odd-dimensional case.

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