AFFINE RECURSIONS IN LINEAR SPACES WITH AN APPLICATION IN COMBINATORIAL CHEMISTRY

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Abstract. In terms of powers of hypermatrices, we give closed explicit formulas for vector vector sequences $v_1, v_2, \ldots \in \mathbb{C}^N \equiv \mathrm{Mat}(1, N, \mathbb{C})$ with a recursion property $v_n = \sum_{p=1} v_{n-p} A_p + b$, $n > K$ where $A_1, \ldots, A_N \in \mathbb{C}^{N\times N} \equiv \mathrm{Mat}(N, N, \mathbb{C})$ and $b \in \mathbb{C}^N$. We apply the results to solve a problem raised by combinatorial chemists on the number of torsion angle distribution for conformers of n-alkalines. We also deduce consequences on the algebraic expressions of the Taylor coefficients of rational functions in non-commutative matrix algebras.

Key words and phrases. Vector sequence, linear recursion, affine recursion, abstract Jordan decomposition, rational vector mapping.

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1 Introduction

Recent quantum chemical studies [2,3] have established that n-alkaline conformers can be divided into four disjoint finite classes $\mathcal{A}_n, \mathcal{B}_n, \mathcal{C}_n, \mathcal{D}_n$ in a manner such that, by writing a_n, b_n, c_n, d_n for their cardinality, we have

$$\begin{aligned} a_n &= a_{n-1} + b_{n-1} + d_{n-1} \\ b_n &= 2a_{n-1} + b_{n-1} + b_{n-3} + c_{n-3} + c_{n-4} \\ c_n &= 2a_{n-1} + b_{n-1} + b_{n-2} + b_{n-3} + 2c_{n-3} + c_{n-4} \\ d_n &= b_{n-1} + b_{n-2} + c_{n-1} + 2c_{n-2} + c_{n-3}. \end{aligned} \tag{1.1}$$

In [3] explicit interest is expressed for a finite formula for the resulting sequence of integer vectors $\widehat{v}_n := (a_n, b_n, c_n, d_n)$ with the starting values $\widehat{v}_{-3}, \widehat{v}_{-2}, v_{-1}, \widehat{v}_0 = (0, 0, 0, 0)$ and $\widehat{v}_1 = (1, 2, 2, 0)$. In [2] one only could handle some fortunately chosen numerical valued recursive sequences concerning the number of certain conformal geometries. We can achieve a minor reduction that it suffices to restrict our attention to the vectors $v_n := (a_n, b_n, c_n)$ because the component $d_n = b_{n-1} + b_{n-2} + c_{n-1} + 2c_{n-2} + c_{n-3}$ depends only on the components b and c while the componets b, c do not depend on the d in (1.1). In this case we have the *vector valued linear* recursion

$$v_n = v_{n-1}A_1 + v_{n-2}A_2 + v_{n-3}A_3 + v_{n-4}A_4 \tag{1.2}$$

where

$$A_1 := \begin{pmatrix} 1 & 2 & 2 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \ A_2 := \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \ A_3 := \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ 2 & 1 & 2 \end{pmatrix}, \ A_4 := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}.$$

We deduce easily from (1.2) that the vector valued generator function $g(t) := \sum_{n=0}^{\infty} t^n v_n$ satisfies an identity of the form $g(t) - \sum_{p=1}^{4} t^p g(t) A_p = \sum_{p=1}^{4} t^p b_p$ and hence it has the rational form $g(t) = \left[\sum_{p=1}^{3} t^p b_p\right]\left[I - \sum_{p=1}^{4} t^p A_p\right]$ for suitable vectors $b_1, \ldots, b_4 \in \mathbb{R}^3$. However, a Taylor expansion by means of partial fractions as it is a routine task in the scalar case is not practicable now because of the non-commutative character of the algebra of 3×3 matrices. Instead we propose a different treatment of problems analogous to (1.2) by rewriting it in the form

$$(v_n, v_{n-1}, v_{n-2}, v_{n-3}) = (v_{n-1}, v_{n-2}, v_{n-3}, v_{n-4})\mathbf{A}, \quad n > 4 \tag{1.3}$$

in terms of the $12 \times 12 (= [4 \cdot 3] \times [3 \cdot 3])$ matrix

$$\mathbf{A} := \begin{pmatrix} A_1 & I & 0 & 0 \\ A_2 & 0 & I & 0 \\ A_3 & 0 & 0 & I \\ A_4 & 0 & 0 & 0 \end{pmatrix}.$$

In this setting, an analogous role to the decomposition of the generator function to elementary fractions in the scalar case can be played by the Jordan decomposition of matrices. In Section 2 we present this idea in the framework of general complex vector spaces for affine recursions with algebraic linear part. In Section 3 we interpret the results for vector valued generator functions and hence obtain Taylor coefficients for general vector valued functions $\mathbb{R} \to \mathbb{C}^N$ of the rational type $t \mapsto \left[\sum_{p=0}^{K} t^p b_p\right]\left[\sum_{p=0}^{K} t^p A_p\right]^{-1}$. Finally, in Section 3 we discuss some related numerical problems presented with the example of (1.2) as treated in our recent paper [4] in chemistry.

2 Affine recursions with algebraic linear part

Let V be a vector space, possibly with infinite dimensions and over any field for the moment. As usually in the literature, we shall write vA for the value assumed by a linear mapping $A : V \to V$ at the vector $v \in V$. Given any natural number K along with a collection of vectors $b, v_1, \ldots, v_k \in V$ and linear maps $A_1, \ldots, A_K : V \to V$, obviously there is a unique sequence satisfying the recursion $v_{K+1}, v_{k+2}, \ldots \in V$ such that

$$v_n = b + \sum_{p=1}^{K} v_{n-p} A_p, \qquad n > K. \tag{2.1}$$

Observe that, by introducing the linear map $\mathbf{A} : V^{K+1} \to V^{K+1}$ corresponding to the operator matrix

$$\mathbf{A} := \begin{pmatrix} I & I & 0 & & & \\ 0 & A_1 & I & & & \\ & A_2 & 0 & \ddots & & \\ & \vdots & & \ddots & & \\ & A_{K-1} & & \ddots & 0 & I \\ & A_K & & & & 0 \end{pmatrix} \tag{2.2}$$

where I denotes the identity on V and we have $\mathbf{A}_{pq} = 0$ at all entries with row-column index pairs $(p,q) \notin \big\{(1,1),(p,p+1),(p+1,2):\ p=1,\ldots,K\big\}$, the vectors

$$x_n := (b, v_{K+n}, v_{n-1}, \ldots, v_{n+1}), \qquad n \geq 0$$

in V^{K+1} satisfy the linear recursion $x_n = x_{n-1}\mathbf{A}$, $n > K$. Thus simply

$$\begin{aligned} &x_n = x_0 \mathbf{A}^{n-K}, \\ &v_{K+n} = (b, v_K, v_{K-1}, \ldots, v_1)\mathbf{A}^n \mathbf{P} \quad \text{for} \quad n = 0, 1, \ldots \end{aligned} \tag{2.3}$$

where $\mathbf{P}$ denotes the coordinate projection $(w_1, \ldots, w_{K+1}) \mapsto w_2$ on V^{K+1} with $\mathbf{P}_{22} = I$ and $\mathbf{P}_{pq} = 0$ else. Though (2.3) is a closed explicit formula for the sequence $v_{K+1}, v_{K+2}, \ldots$, it is not fine enough even for purely theoretical considerations. Here we restrict our attention to an important special case, including the classical setting of $V = \mathbb{C}^N$. Recall a linear operator $T : W \to W$ over a vector space W is *algebraic* if some of its non-trivial polynomials vanishes i.e. $T^m + \sum_{p=0}^{m-1} \alpha_p T^p = 0$ with some (non-empty) finite sequence of constants $\alpha_0, \ldots, \alpha_{m-1}$. It is remarkable [1] that T admits an *abstract Jordan decomposition*

$$T = T_0 + T_1 \qquad \text{where} \quad \begin{aligned} &T_0, T_1 \text{ are polynomials of } T, \\ &T_0 \text{ is semisimple, } T_1 \text{ is nilpotent} \end{aligned}$$

if and only if $\prod_{p=1}^n (T - \lambda_p I) = 0$ for some finite sequence $\lambda_1, \ldots, \lambda_n$ of (not necessarily different) scalars.[1]By definition, $T : W \to W$ is semisimple if it has finitely many eigenvalues and its eigenvectors span the whole underlying space W, while T is nilpotent if $T^n = 0$ for some $n > 0$. In the classical case if $T = SJS^{-1}$ where S is some invertible matrix and J is a matrix consisting of Jordan blocks then $T_q = SJ_qS^{-1}$, $q = 0, 1$ where J_0 and J_1 are the diagonal and off-diagonal parts of J, respectively. E.g. for $T := S\big(\begin{smallmatrix}\lambda 1\\ 0\lambda\end{smallmatrix}\big)S^{-1}$ we have $T_0 := S\big(\begin{smallmatrix}\lambda 0\\ 0\lambda\end{smallmatrix}\big)S^{-1}$, $T_1 := S\big(\begin{smallmatrix}01\\ 00\end{smallmatrix}\big)S^{-1}$.

Henceforth we assume that the matrix $\mathbf{A}$ in (2.2) associated with the vector recursion (2.1) is algebraic, moreover it admits the abstract Jordan decomposition $\mathbf{A} = \mathbf{A}_0 + \mathbf{A}_1$ where $\mathbf{A}_1^{R+1} = 0$ for some $R \geq 0$. Since $\mathbf{A}_0$ commutes with $\mathbf{A}_1$, we have

$$\mathbf{A}^n = \sum_{p=0}^{n} \binom{n}{p} \mathbf{A}_0^{n-p} \mathbf{A}_1^p = \sum_{p=0}^{\max\{R,n\}} \binom{n}{p} \mathbf{A}_0^{n-p} \mathbf{A}_1^p, \quad n = 1, 2, \ldots.$$

Actually, by denoting by $\lambda_1, \ldots, \lambda_N$ the different eigenvalues of $\mathbf{A}$, the domain space V^{K+1} of $\mathbf{A}$ is the direct sum of the higher order eigenvectors of $\mathbf{A}$ as

$$V^{K+1} = \oplus_{q=1}^N \mathbf{V}^{(q)} \quad \text{where} \ \ \mathbf{V}^{(q)} := \big\{ v \in V :\ (\mathbf{A} - \lambda_q)^R v = 0 \big\}.$$

[1] *

The effect of $\mathbf{A}_0$ on the subspace $\mathbf{V}^{(q)}$ is just the multiplication with λ_q, while $\mathbf{A}_1$ maps $\mathbf{V}^{(q)}$ into itself and $\mathbf{A}_1^p$ vanishes on $\mathbf{V}^{(q)}$ for $p > R$. Let us write $\mathbf{Q}^{(q)}$ for the projection of the space V^{K+1} onto $\mathbf{V}^{(q)}$ along the complementary subspace $\oplus_{s:\ s\neq q}\mathbf{V}^{(s)}$. Notice that these projections commute with $\mathbf{A}$ and hence with both $\mathbf{A}_0$ and $\mathbf{A}_1$ (actually they are polynomials of $\mathbf{A}$). Therefore, for large indices $n > R$, from (2.3) it follows

$$\begin{aligned}
v_{K+n} &= (b, v_K, \ldots, v_1)\mathbf{A}^n\mathbf{P} = (b, v_K, \ldots, v_1)\sum_{p=0}^{R}\binom{n}{p}\mathbf{A}_1^{n-p}\mathbf{A}_0^p\mathbf{P} = \\
&= \Big[\sum_{q=1}^{N}(b, v_K, \ldots, v_1)\mathbf{Q}^{(q)}\Big]\sum_{p=0}^{R}\binom{n}{p}\mathbf{A}_0^{n-p}\mathbf{A}_1^p\mathbf{P} = \\
&= \sum_{p=0}^{R}\sum_{q=1}^{N}\binom{n}{p}(b, v_K, \ldots, v_1)\mathbf{A}_0^{n-p}\mathbf{Q}^q\mathbf{A}_1^p\mathbf{P} = \\
&= \sum_{\substack{0\leq p\leq R\\ 1\leq q\leq N}}\binom{n}{p}\lambda_q^{n-p}w^{(p,q)}
\end{aligned}$$

with the vectors $w^{(p,q)} := (b, v_K, \ldots, v_1)\mathbf{Q}^q\mathbf{A}_1^p\mathbf{P},\ 1 \leq q \leq N,\ 0 \leq p \leq R$ in V. The eigenvalue 0 (if occurs) plays a special role because $\lambda_q = 0$ implies $\lambda_q^s = 0$ for $s > 0$ and $\lambda_q \neq 0$ implies always that $\lambda_q^{n-p}w^{(p,q)} = \lambda_q^n\big[(1/\lambda_q)^p w^{(p,q)}\big]$. Moreover, if the minimal polynomial of $\mathbf{A}$ has the form $t \mapsto \prod_{q=1}^{N}(t-\lambda_q)^{m_q}$ then the powers $\mathbf{A}^s$, $s > m_q$ vanish on the subspace $\mathbf{V}^{(q)}$. Hence we conclude the following theorem.

Theorem 2.4. *Let V be a vector space (over any field $\mathbb{F}$) and let $b, v_1, \ldots, v_K$ be given vectors. Suppose $A_1, \ldots, A_k : V \to V$ are linear operators such that the linear operator $\mathbf{A} : V^{K+1} \to V^{K+1}$ given by (2.2) is algebraic, moreover the minimal polynomial of $\mathbf{A}$ admits the root decomposition $t^{m_0}\prod_{q=1}^{N}(t-\lambda_q)^{m_q}$ with suitable scalars $0 \neq \lambda_1, \ldots, \lambda_N \in \mathbb{F}$ and integers $m_0 \geq 0 < m_1, \ldots, m_N$, respectively. Then, the tail of the recursive sequence $v_{K+1}, v_{K+2}, \ldots$ defined by (2.2) has the form*

$$v_{K+n} = v^{(0)} + \sum_{q=1}^{N}\sum_{p=0}^{\min\{n,m_q\}}\binom{n}{p}\lambda_q^n v^{(p,q)}, \qquad n \geq 0$$

for suitable vectors $v^{(0)}, v^{(p,q)} \in V$, $(0 \leq p \leq m_q,\ 1 \leq q \leq M)$ which can be expressed in terms of the vector $(b, v_K, \ldots, v_1)$ and some polynomials of the operator $\mathbf{A}$.

2.5. Remarks. 1) In the classical finite dimensional complex case $V = \mathbb{C}^d$, the hypothesis of Theorem 2.4 hold automatically.

2) If the operator $\mathbf{A}$ is semisimple, that is if $\mathbf{A}$ has finitely many eigenvalues (say $\lambda_1, \ldots, \lambda_N$) and its eigenvectors span V^{K+1} then the minimal polynomial of $\mathbf{A}$ is $\prod_{q=1}^{N}(t-\lambda_q)$ and we have $V^{K+1} = \oplus\mathbf{V}^{(q)}$ with $\mathbf{V}^{(q)} = \{\mathbf{v} :\ \mathbf{A}\mathbf{v} = \lambda_q\mathbf{v}\}$. We can choose a basis for V^{K+1} (infinite if $\dim(V) = \infty$) consisting of vectors from $\bigcup_{q=1}^{N}\mathbf{V}^{(q)}$ and the matrix of $\mathbf{A}$ is necessarily diagonal with values $\lambda_1, \ldots, \lambda_N$ in the diagonal entries. Hence the canonical projection $\mathbf{Q}^{(q)} : V^{K+1} \to \mathbf{V}^{(q)}$ with diagonal matrix with 1 in the diagonal entries where the matrix of $\mathbf{A}$ assumes the value λ_q, can be written as

$$\mathbf{Q}^{(q)} = \ell(\mathbf{A}) \qquad \text{with any polynomial } t \mapsto \ell(t) \text{ such that } \ell(\lambda_p) = \delta_{pq}, \quad \leq p \leq N.$$

To this aim, the Lagrangian interpolation polynomial $\ell(t) := \sum_{p:\ p\neq q} \dfrac{t-\lambda_p}{\lambda_q-\lambda_p}$ is suitable.

3) In general, if the minimal polynomial of $\mathbf{A}$ has the form $t \mapsto \prod_{q=1}^N (t-\lambda_q)^{m_q}$, then

$$\mathbf{Q}^{(m)} = \ell(\mathbf{A}) \quad \text{with any polynomial } t \mapsto \ell(t) \text{ such that } \ell\big(\oplus_{q=1}^N J_{\lambda_q,m_q}\big) = \oplus \delta_{pq} I_{m_q}$$

where $J_{\lambda,m}$ is the $m{\times}m$ Jordan block with diagonal λ and I_m is the $m{\times}m$ identity matrix.

3 Vector valued rational functions via generator functions

Next we turn to the classical finite dimensional complex case $V := \mathbb{C}^d$ and we consider the generator function

$$g(t) := v_1 + tv_2 + t^2 v_3 + \cdots = \sum_{n=0}^{\infty} t^n v_{n+1} \tag{3.1}$$

of a sequence satisfying the recursion (2.1). We have

$$\begin{aligned}
g(t) - \Big[tg(t)A_1 + \cdots + t^K g(t) A_K + \sum_{n=K+1}^{\infty} t^n b \Big] &= \\
= \sum_{n=0}^{\infty} t^n v_{n+1} - \sum_{n=1}^{\infty} t^n v_n A_1 - \sum_{n=2}^{\infty} t^n v_{n-1} A_2 - \cdots - \sum_{n=K}^{\infty} t^n v_{n+1-K} A_K - \sum_{n=K}^{\infty} t^n b &= \\
= v_1 + \sum_{n=1}^{K-1} t^n \big[v_{n+1} - (v_n A_1 + v_{n-1}A_2 + \cdots + v_1 A_n)\big] &+ \\
+ \sum_{n=K}^{\infty} t^n \big[v_{n+1} - (v_n A_1 + v_{n-1}A_2 + \cdots + v_{n+1-K} A_K + b)\big] &= \\
= v_1 + \sum_{n=1}^{K-1} t^n \Big[v_{n+1} - \sum_{r=1}^{n} v_{n+1-r} A_r \Big]
\end{aligned}$$

because the coefficients of the powers t^n, $n \geq K$ vanish due to (2.1). Hence

$$g(t) = \Big[\frac{t^K}{1-t} b + \sum_{n=0}^{K-1} t^n b_n \Big] \Big[I - \sum_{p=1}^{K-1} t^p A_p \Big]^{-1} \quad \text{with} \quad b_n := v_{n+1} - \sum_{1\leq r\leq n} v_{n-r} A_r. \tag{3.2}$$

3.3 Proposition. *Let $f : (-\varepsilon, \varepsilon) \to \mathbb{C}^d$ be a rational function that is $f(t) = u(t)U(t)^{-1}$ with a couple of vector- and matrix-valued polynomials $u : \mathbb{R} \to \mathbb{C}^d$, $U : \mathbb{R} \to \mathbb{C}^{d\times d}$, respectively. Then f coincides with the generator function of some sequence $v_1, v_2, \ldots \in \mathbb{C}^d$ with a recursion property (2.1) for some $K > 0$ and $b = 0$. In particular, for the indices $n \geq K$ the Taylor coefficients of f can be written in the form $n!^{-1} d^n/dt^n|_{t=0} f(t) = v^{(0)} + \sum_{q=1}^N \sum_{p=0}^{\min\{n-K,m_q\}} \binom{n-K}{p} \lambda_q^n v^{(p,q)}$.*

Proof. Observe that we can write $f(t) = \big[\sum_{p=0}^K t^p b_p\big]\big[I - \sum_{p=1}^K t^p A_p\big]^{-1}$ with a suitable index threshold $K > 0$, vectors $b_0, \ldots b_K \in \mathbb{C}^d$ and matrices $A_1, \ldots, A_p \in \mathbb{C}^{d\times d}$. Define

$$v_1 := b_0, \quad v_{n+1} := b_n + \sum_{1\leq r\leq n} v_{n-r} A_r \quad \text{for } n = 1, \ldots, K-1.$$

By (3.2), the function f coincides with the generator function (3.1) corresponding to the recursive sequence (2.1) with $b = 0$. Hence the statements are immediate by Theorem 2.5.

4 Numerical example and problems

In this section we turn back to the numerical solution of the problem of finding an explicit formula for a the recursive vector sequence (1.2) raised by Gy. Tasi et al. [3] with the starting values

$$\begin{array}{ccccc} n & a_n & b_n & c_n & d_n \\ 1 & 1 & 2 & 2 & 0 \\ 2 & 3 & 4 & 4 & 4 \\ 3 & 11 & 10 & 12 & 14 \\ 4 & 35 & 36 & 42 & 36. \end{array} \tag{4.1}$$

As outlined in Section 1, the vectors $v_n := (a_n, b_n, c_n)$ determine the sequence $\big(d_n\big)_{n=1}^\infty$ and satisfy the recursions (1.2), (1.3). As noted, by using the Jordan normal form of $\mathbf{A}$ in (1.3), we may control easily the behavior of the sequence $\mathbf{A}, \mathbf{A}^2, \mathbf{A}^3, \ldots$. Namely, with some suitable invertible 12×12 complex matrix $\mathbf{S}$ along with a complex diagonal matrix Λ and a matrix T commuting with Λ and consisting of entries 0 or 1 which do not vanish only in the first skew row under the main diagonal. However, it is well known that *the Jordan normal form is unstable numerically (because the manifold of all semisimple matrices is dense in the full matrix algebra). Hence we have to carry out very accurate calculations in the sequel.* In this case, the characteristic polynomial of the matrix $\mathbf{A}$ is $t^6(-1 - 3*t - 3*t^2 - 7*t^3 - t^4 - 2*t^5 + t^6)$, and its minimal polynomial is $p(t) := t^4(-1 - 3*t - 3*t^2 - 7*t^3 - t^4 - 2*t^5 + t^6)$. The minimal polynomial p admits only roots of multiplicity one outside 0 two of which are real:

$$p(t) = t^4 \prod_{k=1}^{6} (t - \rho_k), \quad \text{where} \quad \begin{aligned} \rho_1 &\approx -0.3557095133858983812919855455171169070289, \\ \rho_2 &\approx \ 3.151547167817781551626140826491852089269, \\ \rho_3 &\approx -.02315525108563376585899389311326849380159+ \\ &\quad + 0.6993847859701559639410195592015526107355i, \\ \rho_5 &\approx -.3747635761303078192804270673563958561375+ \\ &\quad + 1.296624166536722887410205612984270519321i, \\ \rho_4 &= \overline{\rho_3}, \ \ \rho_6 = \overline{\rho_5}. \end{aligned}$$

These values were calculated with the symbolic computer arithmetics program MAPLE5 starting with a heuristical location of the roots and then refining the results with specially designed Newtonian algorithm. The obtained accuracy is actually within 10^{-38}. Due to the fact that all non-zero eigenvalues of $\mathbf{A}$ are simple, fortunately we can avoid the use of Jordan normal form. Indeed,

$$\mathbb{R}^{12} = \oplus_{k=1}^6 S_k, \quad S_0 := \{\mathbf{v}: \ \mathbf{v}\mathbf{A}^4 = 0\}, \ S_k := \{\mathbf{v}: \ \mathbf{v}\mathbf{A} = \rho_k \mathbf{v}\} \ \ (k > 0).$$

Thus the vectors $\mathbf{v}^{(4+n)} := (v_{8+n}, v_{7+n}, v_{6+n}, v_{5+n}) = (v_4, v_3, v_2, v_1)\mathbf{A}^{4+n}$, $n = 1, 2, \ldots$ are already linear combinations of the eigenvectors (of 1-st order) of $\mathbf{A}$. We can start with the the vector $\mathbf{v}^{(4)} \in \oplus_{k=1}^6 S_k$ which can calculated in an elementary manner with the result

$$\mathbf{v}^{(4)} = [3375, 3558, 4044, 1073, 1124, 1282, 339, 356, 404, 107, 116, 130].$$

The components of $\mathbf{v}^{(4)}$ in the subspaces S_k can be expressed in terms of the Lagrangian interpolation polynomials

$$\ell_k(t) := \prod_{j>0:\ j\neq k} \frac{t-\rho_j}{\rho_k-\rho_j}, \qquad k=1,\dots,6$$

as follows:

$$\mathbf{v}^{(4)} = \sum_{k=1}^{6} \mathbf{w}_k, \quad \mathbf{w}_k := \mathbf{v}^{(4)}\ell_k(\mathbf{A}) \in S_k.$$

Since $\mathbf{w}_k\mathbf{A} = \rho_k\mathbf{w}_k$, as a final result we see that, for any $n \geq 0$,

$$\mathbf{v}^{(4+n)} = \sum_{k=1}^{6} \rho_k^n \mathbf{w}_k,$$

$$(v_{8+n}, v_{7+n}, v_{6+n}, v_{5+n}) = \sum_{k=1}^{6} \rho_k^n (v_8, v_7, v_6, v_5)\ell_k(\mathbf{A}).$$

We are primarily interested in a short expression of $v_{8+n} = (a_{8+n}, b_{8+n}, c_{8+n})$. Since $\rho_1, \rho_2 \in \mathrm{I\!R}$ and $\rho_4 = \overline{\rho_3}$, $\rho_6 = \overline{\rho_5}$ along with $\mathbf{w}_1, \mathbf{w}_2 \in \mathrm{I\!R}^{12}$, $\mathbf{w}_4 = \overline{\mathbf{w}_3}$ and $\mathbf{w}_6 = \overline{\mathbf{w}_5}$, we have

$$v_{8+n} = \mathrm{Re}\big\{\rho_1^n[\mathbf{w}_1]_4 + \rho_2^n[\mathbf{w}_2]_4 + 2\rho_3^n[\mathbf{w}_3]_4 + 2\rho_5^n[\mathbf{w}_5]_4\big\},$$

where $[\mathbf{w}_k]_4$ denotes the last 3 terms from the 12-tuple $\mathbf{w}_k$. Actually

$$a_{8+n} = \mathrm{Re}\sum_{k=\in\{1,2,3,5\}} \rho_k^n\alpha_k, \qquad b_{8+n} = \mathrm{Re}\sum_{k=\in\{1,2,3,5\}} \rho_k^n\beta_k, \qquad c_{8+n} = \mathrm{Re}\sum_{k=\in\{1,2,3,5\}} \rho_k^n\gamma_k$$

with the coefficients (within an accuracy of 10^{-18})

$$\begin{aligned}
\alpha_1 &\approx 0.000101542114709722, & \alpha_2 &\approx 3375.074918465711739716,\\
\beta_1 &\approx -0.000053871918933272, & \beta_2 &\approx 3552.588780491677329343,\\
\gamma_1 &\approx -0.000020657650590910, & \gamma_2 &\approx 4039.314501374481984826,
\end{aligned}$$

$$\begin{aligned}
\alpha_3 &\approx 2\cdot(0.000520869023811889 + 0.003517135820364847i),\\
\beta_3 &\approx 2\cdot(0.013459833065518550 - 0.009827259460330338i),\\
\gamma_3 &\approx 2\cdot(-0.004908927797577404 - 0.004908927797577297i),
\end{aligned}$$

$$\begin{aligned}
\alpha_5 &\approx 2\cdot(-0.038030872937036058 + 1.438861710225747925i),\\
\beta_5 &\approx 2\cdot(2.692176857055283420 - 1.486015867241274322i),\\
\gamma_5 &\approx 2\cdot(2.347668569381880450 + 0.900483694962613136i).
\end{aligned}$$

4.2. Remark. The importance of an explicit algebraic formula is by no means numerical, because we can calculate the sequence $(a_n, b_n, c_n.d_n)$ elementarily even with less effort as far as we want. Such algebraic information may support structural considerations in combinatorial chemistry. Nevertheless it may have interest to see, for how big indices n do our numerical calculations coincide exactly with the real sequence. From the initial data (4.1), by standard rounding to nearest integers, we get exact continuation arriving at the magnitude

$$\big(a_{20}, b_{20}, c_{20}, d_{20}\big) = \big(3240180157,\ 3410598912,\ 3877871274,\ 3560801564\big).$$

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