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ENTIRE FUNCTIONS, PT-SYMMETRY AND VOROS'S QUANTIZATION SCHEME

A. E. Eremenko. *Entire functions, PT-symmetry and Voros's quantization scheme*, Mat. Stud. **54** (2020), 203–210.

In this paper, A. Avila's theorem on convergence of the exact quantization scheme of A. Voros is related to the reality proofs of eigenvalues of certain PT-symmetric boundary value problems. As a result, a special case of a conjecture of C. Bender, S. Boettcher and P. Meisinger on reality of eigenvalues is proved. In particular the following Theorem 2 is proved: *Consider the eigenvalue problem*

$$-w'' + (-1)^{\ell}(iz)^m w = \lambda w,$$

where $m \geq 2$ is real, and $(iz)^m$ is the principal branch, $(iz)^m > 0$ when z is on the negative imaginary ray, with boundary conditions $w(te^{i\beta}) \to 0$, $t \to \infty$, where $\beta = \pi/2 \pm \frac{\ell+1}{m+2}\pi$. If $\ell = 2$, and $m \geq 4$, then all eigenvalues are positive.

1. Introduction. The following two theorems are proved in the article:

Theorem 1. *Consider three rays:*

$$L_j = \{e^{ij\alpha}t\colon t \geq 0\}, \quad j \in \{-1, 0, 1\}, \quad i = \sqrt{-1}.$$

If

$$\alpha \in (0, \pi/3], \tag{1}$$

then there exists an entire function g whose all zeros lie on L_0 and all 1-points on $L_1 \cup L_{-1}$, and having infinitely many zeros and 1-points.

Theorem 2. *Consider the eigenvalue problem*

$$-w'' + (-1)^{\ell}(iz)^m w = \lambda w, \tag{2}$$

where $m \geq 2$ is real, and $(iz)^m$ is the principal branch, $(iz)^m > 0$ when z is on the negative imaginary ray, with boundary conditions

$$w(te^{i\beta}) \to 0, \quad t \to \infty, \tag{3}$$

where

$$\beta = \pi/2 \pm \frac{\ell+1}{m+2}\pi.$$

If $\ell = 2$, and $m \geq 4$, then all eigenvalues are positive.

[1]Supported by NSF grant DMS-1361836.
2010 *Mathematics Subject Classification:* 34A05, 34M60, 81Q05.
Keywords: entire functions; PT-symmetry; exact quantization scheme; Stokes multipliers.
doi:10.30970/ms.54.2.203-210

Theorem 2 is the simplest case of a conjecture of Bender, Boettcher and Meisinger [2, 3]. When $m = 2$, $\ell = 1$, the eigenvalue problem (2), (3) is the harmonic oscillator. When $m = 4$, $\ell = 2$, it is the quartic oscillator. When m is an integer, $m \geq 3$, and ℓ is an integer in $[1, m]$, Theorem 2 was proved by Shin ([12]). Notice that the case $m = 3, \ell = 2$ is not covered by Theorem 2. When $m \geq 2$ and $\ell = 1$ positivity of eigenvalues was proved in [8], section 6.2.

When m is not an integer, the bound for $m \geq 4$ in Theorem 2 seems to be exact: almost all eigenvalues are non-real when $\ell = 2$ and $m \in (2,3) \cup (3,4)$, according to the computation in [2, Figs. 14,15]. Here $m = 3$ is an exceptional value, covered by the theorem of Shin, when all eigenvalues are real.

We recall that an eigenvalue problem for a differential operator is called PT-symmetric if it is invariant with respect to the change of the independent variable $z \mapsto \sigma(z) = -\overline{z}$. This means that the equation and the boundary conditions are invariant. If each of the two boundary conditions is invariant under σ, the problem is equivalent to an Hermitian one. In other PT-symmetric problems the two boundary conditions are interchanged by σ. PT-symmetric problems have eigenvalues symmetric with respect to the real line but not necessarily real. The conjecture of Bender, Boettcher and Meisinger arises from their numerical study of PT-symmetric boundary value problems for the operator (2) with various PT-symmetric boundary conditions. The idea was to connect the potentials z^2, z^3 and z^4 into one continuous family. All our eigenvalue problems (2), (3) are PT-symmetric.

The background of Theorem 1 and its relation with Theorem 2 is the following.

In a conference in Joensuu in summer 2015, Gary Gundersen asked whether there exist entire functions with all zeros positive, while 1-points lie on some rays from the origin, distinct from the positive ray, ([5, Questions 3.1, 3.2]). As a partial answer to this question, Bergweiler, Hinkkanen and the present author ([4]) proved among other things the following fact:

Theorem A. *If there exists an entire function with zeros on the positive ray L_0, and 1-points on the rays L and L' from the origin, which are different from the positive ray, and this function has infinitely many zeros and 1-points, then $\angle(L_0, L) = \angle(L_0, L') < \pi/2$.*

Trying to construct an example of a function with this property, the authors of [4] recalled the functional equation

$$f(\omega\lambda)f(\omega^{-1}\lambda) = 1 - f(\lambda), \quad \omega = e^{2\pi i/5},$$

which was studied by Sibuya and Cameron ([17]) and Sibuya ([16]). This equation is satisfied by the Stokes multiplier of the differential equation

$$-y'' + (z^3 - \lambda)y = 0.$$

On the other hand, it is known that this Stokes multiplier is an entire function with all zeros positive ([7]). So f has positive zeros, and 1-points of f lie on the rays $\operatorname{Arg} z = \pm 2\pi/5$. Considering more general differential equations

$$-y'' + (z^m - \lambda)y = 0, \tag{4}$$

with integer $m \geq 3$ the authors of [4] used the results of Sibuya ([15]) and Shin ([12]) to prove Theorem 1 with $\alpha = 2\pi/(m + 2)$, where $m \geq 3$ is an integer.

It was tempting to consider such differential equations (4) with non-integer $m \geq 2$, with solutions defined on the Riemann surface of the logarithm. The Stokes multiplier of such an equation is still an entire function of λ. However, the numerical experiments and heuristic arguments of Bender, Boettcher and Meisinger ([2, 3]) show that the straightforward generalization of the result of Shin on reality of PT-symmetric eigenvalues does not hold for non-integer m.

This suggested a more general treatment of the required functional equations (Section 2 below) based on a deep result of Avila, where the differential equation does not figure at all. Theorem 2 is proved as a byproduct.

The main message of this paper is that a substantial part of reality proofs for PT-symmetric eigenvalues in [7, 8, 12] can be performed in a more general setting, by working only with entire functions of the spectral parameter λ, without even mentioning the differential equation or the variable z.

A challenging question remains whether Theorem 1 can be extended to angles $\alpha \in (\pi/3, \pi/2)$, besides $2\pi/5$. Notice that Theorem 1 does not cover the case $\alpha = 2\pi/5$ which was proved in [4]. Shin's proof of this result uses the change of the independent variable $z \mapsto -z$ which in the case of equation (2) works only for integer m. Numerical and heuristic results in [2, 3] suggest that the construction described below will not work with $\alpha \in (\pi/3, \pi/2)\backslash\{2\pi/5\}$.

Remark. Figs. 14, 15, 20 in [2] show that for some non-integer $m \geq 2$ and some $\ell \geq 2$ almost all eigenvalues are non-real, and form complex conjugate pairs. This shows that the usual asymptotic expansions of eigenvalues λ_k as a function of k, which are common in one-dimensional eigenvalue problems [13, 11, 9], and which would imply $|\lambda_{k+1}| > |\lambda_k|$, for large k, cannot hold in these cases.

2. Voros's quantization scheme and Avila's theorem. Consider an entire function f of genus zero with positive zeros and $f(0) = 1$, that is

$$f(\lambda) = \prod_{j=1}^{\infty} \left(1 - \frac{\lambda}{E_j}\right), \quad 0 < E_1 < E_2 \ldots. \tag{5}$$

Denote

$$\omega = e^{i\alpha}, \quad \alpha \in (0, \pi/2).$$

Later, in Section 3, we will need to impose a stronger condition (1). Consider the function

$$\operatorname{Arg} f(\omega^{-2}t) = \sum_{j=1}^{\infty} \tan^{-1} \frac{\sin 2\alpha}{E_j/t - \cos 2\alpha}.$$

This is a continuous, strictly increasing function of t which is zero at 0, and tends to $+\infty$ as $t \to +\infty$. We want to find a function f as in (5) with the property

$$\frac{1}{\pi} \operatorname{Arg} f(\omega^{-2}E_k) = k - 1/2, \quad k = 1, 2, 3, \ldots. \tag{6}$$

Avila proved in [1] that such functions f exist. More precisely, Voros proposed to solve equations (6) in the following way. Start with an appropriate sequence $E = (E_k)$. It determines f_E by (5) and the increasing function $t \mapsto \operatorname{Arg} f_E(\omega^{-2}t)$. Let $E' = (E'_k)$ be the solutions of

$$\frac{1}{\pi} \operatorname{Arg} f_E(\omega^{-2}E'_k) = k - 1/2, \quad k = 1, 2, \ldots.$$

These E'_k are uniquely defined because $t \mapsto \operatorname{Arg} f_E(\omega^{-2}t)$ is strictly increasing and maps $[0, +\infty)$ onto itself. This construction defines a map $E \mapsto E'$. Voros conjectured that under an appropriate choice of the initial sequence iterates of this map converge to a solution of (6). He called this the "exact quantization scheme". Avila proved the convergence of the scheme for every $\alpha \in (0, \pi/2)$. (He uses parameter $\theta = \pi - 2\alpha \in (0, \pi)$ instead of α.) The sufficient conditions of convergence and initial conditions are stated on p. 309 in [1]. In fact his assumptions on the right hand side of (6) are flexible: it has to be $k + O(1)$ and $\geq (k - 1/2)(1 - 2\alpha)/\pi$.

3. Functional equations. It follows from (6) that the entire function

$$f(\omega^{-2}\lambda) + f(\omega^2\lambda)$$

has zeros at E_k, and no other positive zeros. Indeed, for $\lambda > 0$ the summands are complex conjugate to each other, so their sum is zero if and only if their arguments are $\pi/2$ modulo π, and this happens exactly for $\lambda = E_k$ according to (6). Therefore,

$$f(\omega^{-2}\lambda) + f(\omega^2\lambda) = C(\lambda)f(\lambda), \tag{7}$$

where C is an entire function *without positive zeros*. This is our first main functional equation.

Equation (7) is equivalent to (6): if f is an entire function of the form (5), satisfying (7) with some entire C having no positive zeros, then f satisfies (6).

Substituting $\lambda \mapsto \omega^2\lambda$ we obtain

$$f(\lambda) + f(\omega^4\lambda) = C(\omega^2\lambda)f(\omega^2\lambda). \tag{8}$$

Elimination of $f(\lambda)$ from (7) and (8) gives

$$f(\omega^{-2}\lambda) = \big(C(\lambda)C(\omega^2\lambda) - 1\big)\, f(\omega^2\lambda) - C(\lambda)f(\omega^4\lambda).$$

By substituting $\lambda \mapsto \omega^{-1}\lambda$ and denoting

$$D(\lambda) = C(\omega^{-1}\lambda)C(\omega\lambda) - 1, \tag{9}$$

we obtain our second main functional equation

$$f(\omega^{-3}\lambda) = D(\lambda)f(\omega\lambda) - C(\omega^{-1}\lambda)f(\omega^3\lambda), \tag{10}$$

which is a direct consequence of (7).

Such functional equations were obtained first by Sibuya ([15]) in his studies of Stokes multipliers (the Stokes multiplier is C). Later it was discovered by Dorey, Dunning and Tateo that the same functional equations occur in the exactly solvable models of statistical mechanics on two-dimensional lattices, as well as in the quantum field theory ([7]). Our new observation here is that all these functional equations can be obtained from (6), without any appeal to differential equations.

In the next proposition we will prove that zeros of C and D are negative. Setting $g(\lambda) = -D(-\lambda)$ we will obtain that zeros of g are positive while 1-points, which are zeros of $C(\omega^{-1}\lambda)C(\omega\lambda)$ lie on $L_1 \cup L_{-1}$ in view of (9), which will prove the Theorem 1.

Proposition 1. *Let f be an entire function of order less than 1 of the form (5), and suppose that (7) is satisfied with some entire function C which has no positive zeros. Then (10) is satisfied with D as in (9) and all zeros of C are negative. If (1) holds then all zeros of D are negative as well.*

Proof. First we prove that zeros of C are real. The idea of this comes from [7], see also [8]. Suppose that $C(\lambda) = 0$. Then (7) implies

$$|f(\omega^2\lambda)| = |f(\omega^{-2}\lambda)|. \tag{11}$$

From the explicit form of f in (5) we see that the function $\theta \mapsto |f(re^{i\theta})|$ is even, 2π-periodic, and strictly increasing on $(0,\pi)$. Therefore (11) can hold only with real λ.

As C has no positive zeros, they are all negative. From (7) we obtain $C(0) = 2$, so

$$C(\lambda) = 2\prod_{k=1}^{\infty}(1+\lambda/\lambda_k), \quad \lambda_1 < \lambda_2 < \dots. \tag{12}$$

Now we prove that zeros of D are real. The following ingenious argument is due to K. Shin ([12, Thm. 11]), but we slightly generalize his result.

Let $D(\tau) = 0$. As D is real by (9), we also have $D(\overline{\tau}) = 0$, so without loss of generality we choose

$$\operatorname{Im}\tau \geq 0. \tag{13}$$

We claim that

$$|C(\omega^{-1}\tau)| = 1. \tag{14}$$

For this we will need the assumption (1). From (9) we obtain

$$|C(\omega^{-1}\tau)C(\omega\tau)| = 1. \tag{15}$$

Then, as $\operatorname{Im}\tau \geq 0$ and $\operatorname{Im}\omega > 0$, we obtain

$$|C(\omega\tau)| = \prod_{k=1}^{\infty}|1+\omega\tau/\lambda_k| \leq \prod_{k=1}^{\infty}\left|1+\omega^{-1}\tau/\lambda_k\right| = |C(\omega^{-1}\tau)|,$$

because

$$|1+\omega\zeta| = |\omega^{-1}+\zeta| \leq |\omega+\zeta| = |1+\omega^{-1}\zeta| \quad \text{when} \quad \operatorname{Im}\zeta \geq 0, \quad \operatorname{Im}\omega > 0.$$

Then (15) gives

$$|C(\omega^{-1}\tau)| \geq 1.$$

On the other hand, when we plug $\lambda = \tau$ to (10), we obtain

$$1 \leq |C(\omega^{-1}\tau)| = \left|\frac{f(\omega^{-3}\tau)}{f(\omega^3\tau)}\right| = \prod_{k=1}^{\infty}\left|\frac{\omega^3\lambda_k - \tau}{\omega^{-3}\lambda_k - \tau}\right| \leq 1,$$

where we used (13) and $\operatorname{Im}\omega^3 \geq 0$, which follow from (1). This establishes the claim (14).

Once (14) is known, we substitute $\lambda = \tau$ to (10) again, and obtain

$$|f(\omega^{-3}\tau)| = |f(\omega^3\tau)|,$$

which is similar to (11), and implies that τ must be real, in the same way as (11) implied that λ was real.

It remains only to show that zeros of D are negative. In view of (9), and (12) we have for $x > 0$

$$D(x) + 1 = C(\omega^{-1}x)C(\omega x) = 4\prod_{k=1}^{\infty}\left(1 + 2(x\cos\alpha)/\lambda_k + (x/\lambda_k)^2\right) > 4,$$

so D has no positive zeros. □

Theorem 1 is an immediate consequence: take $g(\lambda) = -D(-\lambda)$.

Remark 1. For future references we state a slight generalization of the proposition to which the same proof applies.

Let f be given by (5) and suppose that we have

$$kf(\omega^2\lambda) + k^{-1}f(\omega^{-2}\lambda) = C(\lambda)f(\lambda), \tag{16}$$

where $|k| = 1$, and C is an entire function with no positive zeros, and $\omega = e^{i\alpha}$, where $0 < \alpha \leq \pi/3$. Then

$$k^{-3/2}f(\omega^{-3}\lambda) + C(\omega^{-1}\lambda)k^{3/2}f(\omega^3\lambda) = D(\lambda)k^{1/2}f(\omega\lambda), \tag{17}$$

where D is as in (9) and both D and C have all zeros negative.

The proof is the same as for $k = 1$.

Combining (17) with (16) we can eliminate C and express D directly in terms of f:

$$D(\lambda)f(\omega^{-1}\lambda)f(\omega\lambda) = k^{-2}f(\omega^{-3}\lambda)f(\omega^{-1}\lambda) + k^2f(\omega^3\lambda)f(\omega\lambda) + f(\omega^{-3}\lambda)f(\omega^3\lambda). \tag{18}$$

4. Proof of Theorem 2. It is convenient to make the change of the variable $y(z) = w(-iz)$. Then

$$-y'' + \left((-1)^{\ell+1}z^m + \lambda\right)y = 0, \tag{19}$$

and

$$y(z) \to 0, \quad z \to \infty, \quad \arg z = \pm\frac{\ell+1}{m+2}\pi. \tag{20}$$

In the equation (19) the principal branch of z^m is used, so the branch cut is on the negative ray.

According to Sibuya ([15]), there is a unique normalized solution $y_0(z,\lambda)$ of the equation (19) with $\ell = 1$ with the property

$$y_0(z,\lambda) = (1 + o(1))z^{-m/4}\exp\left(-\frac{2}{m+2}z^{(m+2)/2}\right), \tag{21}$$

as $z = te^{i\theta}$, $t > 0$, $t \to \infty$ and $|\theta| < 3\pi/(m+2)$. Moreover, for every fixed z_0, the function $y(z_0,\lambda)$ is an entire function of λ of order $1/2 + 1/m < 1$. Sibuya stated this result only for integer m, but his proof actually does not depend on this assumption, see [18], [8], [6]. Let

$$\omega = \exp(2\pi i/(m+2)). \tag{22}$$

As $m \geq 2$, $\operatorname{Arg}\omega \in (0, \pi/2)$. Then

$$y_k(z,\lambda) = \omega^{k/2}y_0(\omega^{-k}z, \omega^{2k}\lambda),$$

where $\omega^{k/2} := \exp(\pi ik/(m+2))$, satisfies the same differential equation (19) with $\ell = 1$ when k is an integer, and the equation (19) with $\ell = 2$ when k is a half of an odd integer. We use normalization of y_k from [7, 8] which is more convenient than Sibuya's normalization. Any three solutions of the same differential equation must be linearly dependent, so

$$y_1(z,\lambda) = C_0(\lambda)y_0(z,\lambda) - \tilde{C}(\lambda)y_{-1}(z,\lambda).$$

Comparison of the asymptotics of y_1 and y_{-1} gives $\tilde{C} \equiv 1$, so

$$y_1(z,\lambda) = C_0(\lambda)y_0(z,\lambda) - y_{-1}(z,\lambda). \tag{23}$$

One can show that C_0 is an entire function of order $1/2+1/m$, [15, 18]. Substituting $(z,\lambda) \mapsto (\omega^{-1}z, \omega^2\lambda)$ into (23), we obtain

$$y_0(z,\lambda) = C_0(\omega^2\lambda)y_1(z,\lambda) - y_2(z,\lambda), \tag{24}$$

a relation of the form (16). Eliminating $y_0(z,\lambda)$ from (23), (24), we obtain

$$y_{-1}(z,\lambda) = \left(C_0(\lambda)C_0(\omega^2\lambda) - 1\right) y_1(z,\lambda) - C_0(\lambda)y_2(z,\lambda)$$

Finally, substitute $(z,\lambda) \mapsto (\omega^{1/2}z, \omega^{-1}\lambda)$ and multiply on $\omega^{-1/4}$. The result is

$$y_{-3/2}(z,\lambda) = D_0(\lambda)y_{1/2}(z,\lambda) - C_0(\omega^{-1}\lambda)y_{3/2}(z,\lambda), \tag{25}$$

where

$$D_0(\lambda) = C_0(\omega^{-1}\lambda)C_0(\omega\lambda) - 1. \tag{26}$$

Equation (25) is a special case of (17).

We see that functions $y_{3/2}$ and $y_{-3/2}$ satisfy equation (19) with $\ell = 2$, and tend to zero on the rays $\operatorname{Arg} z = 3\pi/(m+2)$ and $\operatorname{Arg} z = -3\pi/(m+2)$, respectively. These functions, as functions of z, are linearly dependent if and only if (19), (20) with $\ell = 2$ have a non-trivial solution. Thus the eigenvalues for $\ell = 2$ are zeros of D_0.

Let us denote

$$f(\lambda) = \lim_{x \to 0+} y_0(x,\lambda);$$

it is easy to see that this is well defined, despite the singularity of (19) at 0. Then f is an entire function of genus 0 and its zeros E_k can be interpreted as eigenvalues of (19) under the boundary conditions

$$\lim_{t \to 0+} y(t) = \lim_{t \to +\infty} y(t) = 0. \tag{27}$$

This problem is self-adjoint, so all eigenvalues are real. Moreover the potential z^m is positive on the positive ray, so the "eigenvalues" λ in (19) with $\ell = 1$ under the conditions (27) are all *negative*. We also notice that $y_0(x,\lambda)$ is real for real x and λ, so $f(0)$ is real, and thus f is a real entire function.

Plugging $z = 0$ in (23) we obtain

$$\omega^{-1/2}f(\omega^{-2}\lambda) + \omega^{1/2}f(\omega^2\lambda) = C_0(\lambda)f(\lambda) \tag{28}$$

which is analogous to (16). Notice that

$$C_0(0) = \omega^{-1/2} + \omega^{1/2}$$

is real. All zeros of C_0 are positive by the results in [8, 6.2] and [10]. Application of the Remark in the previous section gives that all zeros of D_0 are negative, and this completes the proof of Theorem 2.

The author thanks André Voros and Kwang Shin for useful discussions.

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Received 11.09.2020