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On a partial theta function and its spectrum

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The bivariate series $\theta(q,x) := \sum_{j=0}^{\infty} q^{j(j+1)/2}x^j$ defines a *partial theta function*. For fixed q ($|q|<1$), $\theta(q,\cdot)$ is an entire function. For $q \in (-1,0)$ the function $\theta(q,\cdot)$ has infinitely many negative and infinitely many positive real zeros. There exists a sequence $\{\bar{q}_j\}$ of values of q tending to -1^+ such that $\theta(\bar{q}_k,\cdot)$ has a double real zero $\bar{y}_k$ (the rest of its real zeros being simple). For k odd (respectively, k even) $\theta(\bar{q}_k,\cdot)$ has a local minimum (respectively, maximum) at $\bar{y}_k$, and $\bar{y}_k$ is the rightmost of the real negative zeros of $\theta(\bar{q}_k,\cdot)$ (respectively, for k sufficiently large $\bar{y}_k$ is the second from the left of the real negative zeros of $\theta(\bar{q}_k,\cdot)$). For k sufficiently large one has $-1<\bar{q}_{k+1}<\bar{q}_k<0$. One has $\bar{q}_k = 1-(\pi/8k)+o(1/k)$ and $|\bar{y}_k| \to \mathrm{e}^{\pi/2} = 4.810477382\ldots$.

Keywords: partial theta function; spectrum; asymptotics

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1. Introduction

The bivariate series

$$\theta(q,x) := \sum_{j=0}^{\infty} q^{j(j+1)/2}x^j$$

defines an entire function in x for every fixed q from the open unit disc. This function is called a *partial theta function* because $\theta(q^2,x/q) = \sum_{j=0}^{\infty} q^{j^2}x^j$, whereas the Jacobi theta function is defined by the same series with summation performed from $-\infty$ to ∞ (i.e. when summation is not partial).

There are several domains in which the function θ finds applications: in the theory of (mock) modular forms (see [3]); in statistical physics and combinatorics (see [18]); in asymptotic analysis (see [2]) and in Ramanujan-type q-series (see [19]). Recently, it has been considered in the context of problems about hyperbolic polynomials (i.e. real polynomials having all their zeros real; see [4–6, 9, 13, 15, 16]). These problems were studied earlier by Hardy [4], Petrovitch [16] and Hutchinson [5]. For more information about θ, see also [1].

For $q \in \mathbb{C}$, $|q| \leqslant 0.108$, the function $\theta(q,\cdot)$ has no multiple zeros (see [11]). For $q \in [0,1)$ the function θ has been studied in [8–10, 13]. The results are summarized in the following theorem.

Theorem 1.1.

(1) *For any* $q \in (0,1)$ *the function* $\theta(q,\cdot)$ *has infinitely many negative zeros.*

(2) *There exists a sequence of values of* q *(denoted by* $0 < \tilde{q}_1 < \tilde{q}_2 < \cdots$*) tending to* 1^- *such that* $\theta(\tilde{q}_k,\cdot)$ *has a double negative zero,* y_k*, which is the rightmost of its real zeros and which is a local minimum of* $\theta(q,\cdot)$*. One has* $\tilde{q}_1 = 0.3092493386\ldots$*.*

(3) *For the remaining values of* $q \in [0,1)$ *the function* $\theta(q,\cdot)$ *has no multiple real zero.*

(4) *For* $q \in (\tilde{q}_k, \tilde{q}_{k+1})$ *(we set* $\tilde{q}_0 = 0$*) the function* $\theta(q,\cdot)$ *has exactly* k *complex conjugate pairs of zeros counted with multiplicity.*

(5) *One has* $\tilde{q}_k = 1 - (\pi/2k) + o(1/k)$ *and* $y_k \to -\mathrm{e}^{\pi} = -23.1407\ldots$*.*

Definition 1.2. A value of $q \in \mathbb{C}$, $|q| < 1$, is said to belong to the *spectrum* of θ if $\theta(q,\cdot)$ has a multiple zero.

We consider the function θ in the case when $q \in (-1,0]$. In order to use the results about the case $q \in [0,1)$ one may note the following fact. For $q \in (-1,0]$ set $v := -q$. Then

$$\theta(q,x) = \theta(-v,x) = \theta\left(v^4, -\frac{x^2}{v}\right) - vx\theta(v^4, -vx^2). \tag{1.1}$$

We prove the analogue of the above theorem. The following three theorems are proved in §§ 3–5, respectively.

Theorem 1.3. *For any* $q \in (-1,0)$ *the function* $\theta(q,\cdot)$ *has infinitely many negative and infinitely many positive real zeros.*

Theorem 1.4.

(1) *There exists a sequence of values of* q *(denoted by* $\bar{q}_j$*) tending to* -1^+ *such that* $\theta(\bar{q}_k,\cdot)$ *has a double real zero,* $\bar{y}_k$ *(the rest of its real zeros being simple). For the remaining values of* $q \in (-1,0)$ *the function* $\theta(q,\cdot)$ *has no multiple real zero.*

(2) *For* k *odd (respectively,* k *even) one has* $\bar{y}_k < 0$*,* $\theta(\bar{q}_k,\cdot)$ *has a local minimum at* $\bar{y}_k$ *and* $\bar{y}_k$ *is the rightmost of the real negative zeros of* $\theta(\bar{q}_k,\cdot)$ *(respectively,* $\bar{y}_k > 0$*,* $\theta(\bar{q}_k,\cdot)$ *has a local maximum at* $\bar{y}_k$ *and for* k *sufficiently large* $\bar{y}_k$ *is the leftmost but one (second from the left) of the real negative zeros of* $\theta(\bar{q}_k,\cdot)$*).*

(3) *For* k *sufficiently large one has* $-1 < \bar{q}_{k+1} < \bar{q}_k < 0$*.*

(4) *For* k *sufficiently large and for* $q \in (\bar{q}_{k+1}, \bar{q}_k)$ *the function* $\theta(q,\cdot)$ *has exactly* k *complex conjugate pairs of zeros counted with multiplicity.*

Remark 1.5. Numerical experience confirms the conjecture that parts (2)–(4) of the theorem are true for any $k \in \mathbb{N}$. Proposition 4.5 clarifies part (2) of the theorem.

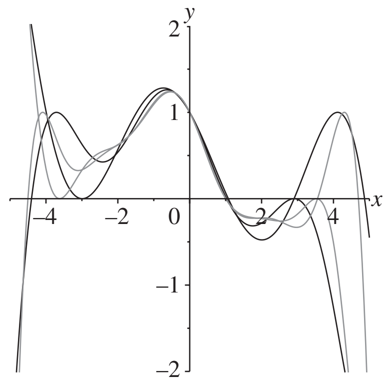

Figure 1. Graphs of the functions $\theta(\bar{q}_k, \cdot)$ for $k = 1, 2, 3, 4$.

THEOREM 1.6. *One has*

$$\bar{q}_k = 1 - \left(\frac{\pi}{8k}\right) + o\left(\frac{1}{k}\right) \quad \textit{and} \quad |\bar{y}_k| \to \mathrm{e}^{\pi/2} = 4.810477382\ldots.$$

REMARK 1.7.

(1) Theorems 1.1 and 1.4 do not us tell whether there are values of $q \in (-1, 1)$ for which $\theta(q, \cdot)$ has a multiple complex conjugate pair of zeros.

(2) It would be interesting to know whether the sequences $\{y_k\}$ and $\{\bar{y}_{2k-1}\}$ are monotone decreasing and $\{\bar{y}_{2k}\}$ is monotone increasing. This is true for at least the five first terms of each sequence.

(3) It would be interesting to know whether there are complex non-real values of q of the open unit disc belonging to the spectrum of θ and (as suggested by Sokal) whether $|\tilde{q}_1|$ is the smallest of the moduli of the spectral values.

(4) The following statement is formulated and proved in [7]:

> the sum of the series $\sum_{j=0}^{\infty} q^{j(j+1)/2} x^j$ (considered for $q \in (0, 1)$ and $x \in \mathbb{C}$) tends to $1/(1 - x)$ (for x fixed and as $q \to 1^-$) exactly when x belongs to the interior of the closed Jordan curve $\{\mathrm{e}^{|s|+\mathrm{i}s}, s \in [-\pi, \pi]\}$.

This statement and (1.1) imply that, as $q \to -1^+$, $\theta(q, x) \to (1-x)/(1+x^2)$ for $x \in (-\mathrm{e}^{\pi/2}, \mathrm{e}^{\pi/2})$, $\mathrm{e}^{\pi/2} = 4.810477381\ldots$. Note that the radius of convergence of the Taylor series at 0 of the function $(1 - x)/(1 + x^2)$ equals 1.

(5) In figures 1 and 2 we show the graphs of $\theta(\bar{q}_k, \cdot)$ for $k = 1, \ldots, 8$. Those for $k = 1, 2, 5, 6$ are shown in black; the others are drawn in grey. One can see by looking at figure 2 that for $x \in [-2.5, 2.5]$ the graphs of $\theta(\bar{q}_k, \cdot)$ for $k \geqslant 5$ are hardly distinguishable from that of $(1 - x)/(1 + x^2)$.

(6) The approximative values of $\bar{q}_k$ and $\bar{y}_k$ for $k = 1, 2, \ldots, 8$ are given in table 1.

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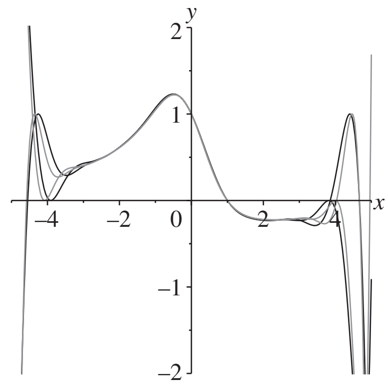

Figure 2. Graphs of the functions $\theta(\bar{q}_k, \cdot)$ for $k = 5, 6, 7, 8$.

Table 1. *Approximative values of* $\bar{q}_k$ *and* $\bar{y}_k$ *for* $k = 1, 2, \ldots, 8$.

k	$-\bar{q}_k$	$\bar{y}_k$
1	0.72713332	−2.991
2	0.78374209	2.907
3	0.84160192	−3.621
4	0.86125727	3.523
5	0.88795282	−3.908
6	0.89790438	3.823
7	0.913191	−4.08
8	0.9192012	4.002

2. Some facts about θ

This section contains properties of the function θ, known or proved in [9]. When a property is valid for all q from the unit disc or for all $q \in (-1, 1)$, we write $\theta(q, x)$. When a property holds true only for $q \in [0, 1)$ or only for $q \in (-1, 0]$, we write $\theta(v, x)$ or $\theta(-v, x)$, where $v \in [0, 1)$.

Theorem 2.1.

(1) *The function* θ *satisfies the following functional equation:*

$$\theta(q, x) = 1 + qx\theta(q, qx), \tag{2.1}$$

and the following differential equation:

$$\frac{2q\partial\theta}{\partial q} = \frac{2x\partial\theta}{\partial x} + \frac{x^2\partial^2\theta}{\partial x^2} = \frac{x\partial^2(x\theta)}{\partial x^2}. \tag{2.2}$$

(2) *For* $k \in \mathbb{N}$ *one has* $\theta(v, -v^{-k}) \in (0, v^k)$.

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(3) *In the following two situations the two conditions* $\operatorname{sgn}(\theta(v, -v^{-k-1/2})) = (-1)^k$ *and* $|\theta(v, -v^{-k-1/2})| > 1$ *hold:*

(i) *for* $k \in \mathbb{N}$ *and* $v > 0$ *small enough;*

(ii) *for any* $v \in (0, 1)$ *fixed and for* $k \in \mathbb{N}$ *large enough.*

The real entire function $\psi(z)$ is said to belong to the Laguerre–Pólya class $\mathcal{L}$–$\mathcal{P}$ if it can be represented as

$$\psi(x) = cx^m \mathrm{e}^{-\alpha x^2 + \beta x} \prod_{k=1}^{\omega} \left(1 + \frac{x}{x_k}\right) \mathrm{e}^{-x/x_k},$$

where ω is a natural number or infinity, c, β and x_k are real, $\alpha \geqslant 0$, m is a non-negative integer and $\sum x_k^{-2} < \infty$. Similarly, the real entire function $\psi_*(x)$ is a function of type I in the Laguerre–Pólya class, written $\psi_* \in \mathcal{L}$–$\mathcal{PI}$, if $\psi_*(x)$ or $\psi_*(-x)$ can be represented in the form

$$\psi_*(x) = cx^m \mathrm{e}^{\sigma x} \prod_{k=1}^{\omega} \left(1 + \frac{x}{x_k}\right), \tag{2.3}$$

where c and σ are real, $\sigma \geqslant 0$, m is a non-negative integer, $x_k > 0$ and $\sum 1/x_k < \infty$. It is clear that $\mathcal{L}$–$\mathcal{PI} \subset \mathcal{L}$–$\mathcal{P}$. The functions in $\mathcal{L}$–$\mathcal{P}$, and only these, are uniform limits, on compact subsets of $\mathbb{C}$, of hyperbolic polynomials (see, for example, [14, ch. 8]). Similarly, $\psi \in \mathcal{L}$–$\mathcal{PI}$ if and only if ψ is a uniform limit on the compact sets of the complex plane of polynomials whose zeros are real and are either all positive or all negative. Thus, the classes $\mathcal{L}$–$\mathcal{P}$ and $\mathcal{L}$–$\mathcal{PI}$ are closed under differentiation; that is, if $\psi \in \mathcal{L}$–$\mathcal{P}$, then $\psi^{(\nu)} \in \mathcal{L}$–$\mathcal{P}$ for every $\nu \in \mathbb{N}$ and, similarly, if $\psi \in \mathcal{L}$–$\mathcal{PI}$, then $\psi^{(\nu)} \in \mathcal{L}$–$\mathcal{PI}$. Pólya and Schur [17] proved that if

$$\psi(x) = \sum_{k=0}^{\infty} \gamma_k \frac{x^k}{k!} \tag{2.4}$$

belongs to $\mathcal{L}$–$\mathcal{P}$ and its Maclaurin coefficients $\gamma_k = \psi^{(k)}(0)$ are all non-negative, then $\psi \in \mathcal{L}$–$\mathcal{PI}$.

The following theorem is the basic result contained in [12].

Theorem 2.2.

(1) *For any fixed* $q \in \mathbb{C}^*$, $|q| < 1$, *and for* k *sufficiently large, the function* $\theta(q, \cdot)$ *has a zero* ζ_k *close to* $-q^{-k}$ *(in the sense that* $|\zeta_k + q^{-k}| \to 0$ *as* $k \to \infty$*). These are all but finitely many of the zeros of* θ*.*

(2) *For any* $q \in \mathbb{C}^*$, $|q| < 1$, *one has* $\theta(q, x) = \prod_k (1 + x/x_k)$, *where* $-x_k$ *are the zeros of* θ *counted with multiplicity.*

(3) *For* $q \in (\tilde{q}_j, \tilde{q}_{j+1}]$ *the function* $\theta(q, \cdot)$ *is a product of a degree* $2j$ *real polynomial without real roots and a function of the Laguerre–Pólya class* $\mathcal{L}$–$\mathcal{PI}$*. Their respective forms are* $\prod_{k=1}^{2j} (1 + x/\eta_k)$ *and* $\prod_k (1 + x/\xi_k)$, *where* $-\eta_k$ *and* $-\xi_k$ *are the complex and real zeros of* θ *counted with multiplicity.*

(4) *For any fixed* $q \in \mathbb{C}^*$, $|q| < 1$, *the function* $\theta(q,\cdot)$ *has at most finitely many multiple zeros.*

(5) *For any* $q \in (-1,0)$ *the function* $\theta(q,\cdot)$ *is a product of the form* $R(q,\cdot)\Lambda(q,\cdot)$, *where*

$$R = \prod_{k=1}^{2j}\left(1 + \frac{x}{\tilde{\eta}_k}\right)$$

is a real polynomial with constant term 1 *and without real zeros and*

$$\Lambda = \prod_{k}\left(1 + \frac{x}{\tilde{\xi}_k}\right), \quad \tilde{\xi}_k \in \mathbb{R}^*,$$

is a function of the Laguerre–Pólya class $\mathcal{L}$–$\mathcal{P}$. *One has* $\tilde{\xi}_k\tilde{\xi}_{k+1} < 0$. *The sequence* $\{|\tilde{\xi}_k|\}$ *is monotone increasing for* k *large enough.*

3. Proof of theorem 1.3

One can use (1.1). By part (3) of theorem 2.1 with v^4 for v, for each $v \in (0,1)$ fixed and for k large enough, if $-x^2/v = -(v^4)^{-k-1/2}$ (i.e. if $|x| = v^{-2k-1/2}$), then $|\theta(v^4, -x^2/v)| > 1$ and $\operatorname{sgn}(\theta(v^4,-x^2/v)) = (-1)^k$. At the same time, part (2) of theorem 2.1 implies that for $-vx^2 = -(v^4)^{-k}$ (i.e. again for $|x| = v^{-2k-1/2}$) one has $\theta(v^4, -vx^2) \in (0, v^{4k})$; hence, $|vx\theta(v^4,-vx^2)| < v^{2k+1/2} < 1$. This means that for $v \in (0,1)$ fixed and for k large enough the equality $\operatorname{sgn}(\theta(v^4,-x^2/v)) = (-1)^k$ holds, i.e. there is a zero of θ on each interval of the form $(-v^{-2k-1/2}, -v^{-2k+1/2})$ and $(v^{-2k+1/2}, v^{-2k-1/2})$.

4. Proof of theorem 1.4

4.1. Properties of the zeros of θ

This subsection contains some preliminary information about the zeros of θ.

LEMMA 4.1. *For* $q \in [-0.108, 0)$ *all zeros of* $\theta(q,\cdot)$ *are real and distinct.*

Proof. Indeed, it is shown in [11] that for $q \in \mathbb{C}$, $|q| \leqslant 0.108$, the zeros of θ are of the form $-q^{-j}\Delta_j$, $\Delta_j \in [0.2118, 1.7882]$. This implies (see [11]) that the moduli of all zeros are distinct for $|q| \leqslant 0.108$. When q is real, as all coefficients of θ are real, each of its zeros either is then real or belongs to a complex conjugate pair. As the moduli of the zeros are distinct, the zeros are all real and distinct. □

NOTATION 4.2. We denote by $0 < x_1 < x_3 < \cdots$ the positive zeros of θ and by $\cdots < x_4 < x_2 < 0$ the negative zeros of θ. For $q \in [-0.108, 0)$ this notation is in line with the fact that x_j is close to $-q^{-j}$.

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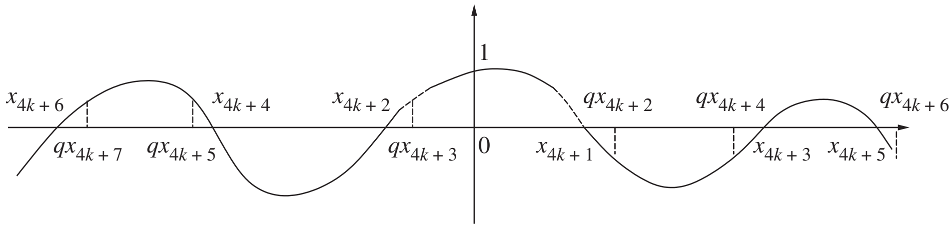

Figure 3. The real zeros of θ for $q \in (-1, 0)$.

Remark 4.3.

(1) The quantities Δ_j are constructed in [11] as convergent Taylor series in q of the form $1 + O(q)$.

(2) For $q \in (-1, 0)$ the function $\theta(q, \cdot)$ has no zeros in $[-1, 0)$. Indeed, this follows from

$$\theta = 1 + q^3x^2 + q^{10}x^4 + \cdots + qx(1 + q^5x^2 + q^{14}x^4 + \cdots).$$

Each of the two series is sign-alternating, with positive first term and with decreasing moduli of its terms for $q \in (-1, 0)$, $x \in [-1, 0)$. Hence, their sums are positive; as $qx > 0$, one has $\theta > 0$.

Lemma 4.4. *For $q \in [-0.108, 0)$ the real zeros of θ and their products with q are arranged on the real line, as shown in figure 3.*

Proof. The lemma follows from (2.1). Indeed,

$$0 = \theta(q, x_{4k+2}) = 1 + qx_{4k+2}\theta(q, qx_{4k+2}), \quad x_{4k+2} < 0 \text{ and } q < 0;$$
$$\text{hence, } \theta(q, qx_{4k+2}) < 0.$$

For small values of q the quantity qx_{4k+2} is close to $-q^{-4k-1}$ (see lemma 4.1 and remark 4.3(1)), i.e. close to x_{4k+1} and as $\theta(q, qx_{4k+2}) < 0$ one must have $x_{4k+1} < qx_{4k+2} < x_{4k+3}$. By continuity, these inequalities hold for all $q < 0$ for which the zeros $x_{4k+1} < x_{4k+3}$ are real and distinct.

In the same way one can justify the disposition of the other points of the form qx_j with respect to (w.r.t.) the points x_j. □

Proposition 4.5. *The function $\theta(q, \cdot)$ with $q \in (-1, 0)$ has a zero in the interval $(0, -1/q)$. More precisely, one has $\theta(q, -1/q) < 0$.*

Proof. Setting $v = -q$, as above, one gets

$$\theta\left(-v, \frac{1}{v}\right) = -v\Phi(v) + v^3\Psi(v),$$

where

$$\Phi(v) = \sum_{j=0}^{\infty}(-1)^j v^{2j^2+3j}, \qquad \Psi(v) = \sum_{j=0}^{\infty}(-1)^j v^{2j^2+5j}.$$

Furthermore, we use some results of [9]. Consider the functions

$$\varphi_k(\tau) := \sum_{j=0}^{\infty}(-1)^j\tau^{kj+j(j-1)/2} = \theta(\tau, -\tau^{k-1})$$

and $\xi_k(\tau) := 1/(1+\tau^k)$, $\tau \in [0,1)$, $k > 0$.

We then use the following proposition.

Proposition 4.6.

(1) *The functions φ_k are real analytic on $[0,1)$; when $k>0$, $\varphi_k < \xi_k$; when $k>1$, $\varphi_k > \xi_{k-1}$; one has $\lim_{\tau\to 1^-}\varphi_k(\tau) = \frac{1}{2}$.*

(2) *Consider the function φ_k as a function of the two variables (k,τ). One has $\partial\varphi_k/\partial k > 0$ for $k > 0$.*

(3) *For $q \in (0,1)$, $x \in (-q^{-1}, \infty)$ one has $\partial\theta/\partial x > 0$.*

(4) *For $q \in (0,1)$, $x \in (-q^{-1/2}, \infty)$ one has $\theta > \frac{1}{2}$.*

Proposition 4.6(2) implies $\varphi_{3/4}(v^4) > \varphi_{1/4}(v^4)$. As $-v\Phi(v) = \varphi_{1/4}(v^4) - 1$ and $-v^3\Psi(v) = \varphi_{3/4}(v^4) - 1$, this means that $\theta(-v, 1/v) < 0$, i.e. $\theta(q, -1/q) < 0$. This completes the proof of proposition 4.5. □

Proof of proposition 4.6. Part (1) of the proposition is proved in [9].

To prove part (2), observe that

$$\begin{aligned}\partial\varphi_k/\partial k &= (-\log\tau)\sum_{j=1}^{\infty}(-1)^{j-1}j\tau^{kj+j(j-1)/2} \\ &= (-\log\tau)\sum_{j=1}^{\infty}(\varphi_{k+2j-1} - \tau^{k+2j-1}\varphi_{k+2j})\tau^{(2j-1)k+(j-1)(2j-1)}.\end{aligned}$$

As $\varphi_{k+2j-1} - \tau^{k+2j-1}\varphi_{k+2j} = 2\varphi_{k+2j-1} - 1$ and (see part (1) of the proposition) as $\varphi_{k+2j-1}(\tau) > \xi_{k+2j-2}(\tau) \geqslant \frac{1}{2}$, each difference $\varphi_{k+2j-1} - \tau^{k+2j-1}\varphi_{k+2j}$ is positive on $[0,1)$. The factors $-\log\tau$ and $\tau^{(2j-1)k+(j-1)(2j-1)}$ are also positive.

For $x \in (-q^{-1}, 0]$ part (3) follows from part (2) and from $\varphi_k(\tau) = \theta(\tau, -\tau^{k-1})$. Indeed, one can represent x as $-\tau^{k-1}$ for some $k > 0$; for fixed τ, as x increases, k also increases. One has

$$0 < \frac{\partial\varphi_k}{\partial k} = (-\log\tau)\frac{\partial\theta}{\partial x}\bigg|_{x=-\tau^{k-1}} \quad \text{and} \quad -\log\tau > 0.$$

For $x > 0$ part (3) results from all coefficients of $\theta(v,x)$ considered as a series in x being positive.

For $x \in (-q^{-1/2}, 0]$ part (4) follows from part (3). Indeed, consider the function

$$\psi := 1 + 2\sum_{j=1}^{\infty}(-1)^j\tau^{j^2}, \quad \tau \in [0,1).$$

This function is positive valued, decreasing and tending to 0 as $\tau \to 1^-$ (see [8]). As $0 < \frac{1}{2}\psi(\tau^{1/2}) = \varphi_{1/2}(\tau) - \frac{1}{2}$ for $k \geqslant \frac{1}{2}$, part (2) implies

$$\theta(\tau, -\tau^{k-1}) = \varphi_k(\tau) \geqslant \varphi_{1/2}(\tau) > \tfrac{1}{2}.$$

For $x = 0$ one has $\theta = 1$; hence, for $x > 0$, part (4) follows from part (2). □

The following lemma follows immediately from the result of Katsnelson cited in remark 1.7(4) and from proposition 4.5.

LEMMA 4.7. *For any $\varepsilon > 0$ sufficiently small there exists $\delta > 0$ such that for $q \in (-1, -1+\delta]$ the function $\theta(q, \cdot)$ has a single real zero in the interval $(-\mathrm{e}^{\pi/2} + \varepsilon, \mathrm{e}^{\pi/2} - \varepsilon)$. This zero is simple and positive.*

4.2. How do the zeros of θ coalesce?

We next describe the way in which multiple zeros are formed when q decreases from 0 to -1.

DEFINITION 4.8. We say that phenomenon A happens before phenomenon B if A takes place for $q = q_1$, B takes place for $q = q_2$ and $-1 < q_2 < q_1 < 0$. By phenomena we mean that certain zeros of θ or another function coalesce.

NOTATION 4.9. We denote by $x_j \prec x_k$ the following statement:

> the zeros x_k and x_{k+2} of θ can coalesce only after x_j and x_{j+2} have coalesced.

LEMMA 4.10. *One has $x_{4k+2} \prec x_{4k+3}$, $x_{4k+2} \prec x_{4k+1}$, $x_{4k+3} \prec x_{4k+4}$ and $x_{4k+5} \prec x_{4k+4}$, $k \in \mathbb{N} \cup 0$.*

Proof. The statements follow from

$$qx_{4k+5} < x_{4k+4} < x_{4k+2} < qx_{4k+3}, \qquad x_{4k+1} < qx_{4k+2} < qx_{4k+4} < x_{4k+3},$$
$$qx_{4k+4} < x_{4k+3} < x_{4k+5} < qx_{4k+6}, \qquad x_{4k+6} < qx_{4k+7} < qx_{4k+5} < x_{4k+4},$$

respectively. □

LEMMA 4.11. *One has $x_{4k+2} \prec x_{4k+6}$, $k \in \mathbb{N} \cup 0$.*

Proof. Indeed, (2.1) implies

$$\theta(q, x) = 1 + qx + q^3x^2 + q^6x^3 + q^{10}x^4\theta(q, q^4x). \tag{4.1}$$

For $x = x_{4k+2}/q^4$ one obtains

$$\theta\biggl(q, \frac{x_{4k+2}}{q^4}\biggr) = 1 + \frac{x_{4k+2}}{q^3} + \frac{x_{4k+2}^2}{q^5} + \frac{x_{4k+2}^3}{q^6} = \biggl(1 + \frac{x_{4k+2}^2}{q^5}\biggr) + \biggl(\frac{x_{4k+2}}{q^3} + \frac{x_{4k+2}^3}{q^6}\biggr).$$

Each of the two sums is negative due to $q \in (-1, 0)$, $x_{4k+2} < -1$ (see remark 4.3(2)). For small values of $|q|$ one has $x_{4k+2}/q^4 \in (x_{4k+8}, x_{4k+6})$ because $x_j = -q^{-j}(1 + O(q))$ and $\theta(q, x_{4k+2}/q^4) < 0$. By continuity, this holds true for all $q \in (-1, 0)$ for which the zeros x_{4k+8}, x_{4k+6}, x_{4k+4} and x_{4k+2} are real and distinct. Hence, if x_{4k+2} and x_{4k+4} have not coalesced, then x_{4k+6} and x_{4k+8} are real and distinct. □

Remark 4.12.

(1) Recall that for $q \in (-1, 0)$ we set $v := -q$ and that (1.1) holds true.

(2) Equation (2.2) implies that the values of θ at its local maxima decrease and its values at local minima increase as q decreases in $(-1, 0)$. Indeed, at a critical point one has $\partial\theta/\partial x = 0$, so $2q\partial\theta/\partial q = x^2\partial^2\theta/\partial x^2$. At a minimum one has $\partial^2\theta/\partial x^2 \geqslant 0$, so $\partial\theta/\partial q \leqslant 0$ and the value of θ increases as q decreases (and similarly for a maximum).

(3) In particular, this means that θ can lose real zeros, but not acquire them as q decreases on $(-1, 0)$. Indeed, the zeros of θ depend continuously on q. If at some point on the real axis a new zero of even multiplicity appears, it cannot be a maximum because the critical value must decrease, and it cannot be a minimum because its value must increase.

(4) To treat the cases of odd multiplicities of the zeros, it suffices to differentiate both sides of (2.2) w.r.t. x. For example, a simple zero x_0 of θ cannot become a triple one because

$$\frac{2q\partial}{\partial q}\left(\frac{\partial\theta}{\partial x}\right) = \frac{2\partial\theta}{\partial x} + 4x\frac{\partial^2\theta}{\partial x^2} + x^2\frac{\partial^3\theta}{\partial x^3},$$

which means that, as

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=x_0} = \left.\frac{\partial^2\theta}{\partial x^2}\right|_{x=x_0} = 0,$$

either $\partial^3\theta/\partial x^3|_{x=x_0} > 0$ (and hence, in a neighbourhood of x_0 one has $\partial\theta/\partial x \geqslant 0$ and $(\partial/\partial q)(\partial\theta/\partial x) < 0$) or $\partial^3\theta/\partial x^3|_{x=x_0} < 0$ and hence $\partial\theta/\partial x \leqslant 0$ and $(\partial/\partial q)(\partial\theta/\partial x) > 0$ (in a neighbourhood of x_0), so in both cases the triple zero bifurcates into a simple one and a complex pair as q decreases. The case of a zero of multiplicity $2m + 1$, $m \in \mathbb{N}$, is treated by analogy.

(5) In (1.1) the first argument of both functions $\theta(v^4, -x^2/v)$ and $\theta(v^4, -vx^2)$ (i.e. v^4) is the same, so when one of them has a double zero they both have double zeros. If the double zero of the first one is at $x = a$, then that of the second is at $x = a/v$.

Proposition 4.13. *For any $k \in \mathbb{N} \cup 0$ there exists $q_k^* \in (-1, 0)$ such that for $q = q_k^*$ the zeros x_{4k+2} and x_{4k+4} coalesce.*

Notation 4.14. We denote the functions $\theta(v^4, -x^2/v)$ and $-vx\theta(v^4, -vx^2)$ by ψ_1 and ψ_2, respectively. By $y_{\pm k}$ and $z_{\pm k}$ we denote their real zeros for $v^4 \in (0, 0.108]$, their moduli increasing with $k \in \mathbb{N}$, $y_k > 0$, $y_{-k} < 0$, $z_k > 0$ and $z_{-k} < 0$. We set $z_0 = 0$.

Proof of proposition 4.13. In figure 4 we show for $v^4 \in (0, 0.108]$ what the graphs of the functions ψ_1 and ψ_2 (drawn as solid and dashed lines, respectively) look like, the former being even, and the latter odd (see remark 4.12(1)). The signs + and −

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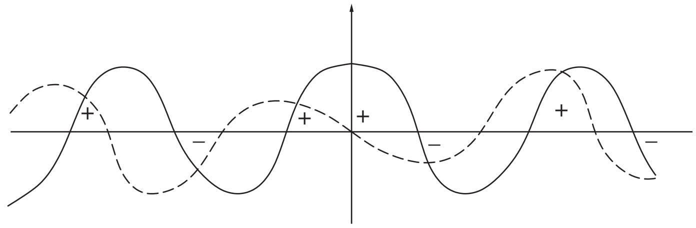

Figure 4. The graphs of ψ_1 (solid line) and ψ_2 (dashed line).

indicate places where it is certain that their sum $\theta(-v,x)$ is positive and negative, respectively. It is positive (respectively, negative) if both functions are of this sign. It is positive near the origin because $\psi_1|_{x=0} > 0$, while $\psi_2|_{x=0} = 0$.

For values of v close to 0 the zeros $y_{\pm k}$ of ψ_1 (respectively, the zeros $z_{\pm k}$ of ψ_2/x) are close to the numbers $\pm v^{-(4k-1)/2}$ (respectively, $\pm v^{-(4k+1)/2}$), $k \in \mathbb{N}$ (see remark 4.3(1)). From these remarks it also follows that for small positive values of v the zeros of $\theta(-v,x)$ are close to the numbers $-v^{-k}$, $k \in \mathbb{N}$. Hence, on the negative half-axis x one obtains the following arrangement of these numbers:

$$\begin{array}{ccccc} \cdots & < -v^{-11/2} & < -v^{-9/2} & < -v^{-4} & < -v^{-7/2} \\ & y_{-5} & z_{-3} & x_4 & y_{-3} \end{array}$$
$$\begin{array}{ccc} < -v^{-5/2} & < -v^{-2} & < -v^{-3/2} < 0. \\ z_{-1} & x_2 & y_{-1} \end{array}$$

Hence, for $v^4 \in (0, 0.108]$ between a zone marked by a $+$ and one marked by a $-$ there is exactly one zero of $\theta(-v,\cdot)$.

As v increases from 0 to 1, it takes countably many values, at each of which one of the functions ψ_1 and ψ_2 (in turn) has a double zero; when the value is passed, this double zero becomes a conjugate pair (see theorem 1.1). Hence, on the negative real half-line, the regions where the corresponding function ψ_1 or ψ_2 is negative disappear one by one, starting from the right. As two consecutive changes of sign of $\theta(-v,\cdot)$ are lost, $\theta(-v,\cdot)$ has a couple of consecutive real negative zeros replaced by a complex conjugate pair. The quantity of these losses being countable implies the proposition. $\square$

Proposition 4.15. *Any interval of the form* $[\gamma, 0]$, $\gamma \in (-1, 0)$, *contains at most finitely many spectral values of* q.

Proof. Indeed, if $\gamma \geqslant -0.108$, the interval contains no spectral value of q (see lemma 4.1); all zeros of θ are real and distinct and the graphs of the functions $\psi_{1,2}$ look as shown in figure 4.

Suppose that $\gamma < -0.108$. When q decreases in $[\gamma, 0]$, for each of the functions this happens at most finitely many times such that each has a double zero that then gives birth to a complex conjugate pair. This is always the zero which is closest to 0 (see theorem 1.1(2)).

Hence, the presentation of the graphs of $\psi_{1,2}$ changes only on some closed interval containing 0, but outside it the zones marked by $+$ and $-$ continue to exist (but their borders change continuously) and the simple zeros of θ that are to be found

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between two such consecutive zones of opposite sign are still to be found there. In addition, no new real zeros appear (see remark 4.12(3)).

Therefore, there exists $s_0 \in \mathbb{N}$ such that, when q decreases from 0 to γ, the zeros $x_{s_0}, x_{s_0+1}, x_{s_0+2}, \dots$ remain simple and depend continuously on q. Hence, only the rest of the zeros (i.e. $x_1, \dots, x_{s_0-1}$) can participate in the bifurcations. □

PROPOSITION 4.16. *For $q \in (-1, 0)$ the function $\theta(q, \cdot)$ can have only simple and double real zeros. Positive double zeros are local maxima, and negative double zeros are local minima.*

Proof. Equality (2.1) implies

$$\theta\left(q, \frac{x}{q^2}\right) = 1 + \frac{x}{q} + \left(\frac{x^2}{q}\right)\theta(q, x).$$

Set $x = x_{4k+2}$. Hence, $x_{4k+2} < -1$ (remark 4.3(2)). As $\theta(q, x_{4k+2}) = 0$ and $1 + x_{4k+2}/q > 0$, this implies $\theta(q, x_{4k+2}/q^2) > 0$. In the same way $\theta(q, x_{4k+4}/q^2) > 0$.

For q close to 0 the numbers x_{4k+2}/q^2 and x_{4k+4}/q^2 are close to x_{4k+4} and x_{4k+6}, respectively (see remark 4.3(1)). Hence, for such values of q one has

$$x_{4k+6} < \frac{x_{4k+4}}{q^2} < \frac{x_{4k+2}}{q^2} < x_{4k+4}. \tag{4.2}$$

This string of inequalities holds true (by continuity) for q belonging to any interval of the form $(a, 0)$, $a \in (-1, 0)$, for any q of which the zeros x_{4k+6}, x_{4k+4} and x_{4k+2} are real and distinct.

Equation (4.2) implies that x_{4k+6} and x_{4k+4} cannot coalesce if x_{4k+4} and x_{4k+2} are real (but not necessarily distinct). Hence, when negative zeros of θ coalesce for the first time, this occurs with exactly two zeros, and the double zero is a local minimum of θ.

For positive zeros, one obtains in the same way the string of inequalities

$$x_{4k+5} < \frac{x_{4k+3}}{q^2} < \frac{x_{4k+5}}{q^2} < x_{4k+7}.$$

Indeed, one has $1 + x_{4k+3}/q < 0$ because $x_{4k+3} > 1$ (see proposition 4.5) and $q \in (0, 1)$. Hence, $\theta(q, x_{4k+3}/q^2) < 0$ and, in the same way, $\theta(q, x_{4k+5}/q^2) < 0$. Thus, x_{4k+5} and x_{4k+7} cannot coalesce if x_{4k+3} and x_{4k+5} are real (but not necessarily distinct). Hence, when positive zeros of θ coalesce for the first time, this occurs with exactly two zeros, and the double zero is a local maximum of θ.

After a confluence of zeros takes place, one can give new indices to the remaining real zeros, so that the indices of consecutive zeros differ by 2 ($x_{2s+2} < x_{2s} < 0$ and $0 < x_{2s+1} < x_{2s+3}$). After this, for the next confluence, the reasoning is the same. □

LEMMA 4.17. *For $k \in \mathbb{N}$ sufficiently large one has $x_{4k+3} \prec x_{4k+6}$.*

Proof. Suppose that $x_{4k+3} \geqslant 3$. Then

$$\theta\left(q, \frac{x_{4k+3}}{q^3}\right) = 1 + \frac{x_{4k+3}}{q^2} + \frac{x_{4k+3}^2}{q^3} + \left(\frac{x_{4k+3}^3}{q^3}\right)\theta(q, x_{4k+3}) = 1 + \frac{x_{4k+3}}{q^2} + \frac{x_{4k+3}^2}{q^3}.$$

For $x_{4k+3} \geqslant 3$ and $q \in (-1, 0)$ the right-hand side is negative. In the same way, $\theta(q, x_{4k+5}/q^3) < 0$. We prove below that

$$x_{4k+8} < \frac{x_{4k+5}}{q^3} < \frac{x_{4k+3}}{q^3 < x_{4k+6}}. \tag{4.3}$$

Hence, the zeros x_{4k+8} and x_{4k+6} cannot coalesce before x_{4k+5} and x_{4k+3} have coalesced. To prove the string of inequalities (4.3) observe that for q close to 0 the numbers x_{4k+8} and x_{4k+5}/q^3 are close to one another (as are x_{4k+3}/q^3 and x_{4k+6}; see remark 4.3(1)), which implies (4.3). By continuity, as long as $x_{4k+3} \geqslant 3$ and $q \in (-1, 0)$, the string of inequalities also holds true for q not necessarily close to 0.

The result of Katsnelson (see remark 1.7(4)) implies that there exists $a \in (-1, 0)$ such that for $q \in (-1, a]$ the function $\theta(q, x)$ has no zeros in $[-3, 3]$ except for the one that is simple and close to 1 (see proposition 4.5). Hence, for $q \in (-1, a]$ the condition $x_{4k+3} \geqslant 3$ is satisfied if the zero x_{4k+3} is real and simple for $q \in (a, 0)$. On the other hand, for $q \in [a, 0)$ only finitely many real zeros of θ coalesce, and only finitely many belong to the interval $[-3, 3]$ for some value of q (proposition 4.15). Therefore, there exists $k_0 \in \mathbb{N}$ such that for $k \geqslant k_0$ one has $x_{4k+3} \geqslant 3$. □

4.3. Completion of the proof of theorem 1.4

Proposition 4.16 and remark 4.12 show that $\theta(q, \cdot)$ has no real zero of multiplicity higher than 2. Lemma 4.11 implies the string of inequalities $-1 < \cdots < \bar{q}_{2l+2} < \bar{q}_{2l} < \cdots < 0$. For k sufficiently large one has $-1 < \cdots < \bar{q}_{k+1} < \bar{q}_k < \cdots < 0$. This follows from lemmas 4.10 and 4.17. It follows from proposition 4.15 and from the above inequalities that the set of spectral values has -1 as a unique accumulation point. This proves part (3) of the theorem.

Part (2) of the theorem results from proposition 4.16.

Part (4) follows from remark 4.12. These remarks show that real zeros can only be lost and no new real zeros are born.

5. Proof of theorem 1.6

Recall that $\psi_1 = \theta(v^4, -x^2/v)$ and $\psi_2 = -vx\theta(v^4, -vx^2)$ (see notation 4.14). Recall that the spectral values $\tilde{q}_k$ of q for $\theta(q, x)$, $q \in (0, 1)$, satisfy the asymptotic relation $\tilde{q}_k = 1 - \pi/2k + o(1/k)$. Hence, the values of v for which the function $\theta(v^4, x)$ has a double zero are of the form

$$\tilde{v}_k = (\tilde{q}_k)^{1/4} = 1 - \frac{\pi}{8k} + o\left(\frac{1}{k}\right)$$

and the functions $\psi_{1,2}$ have double zeros for $v = \tilde{v}_k$.

Consider three consecutive values of k, the first of which is odd: k_0, $k_0 + 1$ and $k_0 + 2$. Set $v := \tilde{v}_{k_0}$. Denote by $a < b < 0$ the double negative zeros of the functions $\psi_{1,2}|_{v=\tilde{v}_{k_0}}$. These zeros are local minima and on the whole interval $[a, b]$ one has $\theta > 0$. The values of θ at local minima increase (see remark 4.12(2)). Therefore, the double zero of $\theta(\bar{q}_{k_0}, \cdot)$ is obtained for some $|q| < |\tilde{v}_{k_0}|$, i.e. before the functions $\psi_{1,2}|_{v=\tilde{v}_{k_0}}$ have double zeros. This follows from (1.1) in which both summands on the right-hand side have local minima (recall that, as k_0 is odd, the double zero of

θ is negative, so $x < 0$ in (1.1)). Hence,

$$|\bar{q}_{k_0}| < |\tilde{v}_{k_0}| = 1 - \frac{\pi}{8k_0} + o\left(\frac{1}{k_0}\right). \tag{5.1}$$

In the same way,

$$|\bar{q}_{k_0+2}| < |\tilde{v}_{k_0+2}| = 1 - \frac{\pi}{8(k_0+2)} + o\left(\frac{1}{k_0+2}\right). \tag{5.2}$$

In the case of k_0+1 the function $\psi_1|_{v=\tilde{v}_{k_0+1}}$ has a local minimum, while $\psi_2|_{v=\tilde{v}_{k_0+1}}$ has a local maximum (because k_0+1 is even, the double zero of θ is positive, so $x > 0$ in (1.1)). As θ has a local maximum and as the values of θ at local maxima decrease (see remark 4.12(2)), the double zero of $\theta(\bar{q}_{k_0+1}, \cdot)$ is obtained for some $|q| > |\tilde{v}_{k_0+1}|$, i.e. after the functions $\psi_{1,2}|_{v=\tilde{v}_{k_0+1}}$ have double zeros. Therefore,

$$|\bar{q}_{k_0+1}| > |\tilde{v}_{k_0+1}| = 1 - \frac{\pi}{8(k_0+1)} + o\left(\frac{1}{k_0+1}\right). \tag{5.3}$$

When k_0 is sufficiently large one has $|\bar{q}_{k_0}| < |\bar{q}_{k_0+1}| < |\bar{q}_{k_0+2}|$ (this follows from theorem 1.4(3)). Using (5.2) and (5.3), one gets

$$1 - \frac{\pi}{8(k_0+1)} + o\left(\frac{1}{k_0+1}\right) < |\bar{q}_{k_0+1}| < |\bar{q}_{k_0+2}| < 1 - \frac{\pi}{8(k_0+2)} + o\left(\frac{1}{k_0+2}\right).$$

Hence,

$$|\bar{q}_{k_0+1}| = 1 - \frac{\pi}{8(k_0+1)} + o\left(\frac{1}{k_0+1}\right) \quad \text{and} \quad |\bar{q}_{k_0+2}| = 1 - \frac{\pi}{8(k_0+2)} + o\left(\frac{1}{k_0+2}\right).$$

This implies the statement of theorem 1.6.

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