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Proximity of degeneracies and chiral points

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Abstract

For complex 2×2 matrices \mathbf{M} , points of degeneracy (D), and chiral points (C) where the eigenvectors are circularly polarized, coincide when \mathbf{M} is symmetric, and often lie close together when \mathbf{M} is not symmetric. This proximity is explained statistically, by averaging over an ensemble in which the elements of \mathbf{M} are random complex numbers: the standard deviation of the separation between C and D points is less than half the separation of the two D points. If the departure from symmetry is treated as a perturbation of strength ε , the separation between C and D points is of order ε^2 ; the probability distribution of the separation is calculated.

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1. Introduction

Singularities in eigenpolarizations are helpful navigation markers in the high-dimensional parameter space of crystal optics [1]. In the general case of dielectric crystals that are absorbing (dichroic) and chiral (optically active) as well as biaxially anisotropic, there are two singularities of codimension 2—occurring, for example, as points in the space of wavevector directions for a given crystal. First, there are the singular axes [2]; these are degeneracies—we will call them D points (they are also called exceptional points [3])—in the form of branch-point singularities, where the refractive indices (eigenvalues) of the two eigenpolarizations coincide. Second are the chiral points, or C, points, where either of the two polarizations is purely circular. In general, these two singularities are distinct, but they coincide for crystals whose dielectric matrix is symmetric (and not necessarily real) [1, 4].

In numerical calculations, it was observed that even for matrices that are not close to symmetric the C and D points lie close together. Indeed, the fact, obvious in retrospect, that they are distinct was discovered [1] only after magnification of direction-space portraits of the polarization states. My purpose here is to demystify this proximity phenomenon, by calculating the statistics of the separation between C and D points for ensembles of random matrices.

2. C and D singularities

Polarization states are the eigenvectors \mathbf{x}_\pm of 2×2 matrices \mathbf{M} representing the reciprocal of the 3×3 dielectric tensor, projected onto the subspace transverse to the wavevector direction [5]; the states \mathbf{x} represent the electric \mathbf{D} vector, which is always transverse and so has two components (here considered in a Cartesian basis) perpendicular to the wavevector direction. The eigenvalues λ_\pm are the reciprocals of the squares of the corresponding refractive indices. Thus, we consider the eigenproblem

$$\mathbf{M}\mathbf{x} = \lambda\mathbf{x}, \quad (1)$$

where \mathbf{M} is a general complex matrix and \mathbf{x} is a vector with two complex components:

$$\mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad a = a_1 + ia_2, \text{ etc}, \quad \mathbf{x} = \begin{pmatrix} p \\ q \end{pmatrix}. \quad (2)$$

The eigenvalues are

$$\lambda_\pm = \frac{1}{2}(a + d \pm \sqrt{(d - a)^2 + 4bc}), \quad (3)$$

so the D singularities (degeneracies) satisfy

$$(d - a)^2 + 4bc = 0. \quad (4)$$

This is a single complex equation, so the D points have codimension 2.

Circular polarization corresponds to the two Cartesian components of \mathbf{x} being 90° out of phase, so the C singularities correspond to

$$\frac{p}{q} = \pm i, \quad \text{i.e.} \quad \left(\frac{p}{q}\right)^2 + 1 = 0 \quad (5)$$

—again a complex equation, so C points also have codimension 2. A short calculation leads to the condition

$$(d - a)^2 + (b + c)^2 = 0. \quad (6)$$

The C and D conditions involve only $d - a$, corresponding to the traceless part of \mathbf{M} . In physical applications where \mathbf{M} represents absorption, $\text{Tr}\mathbf{M}$ must have a fixed sign (+, say); this can be incorporated without changing any of the results to follow.

It is clear from (4) and (6) that the C and D points coincide if \mathbf{M} is symmetric, that is if $b = c$. To explore how close the singularities are if \mathbf{M} is not symmetric, it is convenient to regard them as points in the complex plane (figure 1)

$$z \equiv d - a \quad (7)$$

representing the traceless part of the diagonal elements of \mathbf{M} . Thus, from (4), the D points are at

$$z_{D\pm} = \pm 2i\sqrt{bc}, \quad (8)$$

and, from (6), the corresponding C points are at

$$z_{C\pm} = \pm i(b + c), \quad (9)$$

where ‘corresponding’ is interpreted in the sense of continuation of branches of the square roots for small $|b - c|$. Each of the two eigenvectors has a single C point z_C , represented by one of the signs in (9).

Thus, the separation of each C point from its corresponding D point is

$$z_{CD\pm} \equiv z_{C\pm} - z_{D\pm} = \pm(\sqrt{b} - \sqrt{c})^2, \quad (10)$$

from which it is again clear that the separation vanishes for symmetric matrices.

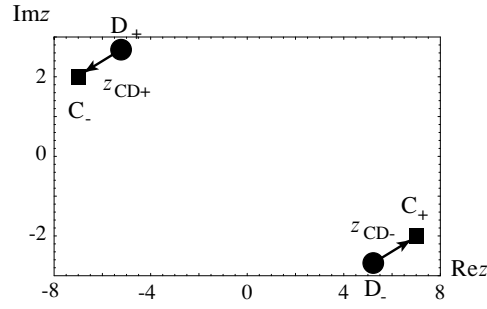


Figure 1. Degeneracy points D_{\pm} (dots) and chiral points C_{\pm} (squares) in the $z = d - a$ plane, for the matrix (2) with $b = 1 + i$, $c = 1 + 6i$, showing separations z_{CD} . Choosing random b and c as in section 2 gives similar pictures, often with D and C points in close proximity even when b and c are very different.

3. Random-matrix theory

A convenient measure of the separation $|z_{CD\pm}|$ of corresponding C and D points is the ratio of this to the separation of the two D points $|z_{D+} - z_{D-}|$. We first calculate the average values of these quantities by considering the real and imaginary parts of the off-diagonal elements of \mathbf{M} as independent Gaussian random variables with variance unity:

$$\langle b_1^2 \rangle = \langle b_2^2 \rangle = \langle c_1^2 \rangle = \langle c_2^2 \rangle = 1. \quad (11)$$

Thus,

$$\langle |b|^2 \rangle = \langle b_1^2 + b_2^2 \rangle = 2, \quad \langle |b| \rangle = \int_0^{\infty} db b^2 \exp\left(-\frac{1}{2}b^2\right) = \sqrt{\frac{\pi}{2}}, \quad (12)$$

and similarly for c .

This gives the variance of the distance between the D points as (cf (8))

$$\langle |z_{D+} - z_{D-}|^2 \rangle = 16\langle |bc| \rangle = 8\pi. \quad (13)$$

The rms distance of each D point from the origin is thus $\sqrt{2\pi}$ —slightly larger than the rms distance of each C point from the origin, which from (9) and (12) is 2.

For the separation between corresponding C and D points, we have, from (10),

$$\begin{aligned} \langle |z_{CD\pm}|^2 \rangle &= \langle |\sqrt{b} - \sqrt{c}|^4 \rangle \\ &= \langle |b|^2 + |c|^2 + 2|b||c| + 4 \operatorname{Re}^2 \sqrt{b^*c} - 4(|b| + |c|) \operatorname{Re} \sqrt{b^*c} \rangle. \end{aligned} \quad (14)$$

This requires the averages

$$4\langle \operatorname{Re}^2 \sqrt{b^*c} \rangle = 4\langle |b||c| \cos^2\left(\frac{1}{2}(\phi_c - \phi_b)\right) \rangle = \pi, \quad (15)$$

and

$$\begin{aligned} 4\langle (|b| + |c|) \operatorname{Re} \sqrt{b^*c} \rangle &= 8\langle |b|^{3/2}|c|^{1/2} \cos\left(\frac{1}{2}(\phi_c - \phi_b)\right) \rangle \\ &= 8 \int_0^{\infty} db b^{5/2} \exp\left(-\frac{1}{2}b^2\right) \int_0^{\infty} dc c^{3/2} \exp\left(-\frac{1}{2}c^2\right) \\ &\quad \times \frac{1}{4\pi^2} \int_0^{2\pi} d\phi_b \int_0^{2\pi} d\phi_c \cos\left(\frac{1}{2}(\phi_c - \phi_b)\right) = \frac{12\sqrt{2}}{\pi} \end{aligned} \quad (16)$$

(both averages are independent of the common choice of origin of the two angles).

Collecting these results, we find the ratio determining the proximity of C and D points as

$$\sqrt{\frac{\langle |z_{CD\pm}|^2 \rangle}{\langle (|z_{D+} - z_{D-}|)^2 \rangle}} = \sqrt{\frac{4 + 2\pi - 12\sqrt{2}/\pi}{8\pi}} = \sqrt{\frac{4.8813}{8\pi}} = 0.441. \quad (17)$$

Thus, the rms separation of corresponding C and D points is less than half the rms separation of the two D points, explaining the observation that C and D points are often close together. (The separation of a C point from the D point that does not correspond to it, e.g. between C_+ and D_- , is 1.793 times greater.)

4. Random-matrix perturbation theory

To explore the proximity phenomenon a little further, we define a different random-matrix ensemble, in which ε measures the departure from symmetry, namely

$$b = u(1 + \varepsilon v), \quad c = u(1 - \varepsilon v), \quad (18)$$

where u and v are independent complex Gaussian variables whose real and imaginary parts have variance unity, and we are interested in $\varepsilon \ll 1$.

From (8),

$$z_{D\pm} = \pm 2iu\sqrt{1 - \varepsilon^2 v^2}, \quad (19)$$

so that the separation of the two D points is

$$\begin{aligned} \langle |z_{D+} - z_{D-}|^2 \rangle &= 16\langle |u|^2 \rangle \langle |1 - \varepsilon^2 v|^2 \exp(2i\phi_v) \rangle \\ &= 32 + O(\varepsilon^2). \end{aligned} \quad (20)$$

For the separation of corresponding C and D points, we have

$$\begin{aligned} \langle |z_{CD\pm}|^2 \rangle &= \langle |u|^2 \rangle \langle |\sqrt{1 + \varepsilon v} - \sqrt{1 - \varepsilon v}|^4 \rangle = 2\varepsilon^4 \langle |v|^4 \rangle + O(\varepsilon^6) \\ &= 16\varepsilon^4 + O(\varepsilon^6). \end{aligned} \quad (21)$$

Thus the ratio analogous to (17) is, for this perturbative situation,

$$\sqrt{\frac{\langle |z_{CD\pm}|^2 \rangle}{\langle (|z_{D+} - z_{D-}|)^2 \rangle}} = \frac{\varepsilon^2}{\sqrt{2}} + O(\varepsilon^4). \quad (22)$$

The fact that this is of order ε^2 , rather than ε as might have been anticipated, further illustrates the proximity of C and D points.

The probability distribution of z_{CD} , of which (21) gives the variance, is

$$\begin{aligned} P(|z_{CD}|)_{\varepsilon \ll 1} &= \int_0^\infty du u \int_0^\infty dv v \exp(-\tfrac{1}{2}(u^2 + v^2)) \delta(|z_{CD}| - |\varepsilon^2 u v^2|) \\ &= \frac{z_{CD}}{\varepsilon^4} \int_0^\infty \frac{dv}{v^3} \exp\left(-\frac{1}{2}\left(v^2 + \frac{|z_{CD}|^2}{\varepsilon^4 v^2}\right)\right) \\ &= \frac{1}{\varepsilon^2} \int_0^\infty dt \exp\left(-2t^2 - \frac{|z_{CD}|}{4\varepsilon^2 t}\right). \end{aligned} \quad (23)$$

The integral is easily evaluated numerically (it can be expressed in terms of Meijer G functions), giving the distribution shown in figure 2.

A close approximation to (23) can be obtained by the saddle-point method:

$$P(|z_{CD}|)_{\varepsilon \ll 1} \approx \frac{1}{\varepsilon^2} \sqrt{\frac{\pi}{6}} \exp\left\{-\frac{3}{4}\left(\frac{2|z_{CD}|^2}{\varepsilon^4}\right)^{1/3}\right\}. \quad (24)$$

This has the normalization integral $\pi/3$ rather than 1, and the (correctly normalized) variance $\langle |z_{CD\pm}|^2 \rangle_{\text{approx}} = \frac{140}{9}\varepsilon^4 \approx 15.55\varepsilon^4$, rather than $16\varepsilon^4$.

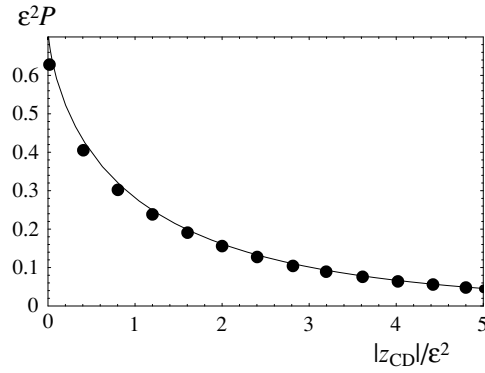


Figure 2. Dots: exact small- ϵ probability distribution (23) for the separation between corresponding D and C points. Curve: the approximate distribution (24).

5. Concluding remarks

The department of C and D points reflects two different types of symmetry breaking. A real symmetric dielectric matrix \mathbf{M} represents a material with both time-reversal and chiral symmetries. Making \mathbf{M} complex while keeping it symmetric (i.e. making \mathbf{M} non-Hermitian) corresponds to adding dissipation, which breaks time-reversal symmetry. Making \mathbf{M} non-symmetric corresponds to breaking chiral symmetry, representing a material with optical activity. If \mathbf{M} is a matrix governing the evolution of a two-component quantum system, the two processes just described represent different kinds of time-reversal symmetry-breaking: adding dissipation when the symmetric matrix \mathbf{M} is made complex (i.e. non-Hermitian), and adding an external magnetic field, or some other kind of non-dissipative time-reversal symmetry-breaking, when \mathbf{M} is made non-symmetric (e.g. complex Hermitian).

The condition (4) for the D points is invariant under similarity transformations of \mathbf{M} , because it involves only the eigenvalues. The condition (6) for the C points is not invariant under similarity or general unitary transformations (though it is invariant under orthogonal transformations). This reflects the fact that the representation of circular polarization is basis-dependent. Therefore, the calculations reported here have meaning only in situations where the requirement for the two components of \mathbf{x} to be 90° out of phase has physical significance. Of course this is the case for polarized light in a dielectric.

The proximity calculations do not apply for bianisotropic materials [6], where each of the electromagnetic \mathbf{D} and \mathbf{B} vectors is coupled to both of the vectors \mathbf{E} and \mathbf{H} . In this case, the governing constitutive matrix is 4×4 , and the eigenvectors have four components: two for the transverse \mathbf{D} vector and two for the transverse \mathbf{B} vector. D points still exist, common to \mathbf{D} and \mathbf{B} , and so do C points, in general different for \mathbf{D} and \mathbf{B} . When the matrix is symmetric, the C and D points no longer coincide. This would appear to violate the theorem [7] on chirality of exceptional points, which holds for general $N \times N$ matrices. But it does not, because when $N > 2$ the theorem concerns not a property of any two-component subvector but a quite different relation, involving factors $\pm i$ in the coefficients of the degenerate N -component eigenvector, when expanded in a basis of states close to the degeneracy.

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