Spectral sets and 3×3 nilpotent matrices

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Abstract

We have conjectured that the numerical range is a 2-spectral set for all bounded operators on a Hilbert space. This paper is an attempt to prove this conjecture in the special case of 3×3 nilpotent matrices.

1 Introduction

Let us denote by $W(A)$ the numerical range of a $d \times d$ matrix A with complex entries. We define

$$\psi(A) := \sup\{\|p(A)\|\,;p \text{ polynomial}, \ |p(z)| \leq 1 \text{ in } W(A)\}.$$

Here we use the operator norm $\|p(A)\| = \sup\{\|p(A)u\|\,; u \in \mathbb{C}^d, \|u\| \leq 1\}$ and the usual Euclidean norm $\|u\| = (\sum |u_i|^2)^{1/2}$ in $\mathbb{C}^d$. It has been proved in [2] that $\psi(A) \leq 2$ if $d = 2$ and conjectured that $\psi(A) \leq 2$ holds independently of the dimension d. In [3], we (have) obtained the uniform bound $\psi(A) \leq 11.08$. The aim of this paper is to show that the bound $\psi(A) \leq 2$ holds in the particular case of 3×3 nilpotent matrices, and furthermore that, for such matrices, $\psi(A) = 2$ implies that the numerical range $W(A)$ is a disk.

It is easily verified that $\psi(\lambda M) = \psi(M)$ if $\lambda \neq 0$, and $\psi(U^*MU) = \psi(M)$ for all unitary matrices U. Therefore we can restrict our analysis to matrices $A = A(\alpha, \beta, \gamma)$ of the form

$$A(\alpha,\beta,\gamma) = \begin{pmatrix} 0 & 2\alpha & 2\gamma \\ 0 & 0 & 2\beta \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{with} \quad \alpha \geq 0, \beta \geq 0, \gamma \geq 0, \ \alpha^2 + \beta^2 + \gamma^2 = 1.$$

Indeed, it is clear in a first time that it suffices to consider upper triangular nilpotent matrices, i.e. matrices of the form $A(\alpha, \beta, \gamma)$. Then, replacing if needed A by $\rho e^{i\theta_1} U^*AU$ with $U = \operatorname{diag}(1, e^{i\theta_2}, e^{i\theta_3})$ and ρ, θ_1, θ_2, θ_3 suitably chosen, we can assume $\alpha \geq 0$, $\beta \geq 0$, $\gamma \geq 0$, and $\alpha^2+\beta^2+\gamma^2 = 1$.

It will be shown in Section 2 that all matrices of this form with $2\alpha\beta\gamma = \tau$ share the same numerical range W_τ and that

$$\max\{\psi(A(\alpha,\beta,\gamma))\,; 2\alpha\beta\gamma = \tau\} = \max\{\psi(A(\alpha,\alpha,\gamma))\,; 2\alpha^2\gamma = \tau\}.$$

This allows us to restrict our analysis to the case of matrices of the form

$$A_s = \begin{pmatrix} 0 & \sqrt{2(1-s^2)} & 2s \\ 0 & 0 & \sqrt{2(1-s^2)} \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{with} \quad 0 \leq s \leq 1.$$

Note that, in the cases $s = 0$ and $s = 1$, the numerical range is the closed unit disk $\mathbb{D}$. Then it follows from a result of Okubo and Ando [7, 1] that $\psi(A) \leq 2$. Noticing that $\|A_0^2\| = \|A_1\| = 2$, it follows that $\psi(A_0) = \psi(A_1) = 2$. For $0 < s < 1$, the numerical range $W(A_s) = W_\tau$ with $\tau = s - s^3$ is no longer a disk, but the convex hull of the algebraic curve with tangential equation

$$w^3 - (u^2+v^2)w + \tau(u^2+v^2)u = 0.$$

We denote by g_τ the Riemann mapping from W_τ onto $\mathbb{D}$ that satisfies $g_\tau(0) = 0$, $g_\tau'(0) > 0$. Then

$$g_\tau(A_s) = M(a(s), b(s)), \qquad \text{with} \quad M(a,b) := \begin{pmatrix} 0 & a & b \\ 0 & 0 & a \\ 0 & 0 & 0 \end{pmatrix},$$

$$a(s) = \sqrt{2(1-s^2)}\, g_\tau'(0), \;\; b(s) = 2s g_\tau'(0) + (1-s^2) g_\tau''(0).$$

It is easily seen, see [2] for instance, that $\psi(A_s) = \psi_{\mathbb{D}}(g_\tau(A_s))$, with

$$\psi_{\mathbb{D}}(M) := \sup\{\|p(M)\|\,; p \text{ polynomial}, |p(z)| \leq 1 \text{ in } \mathbb{D}\}.$$

In Section 3 we will obtain an upper estimate of $\psi_{\mathbb{D}}(M(a,b)$. From this estimate we infer

Lemma 1. *We assume $a > 0$ and $b > 0$. A sufficient condition for $\psi_{\mathbb{D}}(M(a,b)) < 2$ is:*

$$3 - \sqrt{2}\,\sigma(a,b) > 0, \quad \text{with} \quad \sigma(a,b) = \min_{t \geq a} \Big(t + \frac{1}{t} + \frac{(b + a^2 - t^2)^2}{8a^2 t} \Big).$$

We now set

$$C(s) := 3 - \sqrt{2}\,\sigma(a(s), b(s)).$$

In order to settle our restricted conjecture, it suffices to show that $C(s) > 0$ for all $s \in (0,1)$. To this end we will prove that

$$C(s) = \tfrac{3}{1024} s^6 + O(s^8) \quad \text{and} \quad C(s) = \tfrac{1}{2}(1-s)^3 + O((1-s)^4);$$

this shows that the sufficient condition $C(s) > 0$ is realized for s close to 0 and close to 1. For the other values of s, we have computed numerical approximations of $D(s) = 1024\, C(s)/(3s^6)$ for $0 < s < 1/\sqrt{3}$, (and) of $E(s) = 2\, C(s)/(1-s)^3$ for $1/\sqrt{3} < s < 1$ and obtained the following arrays.

s	.03	.09	.15	.21	.27	.33	.39	.45	.51	.57
$D(s)$	1.0037	1.0352	1.1018	1.2111	1.3831	1.6521	2.0856	2.8367	4.3308	8.5866

s	.60	.63	.72	.75	.78	.81	.84	.87	.90	.93	.96	.99
$E(s)$	0.3838	0.6524	0.6513	0.6515	0.6632	0.6752	0.6920	0.7143	0.7431	0.8273	0.8882	0.9679

These arrays show a good agreement of our calculations with the expansions of $C(s)$ for s close to 0 or close to 1, i.e., with the relations $D(s) \to 1$ as $s \to 0$ and $E(s) \to 1$ as $s \to 1$. They also provide numerical evidence that $C(s) > 0$ for $0 < s < 1$ and thus that the inequality $\psi(A_s) < 2$ holds for these s. We have not succeeded to obtain a fully mathematical proof of this.

In order to obtain the expansions of $C(s)$, we first need to get expansions, with respect to τ close to 0, of the values $g_\tau'(0)$ and $g_\tau''(0)$ related to the conformal mapping. This will be the subject of Section 4. Then, we will obtain in Section 5 the expansions of the sufficient condition $C(s)$ close to 0 and 1. Finally, in the last sections we will specify the smoothness of the boundary of the numerical range, and we will describe the method used to compute the numerical approximation of the other values of $C(s)$.

2 The maximum is attained with $\alpha = \beta$

We want to show

$$\max\{\psi(A(\alpha,\beta,\gamma))\,;2\alpha\beta\gamma=\tau\} = \max\{\psi(A(\alpha,\alpha,\gamma))\,;2\alpha^2\gamma=\tau\}. \tag{1}$$

Recall that we consider matrices of the form

$$A = A(\alpha,\beta,\gamma) = \begin{pmatrix} 0 & 2\alpha & 2\gamma \\ 0 & 0 & 2\beta \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{with} \quad \alpha\geq 0, \beta\geq 0, \gamma\geq 0,\ \alpha^2+\beta^2+\gamma^2=1.$$

Since $W(A)$ is a closed convex set, it is the intersection of all the closed half-planes containing it. Therefore there exists a real function $w_m(u,v)$ such that

$$W(A) = \{x{+}iy\,; ux+vy+w_m(u,v)\leq 0,\ \forall (u,v)\in\mathbb{R}^2\setminus(0,0)\}.$$

We introduce the polynomial

$$\begin{aligned} T(u,v,w) &:= \det(\tfrac{u}{2}(A{+}A^*) + \tfrac{v}{2i}(A{-}A^*) + wI), \\ &= w^3 - (u^2{+}v^2)w + \tau\,(u^2{+}v^2)u, \quad \text{with } \tau = 2\alpha\beta\gamma. \end{aligned}$$

It is easily seen that, for all $(u,v)\in\mathbb{R}^2\setminus(0,0)$, $w_m(u,v)$ is the smallest root of the equation $T(u,v,w)=0$ (all the roots are real since they are the eigenvalues of the self-adjoint matrix $-\frac{u}{2}(A{+}A^*) - \frac{v}{2i}(A{-}A^*)$). We set

$$\Omega_\tau := \{(\alpha,\beta,\gamma)\,;\alpha\geq 0,\beta\geq 0,\gamma\geq 0,\ \alpha^2+\beta^2+\gamma^2=1, 2\alpha\beta\gamma=\tau\},$$

(note that, necessarily, $\tau\in[0,\frac{2}{3\sqrt{3}}]$). The numerical range $W(A)$ being the convex hull of the algebraic curve with tangential equation $T(u,v,w)=0$ (see [6]), all the matrices $A(\alpha,\beta,\gamma)$ with $(\alpha,\beta,\gamma)\in\Omega_\tau$ share the same numerical range, which is, from now on, denoted by W_τ.

We then deduce the property (1) from the definition of $\psi(\cdot)$ and from the following lemma

Lemma 2. *Let us consider $\tau\in[0,\frac{2}{3\sqrt{3}}]$. Then, for all polynomials p there holds*

$$\max_{(\alpha,\beta,\gamma)\in\Omega_\tau} \|p(A(\alpha,\beta,\gamma))\| = \max_{(\alpha,\alpha,\gamma)\in\Omega_\tau} \|p(A(\alpha,\alpha,\gamma))\|.$$

Proof. We have, with $A = A(\alpha,\beta,\gamma)$,

$$p(A) = \begin{pmatrix} x & y\alpha & y\gamma+z\alpha\beta \\ 0 & x & y\beta \\ 0 & 0 & x \end{pmatrix} \quad \text{with} \quad x=p(0),\ y=2p'(0),\ z=2p''(0).$$

A simple calculation yields

$$\begin{aligned} \det(\lambda{-}(p(A))^*p(A)) &= \lambda^3 - \big(E+\alpha^2\beta^2|z|^2)\big)\lambda^2 + (F+\alpha^2\beta^2G)\lambda - |x|^6, \\ \text{with} \quad E &= 3|x|^2+|y|^2+\tau\,\mathrm{Re}(y\bar z), \\ F &= |x|^2E - \tau|y|^2\,\mathrm{Re}(x\bar y)), \\ G &= |y|^4+|x|^2|z|^2 - 2\,\mathrm{Re}(\bar x y^2\bar z). \end{aligned}$$

Recall that $\|p(A)\|^2$ is the largest root of $P(\lambda,\alpha\beta) := \det(\lambda{-}(p(A))^*p(A)) = 0$. Let $\tau = \alpha\beta\gamma$ be fixed, and $\lambda_0 = \max_{(\alpha,\beta,\gamma)\in\Omega_\tau}\|p(A(\alpha,\beta,\gamma))\|^2$. We have $P(\lambda_0,\alpha\beta)\geq 0$ for all $(\alpha,\beta,\gamma)\in\Omega_\tau$ and there is a point in Ω_τ where $P(\lambda_0,\alpha\beta)=0$. Since $P(\lambda,\alpha\beta)$ depends linearly on $\alpha^2\beta^2$, we necessarily have $P(\lambda_0,\alpha\beta)=0$ if $\alpha^2\beta^2$ is minimum or if it is maximum. In these two cases we have $\alpha=\beta$. □

3 An estimate in the unit disk

Here we consider matrices of the form $M(a,b) = \left(\begin{smallmatrix} 0 & a & b \\ 0 & 0 & a \\ 0 & 0 & 0 \end{smallmatrix}\right)$, with $a \geq 0$ and $b \geq 0$, and we are looking for an estimate of

$$\psi_{\mathbb{D}}(M) := \sup\{\|p(M)\|\,; p \text{ polynomial}, |p(z)| \leq 1 \text{ in } \mathbb{D}\}.$$

If $b + a^2 \leq 1$, then $M(a,b)$ is a contraction, and it follows from the von Neumann inequality that $\psi_{\mathbb{D}}(M) = 1$. Thus, we assume from now on that $b + a^2 > 1$. From the definition we have the lower estimate

$$\psi_{\mathbb{D}}(M) \geq \max(\|M\|, \|M^2\|) = \max\left(\tfrac{1}{2}(b+\sqrt{b^2+4a^2}, a^2\right),$$

and it is known [2] that

$$\psi_{\mathbb{D}}(M) = \max\{\|(\zeta_1 - M)(1 - \bar{\zeta}_1 M)^{-1}(\zeta_2 - M)(1 - \bar{\zeta}_2 M)^{-1}\|\,; \zeta_1, \zeta_2 \in \mathbb{D}\}, \tag{2}$$

but we do not have a more explicit formula for this quantity. An upper bound for $\psi_{\mathbb{D}}(M)$ is given by the complete bound $\psi_{cb,\mathbb{D}}(M)$ of the map $p \mapsto p(A)$ from the algebra of polynomials on the disk, onto the algebra of 3×3 matrices. From a result due to Paulsen [8], we have the characterization

$$\psi_{cb,\mathbb{D}}(M) = \min\{\|H^{-1}\|\,\|H\|\,; \|H^{-1}MH\| \leq 1\}.$$

Since all matrices are unitarily similar to upper triangular matrices, we can consider only triangular matrices H in the previous formula. For symmetry reasons we have chosen matrices H of the form

$$H_t = \begin{pmatrix} t & v\sqrt{t} & -v^2/2 \\ 0 & 1 & -v/\sqrt{t} \\ 0 & 0 & 1/t \end{pmatrix}; \quad \text{then} \quad H_t^{-1} M H_t = \begin{pmatrix} 0 & a/t & \frac{b}{t^2} - \frac{2av}{t\sqrt{t}} \\ 0 & 0 & a/t \\ 0 & 0 & 0 \end{pmatrix}.$$

If $a > 0$, then for $t \geq a$ and $v = \frac{b+a^2-t^2}{2a\sqrt{t}}$, we have $\|H_t^{-1} M H_t\| = 1$. Therefore $\psi_{\mathbb{D}}(M) \leq \psi_{cb,\mathbb{D}}(M) \leq \|H_t\|\|H_t^{-1}\| = \|H_t\|^2$. A simple computation shows that $\|H_t\|^2$ is the largest root of the polynomial $X^2 - \left((\frac{v^2}{2}+t+\frac{1}{t})^2 - 2\right)X + 1$. We deduce

$$\psi_{cb,\mathbb{D}}(M) \leq \psi_M(a,b) := \tfrac{1}{4}\left(\sigma(a,b) + \sqrt{\sigma(a,b)^2 - 4}\right)^2,$$
$$\text{with} \quad \sigma(a,b) := \min_{t \geq a}\left(\frac{(b + a^2 - t^2)^2}{8a^2 t} + t + \frac{1}{t}\right).$$

It is easily seen that the minimum is attained for $t = a$ if $8a^4 - 8a^2 - 4a^2 b - b^2 \geq 0$, and for $t^2 = \frac{-3a^2+b+2\sqrt{3a^4+b^2+6a^2}}{3}$ otherwise.

We obtain Lemma 1 by noticing that $\psi_M(a,b) < 2$ is equivalent to $\sigma(a,b) < 3/\sqrt{2}$.

Remark 1. We have been convinced by our numerical experiments that $\psi_{\mathbb{D}}(M) = \psi_{cb,\mathbb{D}}(M) = \psi_M(a,b)$. Indeed we have computed a lower bound of $\psi_{\mathbb{D}}(M)$ by using an optimization procedure to approximate the maximum in Formula (2), and noted an equality with the upper bound (up to rounding error). Furthermore, the maximum is attained with two real numbers ζ_1 and ζ_2 in (2), and with $\zeta_1 = 1$ if $8a^4 - 8a^2 - 4a^2 b - b^2 \geq 0$.

Remark 2. These calculations do not work if $a = 0$. In this case, we choose $t = \sqrt{b}$ and $v = 0$. Then we obtain $\psi_{cb,\mathbb{D}}(M(0,b)) \leq \max(1,b)$. Together with the lower bound, this shows that $\psi_{\mathbb{D}}(M(0,b)) = \psi_{cb,\mathbb{D}}(M(0,b)) = \max(1,b)$.

4 Asymptotic expansion of the conformal mapping

Recall that W_τ is the convex hull of the algebraic curve with tangential equation

$$w^3 - (u^2+v^2)w + \tau(u^2+v^2)u = 0,$$

and that $g_\tau(\cdot)$ denotes the Riemann mapping from W_τ onto the unit disk $\mathbb{D}$ that satisfies $g_\tau(0) = 0$ and $g'_\tau(0) > 0$. Note that all the derivatives $g_\tau^{(k)}(0)$ are real-valued since W_τ is symmetric with respect to the real axis.

4.1 Boundary representation

From now on, we use $u = \cos\theta$, $v = \sin\theta$ and we denote by $w_m(\theta)$ the smallest root of $T(\cos\theta, \sin\theta, w) = w^3 - w + \tau\cos\theta = 0$. Then the boundary ∂W_τ is the envelope of the family of straight lines with Cartesian equations

$$x\,\cos\theta + y\,\sin\theta + w_m(\theta) = 0.$$

The corresponding contact points $\sigma(\theta) = x + iy \in \partial W_\tau$ also satisfy

$$-x\,\sin\theta + y\,\cos\theta + w'_m(\theta) = 0.$$

Therefore, we obtain the boundary representation

$$\partial W_\tau = \{\sigma(\theta) = -e^{i\theta}(w_m(\theta) + i\,w'_m(\theta))\,;\theta \in [0, 2\pi]\}.$$

Now, we use that the smallest root $z_m(\delta)$ of $z^3 - z + \delta = 0$ is an analytic function of δ, for δ small enough, and satisfies the asymptotic expansion

$$\begin{aligned} z_m(\delta) &= a_0 + a_1\delta + \cdots + a_k\delta^k + \cdots \\ &= -1 - \tfrac{\delta}{2} + \tfrac{3}{8}\,\delta^2 - \tfrac{1}{2}\delta^3 + \tfrac{105}{128}\delta^4 - \tfrac{3}{2}\delta^5 + \tfrac{3003}{1024}\delta^6 + \cdots . \end{aligned}$$

These coefficients may be recursively computed by using the formula

$$2\,a_k = -\sum_{j_1=1}^{k-1}\sum_{j_2=0}^{k-j_1} a_{j_1}a_{j_2}a_{k-j_1-j_2} + \sum_{j_2=1}^{k-1} a_{j_2}a_{k-j_2}.$$

Clearly, $w_m(\theta) = z_m(\tau\cos\theta)$, whence $\sigma(\theta) = e^{i\theta}\big(-z_m(\tau\cos\theta) + i\tau\sin\theta\, z'_m(\tau\cos\theta)\big)$, and thus

$$\begin{aligned} e^{-i\theta}\sigma(\theta) &= 1 + \textstyle\sum_{k\geq 1} a_k\tau^k\big(\frac{e^{i\theta}+e^{-i\theta}}{2}\big)^{k-1}\big(k\frac{e^{i\theta}-e^{-i\theta}}{2} - \frac{e^{i\theta}+e^{-i\theta}}{2}\big) \\ &= 1 + \textstyle\sum_{k\geq 1}(\tau/2)^k\sigma_k(e^{i\theta}), \end{aligned}$$

with the notation

$$\sigma_k(z) = a_k(z+1/z)^{k-1}\big((k-1)z - (k+1)/z\big).$$

So, we have

$$e^{-i\theta}\sigma(\theta) = 1 + \tfrac{\tau}{2}e^{-i\theta} + \tfrac{\tau^2}{4}\sigma_2(e^{i\theta}) + \cdots + \tfrac{\tau^k}{2^k}\sigma_k(e^{i\theta}) + \cdots$$

with

$$\begin{aligned} &\sigma_1(z) = 1/z, \quad \sigma_2(z) = \tfrac{3}{8}(z^2-2-3z^{-2}), \quad \sigma_3(z) = -z^3+3z^{-1}+2z^{-3}, \\ &\sigma_4(z) = \tfrac{105}{128}(3z^4+4z^2-6 - 12z^{-2}-5z^{-4}), \quad \sigma_5(z) = -3(2z^5+5z^3-10z^{-1}-10z^{-3}-3z^{-5}), \\ &\sigma_6(z) = \tfrac{3003}{1024}(5z^6+18z^4+15z^2-20-45z^{-2} - 30z^{-4}-7z^{-6}), \ldots \end{aligned}$$

Remark. *Note that the function σ depends also on τ. It is easily verified that $\sigma(\theta,\tau) = -\sigma(\theta+\pi, -\tau)$.*

4.2 An integral representation of the conformal mapping

The Riemann mapping may be written as $g_\tau(z) = z\exp(h(z))$. We set $h(x+iy) = u(x,y) + i\,v(x,y)$, with harmonic real-valued functions u, v defined on W_τ ; we have $v(x,y) = -v(x,-y)$. There exists a 2π-periodic real-valued function q such that

$$h(z) = \frac{1}{2\pi}\int_0^{2\pi} \mathcal{L}\mathrm{og}(\sigma(\varphi)-z)\, q(\varphi)\, d\varphi, \qquad \forall\, z \in W_\tau.$$

This function may be obtained by solving the equation $u = -\log|z|$ on the boundary, i.e.,

$$\frac{1}{2\pi}\int_0^{2\pi} \log|\sigma(\varphi)-\sigma(\theta)|\, q(\varphi)\, d\varphi = -\log|\sigma(\theta)|, \qquad \forall\, \theta \in \mathbb{R}, \tag{3}$$

with the condition

$$\frac{1}{2\pi}\int_0^{2\pi} q(\varphi)\, d\varphi = -1.$$

Note that q is an even function since $|\sigma(\cdot)|$ is even. Thus we may look for q of the form

$$q(\varphi) = q(\varphi,\tau) = -1 + q_1(\tau)\cos\varphi + \cdots + q_k(\tau)\cos(k\varphi) + \cdots$$

Recall that

$$\frac{1}{2\pi}\int_0^{2\pi} \log|e^{i\varphi}-e^{i\theta}|\, \cos(k\varphi)\, d\varphi = \begin{cases} -\dfrac{1}{2k}\cos(k\theta), & \text{if } 0 \neq k \in \mathbb{N},\\ 0, & \text{if } k = 0. \end{cases} \tag{4}$$

Using

$$|\sigma(\theta)| = 1 + \tfrac{\tau}{2}\cos\theta + O(\tau^2), \quad \text{and} \quad \frac{\sigma(\theta)-\sigma(\varphi)}{e^{i\theta}-e^{i\varphi}} = 1 + O(\tau^2),$$

we deduce

$$\frac{1}{2\pi}\int_0^{2\pi} \log|e^{i\varphi}-e^{i\theta}|\,(q + 1 - \tau\cos\varphi)\, d\varphi =$$
$$-\log|\sigma(\theta)| - \frac{1}{2\pi}\int_0^{2\pi} \mathrm{Re}\,\mathcal{L}\mathrm{og}\,\frac{\sigma(\theta)-\sigma(\varphi)}{e^{i\theta}-e^{i\varphi}}\, q(\varphi)\, d\varphi + \tfrac{\tau}{2}\cos\theta = O(\tau^2).$$

Therefore, since $\int_0^{2\pi}(q + 1 - \tau\cos\varphi)\, d\varphi = 0$, we infer that $q(\theta) = -1 + \tau\cos\theta + O(\tau^2)$.

We infer from the relation $\sigma(\theta,\tau) = -\sigma(\theta+\pi,-\tau)$ that the function q_k is even or odd in τ, respectively, if k is even or odd, respectively. Therefore, with values of α,β,γ that we will choose appropriately later on,

$$q_1(\tau) = \tau + \alpha\tau^3 + O(\tau^5), \quad q_2(\tau) = \beta\tau^2 + O(\tau^4), \quad q_3(\tau) = \gamma\tau^3 + O(\tau^5), \ldots$$

In order to go further in the expansion of q, we will use expansions of $\log|\sigma(\theta)|$ and of $\mathrm{Re}\,\mathcal{L}\mathrm{og}\,\frac{\sigma(\theta)-\sigma(\varphi)}{e^{i\theta}-e^{i\varphi}}$.

4.3 Expansion of $\log|\sigma(\theta)|$

We note that $\log|\sigma(\theta)| = \operatorname{Re}\mathcal{L}\mathrm{og}(e^{-i\theta}\sigma(\theta))$. Furthermore

$$e^{-i\theta}\sigma(\theta) = 1 + \tfrac{\tau}{2}e^{-i\theta} + \tfrac{\tau^2}{4}\sigma_2(e^{i\theta}) + \cdots + \tfrac{\tau^k}{2^k}\sigma_k(e^{i\theta}) + \cdots ,$$

This gives

$$\begin{aligned}\mathcal{L}\mathrm{og}(e^{-i\theta}\sigma(\theta)) &= \tfrac{\tau}{2}e^{-i\theta} + \textstyle\sum_{k\geq 2}\tfrac{\tau^k}{2^k}\sigma_k(e^{i\theta}) + \sum_{\ell\geq 2}(-1)^{\ell-1}\dfrac{1}{\ell}\Big(\sum_{k\geq 1}\big(\tfrac{\tau}{2}\big)^k\sigma_k(e^{i\theta})\Big)^\ell \\ &= \tfrac{\tau}{2}e^{-i\theta} + \textstyle\sum_{k\geq 2}\Big(\dfrac{\tau}{2}\Big)^k g_k(e^{i\theta}),\end{aligned}$$

with

$$g_k = \sum_{\ell=1}^{k}(-1)^{\ell-1}\frac{1}{\ell}\sum_{r_1+\cdots+r_\ell=k,r_j\geq 1}\sigma_{r_1}\sigma_{r_2}\ldots\sigma_{r_\ell}.$$

Taking the real part, we deduce

$$\log|\sigma(\theta)| = \tfrac{\tau}{2}\cos\theta + \textstyle\sum_{k\geq 2}\Big(\dfrac{\tau}{2}\Big)^k h_k(\theta), \quad \text{by setting } h_k(\theta) = \operatorname{Re} g_k(e^{i\theta}).$$

We have

$$\begin{aligned}&g_1 = \sigma_1, \quad g_2 = \sigma_2 - \tfrac{1}{2}\sigma_1^2, \quad g_3 = \sigma_3 - \sigma_1\sigma_2 + \tfrac{1}{3}\sigma_1^3, \quad g_4 = \sigma_4 - \sigma_1\sigma_3 - \tfrac{1}{2}\sigma_2^2 + \sigma_1^2\sigma_2 - \tfrac{1}{4}\sigma_1^4\\ &g_5 = \sigma_5 - \sigma_1\sigma_4 - \sigma_2\sigma_3 + \sigma_1^2\sigma_3 + \sigma_1\sigma_2^2 - \sigma_1^3\sigma_2 + \tfrac{1}{5}\sigma_1^5,\\ &g_6 = \sigma_6 - \sigma_1\sigma_5 - \sigma_2\sigma_4 - \tfrac{1}{2}\sigma_3^2 + \sigma_1^2\sigma_4 + 2\sigma_1\sigma_2\sigma_3 + \tfrac{1}{3}\sigma_2^3 - \sigma_1^3\sigma_3 - \tfrac{3}{2}\sigma_1^2\sigma_2^2 + \sigma_1^4\sigma_2 - \tfrac{1}{6}\sigma_1^6,\end{aligned}$$

thus

$$\begin{aligned}&g_1(z) = z^{-1}, \quad g_2(z) = \tfrac{3}{8}z^2 - \tfrac{3}{4} - \tfrac{13}{8}z^{-2}, \quad g_3(z) = -z^3 - \tfrac{3}{8}z + \tfrac{15}{4}z^{-1} + \tfrac{83}{24}z^{-3},\\ &g_4(z) = \tfrac{153}{64}z^4 + \tfrac{73}{16}z^2 - \tfrac{141}{32} - \tfrac{231}{16}z^{-2} - \tfrac{519}{64}z^{-4},\\ &g_5(z) = -\tfrac{45}{8}z^5 - \tfrac{2313}{128}z^3 - \tfrac{227}{32}z + \tfrac{2289}{64}z^{-1} + \tfrac{1605}{32}z^{-3} + \tfrac{12763}{640}z^{-5},\\ &g_6(z) = \tfrac{1697}{128}z^6 + \tfrac{3747}{64}z^4 + \tfrac{9327}{128}z^2 - \tfrac{1371}{32} - \tfrac{23697}{128}z^{-2} - \tfrac{10557}{64}z^{-4} - \tfrac{19357}{384}z^{-6}.\end{aligned}$$

Finally we get

$$\begin{aligned}&h_1(\theta) = \cos\theta, \quad h_2(\theta) = -\tfrac{3}{4} - \tfrac{5}{4}\cos 2\theta, \quad h_3(\theta) = \tfrac{27}{8}\cos\theta + \tfrac{59}{24}\cos 3\theta,\\ &h_4(\theta) = -\tfrac{141}{32} - \tfrac{79}{8}\cos 2\theta - \tfrac{183}{32}\cos 4\theta,\\ &h_5(\theta) = \tfrac{1835}{64}\cos\theta + \tfrac{4107}{128}\cos 3\theta + \tfrac{9163}{640}\cos 5\theta,\\ &h_6(\theta) = -\tfrac{1371}{32} - \tfrac{7185}{64}\cos 2\theta - \tfrac{3405}{32}\cos 4\theta - \tfrac{7133}{192}\cos 6\theta.\end{aligned}$$

4.4 Expansion of $\log\frac{|\sigma(\theta)-\sigma(\varphi)|}{|e^{i\theta}-e^{i\varphi}|}$

We have

$$\sigma(\theta) = e^{i\theta} + \tfrac{\tau}{2} + \textstyle\sum_{k\geq 2}\big(\tfrac{\tau}{2}\big)^k e^{i\theta}\sigma_k(e^{i\theta}),$$

thus

$$\frac{\sigma(\theta)-\sigma(\varphi)}{e^{i\theta}-e^{i\varphi}} = 1 + \textstyle\sum_{k\geq 2}\big(\tfrac{\tau}{2}\big)^k d_k(e^{i\theta}, e^{i\varphi}), \quad \text{with} \quad d_k(x,y) = \dfrac{x\sigma_k(x) - y\sigma_k(y)}{x-y},$$

and then

$$\log \frac{|\sigma(\theta)-\sigma(\varphi)|}{|e^{i\theta}-e^{i\varphi}|} = \sum_{k\geq 2} \left(\tfrac{\tau}{2}\right)^k \operatorname{Re}\rho_k(e^{i\theta}, e^{i\varphi}),$$

$$\text{with}\quad \rho_k = \sum_{\ell=1}^{k/2} (-1)^{\ell-1}\frac{1}{\ell}\sum_{r\in\Sigma_k} d_{r_1}d_{r_2}...d_{r_\ell}, \quad \Sigma_k = \{r=(r_1,...,r_\ell)\,;\, r_1+\cdots+r_\ell = k, r_j\geq 2\}.$$

So we have

$$\begin{aligned}
\rho_2 &= d_2 = \tfrac{3}{8}(x^2+y^2+xy+3x^{-1}y^{-1}-2),\\
\rho_3 &= d_3 = -(x^3+y^3+x^2y+xy^2) - 2(x^{-1}y^{-2}+x^{-2}y^{-1}),\\
\rho_4 &= d_4 - \tfrac{1}{2}d_2^2 = \tfrac{1}{128}\big(306(x^4+y^4)+297(x^3y+xy^3)+288x^2y^2+456(x^2+xy+y^2)-720\\
&\qquad +1368x^{-1}y^{-1}-54(xy^{-1}+x^{-1}y)+525(x^{-1}y^{-3}+x^{-3}y^{-1})+444x^{-2}y^{-2}\big),\\
\rho_5 &= d_5 - d_2d_3 = -\tfrac{45}{8}(x^5+y^5)-\tfrac{21}{4}(x^4y+xy^4)-\tfrac{39}{8}(x^3y^2+x^2y^3)-\tfrac{63}{4}(x^3+x^2y+xy^2+y^3)\\
&\qquad +\tfrac{9}{8}(x^2y^{-1}+x^{-1}y^2)+\tfrac{9}{8}(x+y)+\tfrac{3}{2}(x^{-1}+y^{-1})+\tfrac{3}{4}(xy^{-2}+x^{-2}y)\\
&\qquad -\tfrac{63}{2}(x^{-1}y^{-2}+x^{-2}y^{-1}) - \tfrac{27}{4}(x^{-2}y^{-3}+x^{-3}y^{-2})-9(x^{-1}y^{-4}+x^{-4}y^{-1}).
\end{aligned}$$

The following quantities will be needed in the next section

$$\mu_{k,\ell}(\theta) = \tfrac{1}{2\pi}\int_0^{2\pi} \rho_k(e^{i\theta}, e^{i\varphi})\,\cos\ell\varphi\,d\varphi \quad\text{and}\quad \nu_{k,\ell}(\theta) = \operatorname{Re}\mu_{k,\ell}(\theta).$$

We note that $\mu_{k,\ell}=0$ if $\ell>k$, and

$$\begin{aligned}
&\mu_{2,0} = \tfrac{3}{8}(e^{2i\theta}-2),\quad \mu_{2,1} = \tfrac{3}{16}(3e^{-i\theta}+e^{i\theta}),\quad \mu_{2,2} = \tfrac{3}{16},\\
&\mu_{3,0} = -e^{3i\theta},\quad \mu_{3,1} = -\tfrac{1}{2}e^{2i\theta}-e^{-2i\theta},\quad \mu_{3,2} = -\tfrac{1}{2}e^{i\theta}-e^{-i\theta},\quad \mu_{3,3} = -\tfrac{1}{2},\\
&\mu_{4,0} = \tfrac{1}{64}(153e^{4i\theta}+228e^{2i\theta}-360),\quad \mu_{4,1} = \tfrac{1}{256}(297e^{3i\theta}+402e^{i\theta}+1314e^{-i\theta}+525e^{-3i\theta}),\\
&\mu_{4,2} = \tfrac{1}{128}(144e^{2i\theta}+228+222e^{-2i\theta}),\\
&\mu_{5,0} = -\tfrac{45}{8}e^{5i\theta}-\tfrac{63}{4}e^{3i\theta}+\tfrac{9}{8}e^{i\theta}+\tfrac{3}{2}e^{-i\theta},\quad \mu_{5,1} = -\tfrac{21}{8}e^{4i\theta}-\tfrac{117}{16}e^{2i\theta}+\tfrac{21}{16}-\tfrac{123}{8}e^{-2i\theta}-\tfrac{9}{2}e^{-4i\theta}.
\end{aligned}$$

Considering the real parts, we obtain

$$\begin{aligned}
&\nu_{2,0} = \tfrac{3}{8}\cos 2\theta-\tfrac{3}{4},\quad \nu_{2,1} = \tfrac{3}{4}\cos\theta,\quad \nu_{2,2} = \tfrac{3}{16},\\
&\nu_{3,0} = -\cos 3\theta,\quad \nu_{3,1} = -\tfrac{3}{2}\cos 2\theta,\quad \nu_{3,2} = -\tfrac{3}{2}\cos\theta,\quad \nu_{3,3} = -\tfrac{1}{2},\\
&\nu_{4,0} = \tfrac{153}{64}\cos 4\theta+\tfrac{57}{16}\cos 2\theta-\tfrac{45}{8},\quad \nu_{4,1} = \tfrac{411}{128}\cos 3\theta+\tfrac{429}{64}\cos\theta,\quad \nu_{4,2} = \tfrac{183}{64}\cos 2\theta+\tfrac{57}{32},\\
&\nu_{5,0} = -\tfrac{45}{8}\cos 5\theta-\tfrac{63}{4}\cos 3\theta+\tfrac{21}{8}\cos\theta,\quad \nu_{5,1} = -\tfrac{57}{8}\cos 4\theta-\tfrac{363}{16}\cos 2\theta+\tfrac{21}{16}.
\end{aligned}$$

4.5 Asymptotic expansion of q

Recall that

$$q(\varphi) = q_0 + q_1(\tau)\cos\varphi + \cdots + q_k(\tau)\cos(k\varphi) + \cdots \quad\text{with}\quad q_0 = -1.$$

From (3), we deduce

$$-\frac{1}{2\pi}\int_0^{2\pi}\log|e^{i\theta}-e^{i\varphi}|\,q(\varphi)\,d\varphi = \log|\sigma(\theta)| + \frac{1}{2\pi}\int_0^{2\pi}\log\frac{|\sigma(\theta)-\sigma(\varphi)|}{|e^{i\theta}-e^{i\varphi}|}\,q(\varphi)\,d\varphi.$$

Using (4), this may be written

$$\sum_{j\geq 1}\frac{q_j(\tau)}{2j}\cos j\theta = \sum_{j\geq 1}\left(\tfrac{\tau}{2}\right)^j h_j(\theta) + \sum_{k\geq 2}\left(\tfrac{\tau}{2}\right)^k \Big(\sum_{\ell=0}^{k} q_\ell(\tau)\nu_{k,\ell}(\theta)\Big). \tag{5}$$

If j is odd (resp. even), $h_j(\theta)$ is a linear combination of $\cos(\ell\theta)$ with odd ℓ (resp. even ℓ) and $0 \leq \ell \leq k$. Similarly, if $k-j$ is odd (resp. even), $\nu_{k,j}(\theta)$ is a linear combination of $\cos(\ell\theta)$ with odd ℓ (resp. even ℓ) and $0 \leq \ell \leq k-j$. Comparing the coefficients of $\cos j\theta$, for $j = 1, 2, 3$, in (5) and using the oddness or evenness of q_k, we get

$$\frac{q_1(\tau)}{2} = \left(\tfrac{\tau}{2}\right)+\tfrac{27}{8}\left(\tfrac{\tau}{2}\right)^3+\tfrac{1835}{64}\left(\tfrac{\tau}{2}\right)^5+\tfrac{3}{4}q_1(\tau)\left(\tfrac{\tau}{2}\right)^2-\tfrac{3}{2}q_2(\tau)\left(\tfrac{\tau}{2}\right)^3+\tfrac{429}{64}q_1(\tau)\left(\tfrac{\tau}{2}\right)^4-\tfrac{21}{8}\left(\tfrac{\tau}{2}\right)^5+O(\tau^7).$$

This first gives $q_1(\tau) = \tau + O(\tau^3)$ and, by putting it into the right-hand side, $q_1(\tau) = \tau + \frac{39}{4}\left(\frac{\tau}{2}\right)^3 + O(\tau^5)$, and then reinserting it again

$$q_1(\tau) = 2\left(\tfrac{\tau}{2}\right) + \tfrac{39}{4}\left(\tfrac{\tau}{2}\right)^3 + \tfrac{2993}{32}\left(\tfrac{\tau}{2}\right)^5 - 3q_2(\tau)\left(\tfrac{\tau}{2}\right)^3 + O(\tau^7).$$

Similarly, with $j = 2$,

$$\frac{q_2(\tau)}{4} = -\tfrac{5}{4}\left(\tfrac{\tau}{2}\right)^2-\tfrac{79}{8}\left(\tfrac{\tau}{2}\right)^4-\tfrac{3}{8}\left(\tfrac{\tau}{2}\right)^2-\tfrac{3}{2}q_1(\tau)\left(\tfrac{\tau}{2}\right)^3-\left(\tfrac{57}{16}-\tfrac{183}{64}q_2(\tau)\right)\left(\tfrac{\tau}{2}\right)^4+O(\tau^6),$$

and then

$$q_2(\tau) = -\tfrac{13}{2}\left(\tfrac{\tau}{2}\right)^2 - \tfrac{263}{4}\left(\tfrac{\tau}{2}\right)^4 + O(\tau^6),$$
$$q_1(\tau) = 2\left(\tfrac{\tau}{2}\right) + \tfrac{39}{4}\left(\tfrac{\tau}{2}\right)^3 + \tfrac{3617}{32}\left(\tfrac{\tau}{2}\right)^5 + O(\tau^7).$$

Now we turn to the case $j = 3$,

$$\frac{q_3(\tau)}{6} = \tfrac{59}{24}\left(\tfrac{\tau}{2}\right)^3+\left(\tfrac{\tau}{2}\right)^3+O(\tau^5),$$

and obtain

$$q_3(\tau) = \tfrac{83}{4}\left(\tfrac{\tau}{2}\right)^3 + O(\tau^5).$$

In a general way, we have $q_k(\tau) = O(\tau^k)$.

4.6 Asymptotic expansions of $g'_\tau(0)$ and $g''_\tau(0)$

For $x \in \mathbb{R}$, we have $g_\tau(x) = x\,\exp(u(x, 0))$; thus $g'_\tau(0) = \exp(u(0))$ and $g''_\tau(0) = 2g'_\tau(0)u'_x(0)$. We also have

$$u(0) = \tfrac{1}{2\pi}\int_0^{2\pi}\log|\sigma(\theta)|\,q(\theta)\,d\theta \quad\text{and}\quad u'_x(0) = -\tfrac{1}{2\pi}\int_0^{2\pi}\mathrm{Re}\left(\frac{1}{\sigma(\theta)}\right)q(\theta)\,d\theta.$$

From Section 4.3 we have

$$\tfrac{1}{2\pi}\int_0^{2\pi}\log|\sigma(\theta)|\,d\theta = -\tfrac{3}{4}\left(\tfrac{\tau}{2}\right)^2 - \tfrac{141}{32}\left(\tfrac{\tau}{2}\right)^4 - \tfrac{1371}{32}\left(\tfrac{\tau}{2}\right)^6 + O(\tau^8),$$
$$\tfrac{1}{2\pi}\int_0^{2\pi}\log|\sigma(\theta)|\cos\theta\,d\theta = \tfrac{1}{2}\left(\tfrac{\tau}{2}\right) + \tfrac{27}{16}\left(\tfrac{\tau}{2}\right)^3 + \tfrac{1835}{128}\left(\tfrac{\tau}{2}\right)^5 + O(\tau^7),$$
$$\tfrac{1}{2\pi}\int_0^{2\pi}\log|\sigma(\theta)|\cos 2\theta\,d\theta = -\tfrac{5}{8}\left(\tfrac{\tau}{2}\right)^2 - \tfrac{79}{16}\left(\tfrac{\tau}{2}\right)^4 + O(\tau^6),$$
$$\tfrac{1}{2\pi}\int_0^{2\pi}\log|\sigma(\theta)|\cos 3\theta\,d\theta = \tfrac{59}{48}\left(\tfrac{\tau}{2}\right)^3 + O(\tau^5).$$

Note also that $\int_0^{2\pi} \log|\sigma(\theta)| \cos k\theta \, d\theta = O(\tau^k)$. We deduce

$$\begin{aligned} u(0) &= \tfrac{3}{4}\left(\tfrac{\tau}{2}\right)^2 + \tfrac{141}{32}\left(\tfrac{\tau}{2}\right)^4 + \tfrac{1371}{32}\left(\tfrac{\tau}{2}\right)^6 + \left(\tfrac{1}{2}\left(\tfrac{\tau}{2}\right) + \tfrac{27}{16}\left(\tfrac{\tau}{2}\right)^3 + \tfrac{1835}{128}\left(\tfrac{\tau}{2}\right)^5\right)\left(2\left(\tfrac{\tau}{2}\right) + \tfrac{39}{4}\left(\tfrac{\tau}{2}\right)^3 \right. \\ &\qquad \left. + \tfrac{3617}{32}\left(\tfrac{\tau}{2}\right)^5\right) + \left(\tfrac{5}{8}\left(\tfrac{\tau}{2}\right)^2 + \tfrac{79}{16}\left(\tfrac{\tau}{2}\right)^4\right)\left(\tfrac{13}{2}\left(\tfrac{\tau}{2}\right)^2 + \tfrac{263}{4}\left(\tfrac{\tau}{2}\right)^4\right) + \tfrac{59}{48} \times \tfrac{83}{4}\left(\tfrac{\tau}{2}\right)^6 + O(\tau^8) \\ &= \tfrac{7}{4}\left(\tfrac{\tau}{2}\right)^2 + \tfrac{535}{32}\left(\tfrac{\tau}{2}\right)^4 + \tfrac{23345}{96}\left(\tfrac{\tau}{2}\right)^6 + O(\tau^8). \end{aligned}$$

This gives

$$g_\tau'(0) = 1 + \tfrac{7}{16}\tau^2 + \tfrac{73}{64}\tau^4 + \tfrac{17493}{4096}\tau^6 + O(\tau^8).$$

For the expansion of $u_x'(0)$, we will first need an expansion of $1/\sigma(\theta)$. Recall that

$$\begin{aligned} \frac{e^{i\theta}}{\sigma(\theta)} &= \left(1 + \textstyle\sum_{k\geq 1} \sigma_k(e^{i\theta})\left(\tfrac{\tau}{2}\right)^k\right)^{-1} \\ &= 1 - \sigma_1 \tfrac{\tau}{2} + (\sigma_1^2 - \sigma_2)\left(\tfrac{\tau}{2}\right)^2 + (2\sigma_1\sigma_2 - \sigma_3 + -\sigma_1^3)\left(\tfrac{\tau}{2}\right)^3 + (-\sigma_4 + \sigma_2^2 + 2\sigma_1\sigma_3 - 3\sigma_1^2\sigma_2 + \sigma_1^4)\left(\tfrac{\tau}{2}\right)^4 \\ &\qquad + (-\sigma_5 + 2\sigma_1\sigma_4 + 2\sigma_2\sigma_3 - 3\sigma_1^2\sigma_3 - 3\sigma_1\sigma_2^2 + 4\sigma_1^3\sigma_2 + \sigma_1^5)\left(\tfrac{\tau}{2}\right)^5 + O(\tau^6); \end{aligned}$$

therefore

$$\begin{aligned} \frac{1}{\sigma(\theta)} &= e^{-i\theta} - e^{-2i\theta}\tfrac{\tau}{2} + \left(-\tfrac{3}{8}e^{i\theta} + \tfrac{3}{4}e^{-i\theta} + \tfrac{17}{8}e^{-3i\theta}\right)\left(\tfrac{\tau}{2}\right)^2 + \left(e^{2i\theta} + \tfrac{3}{4} - \tfrac{9}{2}e^{-2i\theta} - \tfrac{21}{4}e^{-4i\theta}\right)\left(\tfrac{\tau}{2}\right)^3 \\ &\qquad + \left(\tfrac{297}{64}e^{3i\theta} - \tfrac{187}{32}e^{i\theta} + \tfrac{225}{64}e^{-i\theta} - \tfrac{633}{32}e^{-3i\theta} - \tfrac{1623}{128}e^{-5i\theta}\right)\left(\tfrac{\tau}{2}\right)^4 \\ &\qquad\qquad + \left(-\tfrac{51}{8}e^{4i\theta} - \tfrac{21}{4}e^{2i\theta} + \tfrac{63}{4} + 12e^{-2i\theta} - \tfrac{199}{8}e^{-4i\theta} - \tfrac{39}{4}e^{-6i\theta}\right)\left(\tfrac{\tau}{2}\right)^5 + O(\tau^6), \end{aligned}$$

whence

$$\begin{aligned} \operatorname{Re}\frac{1}{\sigma(\theta)} &= \cos\theta - \cos 2\theta\,\tfrac{\tau}{2} + \left(\tfrac{3}{8}\cos\theta + \tfrac{17}{8}\cos 3\theta\right)\left(\tfrac{\tau}{2}\right)^2 + \left(\tfrac{3}{4} - \tfrac{7}{2}\cos 2\theta - \tfrac{21}{4}\cos 4\theta\right)\left(\tfrac{\tau}{2}\right)^3 \\ &\quad -\left(\tfrac{149}{64}\cos\theta + \tfrac{969}{64}\cos 3\theta + \tfrac{1623}{128}\cos 5\theta\right)\left(\tfrac{\tau}{2}\right)^4 + \left(\tfrac{63}{4} + \tfrac{27}{4}\cos 2\theta - 20\cos 4\theta - \tfrac{39}{4}\cos 6\theta\right)\left(\tfrac{\tau}{2}\right)^5 + O(\tau^6). \end{aligned}$$

This yields

$$\begin{aligned} \tfrac{1}{2\pi}\int_0^{2\pi} \operatorname{Re}\tfrac{1}{\sigma(\theta)}\,d\theta &= \tfrac{3}{4}\left(\tfrac{\tau}{2}\right)^3 + \tfrac{63}{4}\left(\tfrac{\tau}{2}\right)^5 + O(\tau^7), \\ \tfrac{1}{2\pi}\int_0^{2\pi} \operatorname{Re}\tfrac{1}{\sigma(\theta)}\,\cos\theta\,d\theta &= \tfrac{1}{2} + \tfrac{3}{16}\left(\tfrac{\tau}{2}\right)^2 - \tfrac{149}{128}\left(\tfrac{\tau}{2}\right)^4 + O(\tau^6), \\ \tfrac{1}{2\pi}\int_0^{2\pi} \operatorname{Re}\tfrac{1}{\sigma(\theta)}\,\cos 2\theta\,d\theta &= -\tfrac{1}{2}\tfrac{\tau}{2} - \tfrac{7}{4}\left(\tfrac{\tau}{2}\right)^3 + O(\tau^5), \\ \tfrac{1}{2\pi}\int_0^{2\pi} \operatorname{Re}\tfrac{1}{\sigma(\theta)}\,\cos 3\theta\,d\theta &= \tfrac{17}{16}\left(\tfrac{\tau}{2}\right)^2 + O(\tau^4). \end{aligned}$$

Returning to $u_x'(0)$, and using the oddness in τ, we obtain

$$\begin{aligned} u_x'(0) &= \tfrac{3}{4}\left(\tfrac{\tau}{2}\right)^3 + \tfrac{63}{4}\left(\tfrac{\tau}{2}\right)^5 - \left(\tfrac{1}{2} + \tfrac{3}{16}\left(\tfrac{\tau}{2}\right)^2 - \tfrac{149}{128}\left(\tfrac{\tau}{2}\right)^4\right)\left(2\tfrac{\tau}{2} + \tfrac{39}{4}\left(\tfrac{\tau}{2}\right)^3 + \tfrac{3617}{32}\left(\tfrac{\tau}{2}\right)^4\right) \\ &\qquad - \left(\tfrac{1}{2}\tfrac{\tau}{2} + \tfrac{7}{4}\left(\tfrac{\tau}{2}\right)^3\right)\left(\tfrac{13}{2}\left(\tfrac{\tau}{2}\right)^2 + \tfrac{263}{4}\left(\tfrac{\tau}{2}\right)^4\right) - \tfrac{17}{16} \times \tfrac{83}{4}\left(\tfrac{\tau}{2}\right)^5 + O(\tau^7), \end{aligned}$$

and finally

$$u_x'(0) = -\tfrac{\tau}{2} - \tfrac{31}{32}\tau^3 - \tfrac{1705}{512}\tau^5 + O(\tau^7) \quad \text{and} \quad g_\tau''(0) = -\tau - \tfrac{19}{8}\tau^3 - \tfrac{1107}{128}\tau^5 + O(\tau^7).$$

5 Expansion of the sufficient condition $C(s)$

Recall that

$$\begin{aligned} C(s) &:= 3-\sqrt{2}\,\sigma(a(s),b(s)), \quad \text{with} \quad \tau = s - s^3, \\ a(s) &= \sqrt{2(1-s^2)}g'_\tau(0), \;\; b(s) = 2sg'_\tau(0) + (1-s^2)g''_\tau(0), \\ \sigma(a,b) &= \min_{t\geq a}\Big(t+\frac{1}{t}+\frac{(b+a^2-t^2)^2}{8a^2t}\Big). \end{aligned}$$

Using the expansions obtained in the previous section

$$\begin{aligned} g'_\tau(0) &= 1+\tfrac{7}{16}\tau^2+\tfrac{73}{64}\tau^4+\tfrac{17493}{4096}\tau^6+O(\tau^8), \\ g''_\tau(0) &= -\tau-\tfrac{19}{8}\tau^3-\tfrac{1107}{128}\tau^5+O(\tau^7), \end{aligned}$$

we get successively

$$\begin{aligned} g'_\tau(0) &= 1+\tfrac{7}{16}s^2+\tfrac{17}{64}s^4+\tfrac{597}{4096}s^6+O(s^8), \\ g''_\tau(0) &= -s-\tfrac{11}{8}s^3-\tfrac{195}{128}s^5+O(s^7), \\ a(s) &= \sqrt{2}(1-\tfrac{1}{16}s^2-\tfrac{5}{64}s^4-\tfrac{427}{4096}s^6)+O(s^8), \\ b(s) &= s+\tfrac{1}{2}s^3+\tfrac{49}{128}s^5+O(s^7). \end{aligned}$$

We have seen in Section 3 that the minimum in the definition of $\sigma(a,b)$ is attained for $t=a$ if $8a^4-8a^2-4a^2b-b^2 \geq 0$, and for $t^2 = \frac{-3a^2+b+2\sqrt{3a^4+b^2+6a^2}}{3}$ otherwise. Thus, for s close to 0, $t=a$ and

$$\begin{aligned} \sigma(a(s),b(s)) &= a(s)+1/a(s)+b(s)^2/(8a(s)^3), \\ &= \tfrac{1}{\sqrt{2}}\big(3-\tfrac{1}{16}s^2-\tfrac{19}{16}s^4-\tfrac{193}{2048}s^6+O(s^8)\big)+b(s)^2/(8a(s)^3), \\ &= \tfrac{1}{\sqrt{2}}\big(3-\tfrac{3}{1024}s^6+O(s^8)\big). \end{aligned}$$

This gives

$$C(s) = \tfrac{3}{1024}s^6+O(s^8),$$

which shows that the sufficient condition $C(s)>0$ holds for s close to 0.

For s close to 1, we set $\sigma=\sqrt{1-s^2}$; then σ is close to 0, $\tau=\sigma^2\sqrt{1-\sigma^2}=\sigma^2-\frac{1}{2}\sigma^4+O(\sigma^6)$, whence

$$\begin{aligned} g'_\tau(0) &= 1+\tfrac{7}{16}\sigma^4-\tfrac{7}{16}\sigma^6+O(\sigma^8), \qquad & g''_\tau(0) &= -\sigma^2+\tfrac{1}{2}\sigma^4-\tfrac{9}{4}\sigma^6+O(\sigma^8), \\ a(s)^2 &= 2\sigma^2+\tfrac{7}{4}s^6+O(\sigma^8), & b(s) &= 2-\sigma^2-\tfrac{3}{8}\sigma^4-\tfrac{15}{16}\sigma^6+O(\sigma^8). \end{aligned}$$

The minimum in the definition of $\sigma(a,b)$ is attained for $t^2 = \frac{-3a^2+b+2\sqrt{3a^4+b^2+6a^2}}{3}$, whence $b+a^2-t^2 = \frac{4a^2(b+a^2-1)}{b+\sqrt{3a^4+b^2+6a^2}}$. We successively get

$$\begin{aligned} b+a^2-1 &= 1+\sigma^2-\tfrac{3}{8}\sigma^4+O(\sigma^6), \qquad \sqrt{3a^4+b^2+6a^2} = 2(1+\sigma^2+\tfrac{15}{16}\sigma^4)+O(\sigma^6), \\ & b+3a^2+\sqrt{3a^4+b^2+6a^2} = 4+7\sigma^2+\tfrac{3}{2}\sigma^4+O(\sigma^6), \\ \frac{b+a^2-t^2}{a^2} &= \frac{4(b+a^2-1)}{b+3a^2+\sqrt{3a^4+b^2+6a^2}} = 1-\tfrac{3}{4}\sigma^2+\tfrac{9}{16}\sigma^4+O(\sigma^6), \end{aligned}$$

$$
\begin{aligned}
b+a^2-t^2 &= 2\sigma^2 - \tfrac{3}{2}\sigma^4 + \tfrac{23}{8}\sigma^6 + O(\sigma^8),\\
t^2 &= 2 - \sigma^2 + \tfrac{9}{8}\sigma^4 - \tfrac{33}{16}\sigma^6 + O(\sigma^8),\\
t &= \sqrt{2}(1 - \tfrac{1}{4}\sigma^2 + \tfrac{1}{4}\sigma^4 - \tfrac{29}{64}\sigma^6 + O(\sigma^8),\\
\sqrt{2}(t+\frac{1}{t}) &= 3 - \tfrac{1}{4}\sigma^2 + \tfrac{5}{16}\sigma^4 - \tfrac{9}{16}\sigma^6 + O(\sigma^8),\\
\Big(\frac{b+a^2-t^2}{a^2}\Big)^2 &= 1 - \tfrac{3}{2}\sigma^2 + \tfrac{27}{16}\sigma^4 + O(\sigma^6),\\
\frac{(b+a^2-t^2)^2}{a^2} &= 2\sigma^2 - 3\sigma^4 + \tfrac{41}{8}\sigma^6 + O(\sigma^8),\\
\sqrt{2}\frac{(b+a^2-t^2)^2}{8a^2t} &= \tfrac{1}{4}\sigma^2 - \tfrac{5}{16}\sigma^4 + \tfrac{1}{2}\sigma^6 + O(\sigma^8),
\end{aligned}
$$

Finally we obtain

$$
C(s) = 3 - \sqrt{2}\Big(t + \frac{1}{t} + \frac{(b+a^2-t^2)^2}{8a^2t}\Big) = \frac{\sigma^6}{16} + O(\sigma^8) = \frac{(1-s)^3}{2} + O\big((1-s)^4\big).
$$

This shows that the estimate $C(s) > 0$ also holds for s close to 1.

6 About the numerical range

The main geometric and algebraic properties of numerical ranges of matrices are described in the authoritative work of Kippenhahn [6]. Here, we develop a more specific study in our particular case of nilpotent 3×3 matrices, see also [5, section 4]. For the next section, we will need a parametric representation of the boundary of the numerical range. For that, it will be useful to better understand the properties of the algebraic curve $\mathcal{C}_\tau$ with tangential equation

$$
T(u,v,w) = w^3 - (u^2{+}v^2)w + \tau\,(u^2{+}v^2)u = 0, \qquad 0 \le \tau \le \tau_1 := \tfrac{2}{3\sqrt{3}}.
$$

Note that, if w is a double root of $T(\cos\theta, \sin\theta, \cdot)$, then $w^2 = 1/3$, $\tau = \tau_1$ and $\theta = k\pi$, $k \in \mathbb{Z}$.

We first consider the case $0 \le \tau < \tau_1$. Then, we denote (by) $w_m(\theta) < w_i(\theta) < w_M(\theta)$ the roots of $T(\cos\theta, \sin\theta, \cdot)$ (we will also note $w(\theta)$ any one of these roots). They are analytical functions of θ and of τ, and we have explicit formulae, for instance

$$
w_m(\theta) = -\frac{2}{\sqrt{3}}\sin\frac{\pi + \arcsin((3\sqrt{3}\tau\cos\theta)/2)}{3}.
$$

These roots correspond to the points $\sigma_m(\theta) = -e^{i\theta}(w_m(\theta){+}iw_m'(\theta))$, $\sigma_i(\theta) = -e^{i\theta}(w_i(\theta){+}iw_i'(\theta))$ and $\sigma_M(\theta) = -e^{i\theta}(w_M(\theta) + iw_M'(\theta))$ of $\mathcal{C}_\tau$. They satisfy $w_M(\theta) = -w_m(\theta{+}\pi)$ and $w_i(\theta) = -w_i(\theta{+}\pi)$, whence $\sigma_M(\theta) = \sigma_m(\theta{+}\pi)$ and $\sigma_i(\theta) = \sigma_i(\theta{+}\pi)$. For $\tau = 0$, $\sigma_m(\theta) = -\sigma_M(\theta) = -e^{i\theta}$, these points go around the unit circle while the point $\sigma_i(\theta) = 0$ stays fix. For $0 < \tau < \frac{2}{3\sqrt{3}}$, the points $\sigma_m(\theta)$ and $\sigma_M(\theta)$ follow the boundary of W_τ when θ varies from 0 to 2π, while the point $\sigma_i(\theta)$ draws a closed curve $\mathcal{C}_\tau^{(i)} \subset \mathcal{C}_\tau$ interior to W_τ twice. Note that this internal curve has only one tangent orthogonal to a given direction $(\cos\theta, \sin\theta)$.

Remark. *From $T(\cos\theta, \sin\theta, -1/\sqrt{3}) = \tau_1 + \tau\cos\theta > 0$, we deduce $w_m(\theta) < -1/\sqrt{3}$.*

If $\sigma(\theta_0) = -e^{i\theta}(w(\theta_0) + iw'(\theta_0))$ is a singular point of $\mathcal{C}_\tau$, then we have $\sigma'(\theta_0) = 0$, i.e., $w(\theta_0) + w''(\theta_0) = 0$. Combining this with $w(\theta_0)^3 - w(\theta_0) + \tau\cos\theta_0 = 0$,

$(3w^2(\theta_0){-}1)w'(\theta_0) - \tau \sin\theta_0 = 0$, $(3w(\theta_0)^2{-}1)w''(\theta_0) + 6w(\theta_0)w'(\theta_0)^2 - \tau\cos\theta_0 = 0$, we first obtain $(-2w(\theta_0)^2 + 6w'(\theta_0)^2)w(\theta_0) = 0$. This gives

- either $w(\theta_0) = 0$. From the previous remark we have $\sigma(\theta_0) = \sigma_i(\theta_0)$ and $\theta_0 = \pi/2$ (we can assume $\theta_0 \in [0,\pi)$), $w'(\theta_0) = -\tau$. Thus, in this case the singular point is $\sigma(\theta_0) = -\tau$.
- or $w(\theta_0)^2 = 3w'(\theta_0)^2$. Then we have

$$3\tau^2 = 3\tau^2\cos^2\theta_0 + 3\sin^2\theta_0 = 3(w(\theta_0)^3{-}w(\theta_0))2 + (3w(\theta_0)^2{-}1)^2 w(\theta_0)^2, \quad \text{i.e.}$$
$$P(w(\theta_0)^2) = 0, \qquad \text{with} \quad P(X) := 12\,X^3 - 12\,X^2 + 4\,X - 3\tau^2.$$

Note that $P'(X) > 0$ for all $X \in \mathbb{R}$ and $P(0)P(1/3) < 0$; therefore $P(X) = 0$ has only one real solution X_0 and this solution satisfies $0 < X_0 < 1/3$. This shows that $w(\theta_0) = w_i(\theta_0) = \varepsilon\sqrt{X_0}$, $w'(\theta_0) = \varepsilon'\sqrt{X_0/3}$, with $\varepsilon = \pm 1$, $\varepsilon' = \pm 1$. Thus we obtain two singular points

$$\begin{aligned}\sigma(\theta_0) = \sigma_i(\theta_0) &= -e^{i\theta_0}(w(\theta_0) + iw'(\theta_0))\\ &= \frac{1}{\tau}\big(w(\theta_0)^3{-}w(\theta_0) + i(1{-}3w(\theta_0)^2)w'(\theta_0)\big)(w(\theta_0) + iw'(\theta_0))\\ &= \frac{1}{\tau}\big(2X_0^2 - \tfrac{4}{3}X_0 \pm 2i\tfrac{1}{\sqrt{3}}X_0^2\big).\end{aligned}$$

We have found that all singular points of the algebraic curve $\mathcal{C}_\tau$ belong to the internal part $\mathcal{C}_\tau^{(i)}$. Easy to obtain expansions show that these three points are of cusp type. (Such singularities are necessary to obtain a closed curve that has only one tangent parallel to any given direction). Note that, the complex plane being identified to $\mathbb{R}^2$, we have only considered the *real part* of the algebraic curve; if we also consider its *complex part* (i.e., in $\mathbb{C}^2$), there also exist six other singular points.

From Plücker relations (see, for instance, [10, 4]), we know that the Cartesian equation of $\mathcal{C}_\tau$ is polynomial in x, y (and in τ) of degree ≤ 6. Since there is no singular point on the part ∂W_τ, the boundary of the numerical range is analytic. From this we infer that the conformal mapping $g_\tau(\cdot)$ is analytic up to the boundary of W_τ. The dependences of ∂W_τ and of $g_\tau(\cdot)$ on $\tau \in [0,\tau_1)$ are also analytic. In particular $g'_\tau(0)$ and $g''_\tau(0)$ are analytic functions of $\tau \in [0,\tau_1)$.

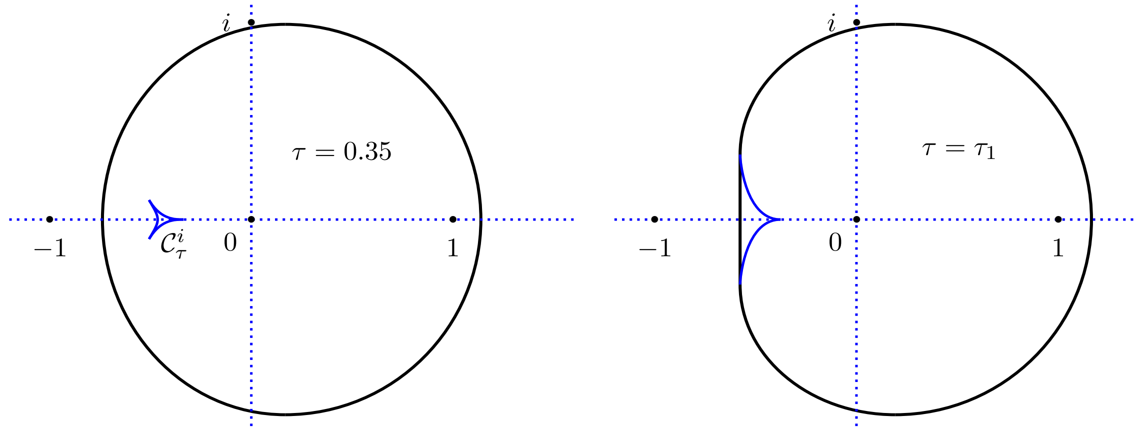

Figure 1: The algebraic curve for $\tau = 0.35$ and for $\tau = \tau_1$.

The case $\tau = \tau_1 = 2/(3\sqrt{3})$. A large part of the previous analysis is valid, except that now the two conjugate singular points

$$\sigma_1 = \frac{1}{\tau_1}\big(2X_0^2 - \tfrac{4}{3}X_0 + 2i\tfrac{1}{\sqrt{3}}X_0^2\big) = \frac{1}{\sqrt{3}} + \frac{i}{3} \qquad \text{and} \quad \sigma_2 = \frac{1}{\sqrt{3}} - \frac{i}{3}$$

of $\mathcal{C}_{\tau_1}^{(i)}$ also belong to ∂W_{τ_1}. The boundary of the numerical range now has a flat part which is the segment $[\sigma_1, \sigma_2]$. We loose the analyticity of ∂W_{τ_1} in these two points, the boundary now is a C^1- joining of (a part of) an analytic curve and of this segment. The conformal mapping $g_{\tau_1}(\cdot)$ is $C^{1,\alpha}$ for all $0 \le \alpha < 1$ (Kellogg-Warschawski theorem) but not C^2 ; the functions $g_\tau'(0)$ and $g_\tau''(0)$ are continuous for $\tau \in [0, \tau_1]$.

We can remark that the solutions of $T(u, v, w) = 0$ are given (up to multiplication by a constant) by $u = 1{-}3t^2$, $v = 3t{-}t^3$, $w = -3\tau_1(1{+}t^2)$, with a parameter $t \in \mathbb{R}$, or by $(u, v, w) = (0, 1, 0)$. This provides a parametric representation of $\mathcal{C}_{\tau_1} = \{x(t){+}iy(t)\,; t \in \mathbb{R}{\cup}\{\infty\}\}$

$$x(t) = \tau_1 \frac{3 - 6t^2 - t^4}{(1 + t^2)^2} \quad \text{and} \quad y(t) = \tau_1 \frac{8t}{(1 + t^2)^2}.$$

This curve is a cardioid ; its Cartesian equation is polynomial of degree 4. The part of $\mathcal{C}_{\tau_1}$ shared with ∂W_{τ_1} corresponds to $t \in [-\sqrt{3}, \sqrt{3}]$.

7 About the numerical computation

We now turn to describe our numerical computation of the conformal mapping. We deduce from the previous section a parametric representation of the boundary of the numerical range: $\partial W_\tau = \{s(\theta)\,; \theta \in [0, 2\pi)\}$. As in Section 4, we write $g_\tau(z) = z \exp(h(z))$ and use the fact that there exists a 2π-periodic real-valued function q such that

$$h(z) = \frac{1}{2\pi}\int_0^{2\pi} \mathcal{L}\mathrm{og}(s(\varphi){-}z)\, q(\varphi)\, d\varphi, \qquad \forall\, z \in W_\tau.$$

This function may be obtained by solving the integral equation

$$\frac{1}{2\pi}\int_0^{2\pi} \log|s(\varphi){-}s(\theta)|\, q(\varphi)\, d\varphi = -\log|s(\theta)|, \qquad \forall\, \theta \in \mathbb{R}.$$

Let us introduce the values $\theta_j = 2j\pi/(2n{+}1)$, $j = 1, \dots, 2n{+}1$. To compute a numerical approximation q_j of $q(\theta_j)$, we solve the linear system (in the least square sense if the matrix is singular)

$$\tfrac{1}{2n+1} \sum_{j=1}^{2n+1} \log|s(\theta_j){-}s(\theta_k)|\; q_j = -\log|s(\theta_k)|, \qquad k = 1, \dots, n{+}1.$$

We obtain approximations of the values of $g_\tau'(0)$ and $g_\tau''(0)$ required for the computation of $C(s)$ by using the formulae

$$g_\tau'(0) = \exp(h(0)) \simeq g_0' := \exp\Big(\tfrac{1}{2n+1} \sum_{j=1}^{2n+1} q_j \log|s(\theta_j)|\Big),$$

$$g_\tau''(0) = 2g_\tau'(0)h'(0)) \simeq g_0'' := -\tfrac{2}{2n+1}\, g_0' \sum_{j=1}^{2n+1} q_j\, \mathrm{Re}(1/s(\theta_j)).$$

We refer to [9] for the study of this numerical method, which is of collocation type. While the boundary is analytic, this method is very accurate, we have a geometric convergence $O(e^{-\alpha n})$ for some $\alpha > 0$; this accuracy deteriorates as τ tends to τ_1 but we keep a polynomial convergence in $O(n^{-2})$, which is sufficient to convince ourselves that $C(\cdot)$ is strictly positive.

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