Propagation of Singularities in Hexagonal Media

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This is a talk on joint work with N. Ortner [6]. We shall first briefly recapitulate the theory created by Atiyah, Bott, and Gårding in [1], [2] concerning the propagation of singularities for *scalar* hyperbolic operators with constant coefficients. We shall then give some observations on *systems*, and finally consider the particular case of the propagation of waves in *hexagonal* linear elastic media.

1. Some facts from Atiyah–Bott–Gårding

We fix $N \in \mathbf{R}^n \setminus \{0\}$ and we assume that the linear partial differential operator with constant coefficients $Q(D) = \sum c_\alpha D^\alpha$, $D = -\mathrm{i}\partial$, is *hyperbolic* with respect to N. If $m = \deg Q$, we write $Q^{\mathrm{pr}}(\eta) = \sum_{|\alpha|=m} c_\alpha \eta^\alpha$ for the *principal part* of Q. We denote by $E(Q(D))$ the *fundamental solution* of $Q(D)$ with support in $H = \{y \in \mathbf{R}^n;\, y \cdot N \geq 0\}$, by $\Gamma(Q(D))$ the *hyperbolicity cone*, i.e., the connectivity component containing N in $\{\eta \in \mathbf{R}^n;\, Q^{\mathrm{pr}}(\eta) \neq 0\}$, and by $K(Q(D))$ the cone dual to $\Gamma(Q(D))$, the so-called *propagation cone*: $K(Q(D)) = \{y \in \mathbf{R}^n;\, \forall \eta \in \Gamma(Q(D)) : \eta \cdot y \geq 0\}$.

For $\eta \in \mathbf{R}^n$, $Q_\eta(\zeta)$ denotes the *localization* of Q at infinity in the direction $\eta \in \mathbf{R}^n$, i.e., the lowest (non-vanishing) coefficient with respect to s in the MacLaurin series of $s^m Q(\zeta + \frac{\eta}{s})$. The operators $Q_\eta(D)$ are again hyperbolic. The set $W(Q(D)) = \cup_{\eta \in \mathbf{R}^n \setminus \{0\}} K(Q_\eta(D))$ is called the *wavefront surface* of $Q(D)$. One of the central results of Atiyah–Bott–Gårding is the following series of inclusions:

$$(1) \qquad \bigcup_{\eta \in \mathbf{R}^n \setminus \{0\}} \operatorname{supp} E(Q_\eta(D)) \subset \operatorname{sing\,supp} E(Q(D)) \subset W(Q(D)),$$

cf. [1, Thm. 4.10, p. 144; Thm. 7.24, p. 177]. In the physically relevant cases, in particular if $n \leq 4$, both of the inclusions in (1) are identities, cf. [2, Thm. 7.7, p. 175].

If $\Xi = \{\eta \in \mathbf{R}^n;\, Q^{\mathrm{pr}}(\eta) = 0\}$ is the *slowness surface* of $Q(D)$ and $\eta \in \Xi$ fulfills $\mathrm{d}Q^{\mathrm{pr}}(\eta) \neq 0$ (and η is thus a regular point of Ξ), then Q_η is a first-order polynomial and $K(Q_\eta(D))$ is the half-ray $\mathbf{R} \cdot \mathrm{d}Q^{\mathrm{pr}}(\eta) \cap H$. Hence $\Xi^* \cap H \subset \operatorname{sing\,supp} E(Q(D))$ if Ξ^* denotes the dual algebraic hypersurface of Ξ, the so-called *wave surface*, i.e.,

Ξ^* is the closure of $\{t\mathrm{d}Q^{\mathrm{pr}}(\eta);\, t \in \mathbf{R},\, \eta \in \Xi\}$. (Here we suppose that Q^{pr} does not contain multiple factors.) We shall say that *conical refraction* occurs if $\Xi^* \cap H$ is a proper subset of $\operatorname{sing\,supp} E(Q(D))$. If the inclusions in (1) are identities (as is usually the case), then conical refraction occurs if the set

$$C = \bigcup \{K(Q_\eta(D));\, \eta \in \mathbf{R}^n \setminus \{0\},\, Q^{\mathrm{pr}}(\eta) = 0,\, \mathrm{d}Q^{\mathrm{pr}}(\eta) = 0\} \tag{2}$$

is not already contained in Ξ^*.

Let us elaborate the above on the simple example $Q(D) = (\partial_t^2 - \Delta_3)(\partial_t^2 - 2\Delta_2 - \frac{1}{2}\partial_3^2)$. Here

$$\Xi = \mathbf{R} \cdot \{\eta = (1, \xi) \in \mathbf{R}^4;\, |\xi| = 1 \text{ or } 2(\xi_1^2 + \xi_2^2) + \tfrac{1}{2}\xi_3^2 = 1\}$$

and

$$\Xi^* = \mathbf{R} \cdot \{y = (1, x) \in \mathbf{R}^4;\, |x| = 1 \text{ or } \tfrac{1}{2}(x_1^2 + x_2^2) + 2x_3^2 = 1\}.$$

Furthermore $\mathrm{d}Q(1, \xi) = 0 \Leftrightarrow |\xi| = 1 = 2(\xi_1^2 + \xi_2^2) + \frac{1}{2}\xi_3^2 \Leftrightarrow |\xi| = 1$ and $\xi_3^2 = \frac{2}{3}$. For such points $\eta = (1, \xi)$, we have $Q_\eta(D) = -4(\partial_t - \xi \cdot \nabla)(\partial_t - 2(\xi_1\partial_1 + \xi_2\partial_2) - \frac{1}{2}\xi_3\partial_3)$ and

$$K(Q_\eta(D)) = [0, \infty) \cdot \{(1, x) \in \mathbf{R}^4;\, x = \lambda\xi + (1 - \lambda)(2\xi_1, 2\xi_2, \tfrac{1}{2}\xi_3),\ 0 \le \lambda \le 1\}.$$

Hence C in (2) furnishes two conical frusta on the boundary of the convex hull of the two ellipsoids representing Ξ^*; cf. Fig. 1, where the intersections with $\tau = 1$ and $t = 1$, respectively, are depicted.

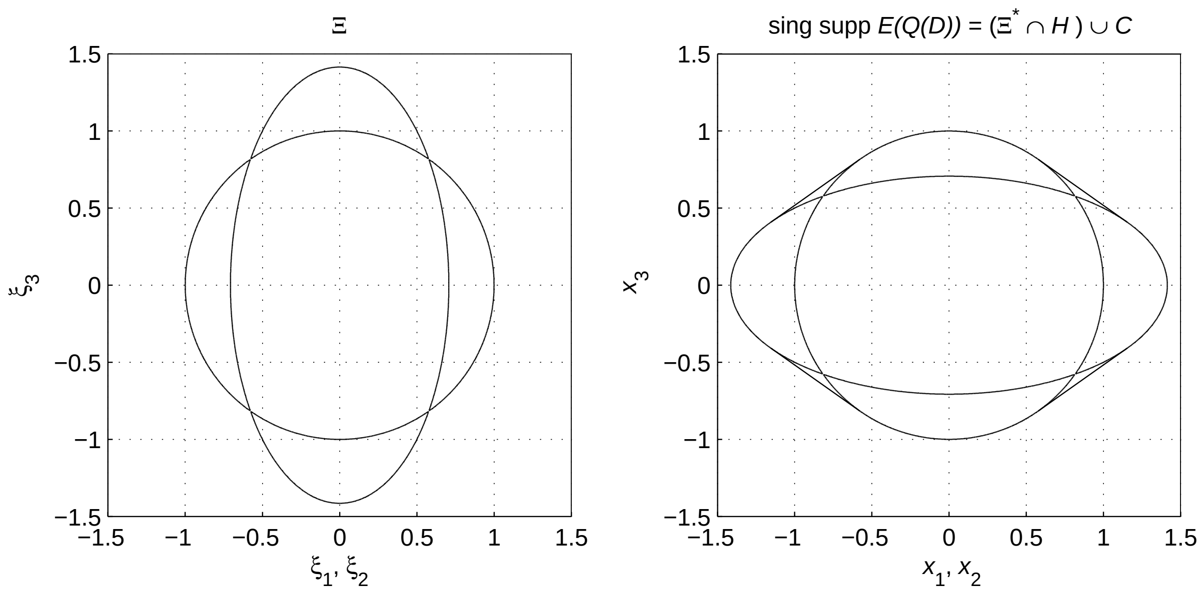

Figure 1: Slowness surface and wavefront surface for $(\partial_t^2 - \Delta_3)(\partial_t^2 - 2\Delta_2 - \frac{1}{2}\partial_3^2)$

2. Hyperbolic systems

The $l\times l-$ matrix $P(D)$ of linear constant coefficient partial differential operators is called *hyperbolic* if this is true for $Q(D)=\det P(D)$. As in the scalar case, $P(D)$ has a unique *fundamental matrix* $E(P(D))$ with support in H, namely $E(P(D))=P^{\mathrm{ad}}(D)E(Q(D))$. For the singular support

$$\operatorname{sing\,supp} E(P(D))=\bigcup_{1\le j,k\le l}\operatorname{sing\,supp} E(P(D))_{jk},$$

we have, instead of (1),

$$\bigcup_{\substack{1\le j,k\le l\\ \eta\in\mathbf{R}^n\setminus\{0\}}}\operatorname{supp}\big[(P^{\mathrm{ad}}_{jk})_\eta(D)E(Q_\eta(D))\big]\subset\operatorname{sing\,supp} E(P(D))\subset W(Q(D)). \tag{3}$$

(This straightforward consequence of (1) is stated in [4, p. 191].)

Unfortunately, in contrast to the scalar case, the inclusion on the right-hand side of (3) can be strict also in physically relevant cases. E.g., if we set $P(D)=\begin{pmatrix}\partial_t^2-\Delta_3 & 0\\ 0 & \partial_t^2-2\Delta_2-\frac12\partial_3^2\end{pmatrix}$, then we obtain for the determinant operator $Q(D)=\det P(D)$ the one in the example of section 1. However, the singular support of

$$E(P(D))=\frac{1}{4\pi t}\begin{pmatrix}\delta(t-|x|) & 0\\ 0 & \frac{1}{\sqrt2}\delta\Big(t-\sqrt{\frac12(x_1^2+x_2^2)+2x_3^2}\Big)\end{pmatrix}$$

consists just of $\Xi^*\cap H$ and no conical refraction occurs.

Let me still sketch how one can use microlocal analysis in order to determine $\operatorname{sing\,supp} E(P(D))$ in the cases where the two bounds in (3) differ. We suppose here that $P(D)$ is homogeneous. Then $T=\lim_{\sigma\nearrow 0}P(\eta+\mathrm{i}\sigma N)^{-1}$ and $E(P(D))=\mathcal{F}^{-1}T$ are both homogeneous. Due to [5, Thm. 8.1.8, p. 258], $(y,\eta)\in(\mathbf{R}^n\setminus\{0\})^2$ belongs to $\operatorname{WF} E(P(D))$, the *wavefront set* of $E(P(D))$, if and only if $(\eta,-y)\in\operatorname{WF} T$. Therefore, $\operatorname{sing\,supp} E(P(D))\setminus\{0\}$ is the negative of the projection of $\operatorname{WF} T$ onto the second factor, cf. the analogous considerations in [9, p. 288]. In particular, the set C, which corresponds to conical refraction, is now given by

$$C=\{y\in\mathbf{R}^n\setminus\{0\};\ \exists\eta\in\Xi:\mathrm{d}Q(\eta)=0\text{ and }(\eta,-y)\in\operatorname{WF} T\}. \tag{4}$$

3. Elastodynamics in hexagonal media

Hexagonal or *transversely isotropic* media are characterized by the property of rotational symmetry with respect to an axis. In [6], we extended R. G. Payton's seminal work [7] in that area by providing qualitative and quantitative information on the fundamental matrix of the elastodynamic system $P(D)=I_3\partial_t^2+A(\nabla)$. With the abbreviations in [3], i.e.,

$$a_1=c_{1111}=c_{11},\quad a_2=c_{3333}=c_{33},\quad a_3=c_{1133}+c_{2323}=c_{13}+c_{44},$$
$$a_4=\tfrac12(c_{1111}-c_{1122})=\tfrac12(c_{11}-c_{12}),\quad a_5=c_{2323}=c_{44},$$

(c_{ij} being the *contracted index notation*), we have

$$A(\nabla) = -\begin{pmatrix} a_1\partial_1^2 + a_4\partial_2^2 + a_5\partial_3^2 & (a_1 - a_4)\partial_1\partial_2 & a_3\partial_1\partial_3 \\ (a_1 - a_4)\partial_1\partial_2 & a_4\partial_1^2 + a_1\partial_2^2 + a_5\partial_3^2 & a_3\partial_2\partial_3 \\ a_3\partial_1\partial_3 & a_3\partial_2\partial_3 & a_5(\partial_1^2 + \partial_2^2) + a_2\partial_3^2 \end{pmatrix}.$$

As observed already by Christoffel in 1877, the determinant $Q = \det P$ splits: $Q = W_1 \cdot R$, with $W_1(D) = \partial_t^2 - a_4\Delta_2 - a_5\partial_3^2$ and

$$R(D) = \partial_t^4 - (a_1 + a_5)\partial_t^2\Delta_2 - (a_2 + a_5)\partial_t^2\partial_3^2 + a_1a_5\Delta_2^2 + a_2a_5\partial_3^4 + (a_1a_2 + a_5^2 - a_3^2)\Delta_2\partial_3^2.$$

$P(D)$ is hyperbolic (with respect to $N = (1, 0, 0, 0)$) iff

$$a_1 \geq 0,\ a_2 \geq 0,\ a_4 \geq 0,\ a_5 \geq 0, \text{ and } a_5 + \sqrt{a_1a_2} \geq |a_3|,$$

see [6, Prop. 2, p. 419]. We assume, moreover, that these inequalities are strict, which is equivalent to $Q(0, \xi) \neq 0$ for $\xi \in \mathbf{R}^3 \setminus \{0\}$, and which, physically, amounts to the positivity of the *propagation speeds.*

Depending on the values of the elastic constants $a_1, \dots, a_5$, the surfaces $W_1 = 0$ and $R = 0$ can intersect along two circular cones around the ξ_3-axis, cf. Fig. 2, left part. (The elastic constants for TiB_2 are (in gigapascal) $a_1 = 690$, $a_2 = 440$, $a_3 = 570$, $a_4 = 140$, $a_5 = 250$.) These ridge points on Ξ imply conical refraction for $Q(D)$, very much so as in the example in section 1. The corresponding parts of $\operatorname{sing\,supp} E(Q(D))$ are represented by the dashed lines in Fig. 2, right part. For the system $P(D)$ however, we showed in [6, Prop. 4, pp. 424, 425] that—similarly as in the example in section 2—no conical refraction can occur in general hexagonal media (to be precise, as long as $a_2 \neq a_5$). Hence the dashed lines in Fig. 2, right part, are not contained in $\operatorname{sing\,supp} E(P(D))$.

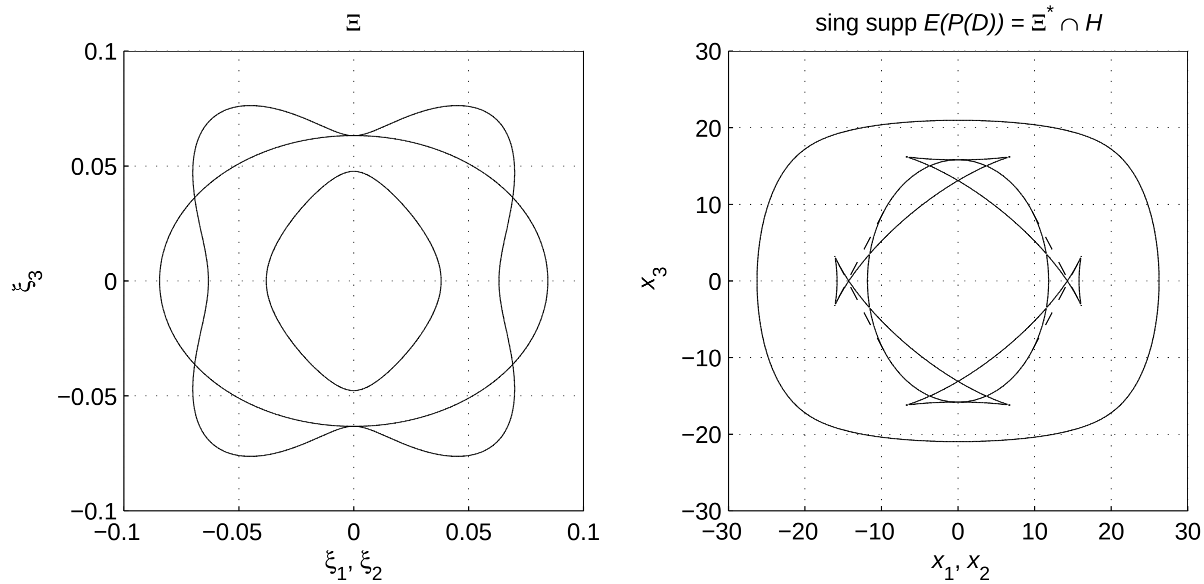

Figure 2: Slowness surface and wavefront surface for titanium boride

Let us explain this fact, which was already conjectured in [7, p. 67], by inspecting $\mathrm{WF}\, E(P(D))$. According to the last paragraph in section 2, we have to consider

$$T(\tau,\xi) = \lim_{\sigma\nearrow 0} P(\tau+\mathrm{i}\sigma,\xi)^{-1} = P(\tau,\xi)^{\mathrm{ad}} \cdot \lim_{\sigma\nearrow 0} Q(\tau+\mathrm{i}\sigma,\xi)^{-1}.$$

For $\rho = \sqrt{\xi_1^2+\xi_2^2} > 0$, an algebraic calculation (see [6, p. 425]) yields $P^{\mathrm{ad}} = W_1 B_1 + R B_2$, where

$$B_1 = \begin{pmatrix} W_4\xi_1^2/\rho^2 & W_4\xi_1\xi_2/\rho^2 & -a_3\xi_1\xi_3 \\ W_4\xi_1\xi_2/\rho^2 & W_4\xi_2^2/\rho^2 & -a_3\xi_2\xi_3 \\ -a_3\xi_1\xi_3 & -a_3\xi_2\xi_3 & W_3 \end{pmatrix} \quad \text{and} \quad B_2 = \begin{pmatrix} \xi_2^2/\rho^2 & -\xi_1\xi_2/\rho^2 & 0 \\ -\xi_1\xi_2/\rho^2 & \xi_1^2/\rho^2 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

with $W_3(\tau,\xi) = -\tau^2 + a_1\rho^2 + a_5\xi_3^2$, $W_4(\tau,\xi) = -\tau^2 + a_5\rho^2 + a_2\xi_3^2$. Due to $Q = W_1 \cdot R$, we conclude that, still for $\rho \neq 0$,

$$T = B_1 \cdot \lim_{\sigma\nearrow 0} R(\tau+\mathrm{i}\sigma,\xi)^{-1} + B_2 \cdot \lim_{\sigma\nearrow 0} W_1(\tau+\mathrm{i}\sigma,\xi)^{-1}.$$

This implies that, for $\eta = (\tau,\xi) \in \Xi$ with $\rho \neq 0$ and $W_1(\eta) = R(\eta) = 0$ (and hence $\mathrm{d}Q(\eta) = 0$),

$$\{y \in \mathbf{R}^4 \setminus \{0\};\ (\eta,-y) \in \mathrm{WF}\, T\} \subset \mathbf{R}\cdot \mathrm{d}R(\eta) \cup \mathbf{R}\cdot \mathrm{d}W_1(\eta).$$

For the points $\eta \in \Xi \setminus \{0\}$ with $\rho = 0$, it is easily seen that the sets $\{y \in \mathbf{R}^4 \setminus \{0\};\ (\eta,-y) \in \mathrm{WF}\, T\}$ are just half-rays. Therefore the set C in (4) is contained in $\Xi^* \cap H$, and thus no conical refraction occurs in general hexagonal media.

Let us finally comment on the exceptional case $a_2 = a_5$. Then the three sheets of Ξ meet along the ξ_3−axis $\rho = 0$, cf. Fig. 3, left part. This leads to conical refraction along two flat circular lids, cf. Fig. 3, right part. This fact is readily verified by evaluating the lower estimate of $\operatorname{sing\,supp} E(P(D))$ in (3). In the special case of $a_1 = a_2 = a_5$, the occurrence of the two lids was proven by explicit calculation of $E(P(D))_{33}$ in [8], cf. also [6, p. 428].

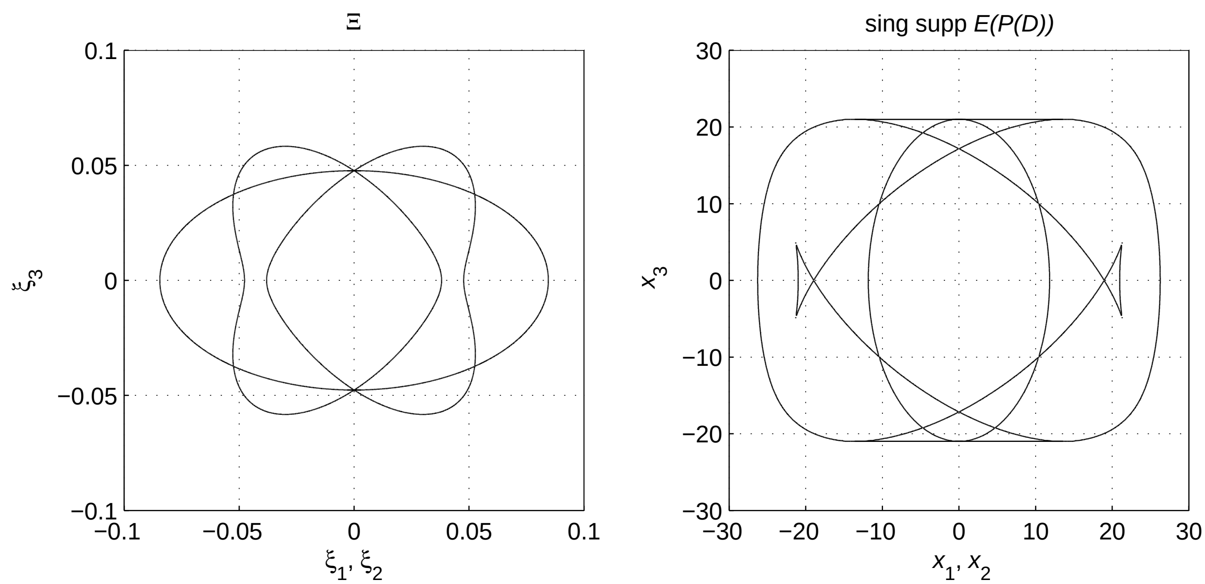

Figure 3: Slowness surface and wavefront surface for $a_2 = a_5$

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