

Singularity Phenomena in Ray Propagation in Anisotropic Media

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Abstract—Propagation of acoustic waves at a high frequency in anisotropic media is considered. In this case, the WKB approximation results in eikonal equations whose Hamiltonians are neither convex nor concave in the impulse variable as it is the case in differential games theory. In this paper the methods of differential games are adopted for the analysis of wave propagation. If the Hamiltonian of a differential game approximates the Hamiltonian of the eikonal equation, then the solution to the game approximates the phase function satisfying the eikonal equation. The method of singular characteristics is used for the analysis of singularities in associated differential games. Numerical results are presented for wave velocity surfaces typical for anisotropic quartz crystals.

I. INTRODUCTION

The study of questions related to the propagation of acoustic waves in anisotropic media is very important for many applications such as the development of acoustic sensors whose operating principle is based on the excitation and detection of acoustic waves in crystals. Propagation of acoustic waves in isotropic media is well investigated and mathematically described by means of geometric optics. The Fermat principle holds in this case, which expresses the fact that the rays, energy propagation trajectories, are minimizers of a functional which is the curve integral of some Lagrangian. In the case of short waves in anisotropic media, one can also utilize geometric optics using WKB approximations. This leads to Hamilton-Jacobi equations describing dynamics of the wave phase. However, one can not find a proper Lagrangian that would realize the Fermat principle in this case because of nonconvexity of the corresponding Hamiltonians in the impulse variable.

The paper studies the case of convex-concave Hamiltonians typical for anisotropic media. We consider the possibility to approximate the Hamiltonians through conflict-controlled systems where the first player chooses the current velocity from an admissible set of velocities with the goal to minimize the signal propagation time whenever the second, opposite, player strives to maximize this time. Although such an approach might look artificial, the point is that solutions to problems with close Hamiltonians must be also close each to other. Thus, the value function of the associated time-optimal differential game satisfies the eikonal equation of the

wave propagation problem. Therefore level sets of the value function represent wave fronts (first arrival) propagating in the anisotropic medium. Like in the Fermat principle, optimal trajectories in the associated differential game can apparently deliver information about the rays representing the energy flow. Note, that the structure of optimal trajectories in differential games is rather complicated because of the so-called singular surfaces, see [1], that can attract, repulse and break the trajectories. In the paper, a preliminary analysis of possible type of singular surfaces is performed for Hamiltonians that correspond to some typical phase velocity contours related to anisotropic crystals.

II. LAGRANGIAN AND HAMILTONIAN FORMALISM IN RAY TRACING

The rays along which disturbances propagate in a medium can be computed as the extremals of the functional (Fermat' principle):

$$J = \int_{t_0}^{t_1} L(x, \dot{x}) dt, \quad L(x, \dot{x}) = \frac{|\dot{x}|}{V(x, \dot{x}/|\dot{x}|)}$$

where V specifies the wave surface \mathcal{V} of the medium. Equivalently, the surface \mathcal{V} can be given as $L(x, v) = 1$. Surface \mathcal{V} is schematically shown in Fig. 1(a).

The wave front propagation can be found by solving the Hamilton-Jacobi equation

$$H(x, \frac{\partial S}{\partial x}) = 1, \quad H(x, p) = |p|W(x, p/|p|)$$

where the function W specifies the velocity surface \mathcal{W} of the medium. Slowness surface profile $N(x, e)$ is defined through $N(x, e)W(x, e) = 1$, where e is a unit (direction) vector. Equivalently, the surface \mathcal{N} can be given as $H(x, n) = 1$ (see Fig. 1(b)).

The Lagrangian $L(x, \dot{x})$ and the Hamiltonian $H(x, p)$ are positively homogeneous of degree one in second variable and

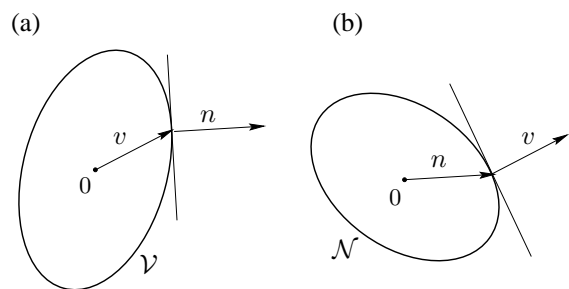


Fig. 1. (a) Wave surface; (b) Slowness surface.

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admit the representation, [2]:

$$L^2(x, \dot{x}) = \langle G(x, \dot{x}), \dot{x} \rangle, \quad H^2(x, p) = \langle Q(x, p), p \rangle$$

where G and Q are positively homogeneous of degree zero symmetric matrices.

Lagrangian and Hamiltonian can be transformed to each other through the formulas

$$Q = G^{-1}(x, \omega(x, p)), \quad G = Q^{-1}(x, \phi(x, \dot{x}))$$

if the following condition is fulfilled:

$$\det G(x, \dot{x}) = \det \left[\frac{1}{2} (L^2)_{\dot{x}\dot{x}} \right] = \det Q^{-1}(x, p) \neq 0$$

The function $\dot{x} = \omega(x, p)$ is defined implicitly by

$$p = \phi(x, \dot{x}) = \frac{1}{2} (L^2)_{\dot{x}} = LL_{\dot{x}} = G(x, \dot{x})\dot{x}.$$

This holds whenever the Hamiltonian and Lagrangian are convex. For anisotropic media the Hamiltonians may be convex-concave like in differential games. For such Hamiltonians the above convexity condition is not fulfilled and one can not transform the Hamiltonian to a single-valued Lagrangian (a typical form of the wave surface in this case is presented in Fig. 2, see e.g. [3]). The constructions using Hamilton-Jacobi equations are possible, though the solution has singularities known in differential games.

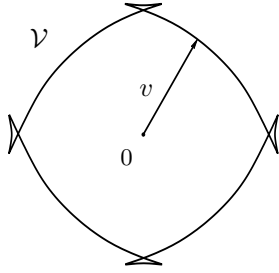


Fig. 2. Schematic picture of a wave surface for a cubic crystal

III. HAMILTON-JACOBI EQUATION IN GEOMETRICAL OPTICS

The Hamilton-Jacobi equation of the form

$$H(x, p) = |p|W(x, \frac{p}{|p|}) = 1 \quad (p = S_x),$$

with W being the phase velocity, arises when applying the WKB-approach (see e.g. [4]) to the elasticity equations for anisotropic inhomogeneous media

$$\rho u_{itt} - \frac{\partial}{\partial x_j} \left(C_{ijkl}(x) \frac{\partial u_l}{\partial x_k} \right) = 0, \quad i, j, k, l = 1, 2, 3.$$

Here u_i are the components of the displacement vector, ρ is the density, and C_{ijkl} is the elastic stiffness tensor. The summation over repeated indices is assumed.

We are looking for solutions of the form

$$u_j^\varepsilon(t, x) = \varepsilon e^{iS(t, x)/\varepsilon} v_j^\varepsilon(t, x)$$

with

$$v_j^\varepsilon(t, x) = v_j^0(t, x) + \varepsilon v_j^1(t, x) + \dots,$$

and the initial conditions

$$u_j^\varepsilon(0, x) = \varepsilon e^{iS(0, x)/\varepsilon} \phi_j(x), \quad x \in R^3,$$

$$u_{jt}^\varepsilon(0, x) = \psi_j(x), \quad x \in R^3.$$

Here ε is a small parameter, $\varepsilon = (\text{length scale} \times \text{wave number})^{-1}$. Assuming $\varepsilon \ll 1$, restrict the analysis to the first term of the expansion for v_j^ε .

Inserting this ansatz into the elasticity equations and collecting terms of the order $1/\varepsilon$ and 1 , respectively, yields the following eikonal and transport equations

$$\det \left[\frac{1}{\rho} C_{ijkl}(x) \frac{\partial S}{\partial x_j} \frac{\partial S}{\partial x_k} - \left(\frac{\partial S}{\partial t} \right)^2 I \right] = 0,$$

$$\rho S_{tt} v_i^0 + 2\rho S_t v_{it}^0 - C_{ijkl}(x) \frac{\partial^2 S}{\partial x_j \partial x_k} v_l^0 - 2C_{ijkl}(x) \frac{\partial S}{\partial x_j} \frac{\partial v_l^0}{\partial x_k} - \left[\frac{\partial}{\partial x_j} C_{ijkl}(x) \right] \frac{\partial S}{\partial x_k} v_l^0 = 0,$$

for $i = 1, 2, 3$. Let functions $c_\alpha(x, n)$, $\alpha = 1, 2, 3$, solve the eigenvalue problem

$$\det \left[\frac{1}{\rho} C_{ijkl}(x) n_j n_k - c^2 I \right] = 0$$

where $|n| = 1$. The functions $c_\alpha(x, n)$ are known to be the phase velocities for three types of waves propagating in anisotropic media in the direction n . The eikonal equation is obviously equivalent to the following three equations

$$S_{\alpha t} - |\nabla S_\alpha| c_\alpha \left(x, \frac{\nabla S_\alpha}{|\nabla S_\alpha|} \right) = 0, \quad \alpha = 1, 2, 3.$$

The substitution $S_\alpha(t, x) = t + T_\alpha(x)$ leads to the equation

$$|\nabla T_\alpha(x)| c_\alpha \left(x, \frac{\nabla T_\alpha(x)}{|\nabla T_\alpha(x)|} \right) = 1, \quad \alpha = 1, 2, 3,$$

which, as we will see in Section IV, determines the propagation times $T_\alpha(x)$ for different wave modes.

IV. DESCRIPTION OF WAVES PROPAGATION USING DIFFERENTIAL GAMES APPROACH

Generally, if the slowness surface \mathcal{N} is non-convex, it is impossible to transform the phase velocity surface \mathcal{W} to the wave surface \mathcal{V} to obtain the related variational problem with a Lagrangian. Therefore, it is necessary to work with the original Hamiltonian constructed on the base of the phase velocity surface \mathcal{W} . Such a Hamiltonian is convex-concave in the impulse variable, which is the reason why this case can not be reduced to an optimal control problem. Note that convex-concave Hamiltonians are typical for differential games [1]. The main goal in the solution of a game is to find the set of optimal trajectories in its complexity, i.e. the optimal phase portrait. Trajectories are not arranged in that regular way as in the calculus of variations or even in the theory of optimal control. There are several specific trajectories, called singular lines, [1], [5], which match regions

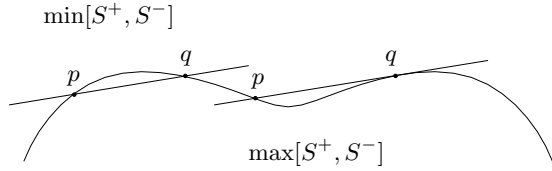


Fig. 5. Dispersal and equivocal situations

Perform a geometrical analysis (see Fig. 4) of the above inequalities using slowness and velocity surfaces. Bear in mind a differential game with the Hamiltonian $H(x, p) = |p|W(x, p/|p|)$. Fix some vectors p and $q \in \mathcal{N}$ and consider the segment AB given by $\lambda q + (1 - \lambda)p$, $0 \leq \lambda \leq 1$.

Consider a point D of that segment and the ray (half-line) passing through O and D . Let R and R' be points of the intersection of the ray with the surfaces \mathcal{N} and \mathcal{W} . Let d , r and r' be the lengths of the vectors OD , OR and OR' , respectively. Since $H(x, p) = |p|W(x, p/|p|)$, we have $H = dr'$. By definition of the surfaces \mathcal{V} and \mathcal{W} it holds $rr' = 1$. Since $d > r$ for the point considered, the relation $dr' > 1$ holds, and, consequently, $H > 1$. This consideration shows that the part $A'B'$ of the segment AB satisfies the inequality $H(x, p) \geq 1$, the parts AA' and $B'B$ satisfy the inequality $H(x, p) \leq 1$.

This property allows us to specify candidate vectors p, q for a potential singular line. Figure 5 demonstrates possible configurations of p, q for dispersal and equivocal type; for the focal type one has tangency at the both points p and q . One can see that unique values of p, q for focal surface can be found through convexification of the surface \mathcal{N} . The tangency of trajectories in Fig. 3 leads to the tangency of the segments at a single point for the equivocal case, and at both points for the focal case provided that the Hamiltonian is smooth in neighborhoods of (x, p) and (x, q) , see [5]. Note, that these singular lines are only potentially allowed by the necessary conditions, but they do not have necessarily to appear in the solution. Which surfaces will be present in the solution depends on boundary conditions. The exact analysis can be done on the base of the complete (numerical) solution of the problem.

There are many publications devoted to ray field and wave front construction using viscosity solutions and classical techniques (see, for example [8], [9], [10]). However, these works consider convex Hamiltonians. This paper utilizes methods of differential games for the analysis of convex-concave Hamiltonians.

V. EQUIVALENT DIFFERENTIAL GAMES, NUMERICAL RESULTS

We demonstrate application of differential games to the problem of propagation of surface acoustic waves in a quartz wafer covered by a thin film made of the isotropic silicon dioxide. Such a structure is typical for acoustic sensors whose operation principle is based on the piezoelectric

excitation of surface acoustic waves and the detection of the phase shift in the waves that arises because of deposition of an additional mass on the sensor surface. The wave propagation velocity in such multi-layered structures is obtained using numerical treatment of dispersion relations derived via substituting plane waves into material equations and matching the interface conditions between the layers, [11].

In Figure 6, the phase velocity contour for shear surface acoustic waves propagating in an ST-quartz wafer covered by a $5 \mu\text{m}$ SiO_2 film is shown. The contour is symmetric with respect to the origin. In fact, surface shear waves exist for directions from the set $\Omega = \{(\cos \phi, \sin \phi) : \phi \in [-\pi/6 + k\pi/2, \pi/6 + k\pi/2], k = \overline{0, 3}\}$. Such directions will be called feasible. For all non-feasible directions, the velocity value is the same and equals to 3739.79 m/s , which corresponds to the velocity of shear bulk waves in the structure considered.

Our next goal is to find constraint sets P and Q for the differential game

$$\dot{x} = u - v, \quad u \in P, \quad v \in Q,$$

so that, for every $\ell \in R^2$, $|\ell| = 1$, the value of the Hamiltonian

$$H(\ell) := \max_{u \in P} \min_{v \in Q} \langle \ell, -u + v \rangle$$

coincides with or is close to the value $W(\ell)$ taken from the velocity surface \mathcal{W} shown in Fig. 6.

Assuming that P and Q are symmetric with respect to the origin, we obtain

$$H(\ell) = \max_{u \in P} \langle \ell, u \rangle - \max_{v \in Q} \langle \ell, v \rangle.$$

Evidently, there exist many sets P and Q satisfying the relation

$$\max_{u \in P} \langle \ell, u \rangle - \max_{v \in Q} \langle \ell, v \rangle = W(\ell), \quad \ell \in R^2.$$

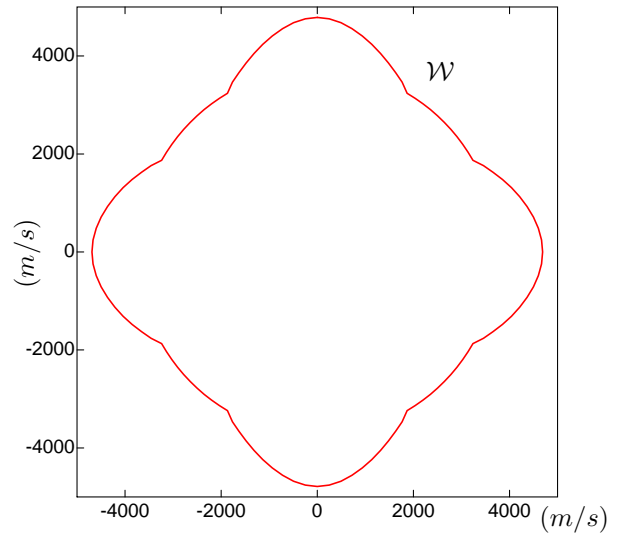


Fig. 6. Velocity contour for shear acoustic waves in ST-quartz covered by a $5 \mu\text{m}$ SiO_2 film

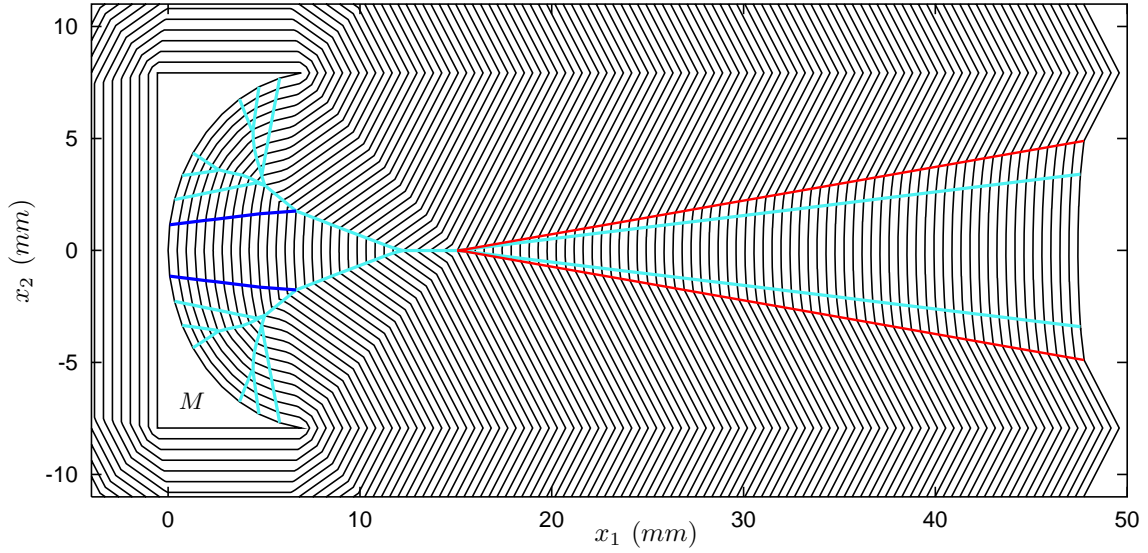


Fig. 8. Wave fronts and singular lines for acoustic sensor-like structure

To approximate the set W along feasible directions, we use the families $P^{\alpha,\beta}$, $\alpha \geq 1$, $\beta \geq 1$, and Q^γ , $\gamma > 0$, having simple analytical description. After an optimization in α, β, γ , the resulting set P^{α_*,β_*} is transformed into the set $\tilde{P}^{\alpha_*,\beta_*}$ that differs from P^{α_*,β_*} along four directions close to $(\cos(\pi/4 + k\pi/2), \sin(\pi/4 + k\pi/2))$, $k = 0, 3$. The result is represented in Fig. 7. The set

$$\tilde{R}^{\alpha_*,\beta_*,\gamma_*} = \max_{u \in P^{\alpha_*,\beta_*}} \langle \ell, u \rangle - \max_{v \in Q^{\gamma_*}} \langle \ell, v \rangle$$

provides a good approximation of W .

Consider now a problem where the first player having the control parameter $u \in P = \tilde{P}^{\alpha_*,\beta_*}$ at his disposal minimizes the time of attaining a given terminal set M , whereas the second player whose control parameter is $v \in Q = Q^{\gamma_*}$

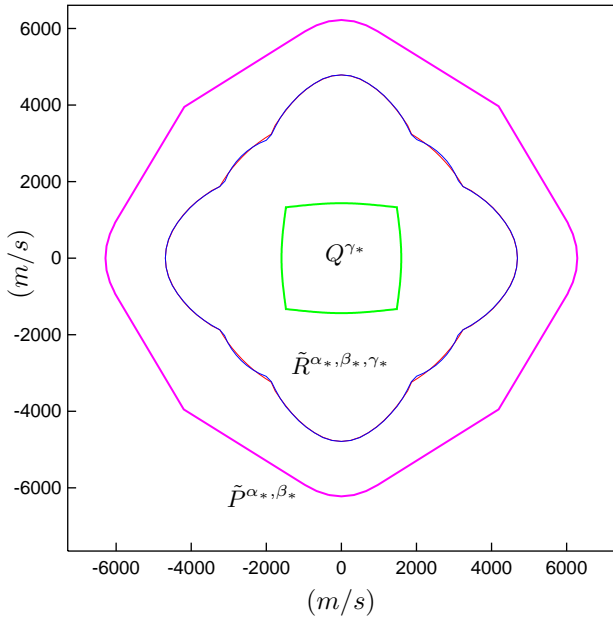


Fig. 7. Sets $\tilde{P}^{\alpha_*,\beta_*}$, Q^{γ_*} , $\tilde{R}^{\alpha_*,\beta_*,\gamma_*}$, and W

maximizes this time. The isochrones or level sets of the value function of this problem are wave fronts in the wave propagation problem with the velocity contour W provided that M is an excitation source that generates shear waves in all directions. Using a further development of algorithms (see [12], [13]) for computation of level sets of value functions for time-optimal game problems, one can obtain a portrait of the propagation of wave fronts for sources with very complicated geometries. The propagation time can also be found very precisely which might be helpful when estimating the sensitivity of acoustic sensors.

In Figure 8, numerically computed wave fronts propagating from a curved source M in x_1 -direction are shown. The computation was performed on the interval $[0, 10^{-5} s]$ with the step $\Delta = 10^{-7} s$. Corner points of the fronts, being connected, form singular lines. These lines can be classified using some additional analysis when computing the wave fronts with the above mentioned algorithm. Red lines in Fig. 8 are equivocal, blue lines are focal, and cyan lines are dispersal. Fig. 9 shows the behavior of optimal trajectories schematically, the arrows indicate the motion in backward time. We expect that singular lines are closely related to the propagation of physical rays. For example, dispersal lines correspond to the intersection of rays (they can be generally continued beyond the first arrival); equivocal lines absorb rays from one side, guide them and radiate to the other side; focal lines guide rays and radiate them to the both sides. This knowledge can be useful for the study of focusing and beam-steering properties of specially designed transducers.

Regular characteristics are known to represent physical rays. We conjecture that the same is true for singular characteristics so that the optimal phase portrait of such a game represents the complete set of rays of first arrival in the corresponding physical problem. The whole picture of rays depends, in addition to the Hamiltonian, upon the initial conditions. Numerical results of the paper show the

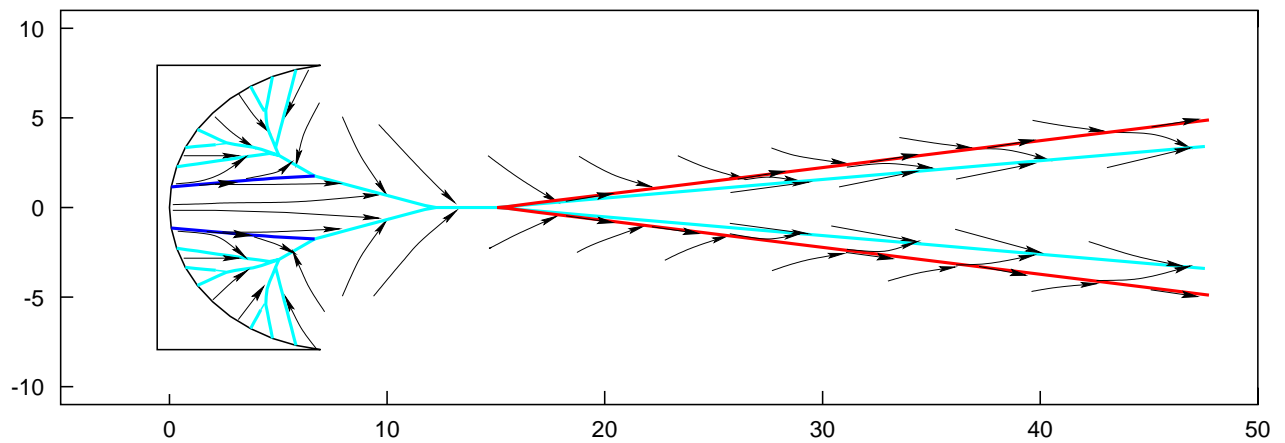


Fig. 9. Behavior of optimal trajectories in reverse time.

realizability of such an approach.

An interesting question for further research is related to physical interpretation of the objectives of the players (minimization and maximization of the propagation time). Physical experiments confirming the structure of ray fields computed seam to be very useful.

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