

PHYSICS NEAR EXCEPTIONAL POINTS

(or: towards systematics of quantum catastrophes)

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Chapter I. INTRODUCTION

EXCEPTIONAL POINTS?

definition 1 (the most elementary one):

The points of the loss of the reality
of **the least stable** pair
of the bound-state energies of H

♡ CHARACTERISTIC ODE MODEL:

see $E = k^2$ in M. Znojil, *PT-symmetric square well*,
Phys. Lett. A 285 (2001) 7-10:

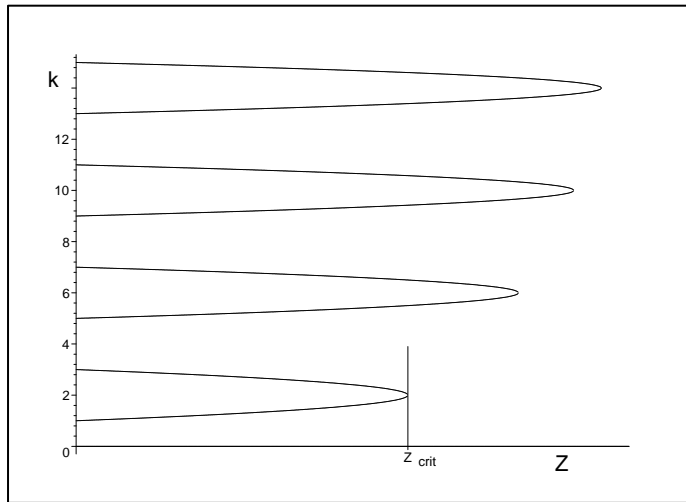


Figure 1: The least stable square-well energies are the lowest ones

◇ AN EVEN MORE ELEMENTARY
SCHEMATIC MATRIX MODEL:

$$\begin{pmatrix} -1 & b \\ -b & 1 \end{pmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = E \begin{pmatrix} \phi \\ \chi \end{pmatrix}$$

$$E = E_{\pm} = \sqrt{1 - b^2},$$

$$\Omega = \mathcal{D}^{(1)} = (-1, 1).$$

EXCEPTIONAL POINTS?

definition 2 (“in physics”):

certain points where “something is happening”

or, often, where “something goes wrong”;

a typical “physical” EP: the $\alpha = 0$ trigger

of the “fall on the center” in $V(r) \sim \frac{\alpha^2 - 1/4}{r^2}$

♠ A SAMPLE OF EPs IN REAL LIFE

catastrophes in strong fields (Dirac equation: Greiner '68),
complex EPs in perturbation theory (BW '69: $\sqrt{\dots}$ for AHOs),
in magnetohydrodynamics (Günther et al, this conference),
in nuclear physics: Scholtz et al, Heiss et al, Rotter et al,
in supersymmetric models: many authors,
in relativistic models: AM '04 etc
etc.

♡ MODELS WITH EP_s LOOK INNOVATIVE

physics can be **unusual** (non-local, superluminal, dissipative, ...)

one could **circumvent** no-go theorems (e.g., in supersymmetry)

relativistic (e.g., Proca) equations appear in a new perspective

MHD models = “physical” inside **as well as** outside Ω

last but, better, first, field theory

math. guide: EP in HO at $\alpha \rightarrow 0$ and all n :

$$E_n^+ = 4n + 2 + 2\alpha \quad \text{merges with} \quad E_n^- = 4n + 2 - 2\alpha,$$

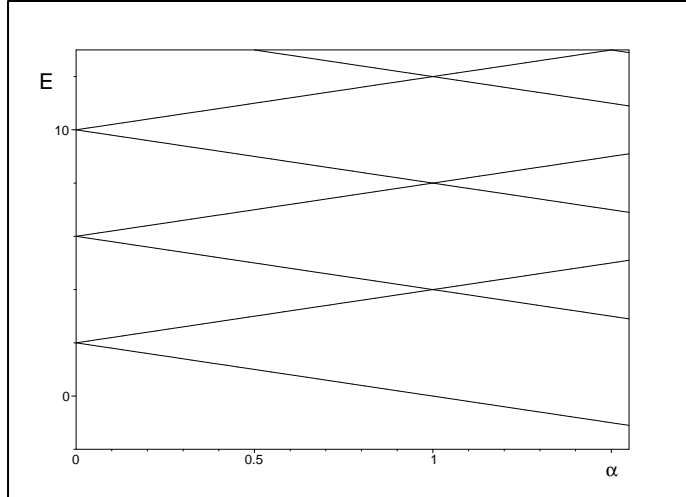


Figure 2: Spectrum of the PT-symmetric harmonic oscillator

♣ **Unfortunately**, HO is **NOT GENERIC**:

all the energies = **suddenly** complex **iff** $\alpha < 0$ (degeneracy)

“isolated” degenerate EPs \exists **periodically** in α

all the energies = **linear** in α

LHO obtained at $\alpha = \frac{1}{2}$ (equidistance, SUSY etc)

M. Znojil, *PT-symmetric harmonic oscillators*,
Phys. Lett. A 259 (1999) 220 - 223).

EXCEPTIONAL POINTS?

definition 3 (*à la* T. Kato):

They form a boundary $\partial\Omega$
of the domain $\Omega = \Omega(H)$
of the quasi-Hermiticity of $H \neq H^\dagger$

an immediate task: *the determination of $\partial\Omega$*

\Rightarrow CHALLENGE TO PHYSICS

EPs are rather rare in Hermitian worlds with $H = H^\dagger$ (Heiss et al)

EP means a singularity in the metric Θ in quasi-Hermitian world

an immediate task: *the determination of $\partial\Omega$*

\implies **CHALLENGE TO MATHEMATICS**

♠ hard life beyond general four-by-four matrices $H^{[N]}$

M. Znojil, *Determination of the domain of the admissible matrix elements in the four-dimensional PT -symmetric anharmonic model,*

Phys. Lett. A, in print, online, quant-ph/0703168 (PTO).

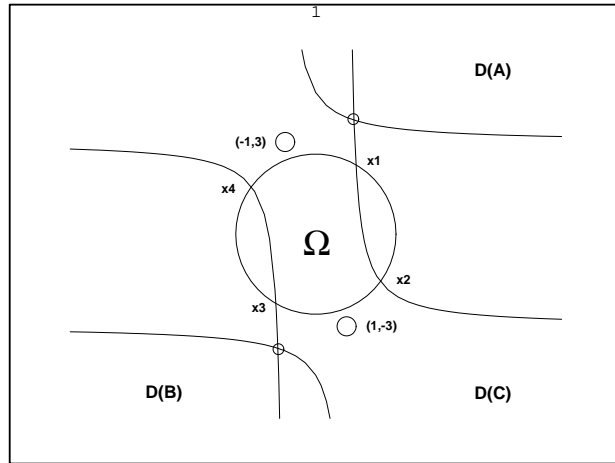


Figure 3: Graphical determination of the three-parametric domain $\Omega^{(4)} = \Omega^{(4)}(a, b, c)$ at a fixed $c = \sqrt{8/5}$, with the four “double” EPs x_1, x_2, x_3, x_4 .

AN AMBITION OF THIS TALK

SIMPLIFY SOME CURRENT HAMILTONIANS $H \neq H^\dagger$

[say, $H = -\Delta + V(\vec{x})$, via a **discretization**, chapter II]

REVIEW BRIEFLY THE GAINS

(results on **matrices** $H = H^\ddagger = \Theta^{-1}H^\dagger\Theta$ inside Ω , ch. III,IV)

while trying to

formulate some generic conjectures on $\partial\Omega$

(method: symbolic manipulations plus extrapolations)

Chapter II. DISCRETIZATIONS

A MENU

(1) RUNGE KUTTA QM

[**any** discrete **one-dimensional** $H = p^2 + V(x) \neq H^\dagger$]

(2) THE OTHER LATTICES OF COORDINATES

[2D here, semi-discrete, coupled channels, **square wells**]

(3) BIORTHOGONAL BASES

[mainly variational, **separably anharmonic oscillators**]

(1) RUNGE KUTTA QM IN 1D

coordinates: $x_k = x_{k-1} + h = -1 + kh$,

$$h = \frac{2}{N}, \quad x_0 = -1, \quad k = 1, 2, \dots, N$$

kinetic energy:

$$-\psi''(x) \approx -\frac{\psi(x_{k+1}) - 2\psi(x_k) + \psi(x_{k-1}))}{h^2}$$

boundary conditions: $\psi(x_0) = \psi(x_N) = 0$

leads to the Weigert's matrix square well model

.

$$\begin{pmatrix} 2 + \frac{1}{4}iZ & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 - \frac{1}{4}iZ \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \gamma \\ \beta_0 \end{pmatrix} = \frac{1}{4}E \begin{pmatrix} \alpha_0 \\ \gamma \\ \beta_0 \end{pmatrix}$$

& its $N > 4$ generalizations **with tridiagonal** H ,

(PTO)

$$\left(\begin{array}{ccc|c|ccc} i\xi - F & -1 & & & & & \\ -1 & i\xi - F & \cdots & & & & \\ & & \cdots & \cdots & -1 & & \\ & & & -1 & i\xi - F & -1 & \\ \hline & & & -1 & -F & -1 & \\ \hline & & & & -1 & -i\xi - F & \cdots \\ & & & & & -1 & \cdots \\ & & & & & & \cdots \end{array} \right)$$

∃ AN EQUIVALENT **REAL FORMULATION OF SE:**

$$\left(\begin{array}{cc|cc|c|c|c}
 -F & -\xi & -1 & 0 & & & \\
 \xi & -F & 0 & -1 & & & \\
 \hline
 -1 & 0 & -F & -\xi & \cdots & & \\
 0 & -1 & \xi & -F & & \cdots & \\
 \hline
 & \cdots & \cdots & \cdots & -1 & 0 & \\
 & & \cdots & \cdots & 0 & -1 & \\
 \hline
 & & -1 & 0 & -F & -\xi & -1 \\
 & & 0 & -1 & \xi & -F & 0 \\
 \hline
 & & & & -2 & 0 & -F
 \end{array} \right) \begin{pmatrix} a_0 \\ b_0 \\ \hline a_1 \\ b_1 \\ \hline \vdots \\ \vdots \\ \hline a_n \\ b_n \\ \hline \gamma \end{pmatrix} = 0.$$

SOLVABLE:

\implies by the matching method

\implies in closed **complex** form (Tschebyshev polynomials)

\implies in closed **real** form (matrix Tschebyshev)

M. Znojil (quant-ph/0605209),

*Matching method and exact solvability of discrete
PT-symmetric square wells*

J. Phys. A: Math. Gen. 39 (2006) 10247 - 10261

MERIT: A PARALLELISM

(i) solvable **differential** Schrödinger equation:

B. Bagchi et al (quant-ph/0503035),

PT-symmetric supersymmetry in a solvable short-range model,

Int. J. Mod. Phys. A 21 (2006) 2173-2190

(ii) parallel solvable **difference** Schrödinger equations:

[$N = 7$ **sample: PTO**]

$$\left(\begin{array}{c|cc|c} i\xi - F & -1 & & \\ \hline -1 & -F & -1 & \\ & -1 & -F & -1 \\ & & -1 & -F & -1 \\ \hline & & & -1 & -i\xi - F \end{array} \right) \begin{pmatrix} \alpha_0 \\ \gamma_0 \\ \gamma \\ \gamma_0^* \\ \alpha_0^* \end{pmatrix} = 0.$$

$$F_0 = 0, \quad F_{\pm, \pm} = \pm \frac{1}{2} \sqrt{8 - 2\xi^2 \pm 2\sqrt{4 + \xi^4}}.$$

$F_{\pm, -}$ responsible for EP, $\xi_{crit} = \sqrt{3/2} \approx 1.2247$ (PTO)

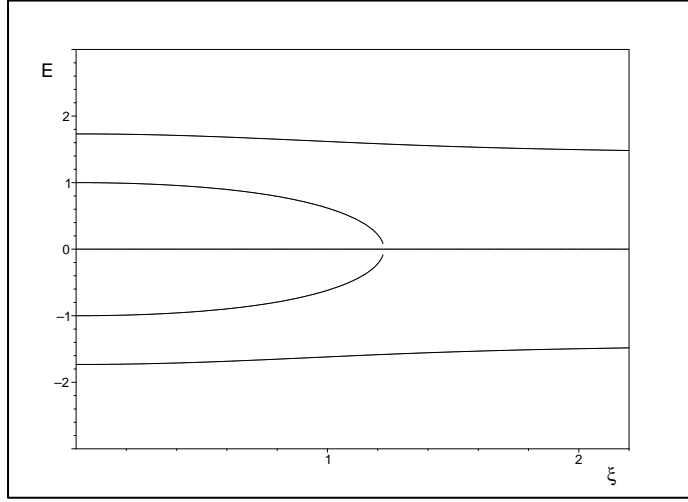


Figure 4: RK spectrum at $N = 7$, single fragile pair of $E_{1,3}$

$$F_{\pm,+} = \pm\sqrt{3} \left[1 - \frac{1}{12} \xi^2 + \frac{5}{288} \xi^4 + \frac{5}{3456} \xi^6 + O(\xi^8) \right]$$

$$F_{\pm,+} = \pm\sqrt{2} \left[1 + \frac{1}{4} y^2 - \frac{1}{32} y^4 - \frac{31}{128} y^6 + O(y^8) \right], \quad y = 1/\xi.$$

RUNGE KUTTA QM: SUMMARY

♡ feasible EP constructions

◇ a useful guidance towards $N \rightarrow \infty$

♠ oversimplified, tuned to 1D dynamics,

♣ not enough structural flexibility in $O\Delta E$

\implies **idea:** try to move to 2D:

$(x, y) \longrightarrow (x, y_n)$ with $n = 1, \dots, K$.

(2) COUPLED-CHANNEL QM

($K = 2$) **two-by-two** Hamiltonian, differential in x :

$$H_{(kinetic)} = \begin{pmatrix} -\frac{d^2}{dx^2} & 0 \\ 0 & -\frac{d^2}{dx^2} \end{pmatrix},$$

$$H_{(interaction)} = \begin{pmatrix} V_a(x) & W_b(x) \\ W_a(x) & V_b(x) \end{pmatrix}.$$

♡ 2D Hamiltonians which are only discretized in y

◇ θ -pseudo-Hermiticity:

$$\theta = \theta^\dagger = \begin{pmatrix} 0 & \mathcal{P} \\ \mathcal{P} & 0 \end{pmatrix} = \theta^{-1}$$

♡ square-well potentials [$x \in (-1, 0)$]:

$$\text{Im } W_a(x) = X > 0,$$

$$\text{Im } W_b(x) = Y > 0,$$

$$\text{Im } V_a(x) = \text{Im } V_b(x) = Z,$$

♠ spin-like ($\sigma = \pm 1$) symmetry:

$$\Omega = \begin{pmatrix} 0 & \omega^{-1} \\ \omega & 0 \end{pmatrix}, \quad \omega = \sqrt{\frac{X}{Y}} > 0.$$

♣ solvable and physical

M. Znojil (quant-ph/0511085),

Coupled-channel version of PT -symmetric square well,

J. Phys. A: Math. Gen. 39 (2006) 441 - 455.

($K = 3$) next, **three-by-three square well:**

$$H_{(kinetic)} = \begin{pmatrix} -\frac{d^2}{dx^2} & 0 & 0 \\ 0 & -\frac{d^2}{dx^2} & 0 \\ 0 & 0 & -\frac{d^2}{dx^2} \end{pmatrix},$$
$$\mathbf{Z}_{(interaction, K=3)} = \begin{pmatrix} Z_{(1,1)} & Z_{(1,2)} & Z_{(1,3)} \\ Z_{(2,1)} & Z_{(2,2)} & Z_{(2,3)} \\ Z_{(3,1)} & Z_{(3,2)} & Z_{(3,3)} \end{pmatrix}.$$

with two “strong” θ -pseudo-Hermiticities:

$$\theta = \theta_{(3,1)} = \begin{pmatrix} 0 & 0 & \mathcal{P} \\ \mathcal{P} & 0 & 0 \\ 0 & \mathcal{P} & 0 \end{pmatrix} = \theta_{(3,2)}^\dagger = \theta_{(3,2)}^{-1} \neq \theta^\dagger,$$

$$\theta_{(3,2)} = \begin{pmatrix} 0 & \mathcal{P} & 0 \\ 0 & 0 & \mathcal{P} \\ \mathcal{P} & 0 & 0 \end{pmatrix} = \theta_{(3,1)}^\dagger = \theta_{(3,1)}^{-1} \neq \theta_{(3,2)}^\dagger.$$

♣ an emergence of a factorized symmetry

In the “strong” case we have $\theta^\dagger \neq \theta = \mathbf{R}$ in

$$H^\dagger = \mathbf{R} H \mathbf{R}^{-1}.$$

A few observations should be made

observation 1

if we wish that

$$H^\dagger = \mathbf{R} H \mathbf{R}^{-1}$$

then

$$H = (H^\dagger)^\dagger = (\mathbf{R}^{-1})^\dagger H^\dagger \mathbf{R}^\dagger$$

observation 2

if we wish that

$$H^\dagger = \mathbf{R} H \mathbf{R}^{-1}$$

then

$$H = (H^\dagger)^\dagger = (\mathbf{R}^{-1})^\dagger H^\dagger \mathbf{R}^\dagger$$

$$H = (H^\dagger)^\dagger = (\mathbf{R}^{-1})^\dagger \mathbf{R} H \mathbf{R}^{-1} \mathbf{R}^\dagger$$

observation 3

if we wish that

$$H^\dagger = \mathbf{R} H \mathbf{R}^{-1}$$

then

$$H = (H^\dagger)^\dagger = (\mathbf{R}^{-1})^\dagger H^\dagger \mathbf{R}^\dagger$$

$$H = (H^\dagger)^\dagger = (\mathbf{R}^{-1})^\dagger \mathbf{R} H \mathbf{R}^{-1} \mathbf{R}^\dagger$$

$$H = (H^\dagger)^\dagger = \mathcal{S} H \mathcal{S}^{-1}$$

♠ This means that

our H must have a **factorized** symmetry,

$$H \mathcal{S} = \mathcal{S} H, \quad \mathcal{S} = (\mathbf{R}^{-1})^\dagger \mathbf{R}$$

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$$H \mathcal{S} = \mathcal{S} H, \quad \mathcal{S} = (\mathbf{R}^{-1})^\dagger \mathbf{R}$$

and we have two possibilities:

- either $\mathcal{S} = I$ (i.e., $\mathbf{R} = \mathbf{R}^\dagger$), *pseudo-Hermiticity*

♠ This means that

our H must have a **factorized** symmetry,

$$H \mathcal{S} = \mathcal{S} H, \quad \mathcal{S} = (\mathbf{R}^{-1})^\dagger \mathbf{R}$$

and we have two possibilities:

- either $\mathcal{S} = I$ (i.e., $\mathbf{R} = \mathbf{R}^\dagger$), *pseudo-Hermiticity*
- or $\mathcal{S} \neq I$ (proper “*factorized symmetry*”).

◇ **factorized symmetry constraints** (for SQWs)

In three channels we get a **unique** 2-parametric set

$$\mathbf{Z}_{(interaction)} = \begin{pmatrix} Z & X & X \\ X & Z & X \\ X & X & Z \end{pmatrix}$$

and define $Z_{(eff)}(m) =$ eigenvalues of \mathbf{Z} ,

$$Z_{eff}(1) = Z + 2X, \quad Z_{eff}(2,3) = Z - X.$$

♡ **all = solvable again, via a ‘new curve’:**

$$t = t^{(\sigma)}(s) = \frac{1}{2s} Z_{eff}(\sigma), \quad \sigma = 1, 2, 3$$

[cf. M. Znojil (quant-ph/0601048),
Strengthened PT-symmetry with $P \neq P^\dagger$
Phys. Lett. A 353 (2006) 463 - 468].

new: degeneracy of levels $\sigma = 2, 3$,

EPs: a boundary $\partial\Omega^{(3)}$ of a triangle (PTO)

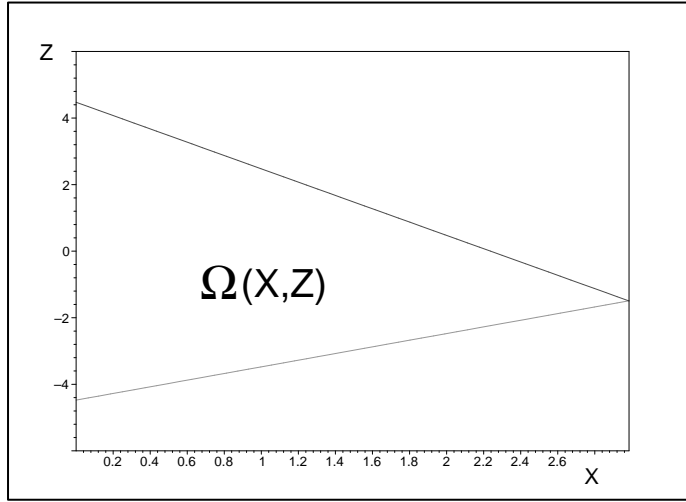


Figure 5: Triangular quasi-Hermiticity domain at $K = 3$

energies real for $X - Z_{crit} \leq Z \leq Z_{crit} - 2X$,

EP vertices $(0, \pm 4.475)$ and $(2.98, -1.49)$.

COUPLED-CHANNEL QM: SUMMARY

♡ an innovation of the concept of symmetries

◇ EPs from a routine square-well solvability

♠ an interpretation of $\mathcal{S} \neq I$ is missing,

♣ not worked out at the higher spins

⇒ an **alternative** natural option:

a universal **biorthogonal basis**

(3) VARIATIONAL QM

initial Schrödinger equation

say, ODE with $x \in (-\infty, \infty)$, \mathcal{PT} -symmetric:

$$H = -\frac{d^2}{dx^2} + U(x) + iW(x) \neq H^\dagger,$$

$$U(x) = U(-x), \quad W(x) = -W(-x)$$

represented in a **partitioned** variational basis,

$$|\psi_+\rangle = \sum_{m=0}^{N_+} |2m\rangle \phi_m, \quad |\psi_-\rangle = \sum_{m=0}^{N_-} |2m+1\rangle \chi_m$$

using the **\mathcal{PT} -symmetric** normalization,

$$|\psi\rangle = |\psi_+\rangle - i|\psi_-\rangle.$$

having to solve **two** Schrödinger equations at once:

$$H|n\rangle = E_n|n\rangle$$

and

$$\langle\langle n|H = E_n\langle\langle n|$$

we arrive at the **partitioned** infinite-dimensional

$$H = \begin{pmatrix} S & +B \\ -B^T & L \end{pmatrix}$$

while **\mathcal{PT} -symmetry** implies that

$$|n\rangle = \begin{pmatrix} \vec{\phi}_n \\ \vec{\chi}_n \end{pmatrix}, \quad |n\rangle\rangle = \begin{pmatrix} \vec{\phi}_n \\ -\vec{\chi}_n \end{pmatrix}.$$

◇ *recipes: linear algebra:*

$$H^\dagger = \Theta H \Theta^{-1}, \quad I \neq \Theta = \Theta^\dagger > 0.$$

$$\text{with } H = \sum_n |n\rangle \frac{E_n}{\langle\langle n|n\rangle} \langle\langle n|$$

$$\text{and } \Theta = \sum_n |n\rangle\langle n| t_n \langle\langle n|$$

♣ *spectra: results, in general, numerical*

illustration: \exists **a nice extension**

of the above-mentioned two-by-two toy problem to dim=3,

$$H^{(3)} = \begin{pmatrix} -1 & a & d \\ -a & 1 & b \\ d & -b & 3+c \end{pmatrix}, \quad \mathcal{P}^{(3)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

♡ **in this model**

Jacobi rotation annihilates $d = 0$,

$$H^{(3)} = \begin{pmatrix} -1 & a & 0 \\ -a & 1 & b \\ 0 & -b & 3+c \end{pmatrix}$$

♡ ♡ **in this model**

all $c \neq -2$ are easy to incorporate in the formulae, and

a two-parametric “representative Hamiltonian” results,

$$H^{(3)} = \begin{pmatrix} -2 & a & 0 \\ -a & 0 & b \\ 0 & -b & 2 \end{pmatrix}$$

♡ ♡ ♡ **in this model**

the EP set $\partial\Omega^{(3)}$ has a “**generic**” shape,

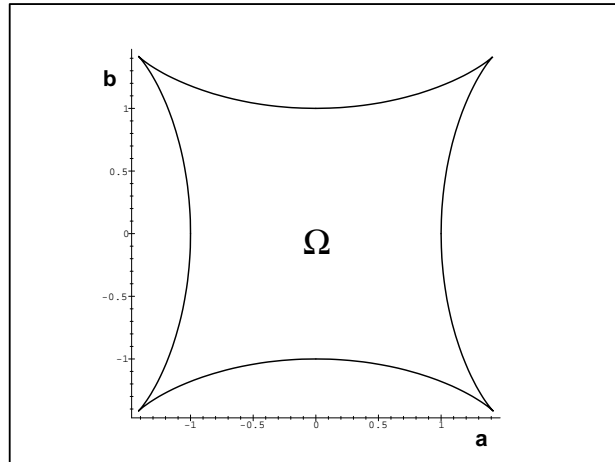


Figure 6: Domain $\Omega(a, b)$ for $H = H^{(3)}$

with two-dimensional **fixed**– b **subdomains** $\Omega_{(b)}^{(2)}(a)$

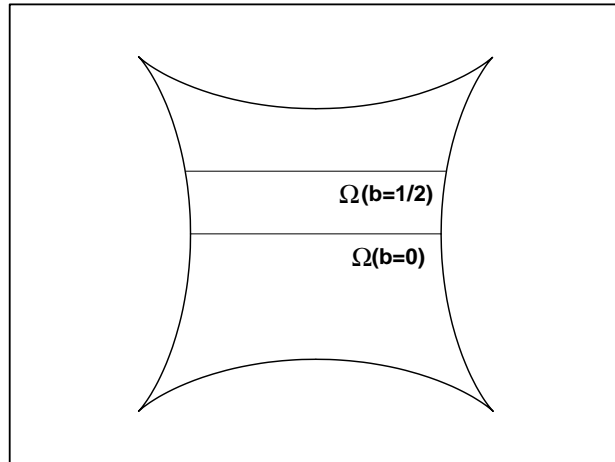


Figure 7: The b –dependence of the interior of $\Omega^{(3)}(a, b)$

♡ ♡ ♡ ♡ **in this model**

conclude: **after a re-coupling**, $b = 0 \longrightarrow b > 0$,

EPs of a “decoupled system” ($= \partial\Omega^{(3)}(a, 0) = \pm 1$),

become physical, **stabilized**, “*regularized*”

by having **moved inside** $\Omega_{(b)}^{(2)}(a) = (-\gamma(b), \gamma(b))$

where, e.g., $\gamma(1/2) \approx 1.04237$.

♡ ♡ ♡ ♡ ♡ **in this model**

$t \in (-1, 1)$ parametrizes the **whole** curve $\partial\Omega^{(3)}$,

$$a = a_{\pm} = \pm \sqrt{\frac{1}{2}(4 - 3t^2 - t^3)},$$

$$b = b_{\pm} = \pm \sqrt{\frac{1}{2}(4 - 3t^2 + t^3)}$$

(trick to be remembered!)

more details:

M. Znojil (quant-ph/0701232),
*A return to observability near exceptional points
in a schematic PT -symmetric model.*
Phys. Lett. B 647 (2007) 225 - 230.

VARIATIONAL QM: SUMMARY

♡ straightforward calculations (linear algebra)

◇ reliable (variational) background at $N \gg 1$

♠ too numerical in general (too many free parameters)

♣ analytic insight ($N = 3$) looks exceptional

⇒ **remedy**: choose some of the parameters in advance.

Chapter III. **TRIDIAGONALIZATIONS:**

K coupled square wells in a chain

THE MENU

(1) RUNGE KUTTA

[tridiagonal by itself in 1D: omitted]

(2) COUPLED CHANNELS

[surprise: \exists **circular-chain** semi-tridiagonalizations !]

(3) BIORTHOGONAL **BASES**

[**main** news on EPs, postponed to ch. IV]

Section III. A. $K > 1$ parallels
to the single-channel case

(i) \exists formulae for wave functions:

square-well ODE with constant coefficients:

$$\begin{aligned} -\frac{d^2}{dx^2} \varphi^{(m)}(x) + \sum_{j=1}^K V_{Z(m,j)}(x) \varphi^{(j)}(x) &= \\ &= E \varphi^{(m)}(x), \quad m = 1, 2, \dots, K \end{aligned}$$

solvable by an ansatz

$$\varphi^{(m)}(x) = \begin{cases} C_L^{(m)} \sin \kappa_L(x + 1), & x < 0, \\ C_R^{(m)} \sin \kappa_R(-x + 1), & x > 0 \end{cases}$$

using $Z_{(eff)}^{(m)}(K)$ as eigenvalues of

$$\begin{pmatrix} Z_{(1,1)} & Z_{(1,2)} & \dots & Z_{(1,K)} \\ Z_{(2,1)} & Z_{(2,2)} & \dots & Z_{(2,K)} \\ \vdots & \ddots & \ddots & \vdots \\ Z_{(K,1)} & Z_{(K,2)} & \dots & Z_{(K,K)} \end{pmatrix}.$$

(ii) **quantized** easily:

ansatz and its insertion:

$$\kappa_R = s + it = \kappa_L^*, \quad s > 0,$$

$$\rightarrow t = X_{first\ curve} \left[Z_{(eff)}^{(m)}(K), s \right] \equiv \frac{Z_{(eff)}^{(m)}(K)}{2s}$$

plus **matching** condition in the origin:

$$\rightarrow t = Y_{second\ curve}(s)$$

$$Y_{\text{second curve}}(s): \quad \kappa_L \cotan \kappa_L = -\kappa_R \cotan \kappa_R$$

→ implicit definition:

$$2s \sin 2s + 2t \sinh 2t = 0$$

→ **energies:**

$$E_n = s_n^2 - t_n^2, \quad n = 0, 1, \dots$$

= **intersections** (s_n, t_n) of two graphs (PTO)

sample of the graphical recipe:

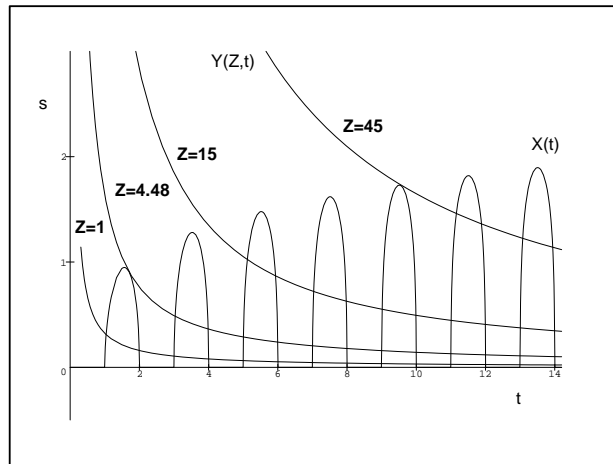


Figure 8: Square-well energies

(iii) the SAME algorithm determining EPs:

$$= \text{hint} \rightarrow 2s = (n+1)\pi + (-1)^n Q$$

$$\frac{Q}{2} \Big|_{crit} \equiv \varepsilon(t_{crit}) = \pi - \frac{Z_{crit}}{2t_{crit}},$$

$$\sin [2\varepsilon(t)] = \frac{t \sinh 2t}{\pi - \varepsilon(t)},$$

$$\varepsilon_{(lower)}(t) = \pi/4 \text{ and } \varepsilon_{(upper)}(t) = 0.$$

Newton's method:

$$\partial_t \varepsilon(t_{crit}) = \frac{Z_{crit}}{2t_{crit}^2},$$

$$\partial_t \varepsilon(t) = \frac{\sinh 2t + 2t \cosh 2t}{2 [\pi - \varepsilon(t)] \cos 2\varepsilon(t) - \sin 2\varepsilon(t)}$$

a sample result:

$$\rightarrow t_{crit} \in (0.839393459, 0.839393461),$$

$$\rightarrow s_{crit} \in (2.665799044, 2.665799069),$$

$$\rightarrow E_{crit} \in (6.401903165, 6.401903294).$$

iteration	$Z_{crit}^{(lower)}$	$Z_{crit}^{(upper)}$
0	4.30	4.66
2	4.461	4.486
4	4.4743	4.4760
6	4.47524	4.47536
8	4.4753038	4.475312
10	4.47530826	4.47530882
12	4.47530856	4.47530861

(iv) formulae in **weakly** non-Hermitian regime:

$$s = s_n = \frac{(n+1)\pi}{2} + \tau \frac{Q_n}{2}, \quad \tau = (-1)^n$$

→ **iterate:**

the first small quantity $\varrho \equiv \frac{1}{L} = \frac{1}{(n+1)\pi}$

the second one $\alpha = \frac{2Z_{eff}(\sigma)}{L}$ or $\beta = \alpha\varrho$

(v) at **intermediate** non-Hermiticities:

→ a “generalized continued fraction”

$$Q = \arcsin \left(2t \frac{\varrho}{1 + \tau Q \varrho} \sinh 2t \right), \quad 2t = \frac{\alpha}{1 + \tau Q \varrho}.$$

$$\rightarrow \arcsin(x) = x + \frac{1}{6}x^3 + \frac{3}{40}x^5 + \dots$$

$$Q = Q(\alpha, \beta) = \alpha\beta \Omega(\alpha, \beta),$$

$$\begin{aligned} \rightarrow \Omega(\alpha, \beta) &= 1 + c_{10} \alpha^2 + c_{01} \beta^2 + \\ &+ c_{20} \alpha^4 + c_{11} \alpha^2 \beta^2 + c_{02} \beta^4 + \mathcal{O}(\alpha^6) \end{aligned}$$

→ equation **re-arranged**:

$$[1 + \tau \beta^2 \Omega(\alpha, \beta)] \operatorname{arcsinh}(\Lambda) = \alpha$$

$$\Lambda = [1 + \tau \beta^2 \Omega(\alpha, \beta)]^2 \frac{1}{\beta} \sin[\alpha \beta \Omega(\alpha, \beta)]$$

(vi) formulae for energies:

→ leading order relation

$$0 = \left(-\frac{1}{6} + c_{10} + c_{01}\varrho^2 + 3\tau\varrho^2\right) \alpha^3 + \dots$$

determines the first two coefficients,

$$c_{10} = \frac{1}{6}, \quad c_{01} = -3\tau,$$

the next-order $O(\alpha^5)$ gives

$$c_{20} = \frac{1}{120}, \quad c_{11} = \frac{1-8\tau}{6}, \quad c_{02} = 15$$

and leads to our **final** $1 + O(\alpha^4)$ formula

$$Q_n = \frac{4 Z_{eff}^2}{(n+1)^3 \pi^3} + \frac{8 Z_{eff}^4}{3 (n+1)^5 \pi^5} \left(1 + \frac{18 (-1)^{n+1}}{(n+1)^2 \pi^2} \right).$$

Section III. B. **There \exists a semi-tridiagonalization
of $2J + 1$ coupled square wells**

At any K , let's use $\mathbf{R}^{-1} = \mathbf{R}^\dagger$, $\mathcal{S} = \mathbf{R}^2$

$$\mathbf{R} = \begin{pmatrix} 0 & \dots & 0 & 0 & \mathcal{P} \\ \mathcal{P} & 0 & \dots & 0 & 0 \\ 0 & \mathcal{P} & 0 & \dots & 0 \\ \vdots & \dots & \dots & \dots & \vdots \\ 0 & \dots & 0 & \mathcal{P} & 0 \end{pmatrix}$$

in **FIVE** channels, *all* choices of **R** lead to *the same*

$$\mathbf{Z}_{(interaction)} = \begin{pmatrix} Z & X & D & D & X \\ X & Z & X & D & D \\ D & X & Z & X & D \\ D & D & X & Z & X \\ X & D & D & X & Z \end{pmatrix}$$

which is “next to tridiagonal” at $D = 0$,

$$\mathbf{Z}_{(interaction)} = \begin{pmatrix} Z & X & & & X \\ X & Z & X & & \\ & X & Z & X & \\ & & X & Z & X \\ X & & & X & Z \end{pmatrix}.$$

For 7 **channels**, similarly, the allowed matrix of couplings

$$\mathbf{Z}_{(interaction)} = \begin{pmatrix} Z & X & Y & D & D & Y & X \\ X & Z & X & Y & D & D & Y \\ Y & X & Z & X & Y & D & D \\ D & Y & X & Z & X & Y & D \\ D & D & Y & X & Z & X & Y \\ Y & D & D & Y & X & Z & X \\ X & Y & D & D & Y & X & Z \end{pmatrix}$$

becomes “almost tridiagonal” at $Y = D = 0$:

$$\mathbf{Z}_{(interaction)} = \begin{pmatrix} Z & X & & & & & X \\ X & Z & X & & & & \\ & X & Z & X & & & \\ & & X & Z & X & & \\ & & & X & Z & X & \\ & & & & X & Z & X \\ X & & & & & X & Z \end{pmatrix} .$$

COUPLED-CHANNEL CHAINS: SUMMARY

♡ an innovation of the concept of the chain model

◇ the solvability extended to the large “spins” $K = 2J + 1$

♠ not so nice at even $K = 2J$ (why? - an open question)

♣ no free parameters: $\partial\Omega^{(EP)} =$ piecewise linear

Chapter IV.

**SEPARABLY ANHARMONIC OSCILLATORS
AND THEIR EXCEPTIONAL POINTS**

THE MENU

(A) COUPLED HARMONIC-OSCILLATOR LEVELS

[$N < \infty$, an **auxiliary** upside-down symmetry]

(B) FULL, MAXIMAL CONFLUENCE OF EPs

[the results of **symbolic manipulations**]

(C) THE PATTERN OF DECONFLUENCE

[the shape of $\partial\Omega^{(N)}$, **strong-coupling regime**]

Section IV. A. **The family of models**

The separable AHO bound-state problem with

$$H_{(int)} = i g (|0\rangle \langle 1| + |1\rangle \langle 0|)$$

is equivalent to the above-mentioned matrix model

$$\begin{pmatrix} -1 & g \\ -g & 1 \end{pmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = E \begin{pmatrix} \phi \\ \chi \end{pmatrix}$$

M. Znojil and H. B. Geyer (quant-ph/0607104),

*Construction of a unique metric
in quasi-Hermitian quantum mechanics.*

Phys. Lett. B 640 (2006) 52 - 56

For the same toy problem

$$H^{(2)} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = E \begin{pmatrix} \phi \\ \chi \end{pmatrix}, \quad H^{(2)} = \begin{pmatrix} -1 & a \\ -a & 1 \end{pmatrix}$$

\exists a straightforward generalization (PTO):

♡ the chain-model family ♡

$$H^{(N)} = \begin{bmatrix} 1 - N & a & 0 & 0 & \dots & 0 \\ -a & 3 - N & b & 0 & \dots & 0 \\ 0 & -b & 5 - N & \ddots & \ddots & \vdots \\ 0 & 0 & \ddots & \ddots & b & 0 \\ \vdots & \vdots & \ddots & -b & N - 3 & a \\ 0 & 0 & \dots & 0 & -a & N - 1 \end{bmatrix} .$$

♡ sample: the **four by four** secular equation

$$\det \begin{bmatrix} 3 - E & b & 0 & 0 \\ -b & 1 - E & a & 0 \\ 0 & -a & -1 - E & b \\ 0 & 0 & -b & -3 - E \end{bmatrix} = 0$$

with $a = \pm\sqrt{A}$, $b = \pm\sqrt{B}$ gives $E = \pm\sqrt{s}$.

This facilitates the study of EPs, e.g., via the

brute-force numerical determination of $\partial\Omega^{(4)}$:

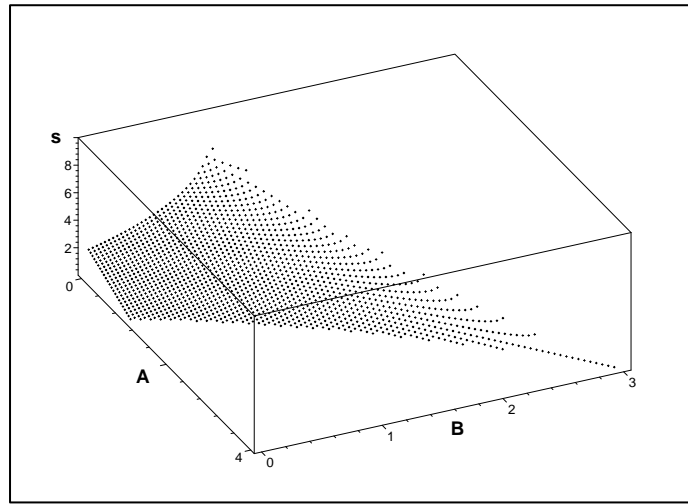


Figure 9: The least stable energy pair $E_{\pm} = \pm\sqrt{s(A, B)}$

Section IV. B. **A** *maximal* **confluence of EPs**

Figure 9 indicates that the EP shape $\partial\Omega^{(4)}$ for

$$H^{(4)} = \begin{pmatrix} 3 - E & b & 0 & 0 \\ -b & 1 - E & a & 0 \\ 0 & -a & -1 - E & b \\ 0 & 0 & -b & -3 - E \end{pmatrix}$$

is **sharply spiked** near $a_{max}^{(EEP)} \approx 2$ and $b_{max}^{(EEP)} \approx \sqrt{3}$.

We intend to demonstrate that this feature is **generic**.

The $N = 4$ **EEP construction** using secular equation

$$s^2 + (-10 + 2b^2 + a^2)s + 9 + 6b^2 - 9a^2 + b^4 = 0$$

compared with $s^2 = 0$ at an extreme EP (EEP).

Gröbner-solvable two conditions:

$$A + 2B = 10, \quad (3 + B)^2 = 9A$$

spurious solution: $A = 64, B = -27,$

the acceptable pair is unique: $A^{(EEP)} = 4, B^{(EEP)} = 3.$

EEP construction at any other N : **the method**:

(a) split the models $H^{(N)}$ in **two series**:

with $N = 2K$ and with $N = 2J + 1$

(b) construct explicit **Gröbner** EEP solutions

(at the first few N)

(c) **extrapolate** to all N

(and verify at the next few N).

◇ ♠ ◇ **the result:** ◇ ♠ ◇

a re-parametrization of the couplings:

$$a^2 = G_1^{(N)} (1 - \alpha) , \quad b^2 = G_2^{(N)} (1 - \beta) , \quad \dots ,$$

$$G_k^{(N)} = k (N - k) .$$

with the innovated Greek-letter parameters $\in (0, 1)$.

♣ **sampling the proof:** $N = 8$:

(1) **consider** secular equation

$$s^4 + P_3 s^3 + P_2 s^2 + P_1 s + P_0 = 0$$

$\implies \Omega^{(8)}(A, B, C, D)$ circumscribed by the simplex

$$A + 2B + 2C + 2D = 84.$$

(2) **take** quadratic P_2 , cubic P_1 and quartic P_0 containing 13, 19 and 20 individual terms, respectively, **reduce**, e.g.

$$P_2 = 1974 + (B + C + D)^2 + 2AD + 2BD + 2AC + \\ + 50D - (83A + 142B + 70C)$$

& Gröbner-solve the EEP set of nonlinear equations

$$P_2(A, B, C, D) = 0, \quad P_1(A, B, C, D) = 0, \quad P_0(A, B, C, D) = 0$$

(3) **find and factorize** the resulting polynomial

$$\begin{aligned} & 314432 D^{17} - 5932158016 D^{16} + 4574211144896 D^{15} + \\ & + 3133529909492864 D^{14} + 917318495163561932 D^{13} + \dots \\ & \dots + 235326754101824439936800228806905073 D^2 - \\ & - 453762279414621179815552897029039797 D + \\ & + 153712881941946532798614648361265167 = 0 \end{aligned}$$

(4) **demonstrate** that 16 roots are spurious:

(i) easy for all the complex roots;

(ii) easy for the three real but manifestly spurious negative roots

$$D = -203.9147095, -156.6667001, -55.49992441.$$

(iii) most complicated for the four real and positive roots

$$D = 0.4192854385, 5.354156128, 1354.675195 \text{ and } 18028.16789.$$

In the latter case, for example, one finds the spurious negative value for

$$\Upsilon^2 \times A = (\text{a polynomial in } D \text{ of 16th degree}).$$

No chance without computers: the number of digits in Υ^2 exceeds one hundred.

(5) **conclude** that the remaining closed solution

$$A^{(EEP)} = 16, B^{(EEP)} = 15, C^{(EEP)} = 12, D^{(EEP)} = 7$$

is unique.

QED.

Summary of the merits of the model:

- provides *all* types of the **confluence of EPs**
- *precisely* the necessary number of parameters.

More details:

M. Znojil (math-ph/0703070),
*Maximal couplings in PT -symmetric chain-models
with the real spectrum of energies.*

J. Phys. A: Math. Theor. 40 (2007) 4863 - 4875

Section IV. C.

**The strong-coupling mechanism of the split
of the EPs near EEPs**

Let's recollect the **smoothness** of the surface $s(A, B) = E^2$,

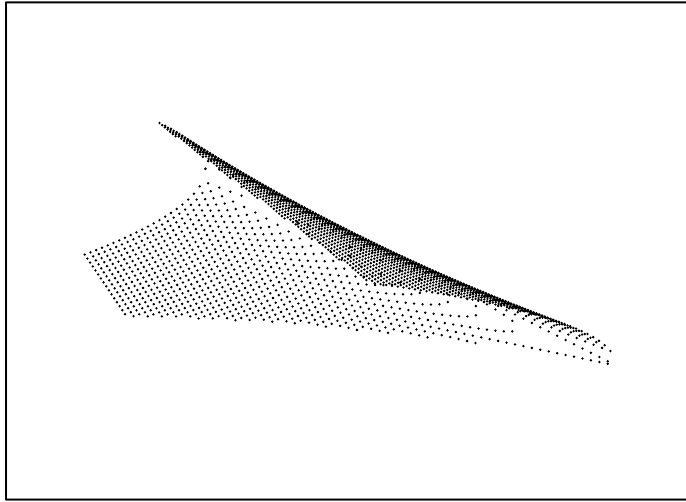


Figure 10: Second sheet of $s(A, B) (\leq 14)$ added to Fig. 9.

reparametrize the matrix elements of $H^{(4)}$ accordingly,

$$\begin{pmatrix} -3 & \sqrt{3}\sqrt{1-\beta} & 0 & 0 \\ -\sqrt{3}\sqrt{1-\beta} & -1 & 2\sqrt{1-\alpha} & 0 \\ 0 & -2\sqrt{1-\alpha} & 1 & \sqrt{3}\sqrt{1-\beta} \\ 0 & 0 & -\sqrt{3}\sqrt{1-\beta} & 3 \end{pmatrix}$$

and reparametrize **also its QH domain** $\Omega^{(4)}$,

$$\beta \geq \beta_{\text{minimal}} = \frac{9\alpha - \alpha^2}{9 + 3\alpha}, \quad \alpha \in (0, 1)$$

$$\alpha \geq \alpha_{\text{minimal}} = \beta - \frac{\beta^2}{4}, \quad \beta \in (0, 1)$$

$$\beta = t + t^2 B(t), \quad \alpha = t + t^2 A(t)$$

M. Znojil, *Conditional observability*,

Phys. Lett. B, to appear (arXiv:0704.3812v1 [hep-th] 28 Apr 2007)

◇ beyond the EEP we can get a “big bang” phenomenon,

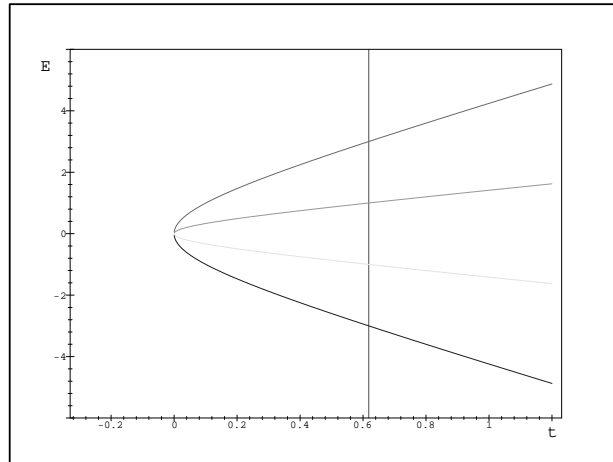


Figure 11: The t -dependence of the energy levels at $A = B = 1$.

Note that $\alpha = \beta = 1$ at the Hermiticity boundary

$$t_{Herm.} = (\sqrt{5} - 1)/2 \approx 0.618033989.$$

◇ ◇ at $A = 2$, $B = 1$ we get a non-EEP pattern,

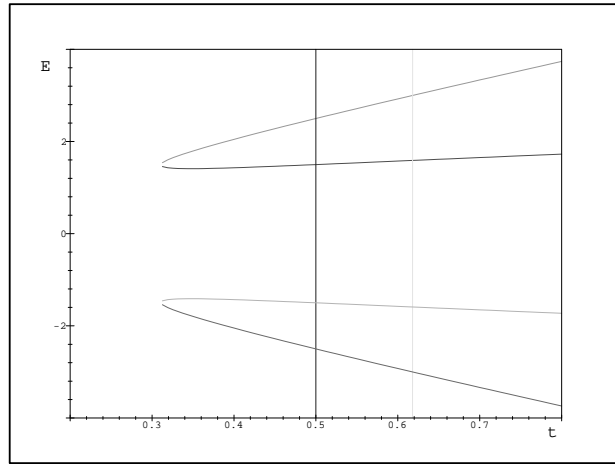


Figure 12: Two “simultaneous small bangs” at an EP value $t_{(EP)} > 0$.

Note that the $\alpha(t) = 1$ line (i.e., the end of PT-symmetry)

comes earlier than $\beta(t) = 1$ (i.e., the Hermiticity boundary).

◇ ◇ ◇ at $A = 1$, $B = 1.5$ we have

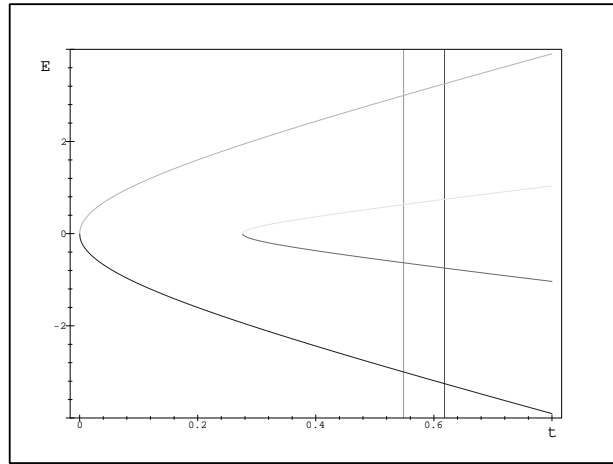


Figure 13: Quasi-Hermiticity established at $t_{(EP)} > 0.2$.

subconclusions: inside Ω ,

\exists **a fine-tuned balance** between $\alpha(t)$ and $\beta(t)$,

\exists **all the possible** patterns of mergers between levels.

conjecture:

both properties are, *mutatis mutandis*, valid at all N

♡ test at the **six by six** $H^{(6)}$,

$$g_1 = c = \sqrt{5(1 - \gamma)}, \quad g_2 = b = 2\sqrt{2(1 - \beta)},$$

$$g_3 = a = 3\sqrt{1 - \alpha}$$

with

$$\alpha = t + t^2 + At^3, \quad \beta = t + t^2 + Bt^3, \quad \gamma = t + t^2 + Ct^3.$$

◇ the “big bang” spectrum beyond the EEP again,

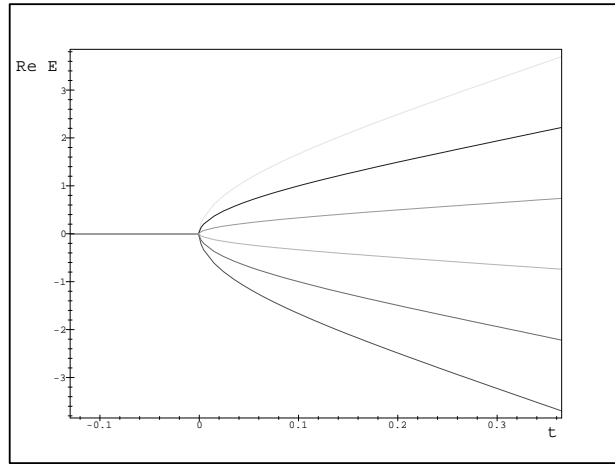


Figure 14: Energy levels at $A = B = C = 1$.

◇ ◇ the choice of $A = 1$, $B = 2$, $C = 1$ gives

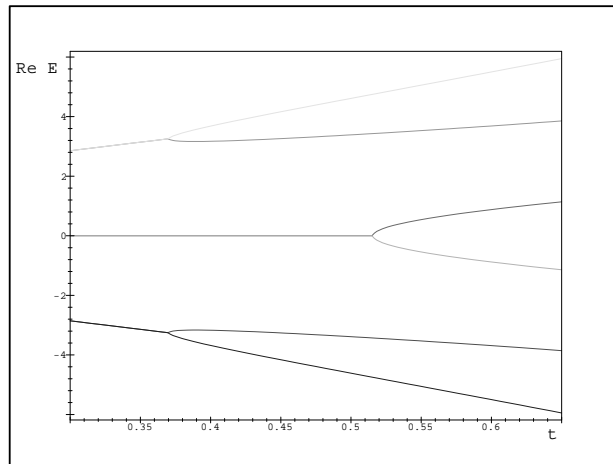


Figure 15: Real parts of the energies, “central” $t_{(EP)} > 0.5$.

◇ ◇ ◇ at $A = 3$, $B = 5$, $C = 1$ one gets

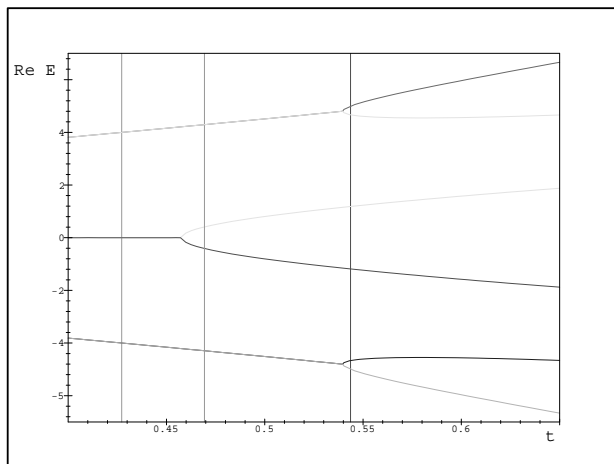


Figure 16: Quasi-Hermiticity established at the ground state.

conclusions: conjecture confirmed at $N = 6$:

∃ **a fine-tuned balance** between α , β and γ

∃ **all the possible** merging patterns again.

conjecture: at any $N = 2J (+1)$ one should parametrize

$$g_n = \sqrt{n(N-n)(1-\xi_n)}, \quad \xi_n = t + t^2 + \dots + t^{J-1} + G_n t^J,$$

$$n = 1, 2, \dots, J.$$

SUMMARY OF THE MODEL:

IT IS

- friendly:** maximal (EEP) couplings = *integers*,
- sufficient:** *all* the EP-merging patterns are encountered
- representative:** its *symmetry* is “maximal”
- necessary:** *couldn't* manage with *less* free parameters

Chapter V.

IN PLACE OF AN OVERALL SUMMARY

FOUR KEY MESSAGES

to take home:

(α) *DISCRETIZATIONS* REVIEWED
(**main merit: the variability of N**)

(β) *CHAIN-MODELS* PROMOTED
(**facilitated treatment, due to tridiagonality**)

(γ) *BRUTE-FORCE CALCULATIONS* REPORTED
(**an insight in EPs, based on symbolic manipulations**)

(δ) *EXTRAPOLATIONS* PERFORMED/RECOMMENDED
(**EP systematics**)

END OF THE STORY

appendices

A BRIEF INTRODUCTION IN QUASI-HERMITIAN QUANTUM MECHANICS

(1) Two Schroedinger equations in place of one,

$$H|n\rangle = E_n|n\rangle \text{ and } \langle\langle n|H = E_n\langle\langle n|.$$

(2) Quasi-Hermiticity in place of Hermiticity,

$$H^\dagger = \Theta H \Theta^{-1}, \quad I \neq \Theta = \Theta^\dagger > 0.$$

(3) A “generalized Dirac” notation,

$$H = \sum_n |n\rangle \frac{E_n}{\langle\langle n|n\rangle} \langle\langle n|$$

(4) The multiparametric “**choice of physics**”,

$$\Theta = \sum_n |n\rangle\rangle \theta_n \langle\langle n|, \quad \theta_n > 0.$$

Illustration:

construction of the metric Θ for a 2×2 Hamiltonian,

$$H = \begin{pmatrix} -T & B \\ -B & T \end{pmatrix}, \quad \Theta = \begin{pmatrix} a & b \\ b & d \end{pmatrix}$$

$$\Theta H = H^T \Theta \implies 2bT = -B(a + d)$$

$$E \in \mathcal{R} \iff |T| \geq |B|, \quad B = T \sin \alpha$$

ambiguity (the whole **interval** of a free parameter):

setting $T = 1$ and $a + d = 2Z > 0$ we have

$$H = \begin{pmatrix} -1 & \sin \alpha \\ -\sin \alpha & 1 \end{pmatrix}, \quad \Theta/Z = \begin{pmatrix} 1 + \xi & \sin \alpha \\ \sin \alpha & 1 - \xi \end{pmatrix}$$

positivity $\theta_{1,2}/Z = 1 \pm \sqrt{\xi^2 + \sin^2 \alpha} > 0$ means $1 > \sqrt{\xi^2 + \sin^2 \alpha}$

solutions $\Theta = \Theta(\xi)$ are numbered by $0 < \xi < \cos \alpha$.

interpretation:

In 2D with biorthogonal “brabacket” basis,

$$\langle\langle n| H = \langle\langle n| E_n, \quad H |n\rangle = E_n |n\rangle$$

ambiguity is compatible with the universal formula

$$\Theta = \sum |n\rangle\rangle s_n \langle\langle n|, \quad s_k > 0.$$