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Classical and quantum polyhedra

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Quantum polyhedra constructed from angular momentum operators are the building blocks of space in its quantum description as advocated by loop quantum gravity. Here we extend previous results on the semiclassical properties of quantum polyhedra. Regarding tetrahedra, we compare the results from a canonical quantization of the classical system with a recent wave-function-based approach to the large-volume sector of the quantum system. Both methods agree in the leading order of the resulting effective operator (given by an harmonic oscillator), while minor differences occur in higher corrections. Perturbative inclusion of such corrections improves the approximation to the eigenstates. Moreover, the comparison of both methods leads also to a full wave function description of the eigenstates of the (square of the) volume operator at negative eigenvalues of large modulus. For the case of general quantum polyhedra described by discrete angular momentum quantum numbers we formulate a set of quantum operators fulfilling in the semiclassical regime the standard commutation relations between momentum and position. Differently from previous formulations, the position variable here is chosen to have dimension of (Planck) length squared which facilitates the identification of quantum corrections. Finally, we provide expressions for the pentahedral volume in terms of Kapovich-Millson variables.

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I. INTRODUCTION

The quantum volume operator is among the most intensively investigated items in the field of loop quantum gravity and is pivotal for the construction of space-time dynamics within this theoretical framework [1–3]. Traditionally two versions of such an operator are discussed, due to Rovelli and Smolin [4] and to Ashtekar and Lewandowski [5], respectively, and considerable attention has been devoted to their properties and interrelations [6–19]. More recently, Bianchi, Dona, and Speziale [20] offered a third proposal for a volume operator which is closer to the concept of spin foams [3]. It relies on an older geometric theorem due to Minkowski [21] stating that N face areas A_i, $i \in \{1, \dots, N\}$, with normal vectors $\vec{n}_i$ such that

$$\sum_{i=1}^{N} \vec{A}_i = 0 \tag{1}$$

for $\vec{A}_i = \vec{n}_i A_i$ uniquely define a convex polyhedron of N faces with areas A_i. The approach of Ref. [20] amounts to expressing the volume of a classical polyhedron in terms of its face areas, which are in turn promoted to be operators. Minkowski's proof, however, is not constructive, and a remaining obstacle of the above route to a volume operator is to actually find the shape of a general polyhedron given its face areas and face normals [20,22–25].

Such difficulties do not occur in the simplest case of a polyhedron, i.e. a tetrahedron consisting of four faces represented by angular momentum operators coupling to a total spin singlet [11,26]. Indeed, for such a quantum tetrahedron all three definitions of the volume operator coincide. On the other hand, for a classical tetrahedron the general phase space parametrization devised by Kapovich and Millson [27] results in just one pair of canonical variables, and the (square of the) volume operator can explicitly formulated in terms of these quantities [23,28]. Moreover, Bianchi and Haggard have performed a Bohr-Sommerfeld quantization of the classical tetrahedron where the role of a Hamiltonian generating classical orbits is played by the volume operator squared. The resulting semiclassical eigenvalues agree extremely well with exact numerical data [22,23]. The above observations make clear that classical tetrahedra, arguably the simplest structures a volume can be ascribed to, should be considered as perfectly integrable systems. In turn, a quantum tetrahedron can be viewed as the "hydrogen atom" of quantum spacetime, whereas the next complicated case of a pentahedron might be referred to as the "helium atom" [25].

Most recently, the present author has put forward yet another approach to the semiclassical regime of quantum tetrahedra [29]. Here, by combining observations on the volume operator squared and its eigenfunctions (as opposed to the eigenvalues), an effective operator in terms of a quantum harmonic oscillator was derived, providing an accurate as well as transparent description of the large-volume sector. One of the purposes of the present work is to demonstrate the relation between the different treatments of quantum tetrahedra sketched above.

The outline of this paper is as follows. In Sec. II we first summarize the Kapovich-Millson phase space parametrization of general classical polyhedra (Sec. II A) before reviewing and extending in Sec. II B results for the classical tetrahedron. In particular, we derive an expansion of the volume squared around its maximum and minimum in up to quadrilinear order. Section III A is devoted to the quantum tetrahedron. We first outline in Sec. III A 1 elementary facts about the volume operator and its Hilbert space, and we point out several relations between appropriate quantum operators which have analogs in the classical tetrahedron. Next the analysis of Ref. [29] is extended to higher corrections to the resulting harmonic oscillator of up to fourth order. The results are compared with the outcome of a canonical quantization of the classical volume expression. The expression of the pentahedral volume in terms of Kapovich-Millson variables is discussed in the Appendix. Finally we construct in Sec. III B a set of quantum operators for general polyhedra whose commutation relations approach in the semiclassical limit the standard commutators between momentum and position.

II. CLASSICAL POLYHEDRA

Let us first recall the essentials of the polyhedral phase space parametrization due to Kapovich and Millson [27].

A. Kapovich-Millson phase space variables

Viewing the vectors $\vec{A}_i$ as angular momenta, the Poisson bracket of arbitrary functions of these variables reads

$$\{f,g\} = \sum_{i=0}^{N} \vec{A}_i \cdot \left(\frac{\partial f}{\partial \vec{A}_i} \times \frac{\partial g}{\partial \vec{A}_i} \right). \tag{2}$$

In order to implement the closure relation (1) one defines

$$\vec{p}_i = \sum_{j=1}^{i+1} \vec{A}_j \tag{3}$$

for $i \in \{1,\ldots,N-3\}$ resulting in $N-3$ momenta $p_i = |\vec{p}_i|$. Defining now

$$\vec{v}_i = \vec{p}_i \times \vec{A}_{i+1}, \qquad \vec{w}_i = \vec{p}_i \times \vec{A}_{i+2}, \tag{4}$$

such that $\vec{v}_{i+1} = \vec{w}_i$ $(i < N-3)$ and

$$\vec{p}_i \cdot \vec{v}_i = \vec{p}_i \cdot \vec{w}_i = 0, \tag{5}$$

the canonical conjugate variables q_i are then given to be the angle between $\vec{v}_i$, $\vec{w}_i$. Indeed, a straightforward calculation shows that these quantities fulfill indeed the canonical Poisson relations [23,27]

$$\{p_i, q_j\} = \delta_{ij}. \tag{6}$$

B. The tetrahedron

The classical volume of a tetrahedron can be expressed as

$$V = \frac{\sqrt{2}}{3}\sqrt{|\vec{A}_1 \cdot (\vec{A}_2 \times \vec{A}_3)|} \tag{7}$$

suggesting to investigate the quantity

$$Q = \vec{A}_1 \cdot (\vec{A}_2 \times \vec{A}_3). \tag{8}$$

The latter can indeed easily be expressed in terms of the phase space variables p_1, q_1 using the observation [23]

$$\vec{v}_1 \times \vec{w}_1 = Q\vec{p}_1. \tag{9}$$

Moreover, it is easily seen that

$$|\vec{v}_1| = |\vec{A}_1 \times \vec{A}_2| = 2\Delta(A_1, A_2, p_1) \tag{10}$$

where $\Delta(a,b,c)$ is the area of a triangle with edges a, b, c expressed via Heron's formula,

$$\Delta(a,b,c) = \frac{1}{4}\sqrt{((a+b)^2 - c^2)(c^2 - (a-b)^2)}. \tag{11}$$

Analogously, using the closure relation (1),

$$|\vec{w}_1| = |\vec{A}_3 \times \vec{A}_4| = 2\Delta(A_3, A_4, p_1) \tag{12}$$

such that

$$Q = 4\frac{\Delta(A_1, A_2, p_1)\Delta(A_3, A_4, p_1)}{p_1} \sin q_1. \tag{13}$$

In order to make closer contact to the quantum tetrahedron to be discussed below, let us introduce the notation

$$A \coloneqq p_1, \qquad p \coloneqq -q_1 + \frac{\pi}{2} \tag{14}$$

fulfilling $\{p, A\} = 1$ and

$$Q = 2\tilde{\beta}(A)\cos p \tag{15}$$

with

$$\tilde{\beta}(A) = 2\frac{\Delta(A_1, A_2, A)\Delta(A_3, A_4, A)}{A}, \tag{16}$$

where A varies according to $A^{\min} \le A \le A^{\max}$ with

$$A^{\min} = \max\{|A_1 - A_2|, |A_3 - A_4|\}, \tag{17}$$

$$A^{\max} = \min\{A_1 + A_2, A_3 + A_4\}. \tag{18}$$

An expression close to (15) was also found in Ref. [28] in the semiclassical limit of a quantum tetrahedron.

Obviously, $\tilde{\beta}(A)$ is a non-negative function with $\tilde{\beta}(A^{\min}) = \tilde{\beta}(A^{\max}) = 0$, and it is not difficult to verify that it has a unique maximum at some $A = \bar{A}$ between $A^{\min}$ and $A^{\max}$ [29]. Thus, Q has a unique maximum at $A = \bar{k}$ and $p = 0$ while the unique minimum lies at $p = \pi$. Expanding around the maximum gives ($x \coloneqq A - \bar{A}$, $|x| \ll 1$, $|p| \ll 1$)

$$Q(p,x) = \tilde{q}\left[1 - \frac{p^2}{2} - \frac{\tilde{\omega}^2}{2}x^2 + \frac{\tilde{c}}{3}x^3 + \frac{\tilde{d}}{4}x^4 + \frac{\tilde{\omega}^2}{4}x^2p^2 + \frac{p^4}{24} + \cdots\right] \tag{19}$$

with

$$\tilde{q} = 2\tilde{\beta}(\bar{A}), \qquad \tilde{\omega}^2 = -\frac{\left(\frac{d^2\tilde{\beta}(A)}{dA^2}\right)_{A=\bar{A}}}{\tilde{\beta}(\bar{A})} > 0 \tag{20}$$

and

$$\tilde{c} = \frac{\left(\frac{d^3\tilde{\beta}(A)}{dA^3}\right)_{A=\bar{A}}}{2\tilde{\beta}(\bar{A})}, \qquad \tilde{d} = \frac{\left(\frac{d^4\tilde{\beta}(A)}{dA^4}\right)_{A=\bar{A}}}{6\tilde{\beta}(\bar{A})}. \tag{21}$$

The analogous expansion around the minimum reads $[p = \pi + (p - \pi),\ |p - \pi| \ll 1]$

$$Q'(p,x) = -\tilde{q}\left[1 - \frac{(p-\pi)^2}{2} - \frac{\tilde{\omega}^2}{2}x^2 + \frac{\tilde{a}}{3}x^3 + \frac{\tilde{b}}{4}x^4 + \frac{\tilde{\omega}^2}{4}x^2(p-\pi)^2 + \frac{(p-\pi)^4}{24} + \cdots\right]. \tag{22}$$

Concentrating in both cases on the quadratic contributions, one obtains two harmonic oscillators,

$$Q_{\mathrm{osc}}(p,x) = \tilde{q}\left[1 - \frac{p^2}{2} - \frac{\tilde{\omega}^2}{2}x^2\right], \tag{23}$$

$$Q'_{\mathrm{osc}}(p,x) = -\tilde{q}\left[1 - \frac{(p-\pi)^2}{2} - \frac{\tilde{\omega}^2}{2}x^2\right]. \tag{24}$$

Finally, it is certainly desirable to also express the volume of higher polyhedra in terms of Kapovich-Millson variables. The Appendix details the case of the pentahedron. As shown there, the above task is certainly feasible, but leads to unpleasantly complicated expressions which inhibit analytical progress.

III. QUANTUM POLYHEDRA

A. The quantum tetrahedron

We begin by reviewing and extending general results of quantum tetrahedra.

1. General properties

A quantum tetrahedron is defined by four angular momentum operators $\hat{\vec{j}}_i$, $i \in \{1,2,3,4\}$, representing its faces and coupling to a total singlet [11,12,22,23,26]; i.e. the Hilbert space consists of all states $|k\rangle$ fulfilling

$$(\hat{\vec{j}}_1 + \hat{\vec{j}}_2 + \hat{\vec{j}}_3 + \hat{\vec{j}}_4)|k\rangle = 0. \tag{25}$$

A usual way to construct this space is to couple first the pairs $\hat{\vec{j}}_1$, $\hat{\vec{j}}_2$ and $\hat{\vec{j}}_3$, $\hat{\vec{j}}_4$ to two irreducible SU(2) representations of dimension $2k+1$ each. For $\hat{\vec{j}}_1$, $\hat{\vec{j}}_2$ this standard construction reads explicitly

$$\hat{\vec{k}} \coloneqq \hat{\vec{j}}_1 + \hat{\vec{j}}_2, \tag{26}$$

$$|km\rangle_{12} = \sum_{m_1+m_2=m} \langle j_1 m_1 j_2 m_2 | km\rangle |j_1 m_1\rangle |j_2 m_2\rangle, \tag{27}$$

such that

$$\hat{k}^z|km\rangle_{12} = m|km\rangle_{12}, \tag{28}$$

$$\hat{\vec{k}}^2|km\rangle_{12} = k(k+1)|km\rangle_{12}, \tag{29}$$

where $\langle j_1 m_1 j_2 m_2 | km\rangle$ are Clebsch-Gordan coefficients following their usual phase convention [30]. Defining analogous states $|km\rangle_{34}$ for $\hat{\vec{j}}_3$, $\hat{\vec{j}}_4$, the quantum number k becomes restricted by $k^{\min} \le k \le k^{\max}$ with

$$k^{\min} = \max\{|j_1 - j_2|, |j_3 - j_4|\}, \tag{30}$$

$$k^{\max} = \min\{j_1 + j_2, j_3 + j_4\}. \tag{31}$$

The two multiplets $|km\rangle_{12}$, $|km\rangle_{34}$ are then coupled to a total singlet,

$$|k\rangle = e^{i\frac{\pi}{2}(k-k^{\min})} \cdot \sum_{m=-k}^{k} \frac{(-1)^{k-m}}{\sqrt{2k+1}} |km\rangle_{12}|k(-m)\rangle_{34}, \tag{32}$$

where the phase factor in front will become useful shortly below. The states $|k\rangle$ span a Hilbert space of dimension $d = k^{\max} - k^{\min} + 1$.

The volume operator of a quantum tetrahedron can be formulated as

$$\hat{V} = \frac{\sqrt{2}}{3}\sqrt{|\hat{\vec{E}}_1 \cdot (\hat{\vec{E}}_2 \times \hat{\vec{E}}_3)|} \tag{33}$$

where the operators

$$\hat{\vec{E}}_i = \ell_P^2 \hat{\vec{j}}_i, \tag{34}$$

$i \in \{1,2,3,4\}$ represent the faces of the tetrahedron with $\ell_P^2 = \hbar G/c^3$ being the Planck length squared. Usually the operators $\hat{\vec{E}}_i$ are defined with additional prefactors proportional to the Immirzi parameter on the r.h.s. of Eq. (34). This establishes contact to the general formalism of loop quantum gravity [1–3] but is unnecessary for our purposes here. What will become important, however, is that ℓ_P^2 is proportional to $\hbar$.

As a result, one is led to consider the operator

$$\hat{R} = \hat{\vec{j}}_1 \cdot (\hat{\vec{j}}_2 \times \hat{\vec{j}}_3), \tag{35}$$

which reads in the basis of the states $|k\rangle$ as [12,23,29–32]

$$\hat{R} = \sum_{k=k^{\min}+1}^{k^{\max}} \alpha(k)(|k\rangle\langle k-1| + |k-1\rangle\langle k|) \tag{36}$$

with

$$\alpha(k) = \frac{2}{\sqrt{k^2 - 1/4}} \Delta(j_1 + 1/2, j_2 + 1/2, k) \cdot \Delta(j_3 + 1/2, j_4 + 1/2, k). \tag{37}$$

Note the close similarity of the expressions (37) and (16). Moreover, in the above basis $\hat{Q}$ couples only states with neighboring labels and is represented by a real matrix. The latter fact depends on the phase factor in the first line of Eq. (32). Indeed, upon striping this factor (which is a unitary operation) $\hat{R}$ becomes antisymmetric and purely imaginary. Thus, for even d, the eigenvalues of Q come in pairs q, $(-q)$, and since

$$u\hat{R}u^+ = -\hat{R} \tag{38}$$

with $u = \mathrm{diag}(1,-1,1,-1,\ldots)$, the corresponding eigenstates $|\phi_q\rangle$, $|\phi_{-q}\rangle$ fulfill

$$|\phi_{-q}\rangle = u|\phi_q\rangle, \tag{39}$$

i.e. eigenvectors of eigenvalues differing just in sign are related to each other by changing the sign of any other component. For odd d an additional zero eigenvalue occurs [13].

To make further contact between the classical and the quantum tetrahedron we define in analogy to Eqs. (4)

$$\hat{\vec{v}} = \frac{1}{2}(\hat{\vec{k}} \times \hat{\vec{j}}_2 - \hat{\vec{j}}_2 \times \hat{\vec{k}}) = \hat{\vec{j}}_1 \times \hat{\vec{j}}_2, \tag{40}$$

$$\hat{\vec{w}} = \hat{\vec{k}} \times \hat{\vec{j}}_3 \tag{41}$$

fulfilling

$$\frac{1}{2}(\hat{\vec{v}} \times \hat{\vec{w}} - \hat{\vec{w}} \times \hat{\vec{v}}) = \frac{1}{2}(\hat{R}\,\hat{\vec{k}} + \hat{\vec{k}}\,\hat{R}), \tag{42}$$

which is the operator analog of Eq. (9). Moreover, one straightforwardly obtains

$$\hat{\vec{v}}^2 = 4\left(\Delta\left(\sqrt{j_1(j_1+1)}, \sqrt{j_2(j_2+1)}, \hat{\vec{k}}\right)\right)^2 \tag{43}$$

and

$$\hat{\Pi}\hat{\vec{w}}^2\hat{\Pi} = 4\hat{\Pi}\left(\Delta\left(\sqrt{j_3(j_3+1)}, \sqrt{j_4(j_4+1)}, \hat{\vec{k}}\right)\right)^2\hat{\Pi}, \tag{44}$$

where

$$\hat{\Pi} = \sum_{k=k^{\min}}^{k^{\max}} |k\rangle\langle k| \tag{45}$$

is the projector onto the singlet space. Equations (43) and (44) are the operator analogs of Eqs. (10) and (12).

2. Rescaling to dimensionful variables

So far we have followed the formalism common to the literature and parametrized the Hilbert space of the quantum tetrahedron by a dimensionless quantum number k, whereas the phase space variable A of the classical tetrahedron has dimension of area. In order to establish closer contact between both descriptions let us rescale the involved quantum numbers by the Planck length squared according to

$$k \mapsto a = \ell_P^2 k, \qquad j_i \mapsto E_i = \ell_P^2 j_i \tag{46}$$

to quantities having also dimension of area. As we shall see below, this step will also provide a close analogy to standard quantum mechanics in the Schrödinger representation. The analog of the classical expression (8) reads

$$\hat{Q} = \ell_P^6 \hat{R} = \hat{\vec{E}}_1 \cdot (\hat{\vec{E}}_2 \times \hat{\vec{E}}_3) \tag{47}$$

$$= \sum_{a=a^{\min}+\ell_P^2}^{a^{\max}} \beta(a)(|a\rangle\langle a-\ell_P^2| + |a-\ell_P^2\rangle\langle a|) \tag{48}$$

with

$$\beta(a) = \ell_P^6 \alpha(k) \tag{49}$$

$$= \frac{2}{\sqrt{a^2 - \ell_P^4/4}} \Delta(E_1 + \ell_P^2/2, E_2 + \ell_P^2/2, a) \cdot \Delta(E_3 + \ell_P^2/2, E_4 + \ell_P^2/2, a). \tag{50}$$

The latter quantity shares the essential properties of $\tilde{\beta}(A)$ in Eq. (16). In particular $\beta(a)$ has a unique maximum at some $a = \bar{a}$.

3. Large volumes

In Ref. [29] the present author has shown how to accurately describe the large-volume (semiclassical) regime of $\hat{Q}$ (or $\hat{R}$) by a quantum harmonic oscillator in real-space representation with respect to a (or k, respectively). Here we shall extend this analysis taking into account higher-order corrections within the rescaled variables introduced in the previous section.

Let us label the eigenstates of $\hat{Q}$ by $|n\rangle$, $n \in \{0,1,2,\ldots\}$, in descending order of eigenvalues with $|0\rangle$ being the state of the largest eigenvalue. With respect to the basis states $|k\rangle$ they can be expressed as

$$|n\rangle = \sum_{a=a_{\min}}^{a_{\max}} \langle a|n\rangle |a\rangle. \tag{51}$$

Thus, taking the view of the standard Schrödinger formalism of elementary quantum mechanics, the coefficients $\langle a|n\rangle$ are the "wave function" of the state $|n\rangle$ with respect to the "coordinate" a. The approach of Ref. [29] starts from evaluating matrix elements

$$\langle\Phi|Q|\Psi\rangle = \sum_a \beta(a)(\langle\Phi|a\rangle\langle a-\ell_P^2|\Psi\rangle + \langle\Phi|a-\ell_P^2\rangle\langle a|\Psi\rangle) \tag{52}$$

between states lying predominantly in the sector of large eigenvalues by approximating the sum by an integral introducing the integration variable $x := a - \bar{a}$,

$$\langle\Phi|Q|\Psi\rangle \approx \frac{1}{\ell_P^2}\int dx\beta(\bar{a}+x)(\tilde{\Phi}^*(x)\tilde{\Psi}(x-\ell_P^2)| + \tilde{\Phi}^*(x-\ell_P^2)\tilde{\Psi}(x)) \tag{53}$$

with $\tilde{\Phi}(x) = \langle\bar{a}+x|\Phi\rangle$, $\tilde{\Psi}(x) = \langle\bar{a}+x|\Psi\rangle$. Expanding now $\beta(\bar{a}+x)$ around its maximum at $\bar{a}$ and the wave functions $\tilde{\Phi}^*(x-\ell_P^2)$, $\tilde{\Psi}(x-\ell_P^2)$ around x, one obtains in up to fourth order the expansions

$$\begin{aligned}\langle\Phi|Q|\Psi\rangle \approx \int dx\Phi^*(x)\bar{q}\Bigg[1-\left(-\frac{\ell_P^4}{2}\frac{d^2}{dx^2}+\frac{\omega^2}{2}x^2\right) \\ +\frac{c}{3}x^3+\frac{d}{4}x^4-\frac{\omega^2}{8}\ell_P^4\left(x^2\frac{d^2}{dx^2}+\frac{d^2}{dx^2}x^2\right) \\ +\frac{\ell_P^8}{24}\frac{d^4}{dx^4}+\frac{\omega^2}{2}\ell_P^2\left[\frac{d}{dx},x^2\right]+\frac{c}{3}\ell_P^2\left[\frac{d}{dx},x^3\right]\Bigg]\Psi(x)\end{aligned} \tag{54}$$

with $\Phi(x) = \tilde{\Phi}(x)/\ell_P$, $\Psi(x) = \tilde{\Psi}(x)/\ell_P$ and

$$\bar{q} = 2\beta(\bar{a}), \qquad \omega^2 = -\frac{\left(\frac{d^2\beta(a)}{da^2}\right)_{a=\bar{a}}}{\beta(\bar{a})} > 0, \tag{55}$$

$$c = \frac{\left(\frac{d^3\beta(a)}{da^3}\right)_{a=\bar{a}}}{2\beta(\bar{a})}, \qquad d = \frac{\left(\frac{d^4\beta(a)}{da^4}\right)_{a=\bar{a}}}{6\beta(\bar{a})}. \tag{56}$$

In calculating the r.h.s. of Eq. (54) we have repeatedly performed integration by parts and assumed the boundary terms to vanish. Introducing now the operators

$$\hat{p} = \frac{\ell_P^2}{i}\frac{d}{dx}, \qquad \hat{x} = x \tag{57}$$

one easily reads off the effective operator expression

$$\begin{aligned}\hat{Q}(\hat{p},\hat{x}) = \bar{q}\Bigg[1-\frac{\hat{p}^2}{2}-\frac{\omega^2}{2}\hat{x}^2+\frac{c}{3}\hat{x}^3+\frac{d}{4}\hat{x}^4 \\ +\frac{\omega^2}{8}(\hat{x}^2\hat{p}^2+\hat{p}^2\hat{x}^2)+\frac{\hat{p}^4}{24}+i\frac{\omega^2}{2}[\hat{p},\hat{x}^2] \\ +i\frac{c}{3}[\hat{p},\hat{x}^3]\Bigg].\end{aligned} \tag{58}$$

This result extends the findings of Ref. [29] to higher corrections in the operators $\hat{p}$, $\hat{x}$. The contribution in Eq. (54) involving only derivatives with respect to x can be viewed as the result of a continuum approximation according to

$$\langle a+\ell_P^2|\Psi\rangle + \langle a-\ell_P^2|\Psi\rangle - 2\langle a|\Psi\rangle \approx \ell_P^4\frac{d^2\tilde{\Psi}(x)}{dx^2}+\frac{\ell_P^8}{12}\frac{d^4\tilde{\Psi}(x)}{dx^4}. \tag{59}$$

Note also that the symmetric operator ordering in the last term of the second line in Eq. (54) [i.e. the middle contribution in the second line in Eq. (58)] emerges from the calculation and not an additional assumption.

As a result, the operator (58) perfectly matches the classical expression (19) taking into account the correct operator ordering and the vanishing of the commutators

$$[\hat{p},\hat{x}^2] = -2i\ell_P^2\hat{x}, \qquad [\hat{p},\hat{x}^3] = -3i\ell_P^2\hat{x}^2 \tag{60}$$

which are indeed small compared to the other contributions in (58) as they are proportional to $\hbar$. Alternatively, the matrix elements of such commutators can be viewed to be of higher order in derivatives since

$$\frac{\omega^2}{2}\int dx\Phi^*(x)[\hat{p},\hat{x}^2]\Psi(x) = \frac{\omega^2}{2}\int dx((\hat{p}\Phi)^*\hat{x}^2\Psi - \Phi^*\hat{x}^2(\hat{p}\Psi)), \tag{61}$$

where the r.h.s contains in total three derivatives with respect to a or x. Finally the coefficients in the expansions (58) and (19) obviously coincide in the limit of large quantum volumes, $\bar{a} \gg \ell_P^2$. In summary, up to the commutators discussed above, the operator (58) is the result of the canonical quantization of the classical expression (19) via the standard operator replacement (57).

When concentrating on the quadratic contributions in Eq. (58) one recovers the harmonic-oscillator expression of Ref. [29],

$$\hat{Q}_{\rm osc}(\hat{p},\hat{x}) = \bar{q}\left[1-\left(\frac{\hat{p}^2}{2}+\frac{\omega^2}{2}\hat{x}^2\right)\right] \tag{62}$$

with eigenvalues

$$q_n^{\rm osc} = \bar{q}(1-\ell_P^2\omega(n+1/2)) \tag{63}$$

and corresponding eigenfunctions

$$\psi_n(x;\omega) = \sqrt{\frac{1}{n!2^n}\sqrt{\frac{\omega}{\pi\ell_P^2}}}H_n(\sqrt{\omega}x/\ell_P)e^{-\frac{\omega}{2\ell_P^2}x^2} \tag{64}$$

where $H_n(x)$ are the usual Hermite polynomials. We note that ω has dimension of inverse area while $\ell_P^2\omega$ is dimensionless and can be computed via Eqs. (55) using $\alpha(k)$ given in Eq. (37) instead of $\beta(a)$,

$$\ell_P^4\omega^2 = -\frac{\left(\frac{d^2\alpha(k)}{dk^2}\right)_{k=\bar{k}}}{\alpha(\bar{k})}. \tag{65}$$

As stated in Ref. [29], the expressions (63) and (64) are excellent approximations to the eigenstates and eigenvalues of the (square of the) volume operator for already intermediate lengths of the involved spins. This fact is illustrated again in Fig. 1 for a typical choice of angular momentum quantum numbers all being of the order of a few tens. In addition to Ref. [29] we also plot there the wave function within the lowest-order correction in Eq. (58) arising from $c\hat{x}^3/3$ accounted for by first-order perturbation theory. Figure 2 shows similar data but for smaller spin lengths $j_i \equiv 4$. Here the oscillatorlike features of the wave functions noticeably disappear with increasing n, and the corrections from cubic term are clearly more substantial. In both Figs. 1 and 2 we have used the expression $a-\bar{a}+\ell_P^2/2$ as the argument for the wave functions where the additional increment ℓ_P^2 takes into account that $\beta(\bar{a})$ couples states of the form $|\bar{a}-\ell_P^2\rangle$ and $|\bar{a}\rangle$ and facilitates comparison with finite size data. With increasing angular momentum quantum numbers, this shift becomes more and more obsolete.

4. Negative eigenvalues of $\hat{Q}$

So far we have concentrated on the large and positive eigenvalues of the operator $\hat{Q}$. The regime of negative eigenvalues of large modulus can be explored by canonically quantizing the classical expression (24) according to the standard recipe (57),

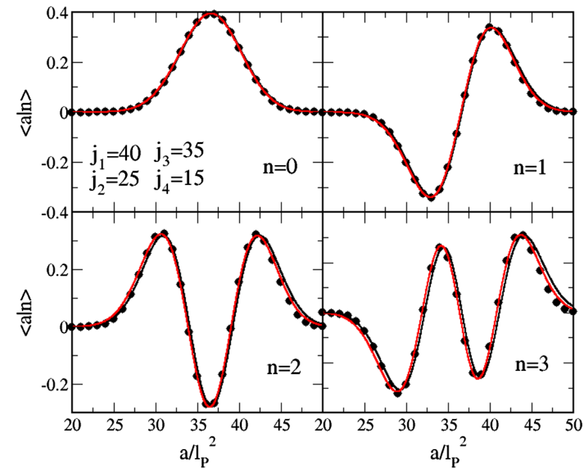

FIG. 1 (color online). The coefficients $\langle a|n\rangle$ (filled circles) for small n and a typical choice of angular momentum quantum numbers. The black solid lines are the unperturbed oscillator wave functions $\psi_n^{(0)}(a-\bar{a}+\ell_P^2/2;\omega)$ (in units of $1/\ell_P$) given in Eq. (64), while the red lines show the eigenfunctions including the first-order perturbation arising from the cubic term $c\hat{x}^3/3$ in Eq. (58).

$$\hat{Q}'_{\rm osc}(\hat{p},\hat{x}) = -\bar{q}\left[1-\left(\frac{(\hat{p}-\pi)^2}{2}+\frac{\omega^2}{2}\hat{x}^2\right)\right], \tag{66}$$

where we have put for simplicity $\tilde{q}=\bar{q}$, $\tilde{\omega}=\bar{\omega}$. This operator is related to $Q_{\rm osc}$ given in Eq. (62) by a gauge transformation along with a change in sign,

$$Q'_{\rm osc} = -e^{i\pi x/\ell_P^2}Q_{\rm osc}e^{-i\pi x/\ell_P^2} \tag{67}$$

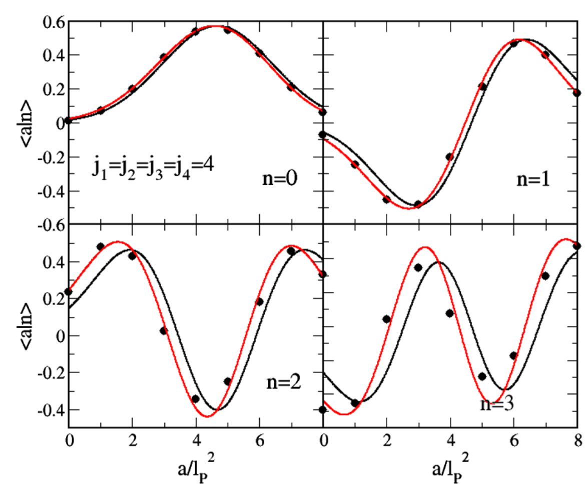

FIG. 2 (color online). The coefficients $\langle a|n\rangle$ (filled circles) for small n and $j_i \equiv 4$. The black solid lines are the unperturbed oscillator wave functions $\psi_n^{(0)}(a-\bar{a}+\ell_P^2/2;\omega)$ (in units of $1/\ell_P$) given in Eq. (64), while the red lines show the eigenfunctions including the first-order perturbation arising from the cubic term $c\hat{x}^3/3$ in Eq. (58).

such that the eigenfunctions are related by

$$\psi'_n(x) = e^{i\pi x/\ell_P^2}\psi_n(x), \tag{68}$$

where the phase factor mimics the change in sign stated in the strict relation (39) between eigenvectors of $\hat{Q}$ to eigenvalues differing in sign only. In fact, based on this analogy, Eq. (68) and, as a consequence, Eqs. (66) and (67) have already been given in Ref. [29]. Here we have provided a more profound derivation based on the canonical quantization of the classical expression (24).

5. Canonical operators in the discrete case

In the operators (57) the variable x (and, in turn, a) is considered to be a continuous quantity. Therefore the question remains how to possibly construct a pair of canonical operators retaining the discrete character of $a = k/\ell_P^2$ with k being (half-)integer. As a step towards this goal we propose the operators

$$\hat{A} = \sum_{a=a^{\min}}^{a^{\max}} a|a\rangle\langle a|. \tag{69}$$

$$\hat{P} = \frac{i}{2}\sum_{a=a^{\min}+\ell_P^2}^{a^{\max}} (|a\rangle\langle a-\ell_P^2| - |a-\ell_P^2\rangle\langle a|) \tag{70}$$

fulfilling

$$[\hat{P},\hat{A}] = \frac{\ell_P^2}{2i}\sum_{a=a^{\min}+\ell_P^2}^{a^{\max}} (|a\rangle\langle a-\ell_P^2| + |a-\ell_P^2\rangle\langle a|). \tag{71}$$

For large volumes, the r.h.s. approaches the unit operator acting on states whose components vary only little on the scale set by ℓ_P^2,

$$\langle\Phi|[\hat{P},\hat{A}]|\Psi\rangle \approx \frac{\ell_P^2}{i}\sum_{a=a^{\min}}^{a^{\max}} \langle\Phi|a\rangle\langle a|\Psi\rangle \tag{72}$$

$$= \frac{\ell_P^2}{i}\langle\Phi|\Psi\rangle. \tag{73}$$

In fact, the expression (70) is obviously a discretization of a differential operator. However, as such discretizations are by no means unique, the question remains open whether there are operators $\hat{P}'$, $\hat{A}'$ which (i) act on the original discretely labeled quantum states, (ii) turn into $\hat{p}$, $\hat{x}$ at large volumes, and (iii) fulfill

$$[\hat{P}',\hat{A}'] = \frac{\ell_P^2}{i} \tag{74}$$

as an exact equation on the entire Hilbert space.

B. General polyhedra

In full analogy to the Kapovich-Millson variables we define for a quantum polyhedron of N faces (angular momenta) the operators

$$\hat{\vec{k}}_i = \sum_{j=1}^{i+1}\hat{\vec{j}}_j \tag{75}$$

for $i \in \{1,\ldots,N-3\}$. As the squares of these quantities commute with each other,

$$[\hat{\vec{k}}_i^2,\hat{\vec{k}}_j^2] = 0, \tag{76}$$

orthonormal basis states of the Hilbert space can be labeled by quantum numbers k_i according to

$$\hat{\vec{k}}_i^2|k_1\ldots k_{N-3}\rangle = k_i(k_i+1)|k_1\ldots k_{N-3}\rangle. \tag{77}$$

The closure relation (1) translates to

$$\sum_{i=1}^{N}\hat{\vec{j}}_i|k_1\ldots k_{N-3}\rangle = 0, \tag{78}$$

i.e. the angular momentum operator $\hat{\vec{k}}_{N-3}$ couples with the remaining spins $\hat{\vec{j}}_{N-1}$, $\hat{\vec{j}}_N$ to a total singlet implying $k_{N-3}^{\min} \leq k_{N-3} \leq k_{N-3}^{\max}$ with

$$k_{N-3}^{\min} \geq |j_{N-1} - j_N|, \tag{79}$$

$$k_{N-3}^{\max} \leq j_{N-1} + j_N, \tag{80}$$

Consider now two total singlet states with $k_i = k_i^{(1)}$ and $k_i = k_i^{(2)}$, $i < N-3$, $k_i^{(1)} < k_i^{(2)}$ and all other quantum numbers k_j, $j \neq i$ identical. Then states with $k_i = k_i^{(1)} + 1,\ldots,k_i^{(2)} - 1$ (and all other k_j the same as before) are also singlets, since $\hat{\vec{k}}_{i-1}$ and $\hat{\vec{j}}_{i+1}$ can couple to these values of k_i, and $\hat{\vec{k}}_i$ with the above quantum numbers and $\hat{\vec{j}}_{i+2}$ can couple to the given value of k_{i+1}. Thus, also the other quantum numbers k_i, $i < N-3$, vary within intervals, $k_i^{\min} \leq k_i \leq k_i^{\max}$, and the representation theory of the angular momentum algebra implies

$$k_i^{\min} \geq \max\{k_{i-1}^{\min} - j_{i+1}, 0, j_{i+1} - k_{i-1}^{\max}\}, \tag{81}$$

$$k_i^{\max} \leq k_{i-1} + j_{i+1} \tag{82}$$

with $k_0 = j_1$ for $i = 1$. Without the additional conditions (79) and (80) the inequalities (81) and (82) would hold as equalities. We note, however, that the structure of the quantum numbers k_i is in general quite complex. For instance, the limiting values $k_i^{\min}$, $k_i^{\max}$ can depend on other quantum numbers k_j, $j \neq i$, and the entire structure depends obviously also on the coupling scheme, i.e. the labeling of the operators $j_1, \ldots, j_N$. A very simple example is provided by the case $N = 4$ in Eqs. (30) and (31); for $N > 4$ explicit expressions for $k_i^{\min}$, $k_i^{\max}$ become increasingly tedious.

Now rescaling the quantum numbers k_i to dimensionful quantities as in Sec. III A 2, $k_i \mapsto a_i = k_i \ell_P^2$, we define analogous to Eqs. (69) and (70) the operators

$$\hat{A}_i = \sum_{a_1 \ldots a_{N-3}} a_i |a_1 \ldots a_{N-3}\rangle\langle a_1 \ldots a_{N-3}|, \tag{83}$$

$$\hat{P}_i = \frac{i}{2} \sum_{a_1 \ldots a_{N-3}} (|a_1 \ldots a_{N-3}\rangle\langle a_1 \ldots (a_i - \ell_P^2) \ldots a_{N-3}| - |a_1 \ldots (a_i - \ell_P^2) \ldots a_{N-3}\rangle\langle a_1 \ldots a_{N-3}|) \tag{84}$$

fulfilling the commutation relations

$$[\hat{P}_i, \hat{A}_j] = \frac{\delta_{ij}\ell_P^2}{2i} \cdot \sum_{a_1 \ldots a_{N-3}} (|a_1 \ldots a_{N-3}\rangle\langle a_1 \ldots (a_i - \ell_P^2) \ldots a_{N-3}| + |a_1 \ldots (a_i - \ell_P^2) \ldots a_{N-3}\rangle\langle a_1 \ldots a_{N-3}|). \tag{85}$$

In the limit of large volumes, the above r.h.s. approaches the unit operator in just the same way as in Eq. (71).

IV. CONCLUSIONS AND OUTLOOK

The investigation of the semiclassical limit of loop quantum gravity is one of the key issues in that approach towards a quantum theory of gravitation. In the present work we have focused on semiclassical properties of quantum polyhedra. Regarding tetrahedra, as their simplest examples, Eqs. (41)–(45) provide operator analogs of classical geometric relations for tetrahedra. These classical relations are the key ingredient to the Bohr-Sommerfeld analysis of Refs. [22,23].

The expansion of the classical volume squared in up to fourth order in the canonical variables are given in Eqs. (19) and (22). We have explicitly established the connection between a canonical quantization of these expressions with a recent wave-function-based approach by the present author [29] to the large-volume sector of the quantum system. In the leading order both routes concur, yielding a quantum harmonic oscillator as an effective description for the (square of the) volume operator. As regards higher orders, the approach of Ref. [29] leads to additional corrections in terms of commutators which are naturally absent in the classical expressions. Including the third-order correction perturbatively leads to improvements of the approximate wave functions. In fact, it is a distinctive feature of the present work (and Ref. [29]) that it addresses not only the *eigenvalues* of the volume operator squared, but also provides very accurate approximations to the *eigenstates*. Furthermore, the comparison of both methods leads also to a full wave function description of the eigenstates of negative eigenvalues of large modulus, a result which could only be conjectured in Ref. [29].

Differently from previous formulations, the position variable used here is chosen to have dimension of (Planck) length squared, $\ell_P^2 = \hbar G/c^3$. This definitional detail is by no means necessary but facilitates the identification of quantum corrections. The ultimate reason for the latter observation is the fact that Planck's constant $\hbar$ itself is dimensionful.

A further interesting point is the zero eigenvalue occurring for tetrahedra with odd Hilbert space dimension d where the eigenstate can be given, up to normalization, in a closed form [13]. Moreover, the Bohr-Sommerfeld quantization carried out by Bianchi and Haggard [22,23] yields also surprisingly accurate results for eigenvalues of such small modulus. Thus the question arises whether the eigenstates corresponding to zero eigenvalues can also be cast, for large angular momenta $j_i \gg 1$, in a wave function of a continuous variable.

An important step towards extending the results for the tetrahedron to higher polyhedra is to express their volume in terms of canonical variables. In the Appendix we have achieved this goal for the case of pentahedra. However, the resulting expressions are particularly lengthy and complex such that further practical progress seems to require dedicated numerics and/or extensive but judicious use of computer algebra, which is beyond the scope of the present investigation.

For general quantum polyhedra described by discrete angular momentum quantum numbers we have formulated a set of quantum operators fulfilling in the semiclassical regime the standard commutation relations between momentum and position. Indeed a major challenge is of course the analysis of the volume operator(s) for higher polyhedra. Results towards this goal were obtained in Refs. [24,25] for pentahedra, and for the general case the operators constructed in the present paper in analogy to the Kapovich-Millson variables of the classical phase space

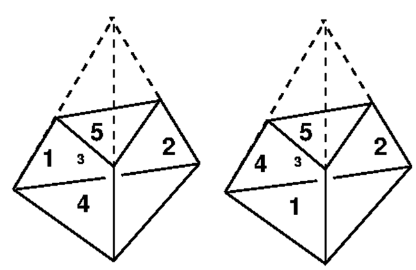

FIG. 3. A pentahedron of dominant type (trigonal prism) extended to a tetrahedron. Two different labelings of faces are shown.

might, although fairly straightforward, provide a useful step. Yet another possible route for generalizing the present investigations is to study polytopes in higher dimensions which also allow for a description in terms of SU(2) intertwiners [33].

APPENDIX: THE CLASSICAL PENTAHEDRON AND CANONICAL VARIABLES

In this Appendix we discuss the volume of a classical pentahedron in terms of Kapovich-Millson variables. We concentrate on the dominant type of pentahedra which define the submanifold of maximal dimension in the phase space of the variables $\vec{A}_i$ [20]. These pentahedra are trigonal prisms whereas a subdominant type is given by pyramidal pentahedra. These can be generated from the former type by collapsing an edge connecting the two trigonal faces onto a single point and forming therefore a submanifold of lower dimension.

1. Volume

An expression for the volume of a trigonal prism has been devised by Haggard [24] starting from the observation that such an object can always be extended to a tetrahedron. Using the labeling on the left of Fig. 3 this extended body fulfills the closure relation

$$\alpha\vec{A}_1 + \beta\vec{A}_2 + \gamma\vec{A}_3 + \vec{A}_4 = 0, \tag{A1}$$

and by projecting this equation onto appropriate cross products the above coefficients are easily obtained as

$$\alpha = -\frac{W_{234}}{W_{123}}, \qquad \beta = \frac{W_{134}}{W_{123}}, \qquad \gamma = -\frac{W_{124}}{W_{123}} \tag{A2}$$

with $W_{ijk} = \vec{A}_i \cdot (\vec{A}_j \times \vec{A}_k)$. The volume can now be expressed as the difference of two tetrahedral volumes,

$$V = \frac{\sqrt{2}}{3}\left(\sqrt{\alpha\beta\gamma} - \sqrt{(\alpha-1)(\beta-1)(\gamma-1)}\right)\sqrt{W_{123}}. \tag{A3}$$

2. Canonical variables

Our goal is now to express the scaling coefficients (A2) occurring along W_{123} in Eq. (A3) in terms of standard Kapovich-Millson variables. According to the prescription given in Sec. II A we define

$$\vec{p}_1 = \vec{A}_1 + \vec{A}_2, \tag{A4}$$

$$\vec{p}_2 = \vec{A}_1 + \vec{A}_2 + \vec{A}_3 \tag{A5}$$

and

$$\vec{v}_1 = \vec{p}_1 \times \vec{A}_2, \tag{A6}$$

$$\vec{w}_1 = \vec{v}_2 = \vec{p}_2 \times \vec{A}_3, \tag{A7}$$

$$\vec{w}_2 = \vec{p}_2 \times \vec{A}_4 \tag{A8}$$

such that the variables q_i, $i = 1, 2$, conjugate to $p_i \coloneqq |\vec{p}_i|$, are the angles between $\vec{v}_i$, $\vec{w}_i$. Using the definition (11) one has

$$|\vec{v}_1| = 2\Delta(p_1, A_1, A_2), \tag{A9}$$

$$|\vec{w}_1| = |\vec{v}_2| = 2\Delta(p_1, p_2, A_3), \tag{A10}$$

$$|\vec{w}_2| = 2\Delta(p_2, A_4, A_5). \tag{A11}$$

Moreover, the relations

$$\vec{v}_1 \times \vec{w}_1 = \vec{p}_1 W_{123}, \tag{A12}$$

$$\vec{v}_2 \times \vec{w}_2 = \vec{p}_1 (W_{134} + W_{234}) \tag{A13}$$

allow us to achieve a part of our task in a comparatively compact manner,

$$W_{123} = \frac{4\Delta(p_1, A_1, A_2)\Delta(p_1, p_2, A_3)\sin q_1}{p_1}, \tag{A14}$$

$$\beta - \alpha = \frac{\Delta(p_2, A_4, A_5) p_1 \sin q_2}{\Delta(p_1, A_1, A_2) p_2 \sin q_1}. \tag{A15}$$

Unfortunately, the remaining quantities entering the volume (A3) will turn out to lead to clearly lengthier expressions. To compute them, we shall not aim at accessing further triple products W_{ijk} directly but rather project the closure relation (A1) onto $\vec{p}_i$,

$$\alpha\vec{p}_1 \cdot \vec{A}_1 + \beta\vec{p}_1 \cdot \vec{A}_2 + \gamma\vec{p}_1 \cdot \vec{A}_3 = -\vec{p}_1 \cdot \vec{A}_4, \tag{A16}$$

$$\alpha\vec{p}_2 \cdot \vec{A}_1 + \beta\vec{p}_2 \cdot \vec{A}_2 + \gamma\vec{p}_2 \cdot \vec{A}_3 = -\vec{p}_2 \cdot \vec{A}_4, \tag{A17}$$

providing two further equations for α, β, γ with coefficients we will determine now.

From Eqs. (A4) and (A5) one easily finds

$$\vec{p}_1 \cdot \vec{A}_{1/2} = \frac{1}{2}(p_1^2 \pm (A_1^2 - A_2^2)), \tag{A18}$$

$$\vec{p}_{1/2} \cdot \vec{A}_3 = \frac{1}{2}(p_2^2 - p_1^2 \mp A_3^2), \tag{A19}$$

along with

$$\vec{p}_1 \cdot \vec{p}_2 = \frac{1}{2}(p_1^2 + p_1^2 - A_3^2), \tag{A20}$$

and, via the closure relation (1),

$$\vec{p}_2 \cdot \vec{A}_4 = -\frac{1}{2}(p_2^2 + A_4^2 - A_5^2). \quad \text{(A21)}$$

In order to determine $\vec{p}_2 \cdot \vec{A}_{1/2}$ we calculate, using Eq. (A19),

$$\begin{aligned}\vec{v}_1 \cdot \vec{w}_1 &= ((\vec{A}_1 \times \vec{A}_2) \times \vec{p}_1) \cdot \vec{A}_3 \\ &= -\vec{A}_1 \cdot \vec{A}_3(\vec{p}_1 \cdot \vec{A}_2) + \vec{A}_2 \cdot \vec{A}_3(\vec{p}_1 \cdot \vec{A}_1) \\ &= \frac{1}{2}(A_1^2 - A_2^2)\vec{p}_1 \cdot \vec{A}_3 - \frac{1}{2}p_1^2(\vec{A}_1 - \vec{A}_2) \cdot \vec{A}_3 \quad \text{(A22)}\end{aligned}$$

such that, taking into account Eq. (A20),

$$\vec{A}_{1/2} \cdot \vec{A}_3 = \frac{1}{4}\left(1 \pm \frac{A_1^2 - A_2^2}{p_1^2}\right)(p_1^2 \pm (A_1^2 - A_2^2)) \mp \frac{\vec{v}_1 \cdot \vec{w}_1}{p_1^2} \quad \text{(A23)}$$

and finally

$$\begin{aligned}\vec{p}_2 \cdot \vec{A}_{1/2} &= \vec{p}_1 \cdot \vec{A}_{1/2} + \vec{A}_3 \cdot \vec{A}_{1/2} \\ &= \frac{1}{4}(p_1^2 + p_2^2 + A_3^2) \pm (A_1^2 - A_2^2)\frac{p_1^2 + p_2^2 + A_3^2}{4p_1^2} \\ &\mp \frac{\vec{v}_1 \cdot \vec{w}_1}{p_1^2} \quad \text{(A24)}\end{aligned}$$

where

$$\vec{v}_1 \cdot \vec{w}_1 = 4\Delta(p_1, A_1, A_2)\Delta(p_1, p_2, A_3)\cos q_1. \quad \text{(A25)}$$

Similarly, one finds

$$\vec{v}_2 \cdot \vec{w}_2 = -p_2^2\vec{p}_1 \cdot \vec{A}_4 + \frac{1}{2}(p_2^2 + p_1^2 - A_3^2)\vec{p}_2 \cdot \vec{A}_4, \quad \text{(A26)}$$

which yields in combination with Eq. (A22)

$$\vec{p}_1 \cdot \vec{A}_4 = \frac{p_1^2 + p_2^2 - A_3^2}{4p_2^2}(p_2^2 + A_4^2 - A_5^2) - \frac{\vec{v}_2 \cdot \vec{w}_2}{p_2^2} \quad \text{(A27)}$$

with

$$\vec{v}_2 \cdot \vec{w}_2 = 4\Delta(p_1, p_2, A_3)\Delta(p_2, A_4, A_5)\cos q_2. \quad \text{(A28)}$$

Thus we have expressed all scalar products occurring in Eqs. (A17) and (A18) in terms of the canonical variables p_i, q_i. Taking into account Eq. (A16), these relations can now be formulated as

$$M(p_1, p_2)\begin{pmatrix}\alpha + \beta \\ \gamma\end{pmatrix} = \begin{pmatrix}F(p_i, q_i) \\ G(p_i, q_i)\end{pmatrix} \quad \text{(A29)}$$

with

$$M(p_1, p_2) = \begin{pmatrix} p_1^2 & p_2^2 - p_1^2 - A_3^2 \\ \frac{1}{2}(p_2^2 + p_1^2 + A_3^2) & p_2^2 - p_1^2 + A_3^2 \end{pmatrix} \quad \text{(A30)}$$

and

$$\begin{aligned}F(p_i, q_i) &= \frac{\Delta(p_2, A_4, A_5)p_1 \sin q_2}{\Delta(p_1, A_1, A_2)p_2 \sin q_1}(A_1^2 - A_2^2) \\ &- \frac{p_1^2 + p_2^2 - A_3^2}{2p_2^2}(p_2^2 + A_4^2 - A_5^2) + 2\frac{\vec{v}_2 \cdot \vec{w}_2}{p_2^2}, \quad \text{(A31)}\end{aligned}$$

$$\begin{aligned}G(p_i, q_i) &= \frac{\Delta(p_2, A_4, A_5)p_1 \sin q_2}{\Delta(p_1, A_1, A_2)p_2 \sin q_1} \\ &\times \left[-2\frac{\vec{v}_1 \cdot \vec{w}_1}{p_1^2} + (A_1^2 - A_2^2)\frac{p_1^2 + p_2^2 + A_3^2}{2p_1^2}\right] \\ &+ p_2^2 + A_4^2 - A_5^2. \quad \text{(A32)}\end{aligned}$$

Now, inverting the 2×2 matrix (A31) and using again Eq. (A16) one can explicitly solve for the scaling coefficients α, β, γ. This procedure, however, will obviously result in forbiddingly lengthy and complicated expressions, which is mainly due to the cumbersome structures in the r.h.s of Eq. (A30). We note that these expressions considerably simplify for $A_1 = A_2$ and $A_4 = A_5$, i.e. if the two triangular faces and two of the other faces have pairwise the same area. Then one has

$$F(p_i, q_i) = -\frac{1}{2}(p_1^2 + p_2^2 - A_3^2) + 2\frac{\vec{v}_2 \cdot \vec{w}_2}{p_2^2}, \quad \text{(A33)}$$

$$G(p_i, q_i) = -\frac{8\Delta(p_1, p_2, A_3)\Delta(p_2, A_4, A_4)}{p_1 p_2}\frac{\sin q_2}{\tan q_1} + p_2^2. \quad \text{(A34)}$$

However, also these quantities seem to be too complicated to allow for further practical analytical progress towards, e.g., the extrema of the pentahedral volume and expansions around them.

3. Relabelings and alternative variables

One might suspect that simpler expressions for the pentahedral volume can be obtained by a judicious alternative choice of the canonical variables. For example, an apparently more symmetric arrangement would be to couple the trigonal faces separately with other faces to canonical momenta. Using the labeling given on the right of Fig. 3, this means to use the definitions (A4), (A6), and (A7) as before and put

$$\vec{p}_2' = \vec{A}_4 + \vec{A}_5, \tag{A35}$$

$$\vec{v}_2' = \vec{p}_2' \times \vec{A}_4, \tag{A36}$$

$$\vec{w}_2' = \vec{p}_2' \times \vec{A}_3. \tag{A37}$$

However, the closure relation (1) immediately tells that

$$\vec{p}_2' = -\vec{p}_2, \qquad \vec{v}_2' = -\vec{w}_2, \qquad \vec{w}_2' = -\vec{v}_2. \tag{A38}$$

Thus, up to inessential signs, we end up with the same canonical variables as before. Moreover, the closure relation for the extended tetrahedral volume reads now

$$\vec{A}_1 + \alpha' \vec{A}_2 + \beta' \vec{A}_3 + \gamma' \vec{A}_4 = 0, \tag{A39}$$

where the new scaling coefficients can be expressed in terms of the old ones (A2) as [24]

$$\alpha' = \frac{\beta}{\alpha}, \qquad \beta' = \frac{\gamma}{\alpha}, \qquad \gamma' = \frac{1}{\alpha}. \tag{A40}$$

As a result, we encounter very similar technical difficulties. Furthermore, in Ref. [24] an exhaustive list of pentahedral face labelings and corresponding scaling coefficients has been given. Inspecting these results does also not give rise to the hope that such a change of variables will lead to substantially simpler expressions for the volume.

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