Spectral Analysis of *XX* Quantum Spin Chains

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Universidad de Talca

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Preliminaries

Let $m > 1$ denote the number of sites and let $\alpha,\ \beta \in \mathbb{R}$.

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- Hamiltonian

$$\mathrm{H} = \sum_{l=1}^{m-1} \left(\sigma_l^+ \sigma_{l+1}^- + \sigma_{l+1}^+ \sigma_l^-\right) + \alpha\, \sigma_1^+ \sigma_1^- + \beta\, \sigma_m^+ \sigma_m^-,$$

which acts on the state space $\mathbb{C}^{2m}$. Here, σ_l^- and σ_l^+ denote the lowering and raising operators at site l, respectively.

Single-particle Hamiltonian

The action of H on the single-particle states

$$e_j = |0, \ldots, 0, \underbrace{1}_{j}, 0, \ldots, 0\rangle$$

is represented by the $m \times m$ Jacobi matrix

$$\mathrm{J} = \begin{bmatrix} \alpha & 1 & 0 & \cdots & 0 \\ 1 & 0 & \ddots & \ddots & \vdots \\ 0 & 1 & \ddots & 1 & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \cdots & 0 & 1 & \beta \end{bmatrix}.$$

Characteristic polynomial

The characteristic polynomial of J can be expressed in terms of Chebyshev polynomials of the second kind as

$$\begin{aligned}\chi_m(\mathrm{E}) &= \det(\mathrm{E}\,\mathrm{I} - \mathrm{J}) \\ &= U_m\Big(\frac{\mathrm{E}}{2}\Big) - (\alpha+\beta)\,U_{m-1}\Big(\frac{\mathrm{E}}{2}\Big) + \alpha\beta\,U_{m-2}\Big(\frac{\mathrm{E}}{2}\Big),\end{aligned}$$

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Relation to Bernstein–Szegő orthogonal polynomials

$$\chi_m(\underbrace{z + z^{-1}}_{=\mathrm{E}(z)}) = p_m(z),$$

where

$$p_m(z) = c(z)\, z^m + c(z^{-1})\, z^{-m},$$

with

$$c(z) = \frac{(1 - \alpha z^{-1})(1 - \beta z^{-1})}{1 - z^{-2}}.$$

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Band-state root

Let $\xi_k \in (0, \pi)$ with $k \in \{1, \ldots, m\}$ satisfy

$$\boxed{m\xi + \arctan\left(\frac{1+\alpha}{1-\alpha}\tan\left(\frac{\xi}{2}\right)\right) + \arctan\left(\frac{1+\beta}{1-\beta}\tan\left(\frac{\xi}{2}\right)\right) = \pi k}$$

then $z = e^{i\xi_k}$ is a band-state root of $p_m(z)$.

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then $z = e^{i\xi_k}$ is a band-state root of $p_m(z)$.

Bound-state root

Let $z_- \in (-1,0)$ or $z_+ \in (0,1)$ satisfy

$$\boxed{z^{2m}(z-\alpha)(z-\beta) - (1-\alpha z)(1-\beta z) = 0}$$

then $z = z_\pm$ is a bound-state root of $p_m(z)$.

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Main Results

Theorem (Bernstein–Szegő roots)

If $\alpha > 1$ and $-1 < \beta < 1$, the roots of the Bernstein–Szegő polynomial $p_m(z)$ are given by

$$z = e^{i\xi_k}, \quad k \in \{1, \dots, m-1\},$$

together with

$$z = \begin{cases} e^{i\xi_0^{(m;\alpha,\beta)}} & \text{if } m < 1 - (1-\alpha)^{-1} - (1-\beta)^{-1}, \\ 1 & \text{if } m = 1 - (1-\alpha)^{-1} - (1-\beta)^{-1}, \\ z_+ \in (0,1) & \text{if } m > 1 - (1-\alpha)^{-1} - (1-\beta)^{-1}, \end{cases}$$

where $z_+ \in (0, \alpha^{-1})$ if $\alpha\beta > 1$, $z_+ = \alpha^{-1}$ if $\alpha\beta = 1$, and $z_+ \in (\alpha^{-1}, 1)$ if $\alpha\beta < 1$.

Theorem (NR Approximation of Bound-state Roots)

If $\alpha > 1$ and $-1 < \beta < 1$, then, as $m \to \infty$,

$$z_+ = z_+^{\mathrm{nr}} + o(\alpha^{-2m}),$$

where

$$z_+^{\mathrm{nr}} = \alpha^{-1} + \frac{\alpha^{-1}(\alpha^2 - 1)(\alpha\beta - 1)}{\alpha^{2m+1}(\alpha - \beta) + 2m(\alpha^2 - 1)(\alpha\beta - 1) - (\alpha^2 - 1) - (\alpha\beta - 1)},$$

with

$$\lim_{m\to\infty} \frac{o(\alpha^{-2m})}{\alpha^{-2m}} = 0.$$

Theorem (NR Approximation Band-state roots)

The angle ξ_k^{nr} of the Newton-Raphson approximation for the band-state eigenvalue $\mathrm{E}_k = 2\cos(\xi_k)$ reads:

$$\xi_k^{nr} = \left(\xi + \frac{\pi k - m\xi - \arctan\left(\frac{1+\alpha}{1-\alpha}\tan\left(\frac{\xi}{2}\right)\right) - \arctan\left(\frac{1+\beta}{1-\beta}\tan\left(\frac{\xi}{2}\right)\right)}{m + \frac{\frac{1}{2}(1-\alpha^2)}{1+\alpha^2-2\alpha\cos(\xi)} + \frac{\frac{1}{2}(1-\beta^2)}{1+\beta^2-2\beta\cos(\xi)}} \right) \Bigg|_{\xi=\xi_k^{(0)}}$$

with

$$\xi_k^{(0)} = \begin{cases} \frac{\pi k}{m+1} & \text{if } \max(|\alpha|,|\beta|) < 1, \\ \frac{\pi k}{m} & \text{if } \min(|\alpha|,|\beta|) < 1 \text{ and } \max(|\alpha|,|\beta|) > 1, \\ \frac{\pi k}{m-1} & \text{if } \min(|\alpha|,|\beta|) > 1. \end{cases}$$

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- Hamiltonian

$$\mathrm{H}_T = \sum_{l=1}^{m-1} (\sigma_l^+ \sigma_{l+1}^- + \sigma_{l+1}^+ \sigma_l^-) + \alpha \left(\sigma_1^+ \sigma_1^- + \sigma_m^+ \sigma_m^-\right) + \gamma \left(\sigma_1^+ \sigma_m^- + \sigma_m^+ \sigma_1^-\right)$$

which acts on the state space $\mathbb{C}^{2m}$.

Single-particle Hamiltonian

The action of H on the single-particle states

$$e_j = |0, \dots, 0, \underbrace{1}_{j}, 0, \dots, 0\rangle$$

is represented by the $m \times m$ Jacobi matrix

$$\mathrm{T} = \begin{bmatrix} \alpha & 1 & 0 & \cdots & \gamma \\ 1 & 0 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ \gamma & \cdots & 0 & 1 & \alpha \end{bmatrix}.$$

Characteristic Polynomial

The characteristic polynomial of T can be written in terms of Chebyshev polynomials of the second kind as

$$\mathrm{P}_m^{(\alpha,\gamma)}(\mathrm{E}) = (-1)^m \left[(\mathrm{E} - 2\alpha)\, \mathrm{U}_{m-1}\left(\tfrac{\mathrm{E}}{2}\right) + (\alpha^2 - \gamma^2 - 1)\, \mathrm{U}_{m-2}\left(\tfrac{\mathrm{E}}{2}\right) - 2\gamma \right].$$

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Equivalent Polynomial

$$\mathrm{R}_m^{(\alpha,\gamma)}(z) = z^{2(m+1)}\left(1 - \alpha z^{-1} - \gamma z^{-m}\right)^2 - \left(1 - \alpha z - \gamma z^m\right)^2.$$

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Application of Previous Results to the Spectrum

Consider the following polynomial:

$$\mathrm{R}_m^{\alpha}(z) = z^{2m}(z-\alpha)^2 - (1-\alpha z)^2.$$

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Factorization

$$\mathrm{R}_m^\alpha(z) = \mathrm{R}_{m,-}^\alpha(z)\,\mathrm{R}_{m,+}^\alpha(z),$$

where

$$\mathrm{R}_{m,-}^\alpha(z) = z^{m+1} - \alpha(z^m + z) + 1,$$

and

$$\mathrm{R}_{m,+}^\alpha(z) = z^{m+1} - \alpha(z^m - z) - 1.$$

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$$\mathrm{R}_{m,+}^\alpha(z) = z^{m+1} - \alpha(z^m - z) - 1.$$

Bound-state roots

The polynomials $\mathrm{R}_{m,-}^\alpha(z)$ and $\mathrm{R}_{m,+}^\alpha(z)$ can be used to determine the bound-state roots.

Band-state roots

The equations to determine the band-state roots are

$$\mathrm{V}^{\alpha}_{m,-}(\xi) = m\xi + 2\arctan\left(\frac{1+\alpha}{1-\alpha}\tan\left(\frac{\xi}{2}\right)\right) \in \pi + 2\pi\mathbb{Z},$$

and

$$\mathrm{V}^{\alpha}_{m,+}(\xi) = m\xi + 2\arctan\left(\frac{1+\alpha}{1-\alpha}\tan\left(\frac{\xi}{2}\right)\right) \in 2\pi\mathbb{Z}.$$

Theorem (Roots of $\mathrm{R}_m^{\alpha+\gamma}(z)\mathrm{R}_m^{\alpha-\gamma}(z)$)

If $\alpha-\gamma>1$ and $-1<\alpha+\gamma<1$, then the roots of the polynomial

$$\mathrm{R}_m^{(\alpha,\gamma)}(z)=\mathrm{R}_m^{\alpha+\gamma}(z)\,\mathrm{R}_m^{\alpha-\gamma}(z)$$

are given by

$$z=e^{i\xi_{2k-1}^{(m;\alpha+\gamma)}},\quad k=1,\dots,\left\lfloor\frac{m+1}{2}\right\rfloor,$$

$$z=e^{i\xi_{2k}^{(m;\alpha-\gamma)}},\quad k=1,\dots,\left\lfloor\frac{m}{2}\right\rfloor-1,$$

together with an additional root:

$$z=\begin{cases} e^{i\xi_0^{(m;\alpha-\gamma)}} & \text{if } m<1-2\,(1-\alpha+\gamma)^{-1},\\ 1 & \text{if } m=1-2\,(1-\alpha+\gamma)^{-1},\\ z_+^{(m;\alpha)}\in\left((\alpha-\gamma)^{-1},1\right) & \text{if } m>1-2\,(1-\alpha+\gamma)^{-1}.\end{cases}$$

Theorem (NR Approximation for Bound-state Roots)

- If $\alpha - \gamma \in \mathbb{R} \setminus (-1, 1)$, then as $m \to \infty$:

$$z_{-}^{(m;\alpha+\gamma)} = z_{nr,-}^{(m;\alpha+\gamma)} + o\big((\alpha+\gamma)^{-m}\big)\,,$$

  where

$$z_{nr,-}^{(m;\alpha+\gamma)} = (\alpha-\gamma)^{-1} - \frac{(\alpha+\gamma)^2 - 1}{(\alpha+\gamma)^{m+2} + m\alpha^3 - (m+1)(\alpha+\gamma)}.$$

- If $\alpha + \gamma \in \mathbb{R} \setminus (-1, 1)$, then as $m \to \infty$:

$$z_{+}^{(m;\alpha-\gamma)} = z_{nr,+}^{(m;\alpha-\gamma)} + o\big((\alpha-\gamma)^{-m}\big)\,,$$

  where

$$z_{nr,+}^{(m;\alpha-\gamma)} = (\alpha+\gamma)^{-1} - \frac{1 - (\alpha+\gamma)^2}{(\alpha+\gamma)^{m+2} - m(\alpha+\gamma)^3 - (m+1)(\alpha+\gamma)}.$$

- $$\lim_{m\to\infty} o\big((\alpha\pm\gamma)^{-m}\big)/(\alpha\pm\gamma)^{-m} = 0.$$

Theorem (NR Approximation for Band-state Roots)

The angle $\xi_{k,nr}^{(m;\alpha)}$ of the Newton-Raphson approximation for the band-state eigenvalue $\mathrm{E}_k = 2\cos(\xi_k)$ reads:

$$\xi_{2k-\delta_x^-,nr}^{(m;\alpha)} = \left(\xi + \frac{\pi(2k-\delta_x^-) - m\xi - 2\arctan\left(\frac{1+\alpha}{1-\alpha}\tan\left(\frac{\xi}{2}\right)\right)}{m + \frac{(1-\alpha^2)}{1+\alpha^2-2\alpha\cos(\xi)}} \right)\Bigg|_{\xi=\xi_{2k-\delta_x^-,0}^{(m;\alpha)}},$$

with

$$\xi_{2k-\delta_x^-,0}^{(m;\alpha)} = \begin{cases} \frac{\pi(2k-\delta_x^-)}{m+1} & \text{if } |\alpha| < 1, \\ \frac{\pi(2k-\delta_x^-)}{m-1} & \text{if } |\alpha| > 1. \end{cases}$$

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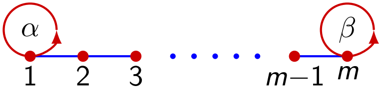
Models Considered Thus Far

Model on $\{1, 2, \ldots, m\}$



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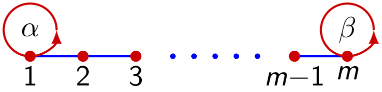
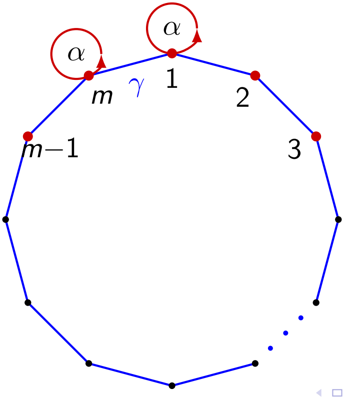


Model on $\mathbb{Z}_m$



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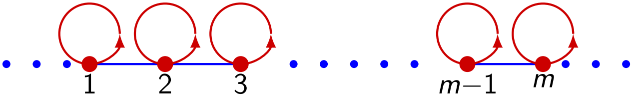
Model We Aim to Study

Model on $\mathbb{Z}$



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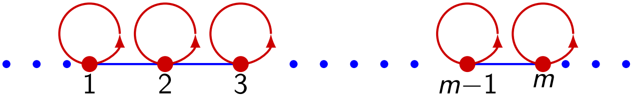

Associated Laplacian

$$(L\psi)(n,z) = a_n\psi(n+1,z) + b_n\psi(n,z) + a_{n-1}\psi(n-1,z), \quad n \in \mathbb{Z},$$

where $\psi : \mathbb{Z} \to \mathbb{C}$ and z denotes a (possibly complex) spectral parameter.

Jacobi matrix

$$\begin{bmatrix} \ddots & \ddots & \ddots & & & \\ \ddots & b_1 & a_1 & 0 & & \\ \ddots & a_1 & b_2 & a_2 & 0 & \\ & 0 & a_2 & b_3 & a_3 & \ddots \\ & & 0 & a_3 & b_4 & \ddots \\ & & & \ddots & \ddots & \ddots \end{bmatrix}$$

Jacobi matrix

$$\begin{bmatrix} \ddots & \ddots & \ddots & & & \\ \ddots & b_1 & a_1 & 0 & & \\ \ddots & a_1 & b_2 & a_2 & 0 & \\ & 0 & a_2 & b_3 & a_3 & \ddots \\ & & 0 & a_3 & b_4 & \ddots \\ & & & \ddots & \ddots & \ddots \end{bmatrix}$$

- When a_n and b_n are constant, the spectrum can be determined explicitly.
- This corresponds to the simplest stationary background of the Toda lattice.

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A single soliton

Coefficients and Jost function for a single soliton

- Coefficients of the associated Jacobi matrix ($-1 < z_1 < 1$):

$$a_n = \frac{\sqrt{(1 - z_1^2 + \nu_1 z_1^{2n+4})(1 - z_1^2 + \nu_1 z_1^{2n})}}{1 - z_1^2 + \nu_1 z_1^{2n+2}},$$

$$b_n = (z_1 - z_1^{-1}) \left[\frac{\nu_1 z_1^{2n+2}}{1 - z_1^2 + \nu_1 z_1^{2n+2}} - \frac{\nu_1 z_1^{2n}}{1 - z_1^2 + \nu_1 z_1^{2n}} \right],$$

$$\nu_1 = \left(\sum_{n \in \mathbb{Z}} \psi_{\text{jost}}^2(n, z_1) \right)^{-1}.$$

- Jost function and asymptotic behavior ($0 < |z| \leq 1$):

$$\psi_{\text{jost}}(n,z) = \frac{z^n\left(1 + \frac{v_1 z_1^{2n+2}}{1-z_1^2}\frac{1-zz_1^{-1}}{1-zz_1}\right)}{\sqrt{\left(1+\frac{v_1 z_1^{2n+2}}{1-z_1^2}\right)\left(1+\frac{v_1 z_1^{2n}}{1-z_1^2}\right)}},$$

$$\psi_{\text{jost}}(n,z) \underset{n\to+\infty}{\longrightarrow} z^n.$$

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Objectives:

Objectives:

- Construct a spin Hamiltonian of the form

$$\mathrm{H} = \sum_{l \in \mathbb{Z}} \left[a_l \left(\sigma_l^+ \sigma_{l+1}^- + \sigma_{l+1}^+ \sigma_l^- \right) + b_l \, \sigma_l^+ \sigma_l^- \right],$$

  with non-constant a_n and b_n given by a soliton solution of the Toda chain.

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  with non-constant a_n and b_n given by a soliton solution of the Toda chain.
- Determine the spectrum and the eigenfunctions of the corresponding spin Hamiltonian.

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Thank you!