Anharmonic oscillators, Fekete points and a conjecture of Shapiro and Tater

Tamara Grava

University of Bristol, UK

Area of Mathematics, *SISSA*, Trieste, Italy

Firenze, April 2022

"Exactly solvable anharmonic oscillator, degenerate orthogonal polynomials and Painlevé II", arXiv:2203.16889

and "The Stieltjes–Fekete problem and degenerate orthogonal polynomials", in preparation **Joint work with Eduardo Chavez-Heredia, Tamara Grava**

Rational solutions of PII

$$\frac{\mathrm{d}^2 u(t)}{\mathrm{d}t^2} = 2u(t)^3 + tu(t) + \alpha, \tag{1}$$

Rational solution iff $\alpha = n \in \mathbb{Z}$;

$$u_n(t) = \frac{\mathrm{d}}{\mathrm{d}t} \log \frac{Y_{n-1}(t)}{Y_n(t)} \tag{2}$$

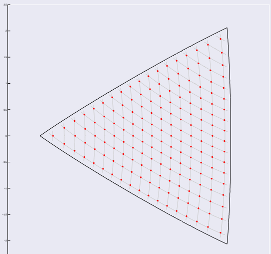
with Y_n the Vorob'ev–Yablonski polynomials of degree $n(n+1)/2$.

$$Y_{n+1}(t)Y_{n-1}(t) = tY_n^2(t) - 4\Big[Y_n''(t)Y_n(t) - \big(Y_n'(t)\big)^2\Big], \qquad n \geqslant 1,\ t \in \mathbb{C} \tag{VY}$$

with $Y_0(t) = 1, Y_1(t) = t$. Or otherwise

$$Y_n(t) = \left(-\frac{4}{3}\right)^{n(n+1)/6} \left(\prod_{k=1}^{n} (2k-1)!!\right) S_{(n,n-1,\dots,1)} \left(\left(-\frac{3}{4}\right)^{\frac{1}{3}} t, 0, 1, 0, 0, \dots\right).$$

The regularity of the pattern of zeroes of $Y_n(t)$ observed numerically by Clarkson ['03], and explained (asymptotically and analytically) by Buckingham–Miller ['14], Bertola-Bothner ['14];



Quartic Anharmonic Oscillators

By this we mean the spectrum of a Sturm–Liouville problem in "physical " form:

$$y''(x) - \left(x^4 + tx^2 + 2Jx\right) y(x) = \Lambda y(x) \tag{3}$$

$$y(x) \to 0 \text{ as } x \to \infty \text{ and } \arg(x) = \pi, \pm\pi/3, \tag{4}$$

Quasi–Exactly–Solvable spectrum

If only two boundary conditions $\Rightarrow$ Bender–Boettcher ['98]. Part of the spectrum (the "Exactly–Solvable") is explicit for $J \in \mathbb{N}$.

Exactly–Solvable spectrum

Three boundary conditions $\Rightarrow$ All the spectrum is explicit for $J \in \mathbb{N}$.

If $J \in \mathbb{N}$ the equation has quasi–polynomial solutions

$$y(x) = p(x)e^{\theta(x;t)} \quad \text{where } \theta(x;t) = \frac{x^3}{3} + \frac{tx}{2} \tag{5}$$

$p(x)$ a polynomial of degree n if and only if $J = n + 1$ and $\lambda = \Lambda - \frac{t^2}{4}$ is an eigenvalue of the operator

$$\widehat{L_J} := \frac{\mathrm{d}^2}{\mathrm{d}x^2} + 2\left(x^2 + \frac{t}{2}\right)\frac{\mathrm{d}}{\mathrm{d}x} - 2(J-1)x \tag{6}$$

acting on the space of polynomials of degree up to n.

Proposition

The Exactly solvable spectrum is characterized by the above boundary value problem; it has solutions if and only if $J = n + 1 \in \mathbb{N}$ and (t, λ) satisfy $\det(\lambda \mathbf{1} - M_n(t)) = 0$ with

$$M_n(t) := \begin{bmatrix} 0 & -2n & & & & & \\ t & 0 & -2(n-1) & & & & \\ 2 & 2t & 0 & & & & \\ & 6 & 3t & 0 & \ddots & & \\ & & 12 & \ddots & \ddots & -4 & \\ & & & \ddots & & 0 & -2 \\ & & & & n(n-1) & nt & 0 \end{bmatrix} \tag{7}$$

The discriminant locus

The ES eigenvalues depend on t: for certain values of t there are coincidences.

Shapiro-Tater $\simeq$'18 (formalized in '22)

What are the (complex) values of $t \in \mathbb{C}$ for which the spectrum is **not simple**?

$$D_n(t) := \mathrm{Disc}_\lambda \left(\det(\lambda \mathbf{1} - M_n(t)) \right) = 0$$

Our problem is non self-adjoint and the spectrum is complex (particularly so for $t \in \mathbb{C}$).

The numerics

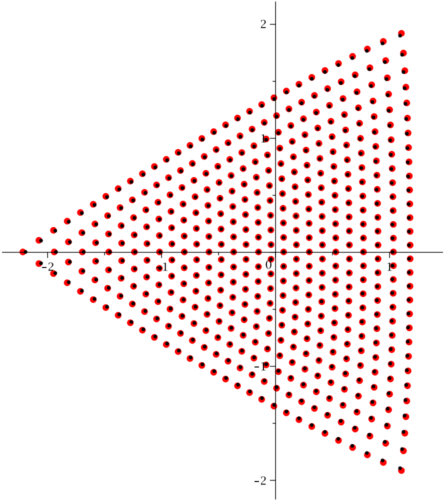


Figure: Scaled roots of the Vorob'ev-Yablonsky polynomials $Y_n(n^{2/3}s)$ in red, and roots of the discriminant $D_n(n^{2/3}s)$ in black, for $n = 30$. This particular scaling was conjectured by [Shapiro–Tater '22].

n	$D_n(t)$
1	t
2	$t^3 + \frac{27}{8}$
3	$t^6 + \frac{35}{2}t^3 - \frac{243}{4}$
4	$t^{10} + \frac{215}{4}t^7 + \frac{89}{8}t^4 + \frac{4084101}{512}t$
5	$t^{15} + \frac{255}{2}t^{12} + \frac{76211}{32}t^9 + \frac{3730405}{64}t^6 - \frac{8700637815}{4096}t^3 - \frac{125005275}{32}$

n	$Y_n(t)$
1	t
2	$t^3 + 4$
3	$t^6 + 20t^3 - 80$
4	$t^{10} + 60t^7 + 11200t$
5	$t^{15} + 140t^{12} + 2800t^9 + 78400t^6 - 3136000t^3 - 6272000$

Table: The first five monic Vorob'ev–Yablonskii polynomials $Y_n(t)$ and discriminant polynomials $D_n(t)$.

Structural results: ES spectrum I

Proposition

The boundary value problem

$$y''(x) - (x^4 + tx^2 + 2Jx + \Lambda)y(x) = 0 \tag{8}$$

$$y(se^{k\pi i/3}) \to 0, \quad s \to +\infty, \; k = 1, 3, 5. \tag{9}$$

has solution if and only if $J = n + 1 \in \mathbb{N}$ and then $y(x) = p(x)e^{\theta(x;t)}$, with $\theta(x;t) = \frac{x^3}{3} + \frac{tx}{2}$, with $p(x)$ a polynomial of degree n satisfying

$$\left(\frac{d^2}{dx^2} + 2\left(x^2 + \frac{t}{2}\right)\frac{d}{dx} - 2(J-1)x\right)p(x) = \lambda p(x), \qquad \lambda = \Lambda - \frac{t^2}{4}.$$

Proposition

If $p(x)$ is a polynomial as above then

- p is a **degenerate orthogonal polynomial**

$$\left(\kappa\int_{\infty_1}^{\infty_3}+\tilde{\kappa}\int_{\infty_5}^{\infty_3}\right)p_n(z)z^k\mathrm{e}^{2\theta(z;t)}\,\mathrm{d}z=0\quad k=0,1,\cdots,n-1,\mathbf{n}. \tag{10}$$

- The coefficients $\kappa,\tilde{\kappa}$ are

$$\kappa=\int_{\infty_2}^{\infty_0}\frac{\mathrm{e}^{-2\theta(z;t)}\,\mathrm{d}z}{p^2(z)}\qquad\tilde{\kappa}=\int_{\infty_0}^{\infty_4}\frac{\mathrm{e}^{-2\theta(z;t)}\,\mathrm{d}z}{p^2(z)}$$

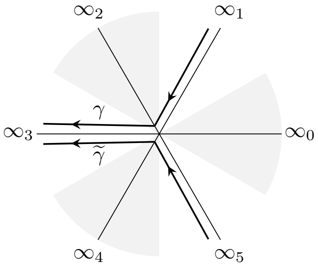


Figure: Directions at infinity ∞_k of argument $k\frac{i\pi}{3}$.

Structural results: ES degenerate spectrum

Theorem

$t \in \mathbb{C}$ is such that the Exactly Solvable spectrum of (8)-(9) *has a repeated eigenvalue iff there is a quasi-polynomial solution $p_n(x)\mathrm{e}^{\theta(x;t)}$ of* (8)-(9) *that* **additionally** *satisfies*

$$\int_{\infty_1}^{\infty_3} p_n^2(z)e^{2\theta(z;a)}\,\mathrm{d}z = 0, \quad \int_{\infty_3}^{\infty_5} p_n^2(z)e^{2\theta(z;a)}\,\mathrm{d}z = 0 \tag{11}$$

Proposition

The zeros of the degenerate orthogonal polynomial $p_n(z)$ satisfies the Fekete type relation

$$\theta'(z_j) = \sum_{k \neq j} \frac{1}{z_k - z_j}, \quad j = 1, \ldots, n.$$

Asymptotic analysis

From Lax pair to scalar ODE

Proposition

The point t is a pole with residue -1 of the rational PII function $u(t)$ with parameter $\alpha = n$ (i.e. a zero of $Y_n(t)$) if and only if there is b such that the ODE (Its-Novokshenov)

$$f(x)'' - V_{JM}(x;t,b)f(x) = 0$$

$$V_{JM}(x;t,b) = x^4 + tx^2 + 2(n + \frac{1}{2})x + \left(\frac{7t^2}{36} + 10b\right)$$

manifests the Stokes' phenomenon indicated below [Buckingham–Miller '14]

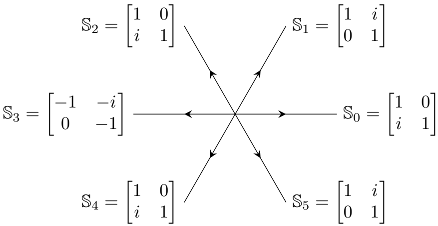


Figure: Stokes data for the Lax pair corresponding to rational solutions of Painlevé II

Proposition

The values t, Λ belong to the ES spectrum iff

$$y''(x) - (x^4 + tx^2 + 2(n+1)x + \Lambda)y(x) = 0 \tag{12}$$

corresponds to the Stokes' phenomenon below. In addition the parameter t is in the discriminant locus if and only if

$$\int_{\infty_1}^{\infty_3} y^2(x)\,\mathrm{d}x = 0 = \int_{\infty_5}^{\infty_3} y^2(x)\,\mathrm{d}x$$

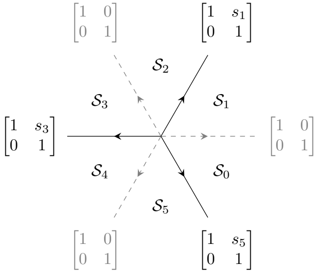


Figure: Stokes matrices and Stokes sectors for the Shapiro-Tater eigenvalue problem: it is necessary $s_1 + s_3 + s_5 = 0$. The Stokes matrices S_0, S_2, S_4 are all the identity.

Strategy

1. Scale t, Λ (and z) with $\hbar = (n+1)^{-1}$ or $\hbar = (n+\frac{1}{2})^{-1}$ to bring the equation to standard singularly perturbed.

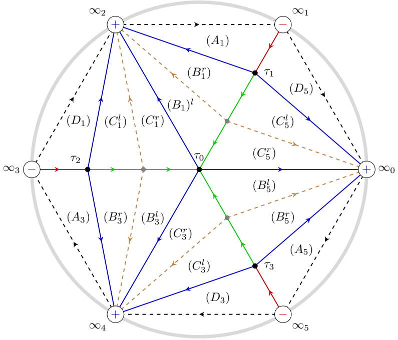
$$y''(z) - \frac{1}{\hbar^2} Q(z; s, E) y(z) = 0, \qquad Q(z; s, E) = z^4 + s z^2 + 2z + E \tag{13}$$

$$s = \hbar^{\frac{2}{3}} t, \quad E = \hbar^{\frac{4}{3}} \Lambda \tag{14}$$

2. Use WKB to compute Stokes' data
3. Match Stokes' data with the figure.
   1. For the VY case the Stokes' parameters are completely determined and this (implicitly) fixes the pair (s, E);
   2. For the ST case we need to **additionally** impose the degeneracy condition, which is equivalent to

$$\int_{\{\gamma_1, \gamma_2\}} p_n^2 \mathrm{e}^{2\theta} \, \mathrm{d}x = 0.$$

These integrals must be estimated using the WKB approximation.



Stokes' complex compatible with the conditions

Figure: Labelled regions in the WKB Riemann-Hilbert problem.

Quantization conditions (leading order)

ST case

$$
\begin{aligned}
2(n+1)\int_{\tau_1}^{\tau_0}\sqrt{Q(z_+;s,E)}\,\mathrm{d}z &= \ln\left(\frac{-1}{1+\boldsymbol{\tau}(s,E)}\right) - 2i\pi(m_1+1)\\
2(n+1)\int_{\tau_2}^{\tau_0}\sqrt{Q(z_+;s,E)}\,\mathrm{d}z &= \ln\left(-1-\frac{1}{\boldsymbol{\tau}(s,E)}\right) - 2i\pi(m_2+1)\\
2(n+1)\int_{\tau_3}^{\tau_0}\sqrt{Q(z_+;s,E)}\,\mathrm{d}z &= \ln\left(\boldsymbol{\tau}(s,E)\right) - 2i\pi(m_3+1)
\end{aligned}
$$

$$
\boldsymbol{\tau}(s,E) = \frac{\displaystyle\int_{\tau_1}^{\tau_0}\frac{\mathrm{d}z}{\sqrt{Q(z_+;s,E)}}}{\displaystyle\int_{\tau_2}^{\tau_0}\frac{\mathrm{d}z}{\sqrt{Q(z_+;s,E)}}}, \quad \Im(\boldsymbol{\tau}(s,E))>0
$$

$$
m_1+m_2+m_3 = n-1. \tag{15}
$$

VY case

$$
(2n+1)\int_{\tau_j}^{\tau_0}\sqrt{Q(z_+;s,E)}\,\mathrm{d}z = -i\pi - 2i\pi k_j
$$

$$
k_1+k_2+k_3 = n-1. \tag{16}
$$

Geometry of the lattices I

$$\omega := \int_{\tau_2}^{\tau_0} \frac{\mathrm{d}z}{\sqrt{Q(z_+; s, E)}}, \quad \omega' := \int_{\tau_1}^{\tau_0} \frac{\mathrm{d}z}{\sqrt{Q(z_+; s, E)}} \tag{17}$$

Proposition

Let (s_0, E_0) correspond to the first-order quantization conditions (15) or (16) in the bulk, namely, $m_j/n \simeq c_j \neq 0$. Then the neighbour points in the s–plane form a slowly modulated hexagonal lattice in the sense that the six closest neighbours of s_0 are

$$s_0 + 2\hbar\left(\omega\Delta m_1 - \omega'\Delta m_2\right) \tag{18}$$

where ω and ω' are the half periods of the holomorphic differentials in (17) and

$$\Delta m_j \in \{-1, 0, 1\}, \qquad |\Delta m_1 + \Delta m_2| \leqslant 1, \qquad |\Delta m_1| + |\Delta m_2| \geqslant 1.$$

Near the origin

If $(s, E) = \mathcal{O}(\hbar)$

Theorem

The rescaled lattices of the zeroes of the VY Polynomials, and the of ST problem coincide to within order $\mathcal{O}(\hbar^2) = \mathcal{O}(n^{-2})$ *in a* $\mathcal{O}(\hbar)$ *neighbourhood of the origin in the* s*–plane. More precisely the quantization conditions corresponding to the triples* $(m_1, m_2, m_3), \quad m_1 + m_2 + m_3 = n - 1$ *and* $(k_1, k_2, k_3), \quad k_1 + k_2 + k_3 = n - 1$ *with* $m_j = k_j$ *single out values of* s, E *that differ by a discrepancy of order* $\mathcal{O}(\hbar^2)$*, provided that* $m_j - \frac{n-1}{3}$ *remain bounded as* $n \to \infty$*.*

Stieljes–Fekete property

The zeroes of the degenerate OP satisfy the following algebraic equations;

$$\theta'(z_j) = z_j^2 + \frac{t}{2} = \sum_{\substack{k=1 \\ k \neq j}}^{n} \frac{1}{z_k - z_j}, \quad j = 1, \ldots, n. \tag{19}$$

$$\text{where } \theta(z;t) = \frac{z^3}{3} + \frac{tz}{2} \tag{20}$$

An old result of Stieltjes

The roots of the n–th Hermite polynomial $H_n(x) = \mathrm{e}^{x^2} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \mathrm{e}^{-x^2}$ are the "Fekete" points, i.e. maximize the function

$$\mathcal{F}(x_1, \ldots, x_n) = \prod_{j<k} (x_j - x_k)^2 \mathrm{e}^{-\frac{x_j^2 + x_k^2}{2}}$$

The variational equations yield

$$x_j = \sum_{\substack{k=1 \\ k \neq j}}^{n} \frac{1}{x_k - x_j}, \quad j = 1, \ldots, n.$$

Similar results for Jacobi and Laguerre polynomials.

Generalization

We consider a *holomorphic* version of the condition of criticality in the form

$$\sum_{k\neq j} \frac{1}{z_j - z_k} = \frac{A(z_j)}{2B(z_j)}, \quad j = 1, \ldots, n,$$

where A, B are two relatively prime polynomials. These turn out to be the stationary equations for

$$\mathscr{F}(z_1, \ldots, z_n) = \prod_{j=1}^{n} \prod_{\substack{k=1 \\ k\neq j}}^{n} (z_j - z_k) \mathrm{e}^{\frac{\theta(z_j)+\theta(z_k)}{2}}$$

where

$$\theta'(z) = -\frac{A(z) + B(z)'}{B(z)}$$

In the excellent review Marcellán–Martínez-Finkelshtein–Martínez-González,

"Electrostatic models for zeros of polynomials: Old, new, and some open problems", *J. Comp. Appl. Math.*, **207** (2007), 258–272.

the following questions were raised, to quote verbatim from loc. cit.: "[...] Reviewing the electrostatic models above several natural questions arise, such as:

- Are there generalizations of these models to other families of polynomials?
- Why necessarily the global minimum of the energy should be considered? Which other types of equilibria described above could be linked to the zeros of the polynomials?
- What is the appropriate model for the complex zeros (when they exist)? [...]"

We address and answer precisely the above three questions

There is a one-to-one correspondence between the solutions of the algebraic system of equations

$$\sum_{k\neq j} \frac{1}{z_j - z_k} = \frac{A(z_j)}{2B(z_j)}, \quad j = 1, \dots, n,$$

and the *maximally degenerate* orthogonal polynomials of degree n for a *semiclassical moment functional* of type (A, B).

Fix two polynomials, $A(z), B(z)$ of degree a, b, respectively, and relatively prime. The moment functional $\mathcal{M} : \mathbb{C}[x] \to \mathbb{C}$ is a *semiclassical moment functional* of type (A, B) if

$$\mathcal{M}\big[B(x)p'(x)\big] = \mathcal{M}\big[A(x)p(x)\big], \qquad \forall p(x) \in \mathbb{C}[x].$$

Studied by Maroni ['87], Ismail-Masson-Rahman ['91], Marcellán-Rocha ['98]: any such moment functional can be represented as:

$$\mathcal{M}[p] = \sum_{\ell=1}^{d} s_\ell \int_{\gamma_\ell} p(x)\mathrm{e}^{\theta(x)}\,\mathrm{d}x \ , \qquad \theta'(x) = -\frac{A(x) + B'(x)}{B(x)}$$

and $d = \max\{a, b-1\}$.

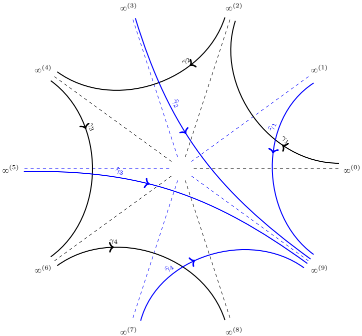


Figure: The contours, and dual contours, for the Freud case θ polynomial of degree 5

Orthogonal Polynomials satisfy

$$\langle P_n, z^k \rangle := \mathcal{M}\Big[P_n(z) z^k\Big] = \sum_{j=1}^{d} s_j \int_{\gamma_j} P_n(z) z^k \mathrm{e}^{\theta} \, \mathrm{d}z = 0,$$

$$k = 0, \ldots, n-1,$$

Let $\mu_k(\mathbf{s}) = \int_\Gamma z^k \mathrm{e}^{\theta} \, \mathrm{d}z, \quad \mathbf{s} = (s_1, \ldots, s_d)$,

$$D_n(\mathbf{s}) := \det \left[\mu_{a+b}(\mathbf{s})\right]_{a,b=0}^{n-1}$$

The polynomials of degree $\leqslant n$ that satisfy the orthogonality are determined

$$P_n(z) = \det \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & & & \\ \mu_{n-1} & \cdots & & \mu_{2n-1} \\ 1 & z & \ldots & z^n \end{bmatrix}$$

Degenerate orthogonality

Definition

The polynomial P_n is called ℓ**–degenerate orthogonal** if, in addition

$$\left\langle P_n, z^k \right\rangle = 0, \quad k = n, n+1, \ldots, n+\ell-1.$$

Lemma

The orthogonal polynomial P_n is ℓ–degenerate if and only if

$$D_{n,k}(\mathbf{s}) := \det H_{n,k} = 0, \qquad k = 0, 1, \ldots, \ell-1,$$

$$H_{n,k} := \left[\begin{array}{cccc} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & & & \\ \mu_{n-1} & \cdots & & \mu_{2n-1} \\ \hline \mu_{n+k} & \mu_{n+k+1} & \cdots & \mu_{2n+k} \end{array} \right].$$

Maximal degeneracy

When $\ell = d-1$: gives $d-1$ **homogeneous polynomial relations on the "weights"** $s_1, \ldots, s_d$

Theorem

Let $\mathscr{X} = \{z_1, \dots, z_n\}$ *be a critical configuration satisfying the equilibrium equations*

$$\sum_{k \neq j} \frac{1}{z_j - z_k} = \frac{A(z_j)}{2B(z_j)}, \quad j = 1, \dots, n,$$

where $A(z), B(z)$ *are relatively prime arbitrary polynomials (and* B *monic). Then*

(1) *the polynomial* $P_n(z) = \prod_{j=1}^n (z - z_j)$ *is a maximally degenerate orthogonal polynomial for a semiclassical moment functional* $\mathcal{M}$ *of type* (A, B)*. For fixed* n *the number of critical configuration is* $(n+1)^{d-1}$ *where* $d =$ *max*$(b-1, a)$*.*

(2) *The quasi-polynomial* $y(z) = P_n(z) \mathrm{e}^{\frac{1}{2}\theta(z)}$*, with*

$$\theta'(z) = -\frac{A(z) + B'(z)}{B(z)}$$

satisfies the differential equation

$$y(z)'' - V(z) y(z) = 0$$

where the function V *is a rational function with poles only at the zeroes of* $B(z)$ *(and a polynomial of degree* $2 \deg A$ *if* $B = 1$*)*

Viceversa, if P_n *is a semiclassical, maximally degenerate orthogonal polynomial of degree* n *for a semiclassical moment functional* $\mathcal{M}$ *of type* (A, B) *then its zeroes satisfy the equilibrium equation and the ODE as above.*

Thank you!