Inhomogeneous XX spin chains and QES models

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Symmetry, Invariants, and their Applications
A celebration of Peter Olver's 70th birthday

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Outline of the talk

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1. QES models
2. $\mathrm{sl}(2)$ QES models and orthogonal polynomials
3. Inhomogeneous XX spin chains
4. XX chains and orthogonal polynomials
5. $\mathrm{sl}(2)$ QES models and XX chains
6. Conclusions

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$\mathrm{sl}(2)$ QES models

sl(2) QES models

- A one-dimensional quantum Hamiltonian

$$H = -\partial_x^2 + V(x) : L^2(\mathbb{R}) \to L^2(\mathbb{R})$$

is said to be quasi-exactly solvable (QES) if there is a *known* finite-dimensional subspace $\mathcal{N} = \operatorname{span}\{\psi_0, \dots, \psi_m\}$ s.t. $H\mathcal{N} \subset \mathcal{N}$

$\implies$ $m+1$ eigenvalues/eigenfunctions algebraically computable!

- Simplest example: $\mathrm{sl}(2)$ QES Hamiltonians

$\exists$ change of variable $z(x)$, gauge factor $\mu(z)$ s.t.

$$H_g := \mu(z)^{-1} H \mu(z) = -\sum_{a\leqslant b} h_{ab} L_a L_b - \sum_a h_a L_a - h_*$$

where h_*, h_a, h_{ab} = constants, $L_-, L_0, L_+ = \mathrm{sl}(2)$ generators

$$L_- = \partial_z\,, \quad L_0 = z\partial_z - \frac{m}{2}, \quad L_+ = z^2\partial_z - mz; \qquad m \in \mathbb{N} \cup \{0\}$$

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  $\implies \boxed{H_g \mathcal{P}_m \subset \mathcal{P}_m} \implies \boxed{H(\mu \mathcal{P}_m) \subset \mu \mathcal{P}_m}$
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$\mathfrak{sl}(2)$ QES models

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Communications in Mathematical Physics

Normalizability of One-dimensional Quasi-exactly Solvable Schrödinger Operators

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[2] Department of Mathematics, McGill University, Montréal, Québec, Canada H3A 2K6
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Abstract. We completely determine necessary and sufficient conditions for the normalizability of the wave functions giving the algebraic part of the spectrum of a quasi-exactly solvable Schrödinger operator on the line. Methods from classical invariant theory are employed to provide a complete list of canonical forms for normalizable quasi-exactly solvable Hamiltonians and explicit normalizability conditions in general coordinate systems.

1. Introduction

Lie algebraic and Lie group theoretic methods have played a significant role in the development of quantum mechanics since its inception. In the classical applications, the Lie group appears as a symmetry group of the Hamiltonian operator, and the associated representation theory provides an algebraic means for computing the spectrum. Of particular importance are the exactly solvable problems, such as the harmonic oscillator or the hydrogen atom, whose point spectrum can be completely determined using purely algebraic methods. In the early 1980's, in order to study molecular spectroscopy, Alhassid, Gürsey, Iachello, Levine, and collaborators, [2, 3, 1, 14], introduced the concept of a "spectrum generating algebra" to construct models for complicated molecules whose point spectrum could be analyzed algebraically. The Schrödinger operators amenable to the algebraic approach to scattering assumed a "Lie algebraic form," meaning that they belong to the universal enveloping algebra of the spectrum generating algebra. Thus, a second order differential operator

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sl(2) QES models

Contemporary Mathematics
Volume 160, 1994

QUASI-EXACT SOLVABILITY

Artemio González-López, Niky Kamran, and Peter J. Olver

Abstract. This paper surveys recent work on quasi-exactly solvable Schrödinger operators and Lie algebras of differential operators.

1. Introduction.

Lie algebraic and Lie group theoretic methods have played a significant role in the development of quantum mechanics since its inception. In the classical applications, the Lie group appears as a symmetry group of the Hamiltonian operator, and the associated representation theory provides an algebraic means for computing the spectrum. Of particular importance are the exactly solvable problems, such as the harmonic oscillator or the hydrogen atom, whose point spectrum can be completely determined using purely algebraic methods. The fundamental concept of a "spectrum generating algebra" was introduced by Arima and Iachello, [4], [5], to study nuclear physics, and subsequently, by Iachello, Alhassid, Gürsey, Levine, Wu and their collaborators, was also successfully applied to molecular dynamics and spectroscopy, [19], [23], and scattering theory, [1], [2], [3]. The Schrödinger operators amenable to the algebraic approach assume a "Lie algebraic form", meaning that they belong to the universal enveloping algebra of the spectrum generating algebra. Lie algebraic operators reappeared in the discovery of Turbiner, Shifman, Ushveridze, and their collaborators, [27], [29], [30], [34], of a new class of physically significant spectral problems, which they named "quasi-exactly solvable", having the property that a (finite) part of the point spectrum can be determined using purely algebraic methods. This is an immediate consequence of the additional requirement that the hidden symmetry algebra preserve a finite-dimensional representation space consisting of smooth wave functions. In this case, the Hamiltonian restricts to a linear transformation on the representation space, and hence the associated eigenvalues can be computed by purely algebraic methods, meaning matrix

1991 *Mathematics Subject Classification.* Primary: 81C05, 81C40; Secondary: 17B15, 17B56.
Key words and phrases. Schrödinger operator, Lie algebra, differential operator, quasi-exactly solvable.
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This paper is in final form and no version of it will be submitted for publication elsewhere

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- $H = \mu H_g \mu^{-1}$ QES, $H_g = -\sum_{a \leqslant b} h_{ab} L_a L_b - \sum_a h_a L_a - h_*$

  Then $\psi = \mu(z)\varphi(z)$ is a formal eigenfunction of H with energy E, i.e., $H\psi = E\psi$, iff $H_g \varphi = E\varphi$.

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Theorem

Let $H_g\varphi = E\varphi$, and write $\varphi(z) = \sum_{n=0}^{\infty} \hat{P}_n(E)\frac{z^n}{n!}$ with $\hat{P}_0 := 1$.

1. The coefficients $\hat{P}_n(E)$ are polynomials of degree n in E satisfying in general a 5-term recursion relation
2. The algebraically computable energies E_k $(0 \leqslant k \leqslant m)$ are the roots of the critical polynomial $\hat{P}_{m+1}(E)$ (and $\hat{P}_{m+j+1} = \hat{P}_{m+1}\hat{Q}_j$, with $\deg \hat{Q}_j = j$)
3. The family $\{\hat{P}_n\}_{n=0}^{m+1}$ is orthogonal, i.e., satisfies a 3-term r.r.
   $A_{n+1}P_{n+1} = (E - B_n)P_n - C_nP_{n-1}$, iff $h_{++} = h_{--} = 0$

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XX spin chains and free fermion systems

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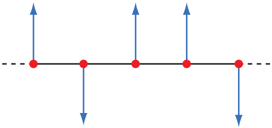
- A spin chain is a one-dimensional lattice whose sites are occupied by particles interacting through their spins (exchange interaction)



- Hamiltonian of free fermion system:

- Jordan–Wigner transformation:

$$c_n = \prod_{i=0}^{n-1} \sigma_i^z \cdot \sigma_n^+ , \quad \{|\uparrow\rangle_n, |\downarrow\rangle_n\} \to \{|0\rangle_n, |1\rangle_n\}$$

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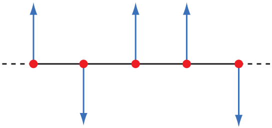

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$$H = \frac{1}{2}\sum_{n=0}^{N-2} J_n\left(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y\right) + \frac{1}{2}\sum_{n=0}^{N-1} B_n\left(1-\sigma_n^z\right)$$

$\sigma_n^\alpha =$ Pauli matrices acting on site n $\qquad (J_n > 0,\ \ B_n \in \mathbb{R})$

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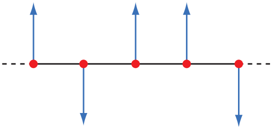

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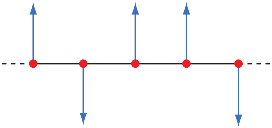

- Hamiltonian of free fermion system:

$$H = \sum_{n=0}^{N-2} J_n \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n\right) - \sum_{n=0}^{N-1} B_n c_n^\dagger c_n$$

$c_n (c_n^\dagger)$ = fermionic annihilation (creation) operator at site n

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XX spin chains and free fermion systems

- Single-particle Hamiltonian:

$$\begin{cases} |n\rangle := c_n^\dagger|\text{vac}\rangle, \ \ 0 \leqslant n \leqslant N-1 \ \ \text{(single spin at site } n\text{)} \\ H|n\rangle = \sum_{j=0}^{N-1} H_{jn}|j\rangle \\ H_{jn} = \langle j|H|n\rangle = J_n\delta_{j,n+1} + J_{n-1}\delta_{j,n-1} + B_n\delta_{jn} \end{cases}$$

- $\mathbb{H} := \left(H_{jn}\right)_{j,n=0}^{N-1}$ is a Jacobi ($\equiv$ real symmetric tridiagonal) matrix
- $\mathbb{H}$ real symmetric $\implies$ it can be diagonalized by a real orthogonal matrix $\Phi = (\Phi_{nk})_{n,k=0}^{N-1}$:

$$\Phi^T \mathbb{H} \Phi = \operatorname{diag}(\varepsilon_0, \dots, \varepsilon_{N-1}), \quad \varepsilon_k = \text{single-particle energy}$$

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- Single-particle energy modes: $\tilde{c}_k := \sum_{n=0}^{N-1} \Phi_{nk} c_n\,, \quad 0 \leqslant k \leqslant N-1$

- $$H = \sum_{n=0}^{N-1} \varepsilon_k \tilde{c}_k^\dagger \tilde{c}_k$$ $\Longrightarrow$ H is diagonal in the basis of energy modes

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(a pure state!). What is the state of a block $X := \{0, \ldots, L-1\}$ of $L < N$ spins?

- *Answer:* the state of X is *not* a pure state, but a density matrix $\rho_X(\mathbf{k}) = \operatorname{tr}_{X^c}(|\mathbf{k}\rangle\langle\mathbf{k}|) \implies$ the state $|\mathbf{k}\rangle$ is entangled (i.e., is not a product of one-particle states for each particle)
- A popular measure of the degree of entanglement of the state $|\mathbf{k}\rangle$ is the (bipartite) Rényi entropy

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Entanglement entropy

- Suppose that the whole chain is in the energy eigenstate

$$|k_0, \dots, k_{M-1}\rangle =: |\mathbf{k}\rangle$$

(a pure state!). What is the state of a block $X := \{0, \dots, L-1\}$ of $L < N$ spins?

- *Answer:* the state of X is *not* a pure state, but a density matrix $\rho_X(\mathbf{k}) = \operatorname{tr}_{X^c}(|\mathbf{k}\rangle\langle\mathbf{k}|) \implies$ the state $|\mathbf{k}\rangle$ is entangled (i.e., is not a product of one-particle states for each particle)
- A popular measure of the degree of entanglement of the state $|\mathbf{k}\rangle$ is the (bipartite) Rényi entropy

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Entanglement entropy

Theorem (Vidal, Latorre, Rico & Kitaev 2003)

Let $\nu_0, \ldots, \nu_{L-1}$:= eigenvalues of the $L \times L$ correlation matrix (two-point function)

$$C_X(\mathbf{k}) := \Big(\langle \mathbf{k}|c_i^\dagger c_j|\mathbf{k}\rangle\Big)_{i,j=0}^{L-1} = \Phi\Phi^T$$

We then have

$$S_\alpha(X;\mathbf{k}) = \sum_{l=0}^{L-1} s_\alpha(\nu_l)\,,$$

where $s_\alpha(x)$ is the binary Rényi entropy

$$s_\alpha(x) = \begin{cases} (1-\alpha)^{-1}\log\big(x^\alpha + (1-x)^\alpha\big), & \alpha \neq 1 \\ -x\log x - (1-x)\log(1-x), & \alpha = 1 \end{cases}$$

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Outline of the talk

XX chains $\leftrightarrow$ orthogonal polynomials

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- The columns $(\Phi_{0k}, \dots, \Phi_{N-1,k})$ of Φ ($\equiv$ eigenvectors of $\mathbb{H}$) can be computed from the eigenvalue equations

$$J_n \Phi_{n+1,k} = (\varepsilon_k - B_n)\Phi_{nk} - J_{n-1}\Phi_{n-1,k}$$

$\implies \Phi_{nk} = \phi_n(\varepsilon_k)\Phi_{0k}$, where $\phi_n(E)$ $(0 \leqslant n \leqslant N-1)$ is the n-th degree polynomial determined by the 3-term recursion relation

$$J_n\phi_{n+1}(E) = (E - B_n)\phi_n(E) - J_{n-1}\phi_{n-1}(E)$$

(with $\phi_{-1} := 0, \ \ \phi_0 := 1$)

- Characteristic equation:

$$0 = (E - B_{N-1})\phi_{N-1}(E) - J_{N-2}\phi_{N-2}(E)$$

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- The monic polynomials $P_n(E) := \prod_{i=0}^{n-1} J_i \cdot \phi_n(E)$ $(0 \leqslant n \leqslant N-1)$ satisfy the canonical recursion relation

$$P_{n+1}(E) = (E - b_n)\, P_n(E) - a_n\, P_{n-1}(E)$$
$$a_n = J_{n-1}^2 > 0, \quad b_n = B_n$$

$\Longrightarrow$ the single-particle energies ε_k are the zeros of the polynomial

$$P_N := (E - b_{N-1})\, P_{N-1}(E) - a_{N-1}\, P_{N-2}$$

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XX chains ↔ orthogonal polynomials

- Conversely, a finite orthogonal polynomial family $\{P_n(E)\}_{0\leqslant n\leqslant N}$ satisfying a 3-term r.r. with coefficients $a_n > 0$, b_n determines an inhomogeneous XX chain Hamiltonian with parameters

$$J_n = \sqrt{a_{n+1}}\,, \quad B_n = b_n$$

- The zeros ε_k of P_N are the single-particle energies ε_k
- $\Phi_{nk} = \sqrt{\frac{w_k}{\gamma_n}}\, P_n(\varepsilon_k)$, with $\gamma_n := \prod_{i=1}^{n} a_i\,,\ \ w_k = \frac{\prod_{n=1}^{N-1} a_n}{P_{N-1}(\varepsilon_k)P_N'(\varepsilon_k)}$

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Outline of the talk

From $\mathrm{sl}(2)$ QES models to inhomogeneous XX chains

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- $H = -\mu\Big(\sum_{a\leqslant b} h_{ab} L_a L_b + \sum_a h_a L_a + h_*\Big)\mu^{-1} \equiv -\mu H_g \mu^{-1}$
- $\varphi_k(z) = \sum_{j=0}^{m} \hat{P}_j(E_k)\frac{z^j}{j!}$ $(0 \leqslant k \leqslant m)$ algebraic eigenfunctions of H_g, where $\{E_0, \dots, E_m\}$ = roots of critical polynomial $\hat{P}_{m+1}$
- $h_{++} = h_{--} = 0 \implies$ the monic polynomials $P_n(E) := \gamma_n \hat{P}_n(E)$ $(0 \leqslant n \leqslant m+1)$ satisfy a canonical 3-term r.r.

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QES model $\to$ XX spin chain

☞ If $a_n > 0$ for $1 \leqslant n \leqslant m$, we can associate to H an XX spin chain Hamiltonian with $N = m+1$ spins and parameters $J_n = \sqrt{a_{n+1}},\ B_n = b_n$

From $\mathfrak{sl}(2)$ QES models to inhomogeneous XX chains

QES model $\leftrightarrow$ XX chain dictionary:

QES model	XX chain
m	$N-1$
Algebraic energies E_k	Single-particle energies ε_k
Algebraic eigenfunctions $\mu\sum_{n=0}^{m}\frac{P_n(E_k)}{\gamma_n}\frac{z^n}{n!}\quad(0\leqslant k\leqslant m)$	Single-particle energy eigenstates $\sum_{n=0}^{N-1}\sqrt{\frac{w_k}{\gamma_n}}\,P_n(\varepsilon_k)\lvert n\rangle\quad(0\leqslant k\leqslant N-1)$

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- The parameters J_n^2 and B_n of XX chains constructed from $\mathrm{sl}(2)$ QES models are polynomials in the site index n, with $\deg J_n^2\leqslant 4$ and $\deg B_n\leqslant 2$.

A classification problem

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Problem

Classify all inequivalent ($\Longleftrightarrow$ non-isomorphic) XX chains obtained from $\mathrm{sl}(2)$ QES models.

- Main idea:

$$H_g = -\sum_{a\leqslant b} h_{ab} L_a L_b - \sum_a h_a L_a - h_* \quad \text{gauge Hamiltonian}$$

$$\Longrightarrow \quad -H_g = p(z)\,\partial_z^2 + q(z)\partial_z + r(z),$$

with $\deg q = 3$, $\deg r = 2$ and

$$p(z) = h_{++}z^4 + 2h_{0+}z^3 + h_{00}z^2 + 2h_{0-}z + h_{--}$$

$$\Longrightarrow \quad \boxed{h_{++} = h_{--} = 0 \iff p(0) = p(\infty) = 0}$$

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A classification problem

- The canonical form for H_g has a residual $\mathrm{gl}(2)$ symmetry

$$z = \frac{\alpha w + \beta}{\gamma w + \delta}, \qquad H_g \mapsto \widetilde{H}_g := (\gamma w + \delta)^m H_g (\gamma w + \delta)^{-m}$$

(with $\Delta := \alpha\beta - \gamma\delta \neq 0$), under which

$$p(z) \mapsto \widetilde{p}(w) = \frac{(\gamma w + \delta)^4}{\Delta^2}\, p\left(\frac{\alpha w + \beta}{\gamma w + \delta}\right) \qquad (*)$$

- It can be shown that H_g and $\tilde{H}_g$ generate isomorphic XX chains. So all we have to do is:

> Classify all fourth-degree polynomials $p(z)$ with $p(\infty) = p(0) = 0$ under the $\mathrm{gl}(2)$ transformation $(*)$.

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2. $\nu z(1-z)$	Trigonometric	3
3. νz^2	Exponential	2
4. z	Sextic oscillator	3
5. $\nu z(1+z)(a+z),\ 0<a<1$	Elliptic $\left(k^2=1-a\right)$	4
6. $\nu z(z^2+2az+1),\ \lvert a\rvert<1$	Elliptic $\left(k^2=\frac{1-a}{2}\right)$	4

Here $\nu>0$ and k is the modulus of the elliptic functions.

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☞ Cases 5 and 6 include the Lamé potential $k^2 l(l+1)\,\mathrm{sn}^2(x;k)$.

Outline of the talk

Conclusions

- $\mathrm{sl}(2)$ QES models with $h_{++} = h_{--} = 0$ determine inhomogeneous XX spin chains through their associated orthogonal polynomial families.
- The QES model's algebraic sector correspond to the chain's single-particle subspace.
- It is possible to classify all inequivalent XX chains that can be constructed in this way, as well as their associated QES potentials.
- The asymptotic behavior of the bipartite entanglement entropy of these chains as the size L of the subsystem $\to \infty$ (relevant to establish their critical behavior) can be determined in closed form. This has been done, for instance, for the chains constructed from the sextic oscillator and Lamé potentials [JSTAT (2020) 093105, JHEP 12 (2021) 184]. In both cases, we find an unusual subleading $\log(\log L)$ term.

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Happy 70th, Peter!!!