Haydock's recursive solution of self-adjoint problems. Discrete spectrum

Alexander Moroz

Wave-scattering.com

wavescattering@yahoo.com

January 3, 2015

Overview

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- Novel numerical method

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- Conclusions

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    - characterization of chaos?

Trivial and always valid statement

For any linear *self-adjoint* $\hat{H}$ there always exists an orthonormal basis $\{\mathbf{e}_n\}_{n=0}^{\infty}$ such that eigenstates $|E\rangle$ of $\hat{H}$

$$\hat{H}|E\rangle = E|E\rangle$$

can be expanded as

$$|E\rangle = \sum_{n=0}^{\infty} p_n(E)\mathbf{e}_n$$

Haydock's recursive solution

- (**H1**) the expansion coefficients $\{p_n(E)\}$ are polynomials with degree $p_n = n$, *orthonormal* with respect to the *density of states* (DOS), $n_0(E)$,

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- (**H2**) energy eigenstates $|E\rangle$ are the *generating function* of the orthogonal polynomials
- (**H3**) the *orthogonality* of the energy eigenstates, $\langle E|E'\rangle = \delta_{EE'}$ yields a *dual* orthogonality relation

$$n_0(E)\sum_{n=0}^{\infty} p_n(E)p_n(E') = \delta_{EE'}$$

where E and E' are both eigenvalues

Tridiagonality is generic

There always exists an orthonormal basis $\{\mathbf{e}_n\}_{n=0}^{\infty}$ such that a given self-adjoint operator takes on a tridiagonal form

$$\mathbf{H}\mathbf{e}_n = a_n\mathbf{e}_n + b_{n+1}\mathbf{e}_{n+1} + b_n\mathbf{e}_{n-1} \tag{1}$$

with *real* recurrence coefficients $\{a_n\}$ and $\{b_n\}$, where $b_n \geq 0, \ n \geq 0$.

Proof of $\mathbf{He}_n = a_n\mathbf{e}_n + b_{n+1}\mathbf{e}_{n+1} + b_n\mathbf{e}_{n-1}$

$n = 0$: find a_0, b_1, $\mathbf{e}_1$

$H\mathbf{e}_0 = a_0\mathbf{e}_0 + b_1\mathbf{e}_1$
$a_0 = \langle \mathbf{e}_0, \mathbf{He}_0 \rangle$
$b_1^2 = \langle (\mathbf{H} - a_0)\mathbf{e}_0, (\mathbf{H} - a_0)\mathbf{e}_0 \rangle$
$\mathbf{e}_1 = (\mathbf{H} - a_0)\mathbf{e}_0 / b_1$

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Induction step to determine a_n, b_{n+1}, $\mathbf{e}_{n+1}$

$\langle \mathbf{e}_{n-1}, \mathbf{H}\mathbf{e}_n \rangle = \langle \mathbf{e}_n, \mathbf{H}\mathbf{e}_{n-1} \rangle \equiv b_n$
$a_n = \langle \mathbf{e}_n, \mathbf{H}\mathbf{e}_n \rangle$
$b_{n+1}\mathbf{e}_{n+1} = (\mathbf{H} - a_n)\mathbf{e}_n - b_n\mathbf{e}_{n-1}$
$b_{n+1}^2 = \langle (\mathbf{H} - a_n)\mathbf{e}_n - b_n\mathbf{e}_{n-1}, (\mathbf{H} - a_n)\mathbf{e}_n - b_n\mathbf{e}_{n-1} \rangle$
$\mathbf{e}_{n+1} = [(\mathbf{H} - a_n)\mathbf{e}_n - b_n\mathbf{e}_{n-1}] / b_{n+1}$
By construction $\mathbf{e}_{n+1}$ normalized to *one* and orthogonal to $\mathbf{e}_n$ and $\mathbf{e}_{n-1}$.

Final check: $\mathbf{e}_{n+1}$ orthogonal to $\mathbf{e}_{n-2},\ldots,\mathbf{e}_0$

Tridiagonality of $\mathbf{He}_n$, self-adjointness, and normalizability

$$b_{n+1}\langle \mathbf{e}_m, \mathbf{e}_{n+1}\rangle = \langle \mathbf{e}_m, \mathbf{He}_n\rangle = \langle \mathbf{He}_m, \mathbf{e}_n\rangle$$

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Tridiagonality for $m < n-1$

$\mathbf{He}_m$ is a linear combination of $\mathbf{e}_{m-1}$, $\mathbf{e}_m$, and $\mathbf{e}_{m+1}$, all of which have zero overlap with $\mathbf{e}_n$ if $m+1<n$.

Relation to orthogonal polynomials I

Wave function expansion

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Three-term recurrence relation (TTRR)

Expansion coefficients satisfy

$$Ep_n(E) = a_n p_n(E) + b_{n+1} p_{n+1}(E) + b_n p_{n-1}(E) \tag{2}$$

with $b_k \geq 0$ and an initial condition $p_0 = 1$ and $p_{-1} = 0$.
$\{p_n(E)\}$ are by the very definition **orthogonal polynomials**.

Favard's theorem (Theorem I-4.4 of Chihara's book)

For given arbitrary sequences of *complex* numbers $\{c_n\}$ and $\{\lambda_n\}$ in the TTRR

$$xP_n = P_{n+1} + c_n P_n + \lambda_n P_{n-1}$$

there always exists a *moment functional*, that is a linear functional $\mathcal{L}$ acting in the space of (complex) monic polynomials $\mathbb{C}[E]$, such that the polynomials P_n defined by the TTRR are *orthogonal* under $\mathcal{L}$:

$$\mathcal{L}(P_k\, P_l) = 0 \qquad k \neq l \in \mathbb{N}$$

The functional $\mathcal{L}$ is *unique* if we impose the normalization condition $\mathcal{L}(P_0) = \mathcal{L}(1) = \mu_0$, where μ_0 is a chosen positive constant.

Relation to orthogonal polynomials II

Shorthand for basis

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Orthogonality relations

$$\langle \mathbf{e}_m, \mathbf{e}_n \rangle = \langle p_m(\mathbf{H})\mathbf{e}_0, p_n(\mathbf{H})\mathbf{e}_0 \rangle = \delta_{mn}$$

Relation to orthogonal polynomials III

Change to the orthonormal basis of eigenstates

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Weight function is the local density of function (DOS)

$$n(E) = \sum_k |\omega_k|^2 \delta(E - E_k)$$

Weight function more rigorously (pp. 62-63 of Chihara's book)

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- **(b)** $-\infty < \xi_1 < \xi_2 < \ldots < \xi_l = \sigma$ for some $l \geq 1$

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- **(c)** $-\infty < \xi_1 < \xi_2 < \ldots < \xi_l < \ldots < \sigma = \infty$

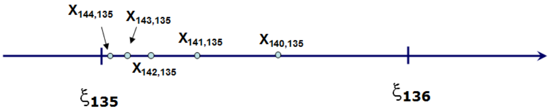
Weight function is the set of limit points of flows of zeros

$$\phi_n = \frac{P_n}{n!}: \qquad \phi_{n+1} + \frac{1}{\kappa(n+1)}[n - \varepsilon \pm (-1)^n \Delta]\phi_n + \frac{1}{n+1}\phi_{n-1} = 0$$

$$P_n = (x - c_{n-1})P_{n-1} - \lambda_{n-1}P_{n-2}, \quad P_{-1} = 0, \quad P_0 = 1,$$

$$c_n = \frac{1}{\kappa}[n \pm (-1)^n \Delta], \quad x = \varepsilon / \kappa = E / g$$

$$\lambda_n = n, \quad \lambda_0 = 1$$



$$\phi_n(\varepsilon) \to 0 \Leftrightarrow \varepsilon \in \Sigma$$

Numerical recipe

- Choose $N_c \geq N_0$ and determine the first N_0 zeros $x_{N_c l}$, $l \leq N_0$, of $P_{N_c}(x)$. Usually a good starting point is to take $N_c \approx N_0 + 20$. Because $P_{N_c}(x)$ has N_c simple zeros, any omission of a zero could be easily identified.

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- Gradually increase the cut-off value of N_c. The latter is what drives the incessant flows of polynomial zeros $x_{N_c l}$, wherein each flow is characterized by the parameter l.
- Monitor convergence of the respective flows induced by the very first n zeros of $P_{N_c}(x)$. Each flow is a monotonically decreasing sequence having necessary a fixed limit point. Terminate your calculations when the N_0-th zero of $P_{N_c}(x)$ converged to ξ_{N_0} within predetermined accuracy. Then as a rule all other flows $x_{N_c l}$ with $l < N_0$ have converged, too.

Rabi model Hamiltonian $\hat{H}_R$

$$\hat{H}_R = \hbar\omega \mathbb{1} \hat{a}^\dagger \hat{a} + \hbar g \sigma_1 (\hat{a}^\dagger + \hat{a}) + \mu\sigma_3$$

ω_0 ... TLS resonance frequency, ω ... cavity mode frequency
$\mu = \hbar\omega_0/2$, $[\hat{a}, \hat{a}^\dagger] = 1$,
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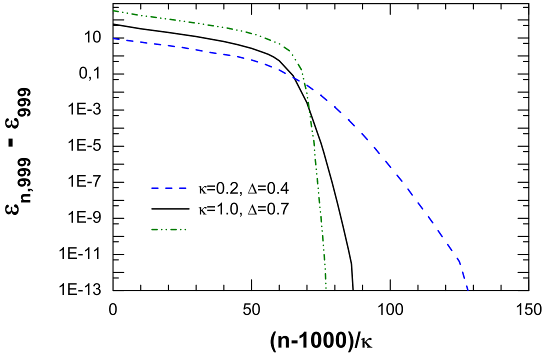
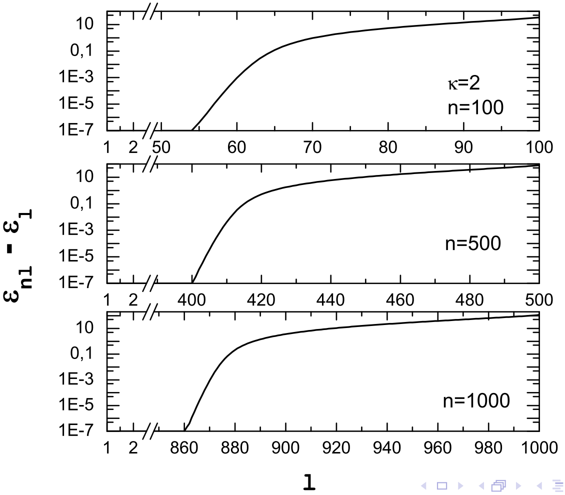
In what follows: $\kappa = g/\omega$, $\Delta = \mu/\omega$, $\hbar = 1$

Convergence toward the 1000th eigenvalue of the Rabi model in positive parity eigenspace



$\epsilon_{999} = 998.907883759510,\ 997.950425260357,\ 973.989087026621$ for $(\kappa, \Delta) = (0.2, 0.4),\ (1, 0.7),\ (5, 0.4)$, respectively

An approximation of the spectrum $\epsilon_l = l - \kappa^2$ of displaced harmonic oscillator by the zeros x_{nl}



I'm looking for somebody to analyze level statistics. My input: Thousands of energy levels per parity subspace.

Comparison with Braak's PRL **107**, 100401 (2011)

A transcendental function is constructed

$$G_{\pm}(\zeta) = \sum_{n=0}^{\infty} K_n(\zeta, \kappa) \left[1 \mp \frac{\Delta}{\zeta - n}\right] \kappa^n$$

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The expansion coefficients K_n are determined by a TTRR

$$\phi_{n+1} - \frac{f_n(\zeta)}{(n+1)}\,\phi_n + \frac{1}{n+1}\,\phi_{n-1} = 0$$

where

$$f_n(\zeta) = 2\kappa + \frac{1}{2\kappa}\left(n - \zeta - \frac{\Delta^2}{n-\zeta}\right).$$

Shortcomings of Braak's approach

Relies heavily on *unproven* hypotheses that $G_{\pm}(\zeta)$ takes on a zero value between its subsequent poles at $\zeta = n$ and $\zeta = n + 1$

- *once* - by implicitly presuming that at one of the poles $G_{\pm}(\zeta)$ goes to $+\infty$ and at the neighboring pole goes to $-\infty$, with a monotonic behavior from $+\infty$ to $-\infty$ between the poles;

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Numerically no advantage over the classical Schweber's solution [Ann. Phys. (N.Y.) **41**, 205 (1967)].

Comparison with Braak's PRL **107**, 100401 (2011) - II

- The TTRR for the coefficients K_n is not a fundamental one, i.e. not of Haydock's type, because of $f_n(\zeta)$ is not a linear function of energy.

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- Any relation with the orthogonal polynomials $\{p_n\}$ is eluded.
- Instead at looking straight at the zeros of p_N of sufficiently large degree, a complicated composite object, $G_\pm(\zeta)$, is formed.

Is Rabi model integrable or solvable?

Divided-difference operator or discrete derivative

$$\mathbb{D}_x f(x) = \frac{f(\iota_+(x)) - f(\iota_-(x))}{\iota_+(x) - \iota_-(x)}$$

Structure relation and bispectral condition

Divided-difference operator or discrete derivative

$$\mathbb{D}_x f(x) = \frac{f(\iota_+(x)) - f(\iota_-(x))}{\iota_+(x) - \iota_-(x)}$$

Structure relation

$$\mathbb{D}_x p_n(x) = -B_n(x) p_n(x) + A_n(x) p_{n-1}(x)$$

where $\mathbb{D}_x : \Pi_n[x] \to \Pi_{n-1}[x]$, $\Pi_n[x]$ being the linear space of polynomials in x over $\mathbb{C}$ with degree at most $n \in \mathbb{Z}_{\geq 0}$

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- a pair of mutually adjoint raising and lowering *ladder operators*
- orthogonal polynomials satisfy in general a second-order difference equation = **bispectral** property
- allows one to introduce a *discrete* analogue of the *Bethe Ansatz* equations
- the polynomials are hypergeometric of **Askey-Wilson** type

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$$\Lambda = \{x \,|\, x = u_2 n^2 + u_1 n + u_0,\ n \in \mathbb{N}\}$$

or

$$\Lambda = \{x \,|\, x = u_2 q^{-n} + u_1 q^n + u_0,\ n \in \mathbb{N}\}$$

where u_j are real constants and the real parameter q satisfies $0 < q < 1$

Is Rabi model integrable or solvable?

Characterization of tridiagonal $\mathbf{H}\mathbf{e}_{n-1} = a_{n-1}\mathbf{e}_{n-1} + b_n\mathbf{e}_n + b_{n-1}\mathbf{e}_{n-2}$

- **(A)** $b_n = 0$ for some $n = \mathcal{N} > 0$

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- (**B**) $b_n \neq 0$ for all $n \geq 0$

$\mathbf{He}_{n-1} = a_{n-1}\mathbf{e}_{n-1} + b_n\mathbf{e}_n + b_{n-1}\mathbf{e}_{n-2}$ with $b_{\mathcal{N}} = 0$ for some $\mathcal{N} > 0$

- $p_{\mathcal{N}}(E)$ enters the TTRR first for $n = \mathcal{N}$. One has

$$p_{n+\mathcal{N}}(E) = p_{\mathcal{N}}(E)Q_n(E) \qquad (n \geq 0)$$

i.e. $p_{\mathcal{N}+1}(E)$ is proportional to $p_{\mathcal{N}}(E)$. The quotient polynomials $Q_n(E)$ form a new orthogonal sequence of polynomials.

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- The polynomials $\{p_n(E)\}_{n=0}^{\mathcal{N}-1}$ *decouple* from $\{p_n(E)\}_{n=\mathcal{N}}^{\infty}$.

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  i.e. $p_{\mathcal{N}+1}(E)$ is proportional to $p_{\mathcal{N}}(E)$. The quotient polynomials $Q_n(E)$ form a new orthogonal sequence of polynomials.
- The polynomials $\{p_n(E)\}_{n=0}^{\mathcal{N}-1}$ *decouple* from $\{p_n(E)\}_{n=\mathcal{N}}^{\infty}$.
- The operator $\hat{H}$ has necessary a *finite dimensional invariant subspace* $\mathcal{V}_{\mathcal{N}} = \{\mathbf{e}_n\}_{n=0}^{\mathcal{N}-1}$.

Quasi-exact solvabality of a linear differential operator $\hat{H}$

- $\hat{H}$ preserves a *finite* dimensional subspace $\mathcal{V}_\mathcal{N}$ of a Hilbert space $L^2(S)$ $(S \subset \mathbb{R})$, $\hat{H}\mathcal{V}_\mathcal{N} \subset \mathcal{V}_\mathcal{N}$, $\dim \mathcal{V}_\mathcal{N} = \mathcal{N} < \infty$, on which the operator $\hat{H}$ is naturally defined

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- The basis of $\mathcal{V}_{\mathcal{N}}$ admits an *explicit analytic form* $\mathcal{V}_{\mathcal{N}} = \text{span } \{\mathbf{e}_0(x), \ldots, \mathbf{e}_{\mathcal{N}-1}(x)\}$

Basic properties of finite OPS defined by $xP_n = P_{n+1} + c_nP_n + \lambda_nP_{n-1}$

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- $w_k > 0$ for $0 \le k < \mathcal{N}$
- $d\nu_P(E)$ is unique

Normalization paradox

Orthogonality

$$\mathcal{L}[\pi(x)p_n(x)] = 0$$

for every polynomial $\pi(x)$ of degree $k < n$. Hence the norm of $p_n(E)$ for $n \geq \mathcal{N}$ vanishes, i.e.

$$0 \equiv \frac{1}{b_{\mathcal{N}+1}} \mathcal{L}[E^{\mathcal{N}} p_{\mathcal{N}}(E)]$$

Paradox

One cannot satisfy (**H1**), i.e. that $\{p_n(E)\}$ are *orthonormal* with respect to the *density of states* (DOS), $n_0(E)$,

$$\int_{-\infty}^{\infty} p_n(E)p_m(E)n_0(E)dE = \delta_{nm}$$

Resolution

Assume that the respective spectra obtained in $\mathcal{V}_{\mathcal{N}}$ and $L^2(S)\backslash\mathcal{V}_{\mathcal{N}}$ form two *disjoint* intervals on the real axis, $S = S_{qes} \cup S_{\infty}$, $\sup S_{qes} < \inf S_{\infty}$.

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- On S_{∞} is $n_0(E)dE$ represented by

$$d\nu_{PQ}(E) = \frac{1}{p_{\mathcal{N}}^2(E)}\, d\nu_Q(E) \qquad (E \in S_{\infty})$$

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  - characterization of chaos?

R. Haydock, p. 217 of his review:

"The generality of this result suggests a new way of looking at quantum mechanics. Since any quantum system can be transformed into a *chain* model, we need only investigate such chain models in order to see the varieties of quantum phenomena that are possible. To understand a particular physical system, we need only find the chain model appropriate to it."

The End

Further reading

This talk has been based on excerpts from my arxiv:1205.3139; EPL **100**, 60010 (2012); AP **338**, 319-340 (2013); AP **340**, 252-266 (2014); J. Phys. A: Math. Theor. **47**(49), 495204 (2014); AP **351**, 960-974 (2014)

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F77 source codes and numerical data files for the Rabi model can be freely downloaded from http://www.wave-scattering.com/rabi.html

My all F77 scattering codes are available at http://www.wave-scattering.com/codes.html

For list of my unfinished projects see http://www.wave-scattering.com/projects.html