Singularity Phenomena in Ray Propagation in Anisotropic Media

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caesar

Multidisciplinary research center employing about 200 researchers

1999 - foundation of caesar;
2003 - moving in the new building

Research areas

- Smart materials combined with nanotechnologies
- Ergonomics: cooperation between humans and machines
- Coupling of biological and electronic systems
Motivation

Development of an acoustic wave sensor for biological and medical applications (microbalance)

Operation principles

1. Excitation of acoustic shear waves due to piezoelectric properties of a substrate

2. Selective binding of the biomolecules from a contacting liquid due to aptamers

3. Mass estimation through the measurement of the phase shift in the electric signal
Methods of modelling

Direct modelling with finite elements (resources consuming because of short wave lengths)

Dispersion relations (dependence of the wave propagation velocity on the frequency) for multi-layered anisotropic structures

Description of wave fronts using Hamilton-Jacobi equations
Waves description using optimality principles

1. Characteristic surfaces

Wave surface

Velocity surface

\( V_e \) energy velocity

\( n \) wave vector

\( V_e \cdot n = |V| - \) phase velocity
Slowness surface
(inverse through the origin to the velocity surface)

\[ m = n / |V| \]

The energy velocity is normal to the slowness surface at all points.
2. Fermat’s principle

\[ T = \int_A^B dt = \int_A^B \frac{ds}{V_e} \rightarrow \min \]

Or, using parametrization

\[ x(\tau), \quad ds = |\dot{x}|d\tau, \]

\[ T = \int_{\tau_0}^{\tau_1} \frac{|\dot{x}|}{V_e(x, x'/|\dot{x}|)}d\tau =: \int_{\tau_0}^{\tau_1} L(x, \dot{x})d\tau \rightarrow \min \]

Thus, feasible rays are solutions of the Euler equation

\[ L_x - \frac{d}{d\tau}L_{\dot{x}} = 0 \]

Applicable if \( V_e \) is a well-defined function.
3. Pontryagin’s maximum principle

\[ \dot{x} = u, \quad u \in \mathbb{R}^2, \quad T = \int_{\tau_0}^{\tau_1} \frac{|u|}{V_e(x, u/|u|)} \, d\tau \to \min_{u(\tau)} \]

\[ p \text{ - adjoint vector,} \]

\[ \max_{u \in \mathbb{R}^2} (\langle p, u \rangle - |u|/V_e(x, u/|u|)) = 0 \]

\[ \max_{u \in B_1} (\langle p, u \rangle - 1/V_e(x, u)) = 0 \]

\[ \max_{u \in B_1} \langle p, uV_e \rangle = 1 \quad \rightarrow \quad \max_{v \in \mathcal{V}} \langle p, v \rangle = 1 \]

\[ \mathcal{V} \text{ - wave surface} \]

Applicable if the wave surface does not have swallow tails.
Complicated structure of wave surfaces

Variation of the curvature of the slowness surface can yield multiple values for the energy velocity (swallow tails in the wave surface).

Example of a wave surface for a crystal with cubic symmetry.
Description of wave propagation using Hamilton-Jacobi equations

Elasticity equations for anisotropic inhomogeneous media

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

WKB-approximation

\[ u_j^\varepsilon(t, x) = \varepsilon e^{iS(t, x)/\varepsilon} v_j^\varepsilon(t, x), \quad x \in \mathbb{R}^3 \]

\[ v_j^\varepsilon(t, x) = v_j^0(t, x) + \varepsilon v_j^1(t, x) + \ldots \]

\[ u_j^\varepsilon(0, x) = \varepsilon e^{iS(0, x)/\varepsilon} \phi_j(x), \quad u_{jt}^\varepsilon(0, x) = \psi_j(x), \]

\[ \varepsilon \ll 1 \quad \text{is a small parameter} \]
Eikonal equation

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

is equivalent to the following three equations

\[
S_{\alpha t} - |\nabla S_{\alpha}| c_{\alpha} \left( x, \frac{\nabla S_{\alpha}}{|\nabla S_{\alpha}|} \right) = 0, \quad \text{where} \quad c_{\alpha}(x, n), \ \alpha = 1, 2, 3,
\]

solve the eigenvalue problem

\[
\det \left| \frac{1}{\rho} C_{ijkl}(x)n_jn_k - c^2 I \right| = 0 \quad \text{with} \quad |n| = 1,
\]

which gives three phase velocities (and three polarizations) for the propagation direction \( n \).

Using the transformation \( S_{\alpha}(t, x) = t - T_{\alpha}(x) \) yields H.-J. equation

\[
|\nabla T_{\alpha}(x)| c_{\alpha} \left( x, \frac{\nabla T_{\alpha}(x)}{|\nabla T_{\alpha}(x)|} \right) = 1
\]
If the wave surface has swallow tails, the Hamiltonian is non-convex in the impulse variable which motivates to use differential games instead of classical optimality principles.
Usage of differential games

\[ \dot{x} = f(x, u, v), \quad u \in P, \quad v \in Q \]

The first player minimizes and the second player maximizes the time of attaining a given terminal set \( M \).

Value function \( T(x) \) satisfies the Hamilton-Jacobi equation

\[
\min_{u \in P} \max_{v \in Q} \left< \nabla T(x), f(x, u, v) \right> = -1
\]

in all points \( x \) where \( T(x) \) is differentiable. In other points, this equation holds in a viscosity sense. If we find a differential game with the dynamics that provides the equality

\[
- \min_{u \in P} \max_{v \in Q} \left< p, f(x, u, v) \right> = |p| c_{\alpha} \left( x, \frac{p}{|p|} \right), \quad p \in \mathbb{R}^2
\]

then level sets of \( T \)

\[ \{ x \in \mathbb{R}^2 : T(x) = r \} \]

yield wave fronts in the wave propagation problem.
Differential games with simple dynamics are appropriate

\[ \dot{x} = u + v, \quad u \in P, \quad v \in Q, \]

\(P\) and \(Q\) are symmetric about the origin convex sets

Hamilton-Jacobi equation

\[
\min_{u \in P} \max_{v \in Q} \min \max \left\langle \nabla T(x), u + v \right\rangle = -1
\]

can be rewritten as

\[
\max_{u \in P} \left\langle \nabla T(x), u \right\rangle - \max_{v \in Q} \left\langle \nabla T(x), v \right\rangle = 1
\]

or

\[
|\nabla T(x)| \left( \max_{u \in P} \left\langle \frac{\nabla T(x)}{|\nabla T(x)|}, u \right\rangle - \max_{v \in Q} \left\langle \frac{\nabla T(x)}{|\nabla T(x)|}, v \right\rangle \right) = 1
\]

Comparison with the eikonal equation yields the condition on \(P\) and \(Q\):

\[
\max_{u \in P} \left\langle \ell, u \right\rangle - \max_{v \in Q} \left\langle \ell, v \right\rangle = c_\alpha(\ell), \quad \ell \in \mathbb{R}^2, \quad |\ell| = 1
\]
Application to the propagation of surface acoustic waves

Multi-layered structure

- Fluid
- Protein layer
- Gold layer
- SiO₂- guiding layer
- Quartz crystal

Velocity contour for shear surface acoustic waves


Slowness surface
1. Approximation of the phase velocity contour

Choose $P$ | Choose $Q$ | The result

\[ P \]

\[ Q \]
2. Numerical solution to the differential game

\[ \dot{x} = u + v, \quad u \in P, \quad v \in Q, \]

\( u \) minimizes and \( v \) maximizes the time of attaining the terminal set \( M \)

Backward step-by-step computation of the attainability set on interval \([0, \theta]\) with a step \( \Delta \)

3. Investigation of singular lines


\[ H(x, \lambda q + (1 - \lambda)p) \geq 1, \quad 0 \leq \lambda \leq 1, \quad S = \max\{S^+, S^-\} \]

\[ H(x, \lambda q + (1 - \lambda)p) \leq 1, \quad 0 \leq \lambda \leq 1, \quad S = \min\{S^+, S^-\} \]
Wave fronts and singular lines

Behavior of optimal trajectories
Acoustic waves in anisotropic crystals obey differential games!