On eigenvalue surfaces near a diabolic point

O. N. Kirillov, A. A. Mailybaev, and A. P. Seyranian

Abstract— **The paper presents a theory of unfolding of eigenvalue surfaces of real symmetric and Hermitian matrices due to an arbitrary complex perturbation near a diabolic point. General asymptotic formulae describing deformations of a conical surface for different kinds of perturbing matrices are derived. As a physical application, singularities of the surfaces of refractive indices in crystal optics are studied.**

I. INTRODUCTION

Since the papers [1] and [2] it is known that the energy surfaces in quantum physics may cross forming two sheets of a double cone: a diabolo. The apex of the cone is called a diabolic point, see [3]. This kind of crossing is typical for systems described by real symmetric Hamiltonians with at least two parameters and Hermitian Hamiltonians depending on three or more parameters. From mathematical point of view the energy surfaces are described by eigenvalues of real symmetric or Hermitian operators dependent on parameters, and the diabolic point is a point of a double eigenvalue with two linearly independent eigenvectors. In modern problems of quantum physics, crystal optics, physical chemistry, acoustics and mechanics it is important to know how the diabolic point bifurcates under arbitrary complex perturbations forming singularities of eigenvalue surfaces like a double coffee filter with two exceptional points or a diabolic circle of exceptional points, see e.g. [4]–[8].

In the present paper following the theory developed in our paper [9] we study effects of complex perturbations in multiparameter families of real symmetric and Hermitian matrices. In case of real symmetric matrices we study unfolding of eigenvalue surfaces near a diabolic point under complex perturbations. Origination of a singularity "double coffee filter" is analytically described. Unfolding of a diabolic point of a Hermitian matrix under an arbitrary complex perturbation is analytically treated. We emphasize that the unfolding of eigenvalue surfaces is described qualitatively as well as quantitatively by using only the information at the diabolic point, including eigenvalues, eigenvectors, and derivatives of the system matrix taken at the diabolic point. As a physical application, singularities of the surfaces of refractive indices in crystal optics are studied.

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II. ASYMPTOTIC EXPRESSIONS FOR EIGENVALUES NEAR A DIABOLIC POINT

Let us consider the eigenvalue problem

$$\mathbf{A}\mathbf{u} = \lambda\mathbf{u} \tag{1}$$

for an $m \times m$ Hermitian matrix $\mathbf{A}$, where λ is an eigenvalue and $\mathbf{u}$ is an eigenvector. Such eigenvalue problems arise in non-dissipative physics with and without time reversal symmetry. Real symmetric and complex Hermitian matrices correspond to these two cases, respectively. We assume that the matrix $\mathbf{A}$ smoothly depends on a vector of n real parameters $\mathbf{p} = (p_1, \dots, p_n)$. Let λ_0 be a double eigenvalue of the matrix $\mathbf{A}_0 = \mathbf{A}(\mathbf{p}_0)$ for some vector $\mathbf{p}_0$. Since $\mathbf{A}_0$ is a Hermitian matrix, the eigenvalue λ_0 is real and possesses two eigenvectors $\mathbf{u}_1$ and $\mathbf{u}_2$. Thus, the point of eigenvalue coupling for Hermitian matrices is diabolic. We choose the eigenvectors satisfying the normalization conditions

$$(\mathbf{u}_1, \mathbf{u}_1) = (\mathbf{u}_2, \mathbf{u}_2) = 1, \quad (\mathbf{u}_1, \mathbf{u}_2) = 0, \tag{2}$$

where the standard inner product of complex vectors is given by $(\mathbf{u}, \mathbf{v}) = \sum_{i=1}^{m} u_i \bar{v}_i$.

Under perturbation of parameters $\mathbf{p} = \mathbf{p}_0 + \Delta\mathbf{p}$, the bifurcation of λ_0 into two simple eigenvalues λ_+ and λ_- occurs. The asymptotic formula for $\lambda_\pm$ under multiparameter perturbation is [9]

$$\lambda_\pm = \lambda_0 + \frac{\langle \mathbf{f}_{11} + \mathbf{f}_{22}, \Delta\mathbf{p}\rangle}{2} \pm$$
$$\pm\sqrt{\frac{\langle \mathbf{f}_{11} - \mathbf{f}_{22}, \Delta\mathbf{p}\rangle^2}{4} + \langle \mathbf{f}_{12}, \Delta\mathbf{p}\rangle\langle \mathbf{f}_{21}, \Delta\mathbf{p}\rangle}. \tag{3}$$

Components of the vector $\mathbf{f}_{ij} = (f_{ij}^1, \dots, f_{ij}^n)$ are

$$f_{ij}^k = \left(\frac{\partial \mathbf{A}}{\partial p_k}\mathbf{u}_i, \mathbf{u}_j\right), \tag{4}$$

where the derivative is taken at $\mathbf{p}_0$, and inner products of vectors in (3) are given by $\langle \mathbf{a}, \mathbf{b}\rangle = \sum_{i=1}^{n} a_i \bar{b}_i$. In expression (3) the higher order terms $o(\|\Delta\mathbf{p}\|)$ and $o(\|\Delta\mathbf{p}\|^2)$ are neglected before and under the square root. Since the matrix $\mathbf{A}$ is Hermitian, the vectors $\mathbf{f}_{11}$ and $\mathbf{f}_{22}$ are real and the vectors $\mathbf{f}_{12} = \bar{\mathbf{f}}_{21}$ are complex conjugate. In case of real symmetric matrices $\mathbf{A} = \mathbf{A}^T$, the vectors $\mathbf{f}_{11}$, $\mathbf{f}_{22}$, and $\mathbf{f}_{12} = \mathbf{f}_{21}$ are real. The asymptotic expression for the eigenvectors corresponding to $\lambda_\pm$ takes the form [9]

$$\mathbf{u}_\pm = \alpha_\pm \mathbf{u}_1 + \beta_\pm \mathbf{u}_2,$$
$$\frac{\alpha_\pm}{\beta_\pm} = \frac{\langle \mathbf{f}_{12}, \Delta\mathbf{p}\rangle}{\lambda_\pm - \lambda_0 - \langle \mathbf{f}_{11}, \Delta\mathbf{p}\rangle} = \frac{\lambda_\pm - \lambda_0 - \langle \mathbf{f}_{22}, \Delta\mathbf{p}\rangle}{\langle \mathbf{f}_{21}, \Delta\mathbf{p}\rangle}. \tag{5}$$

Expressions (5) provide zero order terms for the eigenvectors $\mathbf{u}_\pm$ under perturbation of the parameter vector.

Now, consider an arbitrary complex perturbation of the matrix family $\mathbf{A}(\mathbf{p})+\Delta\mathbf{A}(\mathbf{p})$. Such perturbations appear due to non-conservative effects breaking symmetry of the initial system. We assume that the size of perturbation $\Delta\mathbf{A}(\mathbf{p}) \sim \varepsilon$ is small, where $\varepsilon = \|\Delta\mathbf{A}(\mathbf{p}_0)\|$ is the Frobenius norm of the perturbation at the diabolic point. Behavior of the eigenvalues $\lambda_\pm$ for small $\Delta\mathbf{p}$ and small ε is described by the following asymptotic formula [9]

$$\left(\lambda_\pm - \lambda_0 - \frac{\langle \mathbf{f}_{11}+\mathbf{f}_{22}, \Delta\mathbf{p}\rangle}{2} - \frac{\varepsilon_{11}+\varepsilon_{22}}{2}\right)^2 = \\ = \frac{(\langle \mathbf{f}_{11}-\mathbf{f}_{22}, \Delta\mathbf{p}\rangle + \varepsilon_{11}-\varepsilon_{22})^2}{4} + \\ +(\langle \mathbf{f}_{12}, \Delta\mathbf{p}\rangle + \varepsilon_{12})(\langle \mathbf{f}_{21}, \Delta\mathbf{p}\rangle + \varepsilon_{21}). \quad (6)$$

The quantities ε_{ij} are small complex numbers of order ε given by the expression

$$\varepsilon_{ij} = (\Delta\mathbf{A}(\mathbf{p}_0)\mathbf{u}_i, \mathbf{u}_j)\,. \quad (7)$$

A small variation of the matrix family leads to the following correction of the asymptotic expression for the eigenvectors: $\mathbf{u}_\pm = \alpha^\varepsilon_\pm \mathbf{u}_1 + \beta^\varepsilon_\pm \mathbf{u}_2$, where

$$\frac{\alpha^\varepsilon_\pm}{\beta^\varepsilon_\pm} = \frac{\langle \mathbf{f}_{12}, \Delta\mathbf{p}\rangle + \varepsilon_{12}}{\lambda_\pm - \lambda_0 - \langle \mathbf{f}_{11}, \Delta\mathbf{p}\rangle - \varepsilon_{11}} = \\ = \frac{\lambda_\pm - \lambda_0 - \langle \mathbf{f}_{22}, \Delta\mathbf{p}\rangle - \varepsilon_{22}}{\langle \mathbf{f}_{21}, \Delta\mathbf{p}\rangle + \varepsilon_{21}}. \quad (8)$$

The ratios $\alpha^\varepsilon_+/\beta^\varepsilon_+ = \alpha^\varepsilon_-/\beta^\varepsilon_-$ at the point of coincident eigenvalues $\lambda_+ = \lambda_-$. Hence, the eigenvectors $\mathbf{u}_+ = \mathbf{u}_-$ coincide, and the point of eigenvalue coupling of the perturbed system becomes exceptional.

III. Unfolding of a diabolic singularity for real symmetric matrices

Let us assume that $\mathbf{A}(\mathbf{p})$ is an n-parameter family of real symmetric matrices. Then its eigenvalues λ are real. Let λ_0 be a double eigenvalue of the matrix $\mathbf{A}_0 = \mathbf{A}(\mathbf{p}_0)$ with two real eigenvectors $\mathbf{u}_1$ and $\mathbf{u}_2$. Under perturbation of parameters $\mathbf{p} = \mathbf{p}_0 + \Delta\mathbf{p}$, the eigenvalue λ_0 splits into two simple eigenvalues λ_+ and λ_-. The asymptotic formula for $\lambda_\pm$ under multiparameter perturbation is given by equations (3) and (4), where the vectors $\mathbf{f}_{11}$, $\mathbf{f}_{22}$, and $\mathbf{f}_{12} = \mathbf{f}_{21}$ are real. Then, equation (3) takes the form

$$\left(\lambda_\pm - \lambda_0 - \frac{\langle \mathbf{f}_{11}+\mathbf{f}_{22}, \Delta\mathbf{p}\rangle}{2}\right)^2 - \frac{\langle \mathbf{f}_{11}-\mathbf{f}_{22}, \Delta\mathbf{p}\rangle^2}{4} = \\ = \langle \mathbf{f}_{12}, \Delta\mathbf{p}\rangle^2. \quad (9)$$

Equation (9) describes a surface in the space $(p_1, p_2, \ldots, p_n, \lambda)$, which consists of two sheets $\lambda_+(\mathbf{p})$ and $\lambda_-(\mathbf{p})$. For the two-parameter matrix $\mathbf{A}(p_1, p_2)$ equation (9) defines a double cone with apex at the point $(\mathbf{p}_0, \lambda_0)$ in the space (p_1, p_2, λ). The point $(\mathbf{p}_0, \lambda_0)$ is referred to as a "diabolic point" [3] due to the conical shape of the children's toy "diabolo". The double eigenvalue is a phenomenon of codimension 2 in an n-parameter family of real symmetric matrices [1].

Let us consider a perturbation $\mathbf{A}(\mathbf{p}) + \Delta\mathbf{A}(\mathbf{p})$ of the real symmetric family $\mathbf{A}(\mathbf{p})$ in the vicinity of the diabolic point $\mathbf{p}_0$, where $\Delta\mathbf{A}(\mathbf{p})$ is a complex matrix with the small norm $\varepsilon = \|\Delta\mathbf{A}(\mathbf{p}_0)\|$. Splitting of the double eigenvalue λ_0 due to a change of the vector of parameters $\Delta\mathbf{p}$ and a small complex perturbation $\Delta\mathbf{A}$ is described by equation (6), which acquires the form

$$\lambda_\pm = \lambda'_0 + \mu \pm \sqrt{c}, \quad c = (x+\xi)^2 + (y+\eta)^2 - \zeta^2. \quad (10)$$

In equation (10) the quantities λ'_0, x, and y are real:

$$\lambda'_0 = \lambda_0 + \frac{1}{2}\langle \mathbf{f}_{11}+\mathbf{f}_{22}, \Delta\mathbf{p}\rangle,$$

$$x = \frac{1}{2}\langle \mathbf{f}_{11}-\mathbf{f}_{22}, \Delta\mathbf{p}\rangle, \quad y = \langle \mathbf{f}_{12}, \Delta\mathbf{p}\rangle, \quad (11)$$

while the small coefficients μ, ξ, η, and ζ are complex:

$$\mu = \frac{1}{2}(\varepsilon_{11}+\varepsilon_{22}), \quad \xi = \frac{1}{2}(\varepsilon_{11}-\varepsilon_{22}),$$

$$\eta = \frac{1}{2}(\varepsilon_{12}+\varepsilon_{21}), \quad \zeta = \frac{1}{2}(\varepsilon_{12}-\varepsilon_{21}). \quad (12)$$

From equations (10) and (11) we get the expressions determining the real and imaginary parts of the perturbed eigenvalues

$$\mathrm{Re}\lambda_\pm = \lambda'_0 + \mathrm{Re}\mu \pm \sqrt{\left(\mathrm{Re}c + \sqrt{\mathrm{Re}^2 c + \mathrm{Im}^2 c}\,\right)/2}, \quad (13)$$

$$\mathrm{Im}\lambda_\pm = \mathrm{Im}\mu \pm \sqrt{\left(-\mathrm{Re}c + \sqrt{\mathrm{Re}^2 c + \mathrm{Im}^2 c}\,\right)/2}. \quad (14)$$

Strictly speaking, for the same eigenvalue one should take equal or opposite signs before the square roots in (13), (14) for positive or negative $\mathrm{Im}c$, respectively.

Equations (13) and (14) define surfaces in the spaces $(p_1, p_2, \ldots, p_n, \mathrm{Re}\lambda)$ and $(p_1, p_2, \ldots, p_n, \mathrm{Im}\lambda)$. Two sheets of the surface (13) are connected ($\mathrm{Re}\lambda_+ = \mathrm{Re}\lambda_-$) at the points satisfying the conditions

$$\mathrm{Re}c \le 0, \quad \mathrm{Im}c = 0, \quad \mathrm{Re}\lambda_\pm = \lambda'_0 + \mathrm{Re}\mu, \quad (15)$$

while the sheets $\mathrm{Im}\lambda_+(\mathbf{p})$ and $\mathrm{Im}\lambda_-(\mathbf{p})$ are glued at the set of points satisfying

$$\mathrm{Re}c \ge 0, \quad \mathrm{Im}c = 0, \quad \mathrm{Im}\lambda_\pm = \mathrm{Im}\mu. \quad (16)$$

The eigenvalue remains double under the perturbation of parameters when $c = 0$, which yields two equations $\mathrm{Re}c = 0$ and $\mathrm{Im}c = 0$. Two cases are distinguished according to the sign of the quantity

$$D = \mathrm{Im}^2\xi + \mathrm{Im}^2\eta - \mathrm{Im}^2\zeta. \quad (17)$$

If $D > 0$, then the equations $\mathrm{Re}c = 0$ and $\mathrm{Im}c = 0$ yield two solutions (x_a, y_a) and (x_b, y_b), where

$$x_{a,b} = -\mathrm{Re}\xi + \frac{\mathrm{Im}\xi\mathrm{Re}\zeta\mathrm{Im}\zeta}{\mathrm{Im}^2\xi + \mathrm{Im}^2\eta} \pm$$

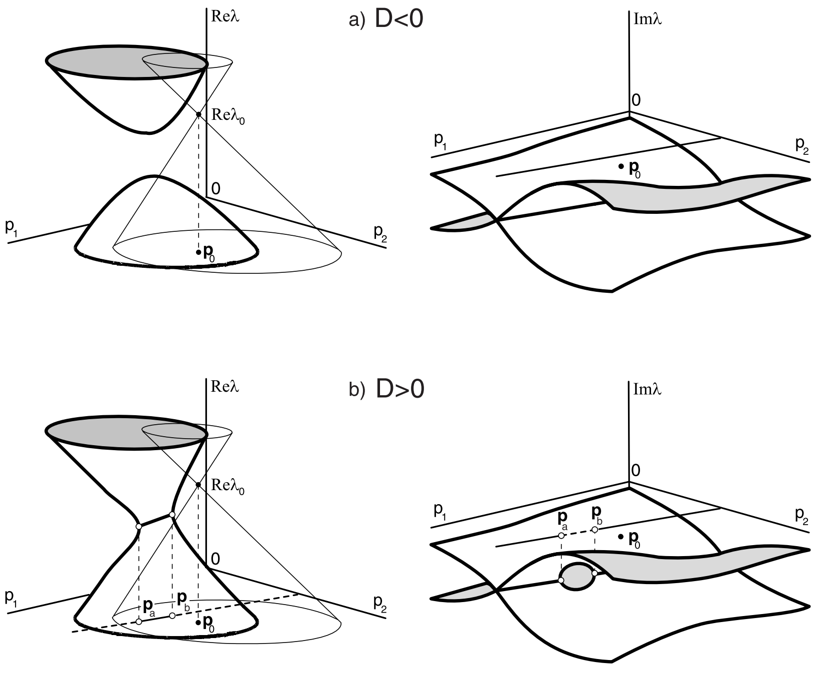

Fig. 1. Unfolding of a diabolic point due to complex perturbation.

$$\pm\frac{\mathrm{Im}\eta\sqrt{(\mathrm{Im}^2\xi{+}\mathrm{Im}^2\eta{+}\mathrm{Re}^2\zeta)(\mathrm{Im}^2\xi{+}\mathrm{Im}^2\eta{-}\mathrm{Im}^2\zeta)}}{\mathrm{Im}^2\xi{+}\mathrm{Im}^2\eta}, \quad (18)$$

$$y_{a,b} = -\mathrm{Re}\eta + \frac{\mathrm{Im}\eta\mathrm{Re}\zeta\mathrm{Im}\zeta}{\mathrm{Im}^2\xi{+}\mathrm{Im}^2\eta}\mp$$

$$\mp\frac{\mathrm{Im}\xi\sqrt{(\mathrm{Im}^2\xi{+}\mathrm{Im}^2\eta{+}\mathrm{Re}^2\zeta)(\mathrm{Im}^2\xi{+}\mathrm{Im}^2\eta{-}\mathrm{Im}^2\zeta)}}{\mathrm{Im}^2\xi{+}\mathrm{Im}^2\eta}. \quad (19)$$

These two solutions determine the points in parameter space, where double eigenvalues appear. When $D = 0$, the two solutions coincide. For $D < 0$, the equations $\mathrm{Re}c = 0$ and $\mathrm{Im}c = 0$ have no real solutions. In the latter case, the eigenvalues λ_+ and λ_- separate for all $\Delta\mathbf{p}$.

Note that the quantities $\mathrm{Im}\xi$ and $\mathrm{Im}\eta$ are expressed by means of the anti-Hermitian part $\Delta\mathbf{A}_N = (\Delta\mathbf{A} - \overline{\Delta\mathbf{A}}^T)/2$ of the matrix $\Delta\mathbf{A}$ as

$$\begin{aligned}\mathrm{Im}\xi &= \frac{(\Delta\mathbf{A}_N(\mathbf{p}_0)\mathbf{u}_1, \mathbf{u}_1) - (\Delta\mathbf{A}_N(\mathbf{p}_0)\mathbf{u}_2, \mathbf{u}_2)}{2i}, \\ \mathrm{Im}\eta &= \frac{(\Delta\mathbf{A}_N(\mathbf{p}_0)\mathbf{u}_1, \mathbf{u}_2) + (\Delta\mathbf{A}_N(\mathbf{p}_0)\mathbf{u}_2, \mathbf{u}_1)}{2i},\end{aligned} \quad (20)$$

while $\mathrm{Im}\zeta$ depends on the Hermitian part $\Delta\mathbf{A}_H = (\Delta\mathbf{A} + \overline{\Delta\mathbf{A}}^T)/2$ as

$$\mathrm{Im}\zeta = \frac{(\Delta\mathbf{A}_H(\mathbf{p}_0)\mathbf{u}_1, \mathbf{u}_2) - (\Delta\mathbf{A}_H(\mathbf{p}_0)\mathbf{u}_2, \mathbf{u}_1)}{2i}. \quad (21)$$

If $D > 0$, one can say that the influence of the anti-Hermitian part of the perturbation $\Delta\mathbf{A}$ is stronger than that of the Hermitian part. If the Hermitian part prevails in the perturbation $\Delta\mathbf{A}$, we have $D < 0$. In particular, $D = -\mathrm{Im}^2\zeta < 0$ for a purely Hermitian perturbation $\Delta\mathbf{A}$.

Let us assume that the vector $\mathbf{p}$ consists of only two components p_1 and p_2, and consider the surfaces (13) and (14) for different kinds of the perturbation $\Delta\mathbf{A}(\mathbf{p})$. Consider first the case $D < 0$. Then, the eigensheets $\mathrm{Re}\lambda_+(\mathbf{p})$ and $\mathrm{Re}\lambda_-(\mathbf{p})$ are separate, see Figure 1a. Equation $\mathrm{Im}c = 0$ defines a line in parameter plane. The sheets $\mathrm{Im}\lambda_+(\mathbf{p})$ and $\mathrm{Im}\lambda_-(\mathbf{p})$ of the eigensurface (14) intersect along the line

$$\mathrm{Im}c/2 = (x{+}\mathrm{Re}\xi)\mathrm{Im}\xi + (y{+}\mathrm{Re}\eta)\mathrm{Im}\eta - \mathrm{Re}\zeta\mathrm{Im}\zeta = 0,$$

$$\mathrm{Im}\lambda_\pm = \mathrm{Im}\mu, \quad (22)$$

given by conditions (16).

In the case $D > 0$ the line $\mathrm{Im}c = 0$ and the ellipse defined by the quation $\mathrm{Re}c = 0$ have common points $\mathbf{p}_a$ and $\mathbf{p}_b$ where the eigenvalues couple. Coordinates of these points can be found from the equations (11), where $x = x_{a,b}$ and $y = y_{a,b}$ are defined by expressions (18) and (19). Here we have assumed that the vectors $\mathbf{f}_{11} - \mathbf{f}_{22}$ and $\mathbf{f}_{12}$ are linearly independent. Note that the points $\mathbf{p}_a$ and $\mathbf{p}_b$ coincide in the degenerate case $D = 0$.

According to conditions (15) the real eigensheets $\mathrm{Re}\lambda_+(\mathbf{p})$ and $\mathrm{Re}\lambda_-(\mathbf{p})$ are glued in the interval $[\mathbf{p}_a, \mathbf{p}_b]$ of the line

$$\mathrm{Im}c/2 = (x{+}\mathrm{Re}\xi)\mathrm{Im}\xi + (y{+}\mathrm{Re}\eta)\mathrm{Im}\eta - \mathrm{Re}\zeta\mathrm{Im}\zeta = 0,$$

$$\mathrm{Re}\lambda_\pm = \lambda_0' + \mathrm{Re}\mu. \quad (23)$$

The surface of real eigenvalues (13) is called a "double coffee filter" [6]. The unfolding of a diabolic point into the double coffee filter is shown in Figure 1b. Note that in crystal optics and acoustics the interval $[\mathbf{p}_a, \mathbf{p}_b]$ is referred to as a "branch cut", and the points $\mathbf{p}_a$, $\mathbf{p}_b$ are called "singular axes", see [5], [7]. According to equation (8) the double eigenvalues at

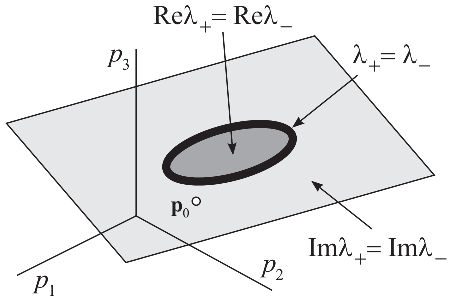

Fig. 2. Unfolding of a diabolic point into an exceptional ring in parameter space.

$\mathbf{p}_a$ and $\mathbf{p}_b$ possess only one eigenvector and, hence, they are exceptional points.

IV. Unfolding of a diabolic singularity for Hermitian matrices

Let us consider a multi-parameter Hermitian matrix $\mathbf{A}(\mathbf{p})$. Assume that $\mathbf{p}_0$ is a diabolic point, where the matrix $\mathbf{A}_0 = \mathbf{A}(\mathbf{p}_0)$ has a double real eigenvalue λ_0 with two eigenvectors. The splitting of λ_0 into a pair of simple real eigenvalues λ_+ and λ_- is described by expressions (3), (4), where the vectors $\mathbf{f}_{11}$ and $\mathbf{f}_{22}$ are real and the vectors $\mathbf{f}_{12} = \overline{\mathbf{f}}_{21}$ are complex conjugate. By using expression (3), we find

$$\lambda_\pm = \lambda_0' \pm \sqrt{x^2 + y^2 + z^2}, \tag{24}$$

where λ_0', x, y, and z are real quantities depending linearly on the perturbation of parameters $\Delta\mathbf{p}$ as follows

$$\lambda_0' = \lambda_0 + \frac{\langle \mathbf{f}_{11} + \mathbf{f}_{22}, \Delta\mathbf{p}\rangle}{2}, \; x = \frac{\langle \mathbf{f}_{11} - \mathbf{f}_{22}, \Delta\mathbf{p}\rangle}{2},$$
$$y = \langle \mathrm{Re}\,\mathbf{f}_{12}, \Delta\mathbf{p}\rangle, \; z = \langle \mathrm{Im}\,\mathbf{f}_{12}, \Delta\mathbf{p}\rangle. \tag{25}$$

The eigenvalues coincide if $x = y = z = 0$. The equations $x = y = z = 0$ with relations (25) provide a plane in parameter space tangent to the set of diabolic points. This plane has dimension $n-3$, which agrees with the well-known fact that the diabolic point is a codimension 3 phenomenon for Hermitian systems [1].

Now let us consider a general non-Hermitian perturbation of the system $\mathbf{A}(\mathbf{p}) + \Delta\mathbf{A}(\mathbf{p})$, assuming that the size of perturbation at the diabolic point $\varepsilon = \|\Delta\mathbf{A}(\mathbf{p}_0)\|$ is small. The two eigenvalues λ_+ and λ_-, which become complex due to non-Hermitian perturbation, are given by asymptotic expressions (6), (7). With the use of the new coordinates (25), we write the expression (6) as

$$\lambda_\pm = \lambda_0' + \mu \pm \sqrt{c}, \tag{26}$$

where

$$c = (x+\xi)^2 + (y+\eta)^2 + (z - i\zeta)^2, \tag{27}$$

and μ, ξ, η, ζ are small complex quantities of order ε given by expressions (12).

The eigenvalues couple ($\lambda_+ = \lambda_-$) if $c = 0$. This yields two equations $\mathrm{Re}c = 0$ and $\mathrm{Im}c = 0$. The first equation defines a sphere in (x, y, z) space with the center at $(-\mathrm{Re}\,\xi, -\mathrm{Re}\,\eta, -\mathrm{Im}\,\zeta)$ and the radius $\sqrt{\mathrm{Im}^2\xi + \mathrm{Im}^2\eta + \mathrm{Re}^2\zeta}$, which are small of order ε. The second equation yields a plane passing through the center of the sphere. The sphere and the plane intersect along a circle. Points of this circle determine values of parameters, for which the eigenvalues $\lambda_\pm$ coincide. Since $c = 0$ at the coupling point, expression (8) for the eigenvectors takes the form

$$\mathbf{u}_\pm = \alpha_\pm^\varepsilon \mathbf{u}_1 + \beta_\pm^\varepsilon \mathbf{u}_2,$$
$$\frac{\alpha_\pm^\varepsilon}{\beta_\pm^\varepsilon} = \frac{y + iz + \eta + \zeta}{-x - \xi} = \frac{x + \xi}{y - iz + \eta - \zeta}. \tag{28}$$

Thus, all points of the circle are exceptional points, where the two eigenvectors $\mathbf{u}_-$ and $\mathbf{u}_+$ merge in addition to the coupling of the eigenvalues λ_+ and λ_-. By using the linear expressions (25), the set of exceptional points is found in the original parameter space $\mathbf{p}$. The exceptional circle in (x, y, z) space is transformed into an exceptional elliptic ring in three-parameter space $\mathbf{p}$, see Figure 2. Let us consider the plane $\mathrm{Im}c = 0$, at which the quantity c is real. By formula (26), the real parts of the eigenvalues $\lambda_\pm$ coincide inside the exceptional ring, where $c < 0$, and the imaginary parts of $\lambda_\pm$ coincide outside the exceptional ring, where $c > 0$, see the dark and light shaded areas in Figure 2.

V. Unfolding of optical singularities of birefringent crystals

Optical properties of a non-magnetic dichroic chiral anisotropic crystal are characterized by the inverse dielectric tensor $\boldsymbol{\eta}$, which relates the vectors of electric field $\mathbf{E}$ and the displacement $\mathbf{D}$ as [10]

$$\mathbf{E} = \boldsymbol{\eta}\mathbf{D}. \tag{29}$$

A monochromatic plane wave of frequency ω that propagates in a direction specified by a real unit vector $\mathbf{s} = (s_1, s_2, s_3)$ has the form

$$\mathbf{D}(\mathbf{r}, t) = \mathbf{D}(\mathbf{s}) \exp i\omega\left(\frac{n(\mathbf{s})}{c}\mathbf{s}^T\mathbf{r} - t\right), \tag{30}$$

where $n(\mathbf{s})$ is a refractive index, and $\mathbf{r}$ is the real vector of spatial coordinates. With the wave (30) and the constitutive relation (29) Maxwell's equations after some elementary manipulations yield

$$\boldsymbol{\eta}\mathbf{D}(\mathbf{s}) - \mathbf{s}\mathbf{s}^T\boldsymbol{\eta}\mathbf{D}(\mathbf{s}) = \frac{1}{n^2(\mathbf{s})}\mathbf{D}(\mathbf{s}). \tag{31}$$

Multiplying equation (31) by the vector $\mathbf{s}^T$ from the left, we find that for plane waves the vector $\mathbf{D}$ is always orthogonal to the direction s, i.e., $\mathbf{s}^T\mathbf{D}(\mathbf{s}) = 0$. By using this condition, we write (31) in the form of the eigenvalue problem

$$\left[(\mathbf{I} - \mathbf{s}\mathbf{s}^T)\boldsymbol{\eta}(\mathbf{I} - \mathbf{s}\mathbf{s}^T)\right]\mathbf{u} = \lambda\mathbf{u}, \tag{32}$$

where $\lambda = n^{-2}$, $\mathbf{u} = \mathbf{D}$, and $\mathbf{I}$ is the identity matrix. Since $\mathbf{I} - \mathbf{s}\mathbf{s}^T$ is a singular matrix, one of the eigenvalues is always zero. Let us denote the other two eigenvalues by λ_+ and λ_-. These eigenvalues determine refractive indices n, and the corresponding eigenvectors yield polarizations.

The inverse dielectric tensor is described by a complex non-Hermitian matrix $\boldsymbol{\eta} = \boldsymbol{\eta}_{transp} + \boldsymbol{\eta}_{dichroic} + \boldsymbol{\eta}_{chiral}$. The symmetric part of $\boldsymbol{\eta}$ consisting of the real matrix $\boldsymbol{\eta}_{transp}$ and imaginary matrix $\boldsymbol{\eta}_{dichroic}$ constitute the anisotropy tensor, which describes the birefringence of the crystal. For a transparent crystal, the anisotropy tensor is real and is represented only by the matrix $\boldsymbol{\eta}_{transp}$; for a crystal with linear dichroism it is complex. Choosing coordinate axes along the principal axes of $\boldsymbol{\eta}_{transp}$, we have

$$\boldsymbol{\eta}_{transp} = \begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_3 \end{pmatrix}. \tag{33}$$

The matrix

$$\boldsymbol{\eta}_{dichroic} = i \begin{pmatrix} \eta_{11}^d & \eta_{12}^d & \eta_{13}^d \\ \eta_{12}^d & \eta_{22}^d & \eta_{23}^d \\ \eta_{13}^d & \eta_{23}^d & \eta_{33}^d \end{pmatrix} \tag{34}$$

describes linear dichroism (absorption). The matrix $\boldsymbol{\eta}_{chiral}$ gives the antisymmetric part of $\boldsymbol{\eta}$ describing chirality (optical activity) of the crystal. It is determined by the optical activity vector $\mathbf{g} = (g_1, g_2, g_3)$ depending linearly on $\mathbf{s}$ as

$$\boldsymbol{\eta}_{chiral} = i \begin{pmatrix} 0 & -g_3 & g_2 \\ g_3 & 0 & -g_1 \\ -g_2 & g_1 & 0 \end{pmatrix},$$

$$\mathbf{g} = \boldsymbol{\gamma}\mathbf{s} = \begin{pmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} \\ \gamma_{12} & \gamma_{22} & \gamma_{23} \\ \gamma_{13} & \gamma_{23} & \gamma_{33} \end{pmatrix} \begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix}, \tag{35}$$

where $\boldsymbol{\gamma}$ is a symmetric optical activity tensor; this tensor has an imaginary part for a material with circular dichroism, see [7] for more details.

First, consider a transparent non-chiral crystal, when $\boldsymbol{\eta}_{dichroic} = 0$ and $\boldsymbol{\gamma} = 0$. Then the matrix

$$\mathbf{A}(\mathbf{p}) = (\mathbf{I} - \mathbf{s}\mathbf{s}^T)\boldsymbol{\eta}_{transp}(\mathbf{I} - \mathbf{s}\mathbf{s}^T) \tag{36}$$

is real symmetric and depends on a vector of two parameters $\mathbf{p} = (s_1, s_2)$. The third component of the direction vector $\mathbf{s}$ is found as $s_3 = \pm\sqrt{1 - s_1^2 - s_2^2}$, where the cases of two different signs should be considered separately. Below we assume that three dielectric constants $\eta_1 > \eta_2 > \eta_3$ are different. This corresponds to biaxial anisotropic crystals.

The nonzero eigenvalues $\lambda_\pm$ of the matrix $\mathbf{A}(\mathbf{p})$ are found explicitly in the form [11]

$$\lambda_\pm = \frac{\operatorname{trace}\mathbf{A}}{2} \pm \frac{1}{2}\sqrt{2\operatorname{trace}(\mathbf{A}^2) - (\operatorname{trace}\mathbf{A})^2}. \tag{37}$$

The eigenvalues $\lambda_\pm$ are the same for opposite directions $\mathbf{s}$ and $-\mathbf{s}$. By using (33) and (36) in (37), it is straightforward to show that two eigenvalues λ_+ and λ_- couple at

$$\mathbf{s}_0 = (S_1, 0, S_3), \ \lambda_0 = \eta_2;$$

$$S_1 = \pm\sqrt{(\eta_1 - \eta_2)/(\eta_1 - \eta_3)}, \ S_3 = \pm\sqrt{1 - S_1^2}, \tag{38}$$

which determine four diabolic points (for two signs of S_1 and S_3), also called optic axes [7]. The double eigenvalue $\lambda_0 = \eta_2$ of the matrix $\mathbf{A}_0 = \mathbf{A}(\mathbf{p}_0)$, $\mathbf{p}_0 = (S_1, 0)$ possesses two eigenvectors

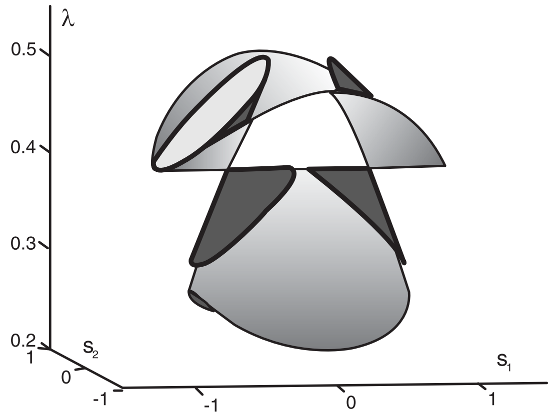

Fig. 3. Diabolic singularities near optic axes and their local approximations.

$$\mathbf{u}_1 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{u}_2 = \begin{pmatrix} S_3 \\ 0 \\ -S_1 \end{pmatrix}, \tag{39}$$

satisfying normalization conditions (2). Using expressions (36) and (39), we evaluate the vectors $\mathbf{f}_{ij}$ with components (4) for optic axes. Substituting them in (9), we obtain the local asymptotic expression for the cone singularities in the space (s_1, s_2, λ) as

$$(\lambda - \eta_2 - (\eta_3 - \eta_1)S_1(s_1 - S_1))^2 =$$
$$= (\eta_3 - \eta_1)^2 S_1^2((s_1 - S_1)^2 + S_3^2 s_2^2). \tag{40}$$

Equation (40) is valid for each of the four optic axes (38).

Now let us assume that the crystal possesses absorption and chirality. Then the matrix family (36) takes a complex perturbation $\mathbf{A}(\mathbf{p}) + \Delta\mathbf{A}(\mathbf{p})$, where

$$\Delta\mathbf{A}(\mathbf{p}) = (\mathbf{I} - \mathbf{s}\mathbf{s}^T)(\boldsymbol{\eta}_{dichroic} + \boldsymbol{\eta}_{chiral})(\mathbf{I} - \mathbf{s}\mathbf{s}^T). \tag{41}$$

Assume that the absorption and chirality are weak, i.e., $\varepsilon = \|\boldsymbol{\eta}_{dichroic}\| + \|\boldsymbol{\eta}_{chiral}\|$ is small. Then we can use asymptotic formulae of Sections 2 and 3 to describe unfolding of diabolic singularities of the eigenvalue surfaces. For this purpose, we need to know only the value of the perturbation $\Delta\mathbf{A}$ at the optic axes of the transparent non-chiral crystal $\mathbf{s}_0$.

Substituting matrix (41) evaluated at optic axes (38) into expression (7), and then using formulae (12), we obtain

$$\begin{aligned} \mu &= i(\eta_{22}^d + \eta_{11}^d S_3^2 - 2\eta_{13}^d S_1 S_3 + \eta_{33}^d S_1^2)/2, \\ \xi &= i(\eta_{22}^d - \eta_{11}^d S_3^2 + 2\eta_{13}^d S_1 S_3 - \eta_{33}^d S_1^2)/2, \\ \eta &= i(\eta_{12}^d S_3 - \eta_{23}^d S_1), \\ \zeta &= -i\left(\gamma_{11} S_1^2 + 2\gamma_{13} S_1 S_3 + \gamma_{33} S_3^2\right). \end{aligned} \tag{42}$$

We see that μ, ξ, and η are purely imaginary numbers depending only on dichroic properties of the crystal (absorption). The quantity ζ depends only on chiral properties of the

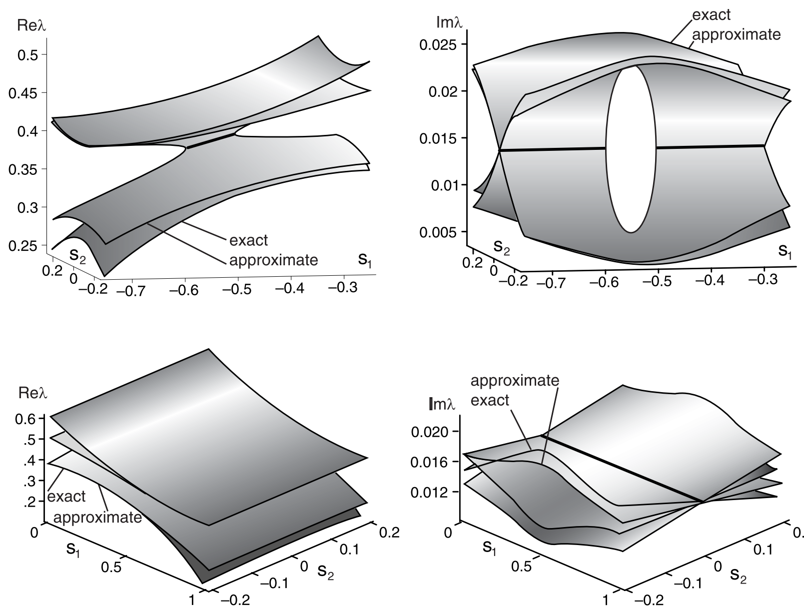

Fig. 4. Unfolding of singularities near optic axes.

crystal; ζ is purely imaginary if the optical activity tensor $\boldsymbol{\gamma}$ is real.

Singularities for crystals with weak dichroism and chirality were studied recently in [7]. It was shown that the double coffee filter singularity arises in absorption-dominated crystals, and the sheets of real parts of eigenvalues are separated in chirality-dominated crystals. According to the results of Section 3, these two cases are explicitly determined by the conditions $D > 0$ and $D < 0$, respectively, where $D = \mathrm{Im}^2\xi + \mathrm{Im}^2\eta - \mathrm{Im}^2\zeta$.

As a numerical example, let us consider a crystal possessing weak absorption and chirality described by the tensors (34), (35) with

$$\boldsymbol{\eta}_{dichroic} = \frac{i}{200}\begin{pmatrix} 3 & 2 & 0 \\ 2 & 3 & 1 \\ 0 & 1 & 3 \end{pmatrix},$$

$$\boldsymbol{\gamma} = \frac{1}{200}\begin{pmatrix} 3 & 1 & 2 \\ 1 & 3 & 1 \\ 2 & 1 & 3 \end{pmatrix}. \tag{43}$$

A corresponding transparent non-chiral crystal is characterized by $\eta_1 = 0.5$, $\eta_2 = 0.4$, $\eta_3 = 0.1$, and its eigenvalue surfaces with two optic axes are presented in Figure 3 together with the conical surfaces (40). The two optic axes shown in Figure 3 are $\mathbf{s}_0 = (\pm 1/2,\, 0,\, \sqrt{3}/2)$ with the double eigenvalue $\lambda_0 = 2/5$.

By using (43) in (42), we find that the condition $D = \frac{7}{160000}(4\sqrt{3} - 5) > 0$ is satisfied for the left optic axis $\mathbf{s}_0 = (-1/2,\, 0,\, \sqrt{3}/2)$. Hence, the diabolic singularity bifurcates into a double coffee filter with two exceptional points. Local approximations of the eigenvalue surfaces are given by expressions (13), (14). Figure 4 shows these local approximations compared with the exact eigenvalue surfaces given by (37). For the right optic axis $\mathbf{s}_0 = (1/2,\, 0,\, \sqrt{3}/2)$, the condition $D = -\frac{7}{160000}(4\sqrt{3} + 5) < 0$ is satisfied. Hence, the eigenvalue sheets (for real parts) separate under the bifurcation of the right diabolic singularity. Approximate and exact eigenvalue surfaces are shown in Figure 4. We observe that the unfolding types are different for different optic axes. As it is seen from Figure 4, the asymptotic formulae provide an accurate description for unfolding of eigenvalue surfaces near diabolic points.

VI. Conclusion

Non-Hermitian Hamiltonians and matrices usually appear in physics when dissipative and other non-conservative effects are taken into account. As it is stated in [8], Hermitian physics differs radically from non-Hermitian physics in case of coalescence (coupling) of eigenvalues. In the present paper we gave analytical description for unfolding of eigenvalue surfaces due to an arbitrary complex perturbation with the singularities known in the literature as a "double coffee-filter" and a "diabolic circle". The developed theory requires only eigenvectors and derivatives of the matrices taken at the singular point, while the size of the matrix and its dependence on parameters are arbitrary. The given physical example from crystal optics demonstrates applicability and accuracy of the theory.

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