

Orthogonal systems with a skew-symmetric differentiation matrix

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joint work with Arie Iserles (Cambridge)

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Cambridge Analysts' Knowledge Exchange

Motivation: Time-dependent PDEs

$$u \in C^\infty([0, \infty); H^1(\mathbb{R})), \quad t \in [0, \infty), \quad x \in \mathbb{R}.$$

- Diffusion:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left[a(t, x, u) \frac{\partial u}{\partial x} \right], \quad a \geq 0$$

- Semi-classical Schrödinger:

$$i\varepsilon \frac{\partial u}{\partial t} = -\varepsilon^2 \frac{\partial^2 u}{\partial x^2} + V(t, x, u)u, \quad 0 < \varepsilon \ll 1, \quad \text{Imag}(V) = 0$$

- Nonlinear advection:

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} + f(u), \quad v \cdot f(v) \leq 0$$

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- Common property? L_2 **stability**:

$$\frac{d}{dt} \int_{-\infty}^{\infty} |u(t, x)|^2 dx \leq 0, \quad \text{for all } t \geq 0.$$

L_2 stability of these PDEs

$$\frac{d}{dt} \int |u(t, x)|^2 dx = \int \frac{\partial}{\partial t} |u(t, x)|^2 dx = 2\operatorname{Re} \int \overline{u(t, x)} \frac{\partial u}{\partial t}(t, x) dx$$

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- Schrödinger:

$$\begin{aligned} \frac{d}{dt} \int_{-\infty}^{\infty} |u|^2 dx &= 2\operatorname{Re} \int_{-\infty}^{\infty} \bar{u} \left(i\varepsilon \frac{\partial^2 u}{\partial x^2} - i\varepsilon^{-1} V(t, x, u) u \right) dx \\ &= -2\operatorname{Re} \int_{-\infty}^{\infty} i\varepsilon \left| \frac{\partial u}{\partial x} \right|^2 + i\varepsilon^{-1} V(t, x, u) |u|^2 dx = 0 \end{aligned}$$

Numerical solution of these PDEs

- Suppose we want a **numerical solution** to the diffusion equation $\partial_t u = \partial_x(a(x) \cdot \partial_x u)$.

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$$\mathbf{u}'(t) = \mathcal{D}\mathcal{A}\mathcal{D}\mathbf{u}(t), \quad \mathbf{u}(0) = \mathbf{u}_0 \in \mathbb{C}^N$$

- E.g. **finite difference method** on a grid x_1, x_2, \dots, x_N

$$\mathbf{u}(t) = (u(t, x_1), u(t, x_2), \dots, u(t, x_N))^T \in \mathbb{C}^N$$

- \mathcal{D} is a matrix encoding a finite-difference approximation to the partial derivative ∂_x .
- \mathcal{A} is a diagonal matrix with entries $(a(x_1), \dots, a(x_N))$.

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- E.g. **spectral method** for a basis $\Phi = \{\varphi_n\}_{n \in \mathbb{Z}_+}$ of $L_2(\mathbb{R})$

$$u(t, \cdot) = \sum_{n=0}^{\infty} u_n(t) \varphi_n$$

- \mathcal{D} and \mathcal{A} are infinite-dimensional matrices encoding:

$$\varphi'_k(x) = \sum_{j=0}^{\infty} D_{k,j} \varphi_j(x), \quad a(x) \varphi_k(x) = \sum_{j=0}^{\infty} A_{k,j} \varphi_j(x)$$

ℓ_2 stability of (semi-)discretised PDEs

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Geometric Numerical Integration

The field of research on **discretisation** of differential equations which **respects qualitative properties** of the analytical solution (see Hairer-Lubich-Wanner 2006)

The joy and pain of skew-symmetry

- The simplest second-order finite difference scheme gives

$$\mathcal{D} = \frac{1}{2\Delta x} \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ -1 & 0 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \cdots & 0 & -1 & 0 \end{pmatrix}$$

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- Looking good! This is the **highest order** skew-symmetric differentiation matrix on an **equispaced grid** (Iserles 2014)
- Higher-order skew-symmetric differentiation matrices on **special grids** are possible but complicated (Hairer-Iserles 2016,2017).

Known example: Fourier spectral methods

Take the Fourier basis:

$$\varphi_0(x) \equiv \frac{1}{(2\pi)^{1/2}}, \quad \varphi_{2n}(x) = \frac{\cos nx}{\pi^{1/2}}, \quad \varphi_{2n+1}(x) = \frac{\sin nx}{\pi^{1/2}}, \quad n \in \mathbb{N}$$

– note that the basis is orthonormal.

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$$\mathcal{D} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & -2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & \cdots \\ 0 & 0 & 0 & 0 & 0 & -3 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

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For **periodic boundary conditions** only.

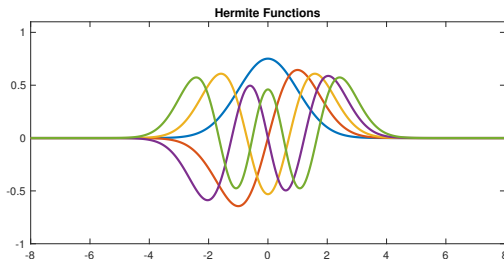
Known example: Hermite spectral methods

- Hermite functions are familiar in mathematical physics:

$$\varphi_n(x) = \frac{(-1)^n}{(2^n n!)^{1/2} \pi^{1/4}} e^{-x^2/2} H_n(x), \quad n \in \mathbb{Z}_+, \quad x \in \mathbb{R},$$

where H_n is the n th *Hermite polynomial*.

- Orthonormal basis for $L_2(\mathbb{R})$
- Uniformly bounded, and smooth
- Eigenfunctions of the Fourier transform



Known example: Hermite spectral methods

Hermite functions obey the ODE

$$\begin{aligned}\varphi_0'(x) &= -\sqrt{\frac{1}{2}}\varphi_1(x), \\ \varphi_n'(x) &= \sqrt{\frac{n}{2}}\varphi_{n-1}(x) - \sqrt{\frac{n+1}{2}}\varphi_{n+1}(x), \quad n \in \mathbb{N}.\end{aligned}$$

In other words,

$$\mathcal{D} = \begin{pmatrix} 0 & -\sqrt{\frac{1}{2}} & 0 & 0 & \cdots \\ \sqrt{\frac{1}{2}} & 0 & -\sqrt{\frac{2}{2}} & 0 & \cdots \\ 0 & \sqrt{\frac{2}{2}} & 0 & -\sqrt{\frac{3}{2}} & \ddots \\ \vdots & 0 & \sqrt{\frac{3}{2}} & \ddots & \ddots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix},$$

a **skew-symmetric, tridiagonal** differentiation matrix.

Nonstandard example: Spherical Bessel Functions

Solutions to the ODE $x^2 \frac{d^2 y}{dx^2} + 2x \frac{dy}{dx} + (x^2 - n(n+1))y = 0$, for each $n \in \mathbb{Z}_+$, are the **spherical Bessel functions** $j_n(x)$.

$$j_0(x) = \frac{\sin(x)}{x}, \quad j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}, \quad j_2(x) = \left(\frac{3}{x^2} - 1\right) \frac{\sin(x)}{x} - \frac{3\cos(x)}{x^2}.$$

Writing $\varphi_n(x) = \sqrt{\frac{2n+1}{\pi}} j_n(x)$, one can obtain the known result

$$\varphi'_n(x) = -\frac{n}{\sqrt{(2n-1)(2n+1)}} \varphi_{n-1}(x) + \frac{n+1}{\sqrt{(2n+1)(2n+3)}} \varphi_{n+1}(x)$$

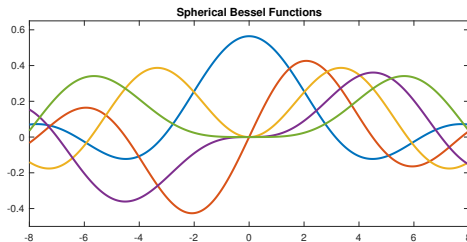
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Aims of the talk

Aim 1

Find a system of functions $\Phi = \{\varphi_n\}_{n \in \mathbb{Z}_+}$, and nonzero scalars $\{b_n\}_{n \in \mathbb{Z}_+}$ such that

$$\begin{aligned}\varphi'_0(x) &= b_0 \varphi_1(x), \\ \varphi'_n(x) &= -b_{n-1} \varphi_{n-1}(x) + b_n \varphi_{n+1}(x), \quad n \in \mathbb{N}.\end{aligned}$$

Φ has **real, skew-symmetric, tridiagonal irreducible differentiation matrix**

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Aim 2

Determine systems which are also **orthonormal** in $L_2(\mathbb{R})$:

$$u(x) = \sum_{n=0}^{\infty} u_n \varphi_n(x) \implies \|\mathbf{u}\|_{\ell_2} = \|u\|_{L_2(\mathbb{R})} \quad (1)$$

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Our continuing mission: to explore strange new bases, to seek out new methods and new special functions, to boldly go...

Elementary construction

Let $\varphi_0 \in C^\infty(\mathbb{R})$ and $\{b_n\}_{n \in \mathbb{Z}_+}$ be given.

$$n = 0 : \quad \varphi_1(x) = \frac{1}{b_0} \varphi'_0(x),$$

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and so on. Easy **induction** confirms that

$$\varphi_n(x) = \frac{1}{b_0 b_1 \cdots b_{n-1}} \sum_{\ell=0}^{\lfloor n/2 \rfloor} \alpha_{n,\ell} \varphi_0^{(n-2\ell)}(x), \quad n \in \mathbb{N},$$

$$\alpha_{n+1,0} = 1, \quad \alpha_{n+1,\ell} = b_{n-1}^2 \alpha_{n-1,\ell-1} + \alpha_{n,\ell}, \quad \ell = 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor.$$

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The Fourier transform

The unitary Fourier transform and its inverse:

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Define the transformed functions

$$\psi_n(\xi) = (-i)^n \mathcal{F}[\varphi_n](\xi).$$

Then

$$\xi \psi_n(\xi) = (-i)^n \xi \mathcal{F}[\varphi_n](\xi) = (-i)^{n+1} (i\xi) \mathcal{F}[\varphi_n](\xi) = (-i)^{n+1} \mathcal{F}[\varphi'_n](\xi).$$

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- Fourier differentiation formula implies

$$\psi_n(\xi) = (-i)^n \mathcal{F}[\varphi_n](\xi), \quad \xi \psi_n(\xi) = (-i)^{n+1} \mathcal{F}[\varphi'_n](\xi), \quad n \in \mathbb{Z}_+.$$

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- Using the skew-symmetric differentiation formula,

$$\begin{aligned} \xi \psi_0(\xi) &= b_0(-i) \mathcal{F}[\varphi_1](\xi) = b_0 \psi_1(\xi), \\ \xi \psi_n(\xi) &= -b_{n-1}(-i)^{n+1} \mathcal{F}[\varphi_{n-1}](\xi) + b_n(-i)^{n+1} \mathcal{F}[\varphi_{n+1}](\xi) \\ &= b_{n-1} \psi_{n-1}(\xi) + b_n \psi_{n+1}(\xi). \end{aligned}$$

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- They satisfy a symmetric recurrence!
- Therefore, they are of the form $\psi_n(\xi) = p_n(\xi) \psi_0(\xi)$, where

$$\begin{aligned} p_0(\xi) &= 1, & p_1(\xi) &= b_0^{-1} \xi \\ p_{n+1}(\xi) &= \frac{\xi}{b_n} p_n(\xi) - \frac{b_{n-1}}{b_n} p_{n-1}(\xi), & n &\in \mathbb{N}. \end{aligned}$$

Favard's Theorem

Theorem (Favard)

Let $P = \{p_n\}_{n \in \mathbb{Z}_+}$ be a sequence of real polynomials such that $\deg(p_n) = n$. P is an **orthogonal system** with respect to the inner product $\langle f, g \rangle_\mu = \int \overline{f(\xi)} g(\xi) d\mu(\xi)$ for some **probability measure** $d\mu$ on the real line if and only if the polynomials satisfy the three-term recurrence,

$$p_{n+1}(\xi) = (\alpha_n - \beta_n \xi) p_n(\xi) - \gamma_n p_{n-1}(\xi), \quad n \in \mathbb{Z}_+,$$

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For us:
$$p_{n+1}(\xi) = \frac{\xi}{b_n} p_n(\xi) - \frac{b_{n-1}}{b_n} p_{n-1}(\xi)$$

Fourier characterisation for Φ

We can now deduce for our $\Phi = \{\varphi_n\}_{n \in \mathbb{Z}_+}$:

$$i^n \mathcal{F}[\varphi_n](\xi) = \psi_n(\xi) = \psi_0(\xi) p_n(\xi), \quad \text{so} \quad \varphi_n(x) = (-i)^n \mathcal{F}^{-1}[\psi_0 \cdot p_n]$$

The mapping can be (carefully) followed both ways:

$$(\{\varphi_n\}_{n \in \mathbb{Z}_+}, \{b_n\}_{n \in \mathbb{Z}_+}) \leftrightarrow (\{p_n\}_{n \in \mathbb{Z}_+}, \psi_0)$$

Theorem (Iserles-Webb 2018)

The sequence $\Phi = \{\varphi_n\}_{n \in \mathbb{Z}_+}$ has a real, skew-symmetric, tridiagonal, irreducible, differentiation matrix if and only if

$$\varphi_n(x) = (-i)^n \mathcal{F}^{-1}[g \cdot p_n],$$

where $P = \{p_n\}_{n \in \mathbb{Z}_+}$ is an orthonormal polynomial system on the real line with respect to a symmetric probability measure $d\mu$, and $g = \psi_0 = \mathcal{F}[\varphi_0]$.

Legendre and Bessel functions

The Legendre polynomials $P = \{P_0, P_1, \dots\}$ satisfy

$$\int_{-1}^1 P_n(\xi) P_m(\xi) d\xi = \left(n + \frac{1}{2}\right)^{-1} \delta_{n,m}$$

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We obtain the **spherical Bessel functions** again! ($g(\xi) = \chi_{[-1,1]}(\xi)$)

Orthogonal systems

- We have the formula, $\varphi_n(x) = (-i)^n \mathcal{F}^{-1}[g \cdot p_n]$, where $g = \mathcal{F}[\varphi_0]$ and $P = \{p_n\}_{n \in \mathbb{Z}_+}$ are orthonormal with respect to a symmetric measure.

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- How can we tell if Φ is an **orthogonal system**?
- **Parseval's Theorem**: For all $\varphi, \psi \in L_2(\mathbb{R})$,

$$\int_{-\infty}^{\infty} \overline{\mathcal{F}[\varphi](\xi)} \mathcal{F}[\psi](\xi) d\xi = \int_{-\infty}^{\infty} \overline{\varphi(x)} \psi(x) dx$$

- Simple!

$$\int_{-\infty}^{\infty} \varphi_n(x) \varphi_m(x) dx = (-i)^{m-n} \int p_n(\xi) p_m(\xi) |g(\xi)|^2 d\xi$$

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Theorem (Iserles-Webb 2018)

Φ is orthogonal in $L_2(\mathbb{R})$ if and only if P is orthogonal with respect to the measure $|g(\xi)|^2 d\xi$. Note, $g = \mathcal{F}[\varphi_0]$.

Hermite revisited

$$\varphi_n(x) = \frac{(-1)^n}{(2^n n!)^{1/2} \pi^{1/4}} e^{-x^2/2} H_n(x), \quad n \in \mathbb{Z}_+, \quad x \in \mathbb{R},$$

- As mentioned earlier, the Hermite functions are **eigenfunctions** of the Fourier transform:

$$\mathcal{F}[\varphi_n](\xi) = (-i)^n \varphi_n(\xi) \tag{2}$$

- Therefore, the Hermite functions are, in a sense, a **fixed point** of our correspondence

Theorem (Iserles-Webb 2018)

Up to trivial rescaling, the only orthogonal system that consists of “quasi-polynomials” is the Hermite system.

Transformed Chebyshev functions

- The Chebyshev polynomials of the second kind, U_0, U_1, U_2, \dots are **orthonormal** with respect to the measure

$$d\mu(\xi) = \frac{2}{\pi} \chi_{[-1,1]}(\xi) \sqrt{1 - \xi^2} d\xi.$$

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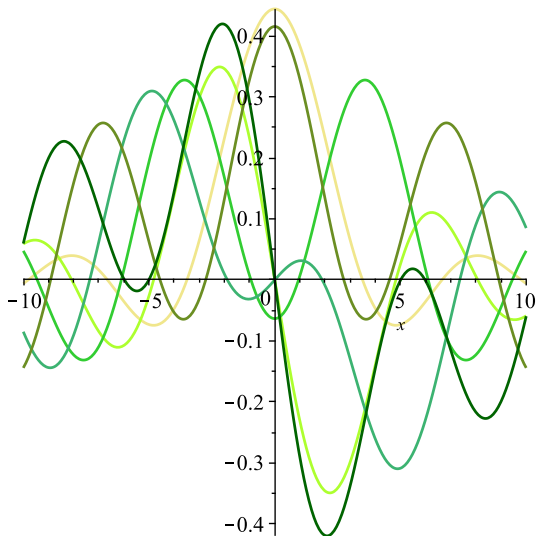
$$d\mu(\xi) = \frac{2}{\pi} \chi_{[-1,1]}(\xi) \sqrt{1 - \xi^2} d\xi.$$

- We have $b_n = \frac{1}{2}$ for all $n \in \mathbb{Z}_+$ (so \mathcal{D} is also a **Toeplitz matrix**)

$$\begin{aligned}\varphi_0(x) &\propto \int_{-1}^1 (1 - \xi^2)^{1/4} e^{ix\xi} d\xi \propto \frac{J_1(x)}{x} \\ \varphi_1(x) &\propto \int_{-1}^1 \xi (1 - \xi^2)^{1/4} e^{ix\xi} d\xi \propto \frac{J_2(x)}{x},\end{aligned}$$

- Here $J_n(x)$ is the Bessel function of degree n .
- The expressions get more complicated...

Transformed Chebyshev functions



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- Clearly, their Fourier transforms are **compactly supported** in $[-1, 1]$
- The **Paley-Wiener spaces** are closed subspaces of $L_2(\mathbb{R})$ obtained by **restricting Fourier transforms** to a set $\Omega \subset \mathbb{R}$:

$$\mathcal{PW}_\Omega(\mathbb{R}) := \{\varphi \in L^2(\mathbb{R}) : \mathcal{F}[\varphi](\xi) = 0 \text{ for a.e. } \xi \in \mathbb{R} \setminus \Omega\},$$

- Keywords: **Band-limiting, band-limited function spaces**. Numerous applications and relevance in signal processing

Transformed Carlitz functions

Consider the **hyperbolic secant** measure

$$d\mu(\xi) = \operatorname{sech}^2(\pi\xi) d\xi$$

This measure (after heroic algebra) is related to the **Carlitz polynomials** on a line in the complex plane.

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$$b_n = \frac{(n+1)^2}{\sqrt{(2n+1)(2n+3)}}$$

Up to a constant scaling,

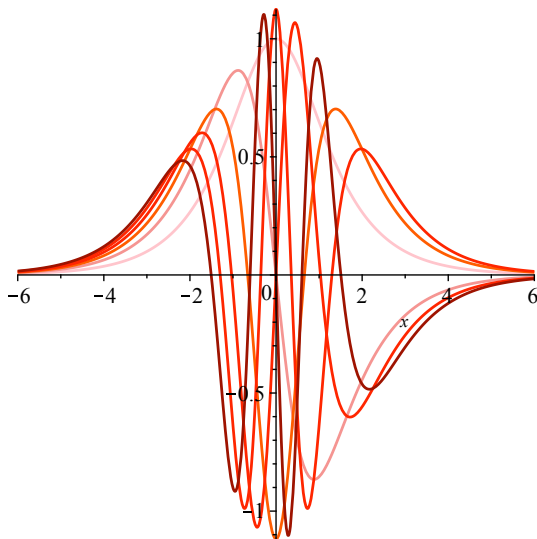
$$\varphi_0(x) = \operatorname{sech}(x)$$

$$\varphi_1(x) = -\sqrt{3} \tanh(x) \operatorname{sech}(x)$$

$$\varphi_2(x) = \frac{\sqrt{5}}{2} (2\operatorname{sech}(x) - 3\operatorname{sech}^3(x))$$

$$\varphi_3(x) = \frac{\sqrt{7}}{2} \tanh(x) (2\operatorname{sech}^2(x) - 5\operatorname{sech}^4(x))$$

Transformed Carlitz functions

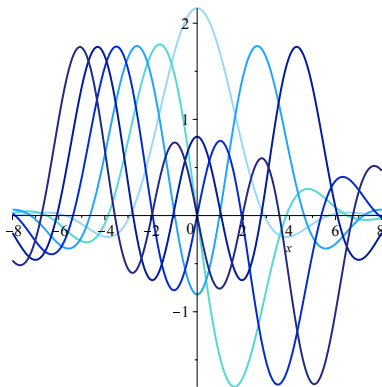


Transformed Freud functions

Polynomials orthogonal with respect to the measure $d\mu(\xi) = e^{-\xi^4} d\xi$ are a particular instance of **Freud polynomials**.

$$\varphi_0(x) = \frac{2^{\frac{3}{4}}}{4\Gamma(\frac{3}{4})} \left\{ 2\pi_0 F_2 \left[\frac{-}{\frac{1}{2}, \frac{3}{4}}; \frac{x^4}{128} \right] - x^2 \Gamma^2 \left(\frac{3}{4} \right) {}_0F_2 \left[\frac{-}{\frac{5}{4}, \frac{3}{2}}; \frac{x^4}{128} \right] \right\},$$

The coefficients $\{b_n\}_{n \in \mathbb{Z}_+}$ satisfy so-called **string relations** (see Clarkson 2016).



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- There is a **one-to-one correspondence** between orthonormal systems with a real, skew-symmetric, tridiagonal, irreducible differentiation matrix and orthonormal polynomials with respect to a symmetric probability measure* $d\mu(\xi) = w(\xi)d\xi$.

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 - Can new, improved, practical, L_2 stable spectral methods for time-dependent PDEs be developed following this work?