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THEORETICAL PHYSICS

Singularities of Energy Surfaces under Non-Hermitian Perturbations

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In [1, 2], it was found that the energy surfaces of quantum systems can cross, forming a conic singularity, which is often called a diabolo and the apex of the cone is called the diabolic point [3]. The energy surfaces are mathematically described by the eigenvalues of real symmetric and Hermitian operators (Hamiltonians) depending on two or more parameters, and the diabolic point is characterized by a double eigenvalue corresponding to two linearly independent eigenvectors. In crystal optics, optical axes characterized by a coincidence of the refractive indices are analogs of diabolic points [4, 5]. In current problems of quantum physics, physical chemistry, crystal optics, and acoustics, it is important to know how the conic singularity of the energy surface is deformed under arbitrary complex perturbation, which describes dissipative and other nonconservative effects, with the formation of singularities corresponding to Jordan blocks [6–9].

In this work, we study singularities of the energy surfaces formed by the eigenvalues of the real symmetric and Hermitian matrices depending on parameters under arbitrary complex perturbation. Using the theory of eigenvalue bifurcations, which was developed in [10], we derive general asymptotic formulas describing the deformation of the energy surface near the conic singularity for various complex perturbations. The deformation of the eigenvalue surfaces appears to be described by the eigenvalues, eigenvectors, and derivatives of the Hamiltonian with respect to the parameters at the diabolic point. As an application, the singularities of the refractive-index surfaces in crystal optics are studied. Explicit expressions are obtained for these surfaces as functions of the properties of a crystal. Singular axes are found for crystals with weak absorption and optical activity. In terms of the components of the inverse dielectric tensor, we obtain a new condition that distinguishes crystals with prevailing absorption and with prevailing optical activity.

1. We 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 appear in reversible and irreversible physical systems without dissipation. These two cases correspond to real symmetric matrices and complex Hermitian matrices [9]. In quantum mechanics, $\mathbf{A}$, λ, and $\mathbf{u}$ correspond to the Hamiltonian, energy level, and vector of state, respectively. The matrix $\mathbf{A}$ is assumed to be a smooth function of the vector $\mathbf{p} = (p_1, p_2, \ldots, p_n)$ of n real parameters.

Let λ_0 be a double eigenvalue of the matrix $\mathbf{A}_0 = \mathbf{A}(\mathbf{p}_0)$ for a certain vector $\mathbf{p}_0$. Since $\mathbf{A}_0$ is a Hermitian matrix, the eigenvalue λ_0 is real and corresponds to two linearly independent eigenvectors $\mathbf{u}_1$ and $\mathbf{u}_2$. Thus, the point of interaction between two eigenvalues is diabolic. Let us take the normalized eigenvectors; i.e.,

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

where $(\mathbf{u}, \mathbf{v}) = \sum_{i=1}^{m} u_i \bar{v}_i$ is the scalar product of the vectors in C^m.

Under the perturbation of the parameters $\mathbf{p} = \mathbf{p}_0 + \Delta\mathbf{p}$, the double eigenvalue λ_0 is split into two single eigenvalues λ_+ and λ_-, which are determined by the asymptotic formula [10]

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

The components of the vector $\mathbf{f}_{ij} = (f_{ij}^1, f_{ij}^2, \ldots, f_{ij}^n)$ are given by the formula

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

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where the derivatives are calculated at the point $\mathbf{p}_0$ and $\langle \mathbf{a}, \mathbf{b} \rangle = \sum_{i=1}^{n} a_i \bar{b}_i$ is the scalar product of vectors in C^n. In Eq. (3), the terms $o(\|\Delta\mathbf{p}\|)$ and $o(\|\Delta\mathbf{p}\|^2)$ are omitted outside and inside the radicand, respectively. Since $\mathbf{A}$ is a Hermitian matrix, the eigenvalues $\mathbf{f}_{11}$ and $\mathbf{f}_{22}$ are real and vectors $\mathbf{f}_{12} = \bar{\mathbf{f}}_{21}$ are complex conjugate. The asymptotic expressions of the zeroth approximation for the eigenvectors $\mathbf{u}_\pm$ corresponding to the eigenvalues $\lambda_\pm$ have the form [10]

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

Let us consider an arbitrary complex perturbation of the family of matrices $\mathbf{A}(\mathbf{p}) + \Delta\mathbf{A}(\mathbf{p})$. Such perturbations appear due to nonconservative effects (such as dissipation), which violate the Hermiticity of the unperturbed problem [9]. Let us assume that the perturbation $\Delta\mathbf{A}(\mathbf{p}) \sim \varepsilon$ is small, where $\varepsilon = \|\Delta\mathbf{A}(\mathbf{p}_0)\|$ is the perturbation norm calculated at the diabolic point. The behavior of the eigenvalues $\lambda_\pm$ for small $\Delta\mathbf{p}$ and ε values is described by the asymptotic expressions [10]

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

where

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

are small complex numbers on the order of ε. The small variation of the family of matrices provides a correction to the asymptotic expression for the eigenvectors $\mathbf{u}_\pm = \alpha_\pm^\varepsilon \mathbf{u}_1 + \beta_\pm^\varepsilon \mathbf{u}_2$, where

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

We emphasize that $\alpha_+^\varepsilon/\beta_+^\varepsilon = \alpha_-^\varepsilon/\beta_-^\varepsilon$ at the point of the coincidence of the eigenvalues $\lambda_+ = \lambda_-$. Thus, at this point, the eigenvectors coincide, $\mathbf{u}_+ = \mathbf{u}_-$, and a Jordan block arises.

2. Let $\mathbf{A}(\mathbf{p})$ be the n-parametric family of real symmetric matrices. In this case, the vectors $\mathbf{f}_{11}$, $\mathbf{f}_{22}$, and $\mathbf{f}_{12} = \mathbf{f}_{21}$ are real and Eq. (3) assumes the form

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

This equation describes the surface consisting of two sheets $\lambda_+(\mathbf{p})$ and $\lambda_-(\mathbf{p})$ in the $(p_1, p_2, \ldots, p_n, \lambda)$ space. For the two-parametric matrix $\mathbf{A}(p_1, p_2)$, Eq. (9) determines a cone with a vertex at the point $(\mathbf{p}_0, \lambda_0)$ in the (p_1, p_2, λ) space [1, 2].

We consider the perturbation $\mathbf{A}(\mathbf{p}) + \Delta\mathbf{A}(\mathbf{p})$ of the real symmetric family $\mathbf{A}(\mathbf{p})$ near the diabolic point $\mathbf{p}_0$, where $\Delta\mathbf{A}(\mathbf{p})$ is a complex matrix with the small norm $\varepsilon = \|\Delta\mathbf{A}(\mathbf{p}_0)\|$. The splitting of the double eigenvalue λ_0 in the presence of the parameter change $\Delta\mathbf{p}$ and small complex perturbation $\Delta\mathbf{A}$ is described by Eq. (6), which assumes the form

$$\lambda_\pm = \lambda_0' + \mu \pm \sqrt{c}, \quad c = (x+\xi)^2 + (y+\eta)^2 - \zeta^2, \quad (10)$$

where

$$\lambda_0' = \lambda_0 + \frac{1}{2}\langle \mathbf{f}_{11} + \mathbf{f}_{22}, \Delta\mathbf{p} \rangle, \quad x = \frac{1}{2}\langle \mathbf{f}_{11} - \mathbf{f}_{22}, \Delta\mathbf{p} \rangle,$$
$$y = \langle \mathbf{f}_{12}, \Delta\mathbf{p} \rangle \quad (11)$$

are real and

$$\mu = \frac{1}{2}(\varepsilon_{11} + \varepsilon_{22}), \quad \xi = \frac{1}{2}(\varepsilon_{11} - \varepsilon_{22}),$$
$$\eta = \frac{1}{2}(\varepsilon_{12} + \varepsilon_{21}), \quad \zeta = \frac{1}{2}(\varepsilon_{12} - \varepsilon_{21}) \quad (12)$$

are small complex coefficients.

From Eqs. (10) and (11), we obtain the following expressions for the real and imaginary parts of the perturbed eigenvalues

$$\mathrm{Re}\lambda_\pm = \lambda_0' + \mathrm{Re}\mu \pm \sqrt{\frac{1}{2}\left(\mathrm{Re}c + \sqrt{\mathrm{Re}^2 c + \mathrm{Im}^2 c}\right)}, \quad (13)$$

$$\mathrm{Im}\lambda_\pm = \mathrm{Im}\mu \pm \sqrt{\frac{1}{2}\left(-\mathrm{Re}c + \sqrt{\mathrm{Re}^2 c + \mathrm{Im}^2 c}\right)}. \quad (14)$$

Equations (13) and (14) determine surfaces in the $(p_1, p_2, \ldots, p_n, \mathrm{Re}\lambda)$ and $(p_1, p_2, \ldots, p_n, \mathrm{Im}\lambda)$ spaces, respectively. Two sheets of the surface given by

Eq. (13) are joined ($\mathrm{Re}\lambda_+ = \mathrm{Re}\lambda_-$) at the points satisfying the conditions

$$\mathrm{Re}c \le 0, \quad \mathrm{Im}c = 0, \quad \mathrm{Re}\lambda_\pm = \lambda_0' + \mathrm{Re}\mu, \tag{15}$$

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

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

When the parameters are perturbed, the eigenvalues continue to be double under the condition $c = 0$, which provides the two equations $\mathrm{Re}c = 0$ and $\mathrm{Im}c = 0$. Depending on the sign of the quantity

$$D = \mathrm{Im}^2\zeta + \mathrm{Im}^2\eta - \mathrm{Im}^2\zeta, \tag{17}$$

two cases can be realized. For $D > 0$, the equations $\mathrm{Re}c = 0$ and $\mathrm{Im}c = 0$ have the two solutions (x_a, y_a) and (x_b, y_b), where

$$x_{a,b} = -\mathrm{Re}\xi + \frac{\mathrm{Im}\xi\mathrm{Re}\zeta\mathrm{Im}\zeta}{\mathrm{Im}^2\xi + \mathrm{Im}^2\eta} \pm \frac{\mathrm{Im}\eta\sqrt{(\mathrm{Im}^2\xi + \mathrm{Im}^2\eta + \mathrm{Re}^2\zeta)D}}{\mathrm{Im}^2\xi + \mathrm{Im}^2\eta}, \tag{18}$$

$$y_{a,b} = -\mathrm{Re}\eta + \frac{\mathrm{Im}\eta\mathrm{Re}\zeta\mathrm{Im}\zeta}{\mathrm{Im}^2\xi + \mathrm{Im}^2\eta} \mp \frac{\mathrm{Im}\xi\sqrt{(\mathrm{Im}^2\xi + \mathrm{Im}^2\eta + \mathrm{Re}^2\zeta)D}}{\mathrm{Im}^2\xi + \mathrm{Im}^2\eta}. \tag{19}$$

These solutions determine the points in the parameter space at which double eigenvalues appear. For $D = 0$, the solutions coincide. For $D < 0$, the equations $\mathrm{Re}c = 0$ and $\mathrm{Im}c = 0$ have no real solutions. In this case, the eigenvalues λ_+ and λ_- are different for all $\Delta\mathbf{p}$ values.

We note that $\mathrm{Im}\xi$ and $\mathrm{Im}\eta$ are expressed in terms of the anti-Hermitian component $\Delta\mathbf{A}_N = \frac{1}{2}(\Delta\mathbf{A} - \overline{\Delta\mathbf{A}}^T)$ of the matrix $\Delta\mathbf{A}$ as

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

whereas $\mathrm{Im}\zeta$ is expressed in terms of the Hermitian component $\Delta\mathbf{A}_H = \frac{1}{2}(\Delta\mathbf{A} + \overline{\Delta\mathbf{A}}^T)$ as

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

For $D > 0$, the effect of the anti-Hermitian part of perturbation $\Delta\mathbf{A}$ is stronger than that of the Hermitian part. If the Hermitian part prevails in perturbation $\Delta\mathbf{A}$, then $D < 0$. In particular, $D = -\mathrm{Im}^2\zeta < 0$ for pure Hermitian perturbation $\Delta\mathbf{A}$.

Let us assume that the vector $\mathbf{p}$ has only two components p_1 and p_2 and consider the surfaces given by Eqs. (13) and (14) for various perturbations $\Delta\mathbf{A}(\mathbf{p})$. First, we consider the case $D < 0$. Then, the eigenvalue surfaces $\mathrm{Re}\lambda_+(\mathbf{p})$ and $\mathrm{Re}\lambda_-(\mathbf{p})$ do not cross (Fig. 1a). The equation $\mathrm{Im}c = 0$ determines a straight line in the parameter plane. According to conditions (16), the sheets $\mathrm{Im}\lambda_+(\mathbf{p})$ and $\mathrm{Im}\lambda_-(\mathbf{p})$ of eigenvalue surfaces (14) cross along the straight line

$$\frac{1}{2}\mathrm{Im}c = (x + \mathrm{Re}\xi)\mathrm{Im}\xi + (y + \mathrm{Re}\eta)\mathrm{Im}\eta - \mathrm{Re}\zeta\mathrm{Im}\zeta = 0, \quad \mathrm{Im}\lambda_\pm = \mathrm{Im}\mu. \tag{22}$$

For $D > 0$, the straight line $\mathrm{Im}c = 0$ contains the points $\mathbf{p}_a$ and $\mathbf{p}_b$, where the eigenvectors coincide. The coordinates of these points are determined from Eqs. (11), where $x = x_{a,b}$ and $y = y_{a,b}$ are given in Eqs. (18) and (19). According to Eqs. (15), the sheets of the real parts $\mathrm{Re}\lambda_+(\mathbf{p})$ and $\mathrm{Re}\lambda_-(\mathbf{p})$ of the eigenvalues are joined along the segment $[\mathbf{p}_a, \mathbf{p}_b]$ of the line

$$\frac{1}{2}\mathrm{Im}c = (x + \mathrm{Re}\xi)\mathrm{Im}\xi + (y + \mathrm{Re}\eta)\mathrm{Im}\eta - \mathrm{Re}\zeta\mathrm{Im}\zeta = 0, \quad \mathrm{Re}\lambda_\pm = \lambda_0' + \mathrm{Re}\mu. \tag{23}$$

The singularity of the surface of the real parts of the eigenvalues described by Eq. (13) for $D > 0$ is called a “coffee filter” [8]. The deformation of the conic singularity to the coffee filter is shown in Fig. 1b. In the optics and acoustics of crystals, the segment $[\mathbf{p}_a, \mathbf{p}_b]$ is called the branch cut, and the points $\mathbf{p}_a$ and $\mathbf{p}_b$ determine “singular axes,” because, according to Eq. (8), each double eigenvalue at these points corresponds to only one eigenvector [4, 5, 7].

3. The optical properties of a nonmagnetic crystal are characterized by the inverse dielectric tensor $\boldsymbol{\eta}$, which relates the electric field strength $\mathbf{E}$ and electric displacement $\mathbf{D}$ [4]

$$\mathbf{E} = \boldsymbol{\eta}\mathbf{D}. \tag{24}$$

For a monochromatic plane wave propagating with frequency ω in the direction $\mathbf{s} = (s_1, s_2, s_3)$, $\|\mathbf{s}\| = 1$, we have

$$\mathbf{D}(\mathbf{r}, t) = \mathbf{D}(\mathbf{s})\exp i\omega\left(\frac{n(\mathbf{s})}{c}\mathbf{s}^T\mathbf{r} - t\right), \tag{25}$$

where $n(\mathbf{s})$ is the refractive index, and $\mathbf{r}$ is the real vector of the spatial coordinates. In view of Eq. (25) for the wave and Eq. (24), Maxwell equations are transformed to the form

$$\boldsymbol{\eta}\mathbf{D}(\mathbf{s}) - \mathbf{s}\mathbf{s}^T\boldsymbol{\eta}\mathbf{D}(\mathbf{s}) = \frac{1}{n^2(\mathbf{s})}\mathbf{D}(\mathbf{s}). \tag{26}$$

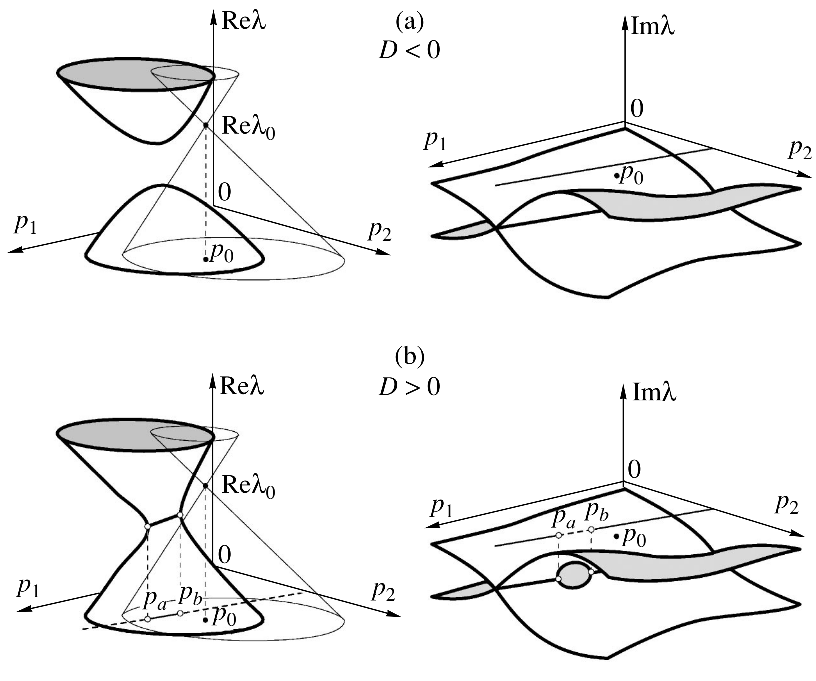

Fig. 1. Unfolding of a conic singularity under complex perturbation.

Multiplying Eq. (26) by the vector $\mathbf{s}^T$ from the left, we find that the vector $\mathbf{D}$ for a plane wave is always orthogonal to the direction vector $\mathbf{s}$; i.e., $\mathbf{s}^T\mathbf{D}(\mathbf{s}) = 0$. Using this condition, we represent Eq. (26) in the form of the eigenvalue problem

$$[(\mathbf{I} - \mathbf{s}\mathbf{s}^T)\boldsymbol{\eta}(\mathbf{I} - \mathbf{s}\mathbf{s}^T)]\mathbf{u} = \lambda\mathbf{u}, \qquad (27)$$

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 eigenvalue is always equal to zero. We denote the other two eigenvalues as λ_+ and λ_-. These eigenvalues determine the refractive index n, and the corresponding eigenvectors determine the polarization [4].

The inverse dielectric tensor is described by the complex non-Hermitian matrix $\boldsymbol{\eta} = \boldsymbol{\eta}_{\text{transp}} + \boldsymbol{\eta}_{\text{dichroic}} + \boldsymbol{\eta}_{\text{chiral}}$. The symmetric part of the matrix $\boldsymbol{\eta}$ consists of the real matrix $\boldsymbol{\eta}_{\text{transp}}$ and imaginary matrix $\boldsymbol{\eta}_{\text{dichroic}}$ and forms the anisotropy tensor describing the birefringence of the crystal. For a transparent crystal, the anisotropy tensor is real and consists only of the matrix $\boldsymbol{\eta}_{\text{transp}}$. For a crystal with linear dichroism, this tensor is represented by a complex matrix. Choosing the coordinate axes along the principal axes of the matrix $\boldsymbol{\eta}_{\text{transp}}$, we obtain $\boldsymbol{\eta}_{\text{transp}} = \text{diag}(\eta_1, \eta_2, \eta_3)$. The matrix

$$\boldsymbol{\eta}_{\text{dichroic}} = i\begin{pmatrix} \eta_{11}^d & \eta_{12}^d & \eta_{13}^d \\ \eta_{12}^d & \eta_{22}^d & \eta_{23}^d \\ \eta_{13}^d & \eta_{23}^d & \eta_{33}^d \end{pmatrix} \qquad (28)$$

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

$$\boldsymbol{\eta}_{\text{chiral}} = i\begin{pmatrix} 0 & -g_3 & g_2 \\ g_3 & 0 & -g_1 \\ -g_2 & g_1 & 0 \end{pmatrix},$$
$$\mathbf{g} = \boldsymbol{\gamma}\mathbf{s} = \begin{pmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} \\ \gamma_{12} & \gamma_{22} & \gamma_{23} \\ \gamma_{13} & \gamma_{23} & \gamma_{33} \end{pmatrix}\begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix}, \qquad (29)$$

where $\boldsymbol{\gamma}$ is the symmetric optical-activity tensor [4, 5].

First, we consider a transparent crystal for which $\boldsymbol{\eta}_{\text{dichroic}} = \boldsymbol{\gamma} = 0$. In this case, the matrix

$$\mathbf{A}(\mathbf{p}) = (\mathbf{I} - \mathbf{s}\mathbf{s}^T)\boldsymbol{\eta}_{\text{transp}}(\mathbf{I} - \mathbf{s}\mathbf{s}^T) \qquad (30)$$

is real and symmetric and depends on the two-component vector $\mathbf{p} = (s_1, s_2)$. The third component of the vector $\mathbf{s}$ is represented as $s_3 = \pm\sqrt{1 - s_1^2 - s_2^2}$, where the cases of two different signs should be analyzed separately. In what follows, we assume that $\eta_1 > \eta_2 > \eta_3$, which corresponds to a biaxial crystal.

Nonzero eigenvalues $\lambda_\pm$ of the matrix $\mathbf{A}(\mathbf{p})$ are found in an explicit form and are identical for opposite directions $\mathbf{s}$ and $-\mathbf{s}$. The eigenvalues λ_+ and λ_- coincide at the points

$$\mathbf{s}_0 = (S_1, 0, S_3)^T, \quad \lambda_0 = \eta_2;$$
$$S_1 = \pm\sqrt{\frac{\eta_1-\eta_2}{\eta_1-\eta_3}}, \quad S_3 = \pm\sqrt{1-S_1^2}, \tag{31}$$

which determine four diabolic points (for two signs of S_1 and S_3), the latter also being called optical axes [4, 5]. A double eigenvalue $\lambda_0 = \eta_2$ of the matrix $\mathbf{A}_0 = \mathbf{A}(\mathbf{p}_0)$, where $\mathbf{p}_0 = (S_1, 0)$, corresponds to two eigenvectors

$$\mathbf{u}_1 = (0, 1, 0)^T, \quad \mathbf{u}_2 = (S_3, 0, -S_1)^T, \tag{32}$$

which satisfy normalization conditions (2). Using Eqs. (30) and (32), we find the vectors $\mathbf{f}_{ij}$ with components (4) for the optical axes. Substituting them into Eq. (9), we obtain the following local asymptotic expressions for conic singularities in the (s_1, s_2, λ) space, which are valid for each of the four optical axes (31):

$$\begin{aligned}&(\lambda-\eta_2-(\eta_3-\eta_1)S_1(s_1-S_1))^2\\ &= (\eta_3-\eta_1)^2S_1^2((s_1-S_1)^2+S_3^2s_2^2).\end{aligned} \tag{33}$$

Let us assume that the crystal is absorptive and optically active. In this case, one can suppose that the family of matrices given by Eq. (30) undergoes complex perturbation $\mathbf{A}(\mathbf{p}) + \Delta\mathbf{A}(\mathbf{p})$, where

$$\Delta\mathbf{A}(\mathbf{p}) = (\mathbf{I}-\mathbf{s}\mathbf{s}^T)(\boldsymbol{\eta}_{\text{dichroic}}+\boldsymbol{\eta}_{\text{chiral}})(\mathbf{I}-\mathbf{s}\mathbf{s}^T). \tag{34}$$

Let us assume that the absorption and optical activity are weak; i.e., the quantity $\varepsilon = \|\boldsymbol{\eta}_{\text{dichroic}}\| + \|\boldsymbol{\eta}_{\text{chiral}}\|$ is small. In this case, the above general asymptotic formulas can be used to describe the rearrangement of the conic singularity of the eigenvalue surface. To this end, it is only necessary to know perturbation $\Delta\boldsymbol{A}$ on the optical axis $\mathbf{s}_0$ of the transparent crystal. Substituting matrix (34), calculated on optical axis (31), into Eq. (7) and using Eq. (12), we obtain

$$\begin{aligned}\mu &= \frac{i}{2}(\eta_{22}^d+\eta_{11}^dS_3^2-2\eta_{13}^dS_1S_3+\eta_{33}^dS_1^2),\\ \xi &= \frac{i}{2}(\eta_{22}^d-\eta_{11}^dS_3^2+2\eta_{13}^dS_1S_3-\eta_{33}^dS_1^2),\\ \eta &= i(\eta_{12}^dS_3-\eta_{23}^dS_1),\\ \zeta &= -i(\gamma_{11}S_1^2+2\gamma_{13}S_1S_3+\gamma_{33}S_3^2).\end{aligned} \tag{35}$$

We note that μ, ξ, and η are imaginary and depend only on absorption and that ζ depends on the optical activity of the crystal.

Singularities in crystals with weak absorption and optical activity were studied in [5]. It was shown that

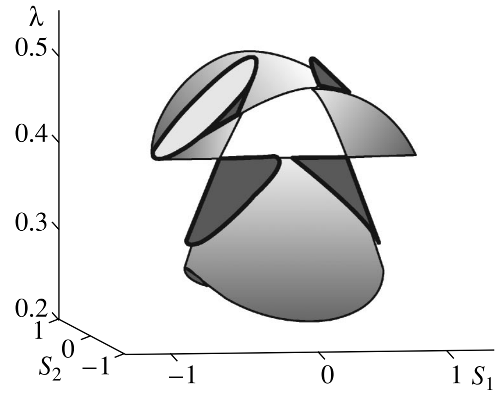

Fig. 2. Conical singularities on optic axes and their local approximations.

the coffee filter singularity appears in crystals with prevailing absorption and that the surfaces of the real parts of eigenvalues for crystals with dominant optical activity do not cross. According to the above general results, these two cases correspond to the conditions $D > 0$ and $D < 0$, where D is given by Eq. (17).

As a numerical example, we analyze a crystal with weak absorption and optical activity, which is described by tensors (28) and (29), where

$$\boldsymbol{\eta}_{\text{dichroic}} = \frac{i}{200}\begin{pmatrix}3&2&0\\2&3&1\\0&1&3\end{pmatrix}, \quad \gamma = \frac{1}{200}\begin{pmatrix}3&1&2\\1&3&1\\2&1&3\end{pmatrix}. \tag{36}$$

The corresponding transparent crystal is characterized by the parameters $\eta_1 = 0.5$, $\eta_2 = 0.4$, and $\eta_3 = 0.1$, and its eigenvalue surfaces with two optical axes are shown in Fig. 2 along with conical surfaces (33). Two optical axes shown in Fig. 2 have the coordinates $\mathbf{s}_0 = \left(\pm\frac{1}{2}, 0, \frac{\sqrt{3}}{2}\right)$ and correspond to the double eigenvalue $\lambda_0 = \frac{2}{5}$. Using Eqs. (36) in Eq. (35), we conclude that the condition $D = \frac{7}{160\,000}(4\sqrt{3}-5) > 0$ is satisfied for the left optical axis $\mathbf{s}_0 = \left(-\frac{1}{2}, 0, \frac{\sqrt{3}}{2}\right)$. Therefore, the conic singularity is transformed into the coffee filter with two singular axes. The local approximation of these surfaces is given by Eqs. (13) and (14). On the right optical axis $\mathbf{s}_0 = \left(\frac{1}{2}, 0, \frac{\sqrt{3}}{2}\right)$, the condition $D = -\frac{7}{160\,000}(4\sqrt{3}+5) < 0$ is satisfied. Thus, the real parts of eigenvalues do not coincide under a perturbation of

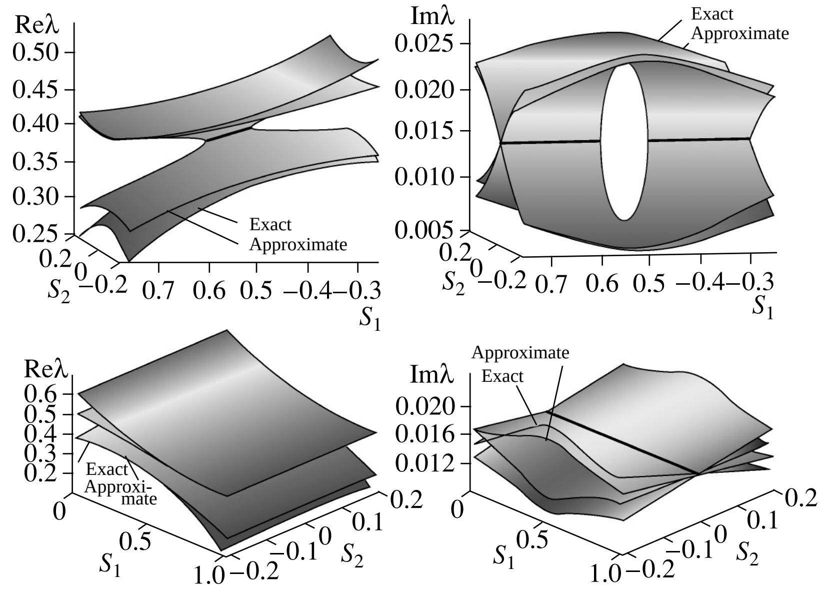

Fig. 3. Refractive-index surfaces for a crystal with weak absorption and optical activity.

the right optical axis. The approximate and exact eigenvalue surfaces are shown in Fig. 3, where it is seen that asymptotic formulas well reproduce the singularities of the refractive-index surfaces of crystals with weak absorption and optical activity.

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