Third-order spectral branch points in Krein space related setups: $\mathcal{PT}$-symmetric matrix toy model, MHD α^2-dynamo and extended Squire equation *)

Uwe Günther, Frank Stefani

Department of Magnetohydrodynamics, Research Center Rossendorf, P.O. Box 510119, D–01314 Dresden, Germany

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The spectra of self-adjoint operators in Krein spaces are known to possess real sectors as well as sectors of pair-wise complex conjugate eigenvalues. Transitions from one spectral sector to the other are a rather generic feature and they usually occur at exceptional points of square root branching type. For certain parameter configurations two or more such exceptional points may happen to coalesce and to form a higher-order branch point. We study the coalescence of two square root branch points semi-analytically for a $\mathcal{PT}$-symmetric 4×4 matrix toy model and illustrate its occurrence numerically in the spectrum of the 2×2 operator matrix of the magneto-hydrodynamic α^2-dynamo and an extended version of the hydrodynamic Squire equation.

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1 Krein space related physical setups and spectral phase transitions

Some basic spectral properties of the Hamiltonians of $\mathcal{PT}$-symmetric Quantum Mechanics (PTSQM) [1] can be easily explained from the fact [2, 3] that these Hamiltonians are self-adjoint operators in Krein spaces [4, 5] — Hilbert spaces with an indefinite metric structure. In contrast to the purely real spectra of self-adjoint operators in "usual" Hilbert spaces (with positive definite metric structure), the spectrum of self-adjoint operators in Krein spaces splits into real sectors and sectors with pair-wise complex conjugate eigenvalues. In physical terms these two types of sectors are equivalent to phases of exact $\mathcal{PT}$-symmetry and spontaneously broken $\mathcal{PT}$-symmetry [1]. The reality of the spectrum of a PTSQM Hamiltonian, e.g., with complex potential ix^3, means that this spectrum is located solely in a real sector and that the operator is quasi-Hermitian[1]) in the sense of Ref. [7]. In

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[1]) Because quasi-Hermitian operators form only a restricted subclass of self-adjoint operators in Krein spaces (pseudo-Hermitian operators in the sense of Ref. [6]), the question for the reality of the spectrum seems up to now to be only partially solved. Apart from the requirement for existing $\mathcal{PT}$-symmetry of the differential expression of the operator, a subtle interplay between the operator domain and some, in general not yet sufficiently clearly identified, additional structural aspects of its differential expression seems to be responsible for the quasi-Hermiticity of the operator (exact $\mathcal{PT}$-symmetry of the corresponding PTSQM setup).

general, the spectrum of a self-adjoint operator in a Krein space is spreading over both sectors.

Considering the spectrum as a Riemann surface depending on model parameters (not necessarily moduli) from a space $\mathcal{M}$, the boundaries between real and complex spectral sectors can be described as an algebraic variety ((multi-component) hypersurface) Υ in $\mathcal{M}$, $\Upsilon \subset \mathcal{M}$, where the Riemann surface has exceptional points of branching type [8–14]. The most generic varieties of this type are those of codimension one, $\text{codim}(\Upsilon) = \dim(\mathcal{M}) - \dim(\Upsilon) = 1$, which can be easily read off, e.g., from a pseudo-Hermitian 2×2-matrix model [15–18]

$$H = \begin{pmatrix} x+y & w \\ -w^* & x-y \end{pmatrix}, \quad H\psi = \lambda\psi\,, \tag{1}$$

where Υ is simply a double cone $y^2 = |w|^2 \subset \mathcal{M} \ni (y, \Re w, \Im w)$. Such codimension-one varieties correspond to a pairwise real-to-complex transition of two eigenvalues what in Riemann surface terms is equivalent to a square root branching of two of its sheets (two spectral branches). At the same time the two (geometric) eigenvectors coalesce into a single (geometric) eigenvector and an additional associated vector (algebraic eigenvector) appears. Instead of *two* eigenvalues of geometric and algebraic multiplicity one (diagonal block), a *single* eigenvalue of geometric multiplicity one, ($m(\lambda) = 1$), and algebraic multiplicity two ($n(\lambda) = 2$), (2×2-Jordan block) forms [18]. When the parameters on this codimension-one variety are further tuned to $y = \Re w = \Im w = 0$ [18] one arrives at a diabolic point [19, 20], where the *single* eigenvalue gets geometric and algebraic multiplicity two ($m(\lambda) = n(\lambda) = 2$, diagonal 2×2 block). In a (more) general setting such configurations correspond to codimension-three varieties [18, 20].

Apart from these generic real-to-complex transitions on codimension-one varieties, there may occur higher-order intersections of more than two Riemann sheets simultaneously — on varieties Υ of higher codimension, $\text{codim}(\Upsilon) \geq 2$, and with larger Jordan blocks in the spectral decomposition [9, 21, 22].

Below we present explicit examples for third-order intersections in three Krein space related physical models. Firstly, we sketch a few aspects of such intersections semi-analytically (algebraically) for a maximally simplified $\mathcal{PT}$-symmetric 4×4-matrix toy model. Afterwards we show numerically that such intersections also occur in the operator spectra of the spherically symmetric α^2-dynamo of magnetohydrodynamics (MHD) [23, 24] and of the recently analyzed $\mathcal{PT}$-symmetric interpolation model of Ref. [25] (which can be understood as a $\mathcal{PT}$-symmetrically extended, rescaled and Wick-rotated version of the Squire equation of hydrodynamics).

2 Spectral triple points in a pseudo-Hermitian 4 × 4-matrix toy model

Similarly to the two different multiplicity contents (Jordan structures) of two-fold degenerate eigenvalues (see, e.g., also [26]), one has to distinguish the following three types of Jordan structures/geometric multiplicities $m(\lambda)$ corresponding to a spectral triple point:

– type I: $m(\lambda) = 1$, $n(\lambda) = 3$; 3×3-Jordan block; e.g., coalescence of two square-root branch points connected by a purely real spectral segment (see Eq. (12) and Figs. 1–3 below),

– type II: $m(\lambda) = 2$, $n(\lambda) = 3$; one 2×2-Jordan block + one simple eigenvalue; e.g., a square-root branch point accidentally coincides with a simple eigenvalue,

– type III: $m(\lambda) = 3$, $n(\lambda) = 3$; diagonal matrix λI_3; e.g., three accidentally coinciding eigenvalues (generalized diabolic point).

Subsequently we concentrate on the physically most interesting case of type I triple points which correspond to pair-wise coalescing square-root branch points.

As maximally simplified toy model we choose a $\mathcal{PT}$-symmetric (pseudo-Hermitian) 4×4-matrix setup in a diagonal representation of the parity (involution) operator $\mathcal{P}$

$$H = \mathcal{P}H^{\dagger}\mathcal{P} = \begin{pmatrix} H_{++} & H_{+-} \\ H_{-+} & H_{--} \end{pmatrix}, \quad \mathcal{P} = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \tag{2}$$

where the 2×2 blocks satisfy the conditions $H_{\pm\pm} = H^{\dagger}_{\pm\pm}, \quad H_{+-} = -H^{\dagger}_{-+}$. In order to keep the demonstration as simple as possible, it suffices to consider a model based on two real (truncated) elementary pseudo-Hermitian 2×2 matrices

$$H_{1,2} = \begin{pmatrix} x_{1,2} + y_{1,2} & w_{1,2} \\ -w_{1,2} & x_{1,2} - y_{1,2} \end{pmatrix}, \qquad x_{1,2}, y_{1,2}, w_{1,2} \in \mathbb{R}, \tag{3}$$

as subsystems, which we embed $\mathcal{PT}$-symmetrically into the also highly reduced[2)] and real pseudo-Hermitian 4×4-matrix H with block structure (2)

$$H_1, H_2 \hookrightarrow H = \begin{pmatrix} x_1 + y_1 & 0 & w_1 & z \\ 0 & x_2 + y_2 & 0 & w_2 \\ -w_1 & 0 & x_1 - y_1 & 0 \\ -z & -w_2 & 0 & x_2 - y_2 \end{pmatrix}. \tag{4}$$

The interaction between the subsystems H_1 and H_2 is controlled by the coupling parameter z. For vanishing coupling, $z = 0$, the characteristic equation $\varDelta(\lambda) = \det(H - \lambda I_4) = 0$ factors as $\varDelta(\lambda) = \det(H_1 - \lambda I_2)\det(H_2 - \lambda I_2) = 0$ and the four eigenvalues of the matrix H are defined by the eigenvalues of H_1 and H_2:

$$\lambda_{1,\pm} = x_1 \pm \sqrt{y_1^2 - w_1^2}, \quad \lambda_{2,\pm} = x_2 \pm \sqrt{y_2^2 - w_2^2}\,. \tag{5}$$

The corresponding two square-root branch points, $\lambda_1 = x_1,\ \lambda_2 = x_2$, with $\varDelta(\lambda) = 0,\ \ \partial_\lambda \varDelta(\lambda) = 0$ are located on the two (reduced) double cones[3)] (crossed lines) defined by

$$y_1^2 = w_1^2, \qquad y_2^2 = w_2^2. \tag{6}$$

[2)] Nine of the 16 effective free real parameters of the pseudo-Hermitian 4×4 matrix H are set to zero.

[3)] The two diabolic points [19, 20] (with eigenvalues of geometric and algebraic multiplicity two) of the subsystems H_1, H_2 are located at $y_1 = w_1 = 0$ and $y_2 = w_2 = 0$, respectively.

For nonvanishing interaction, $z \neq 0$, the eigenvalues of H are given as roots of the quartic equation

$$\varDelta(\lambda) = \lambda^4 + a_3\lambda^3 + a_2\lambda^2 + a_1\lambda + a_0 = 0 \tag{7}$$

with coefficients[4])

$$\begin{aligned} a_3 &= -2(x_1 + x_2)\,, \\ a_2 &= -(y_1^2 - w_1^2) - (y_2^2 - w_2^2) + (x_1 + x_2)^2 + 2x_1x_2 + z^2\,, \\ a_1 &= 2\left[x_1(y_2^2 - w_2^2 - x_2^2) + x_2(y_1^2 - w_1^2 - x_1^2)\right] - z^2(x_1 - y_1 + x_2 + y_2)\,, \\ a_0 &= (y_1^2 - w_1^2 - x_1^2)(y_2^2 - w_2^2 - x_2^2) + z^2(x_1 - y_1)(x_2 + y_2)\,. \end{aligned} \tag{8}$$

A smooth branch point coalescence can be easily arranged by $\mathcal{PT}$-symmetrically blowing up a triple root

$$\lambda_1 = \lambda_2 = \lambda_3 =: \beta_{(c)} \neq \lambda_{4(c)} \tag{9}$$

("inflection point" configuration $\varDelta(\lambda) = \partial_\lambda \varDelta(\lambda) = \partial_\lambda^2 \varDelta(\lambda) = 0$) of the quartic equation (7). For our illustrative purpose it suffices to derive explicitly a suitable parametrization for an arbitrarily chosen triple root[5]) satisfying the additional branch point conditions (6) for the subsystems. Using these conditions together with (8), (9) in Newton's identities (Vieta's formulas) [28]

$$\begin{aligned} \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 &= -a_3\,, \\ \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_1\lambda_4 + \lambda_2\lambda_3 + \lambda_2\lambda_4 + \lambda_3\lambda_4 &= a_2\,, \\ \lambda_1\lambda_2\lambda_3 + \lambda_2\lambda_3\lambda_4 + \lambda_1\lambda_2\lambda_4 + \lambda_1\lambda_3\lambda_4 &= -a_1\,, \\ \lambda_1\lambda_2\lambda_3\lambda_4 &= a_0 \end{aligned} \tag{10}$$

and setting for convenience $\beta_{(c)} = z_{(c)} = 1, \quad x_{1(c)} = 0$ we easily obtain the remaining root $\lambda_{4(c)}$ and the three parameters $x_{2(c)}, y_{1,2(c)}$ as

$$\begin{aligned} \lambda_{4(c)\epsilon} &= 3 + 2^{3/2}\epsilon > 0, \quad \epsilon := \pm 1\,, \\ x_{2(c)\epsilon} &= \tfrac{1}{2}(\lambda_{4(c)\epsilon} + 3) = 3 + 2^{1/2}\epsilon\,, \\ y_{1(c)\epsilon,\delta} &= \tfrac{1}{2}\left[-(3\lambda_{4(c)\epsilon} + 1) + \delta\sqrt{9\lambda_{4(c)\epsilon}^2 + 2\lambda_{4(c)\epsilon} + 1}\right], \quad \delta := \pm 1\,, \\ y_{2(c)\epsilon,\delta} &= \lambda_{4(c)\epsilon} - 1 + \tfrac{1}{2}\delta\sqrt{9\lambda_{4(c)\epsilon}^2 + 2\lambda_{4(c)\epsilon} + 1}\,. \end{aligned} \tag{11}$$

A computer algebraic test shows that the Jordan normal form of H for this triple root configuration is

$$H_{(c)} = S H_{(c)J} S^{-1}, \qquad H_{(c)J} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \lambda_{4(c)\epsilon} \end{pmatrix}, \tag{12}$$

[4]) The reason for restricting to the maximally simplified (truncated) 4×4-matrix setup (4) was in keeping these coefficients $a_k,\ k = 0, \ldots, 3$, in a form sufficiently simple for quick inspection.

[5]) A detailed discriminant-based [27] case analysis and complete classification of possible intersection scenarios for the four roots $\lambda_k,\ k = 1, \ldots, 4$, will be presented elsewhere.

so that the eigenvalue $\beta_{(c)} = 1$ is indeed a type I triple point with geometric multiplicity one and algebraic multiplicity three. For the 2D illustration of the coalescing branch points in Fig. 1 we have chosen a one-parameter matrix parametrization of the type $H(t) = H_{(c)} + h(t), \quad h(t \to 0) \to 0$ providing the blowing-up of the triple root for $t \neq 0$ with

$$\begin{aligned} x_1 &= x_{1(c)}\,, & x_2 &= x_{2(c)} + t\,, \\ y_1 &= y_{1(c)++} + 2t^2\,, & y_2 &= y_{2(c)++} - t^3\,, \\ w_1 &= y_{1(c)++} - t\,, & w_2 &= y_{2(c)++} + 3t^2\,. \end{aligned} \tag{13}$$

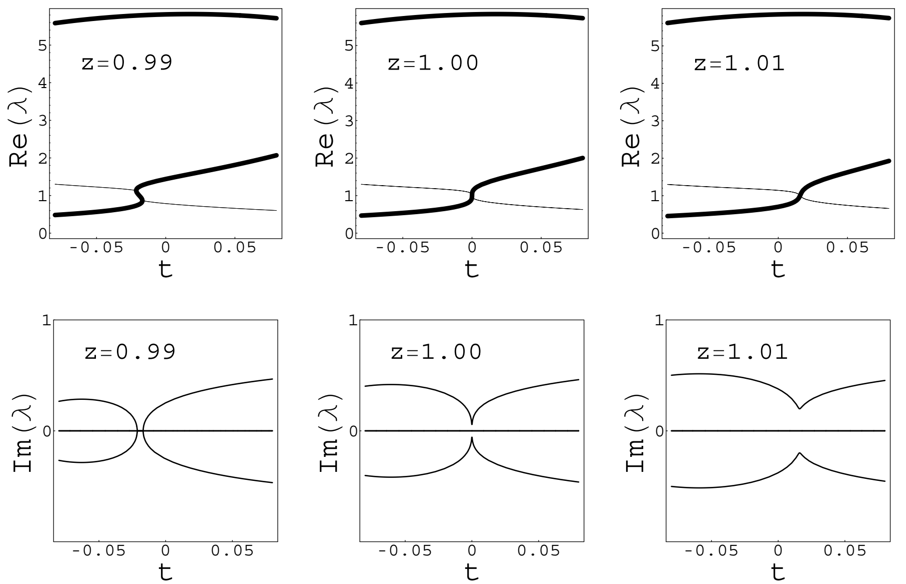

Fig. 1. The four solutions $\lambda_1, \ldots, \lambda_4$ of the quartic equation $\Delta(\lambda) = 0$ (purely real branches highlighted fat) for different subsystem couplings z. For increasing z two of the exceptional points coalesce and disappear [at the inflection point of the inverted purely real branch $t(\Re\lambda_1)$: $\partial^2_{\Re\lambda_1} t(\Re\lambda_1) = 0$]. Simultaneously the originally existing real spectral segment between the exceptional points disappears and the two complex-valued sectors merge into a single one.

A characteristic feature of the present coalescing branch point setup consists in the merging of two originally separated complex spectral sectors (of broken $\mathcal{PT}$-symmetry) into a larger single sector and the simultaneous disappearance of the *real segment* between the two square-root branch points. This is in obvious contrast to coalescing branch point setups in simpler pseudo-Hermitian 2×2 matrix models, where the branch points are connected by *two real or complex branches* which disappear upon branch-point coalescence.

3 Third order spectral transitions of the α^2-dynamo and the extended Squire setup

Based on the information of the previous section, it is easy to identify configurations with coalescing branch points in the spectra of the MHD α^2-dynamo operator and of the operator of the extended Squire setup.

In case of the operator [18, 24, 25] of the spherically symmetric α^2-dynamo [23]

$$\hat{H}_l[\alpha] = \begin{pmatrix} -Q[1] & \alpha \\ Q[\alpha] & -Q[1] \end{pmatrix}, \quad Q[\alpha] := -\left(\partial_r + \frac{1}{r}\right)\alpha(r)\left(\partial_r + \frac{1}{r}\right) + \alpha(r)\frac{l(l+1)}{r^2} \tag{14}$$

with α-profile[6])

$$\begin{aligned} \alpha(r) = C\big[&-(21.465 + 2.467\zeta) + (426.412 + 167.928\zeta)r^2 \\ &- (806.729 + 436.289\zeta)r^3 + (392.276 + 272.991\zeta)r^4\big] \end{aligned} \tag{15}$$

and physical (realistic) boundary conditions [18, 23–25] a triple point transition in the decay-mode sector ($\Re\lambda < 0$) is depicted in Fig. 2. Up to now it is still an open

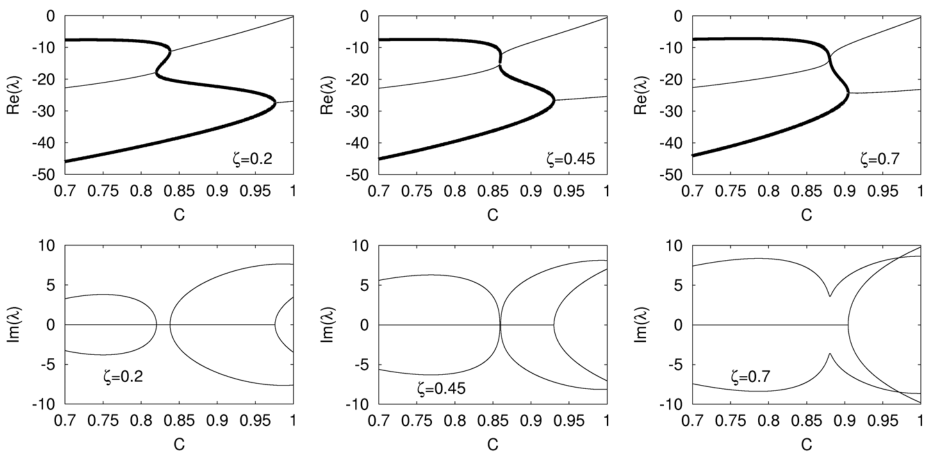

Fig. 2. Coalescing branch points in the spectrum of an α^2-dynamo with α-profile (15) depending on a warp parameter ζ.

question whether such a transition in the sector of growing modes ($\Re\lambda > 0$) has any physical significance, e.g., in dynamo experiments [30, 31].

A different situation occurs in the case of the extended Squire setup of Ref. [25]

$$\left[-\partial_y^2 + g\,y^2(iy)^\nu\right]\psi(y) = E\,\psi(y), \qquad \psi(y = \pm b) = 0\,, \tag{16}$$

[6]) The rather special numerical coefficients in the α-profile are adopted from the recently studied field-reversal scenario for α^2-dynamos [29].

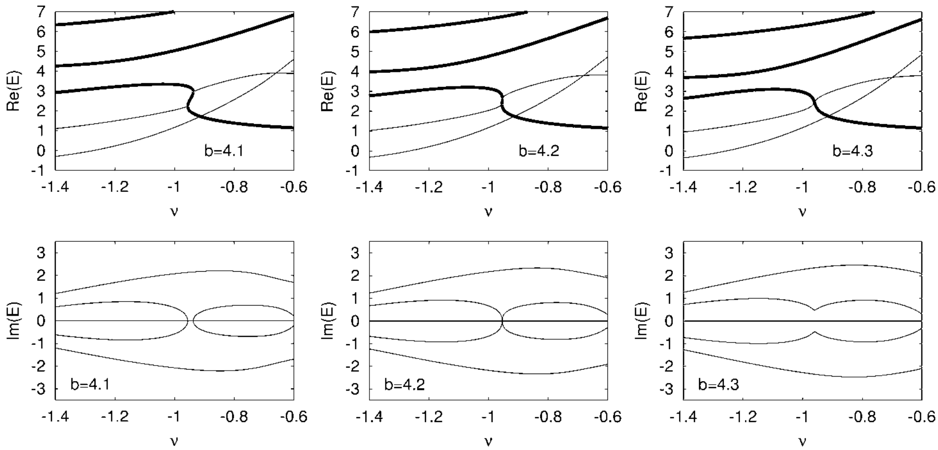

Fig. 3. Coalescing branch points in the spectrum of the extended Squire setup (16) with unit coupling, $g = 1$, in dependence of the cut-off/box length b.

which corresponds to the Bender–Boettcher problem [1] over a finite interval $[-b, b]$. There a coalescence of two square-root branch points occurs close to the real-to-complex transition point in the associated Herbst-box model [25] (Herbst model [32] over a finite interval) located at the low-energy end of a web-like branch structure. An example for the corresponding triple point transition (which supplements the qualitative and graphical analyzes of Ref. [25]) is depicted in Fig. 3.

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