General analytical scheme for determining the characteristic caustic points in phonon focusing patterns of cubic crystals

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Abstract—Phonon focusing patterns are dependent on the existence of concave/saddle regions and acoustic axes in the slowness surface. The main feature of the focusing patterns in cubic crystals can be characterized by the cuspidal and swallowtail points in the symmetry planes. By applying the Stroh formalism, these points are investigated in relation to degeneracies in the Stroh eigenvalue equation. Explicit expressions for these points are derived.

Keywords—caustic point, phonon focusing, cubic crystals

I. INTRODUCTION

Acoustic wave propagation in anisotropic media is governed by the Christoffel equation [1] which yields three-sheeted slowness surface. Two outer slowness sheets can be divided into concave/saddle and convex regions separated by the so-called parabolic line with zero Gaussian-curvature [2,3]. Wave surface, which describes group velocity for bulk waves, is defined by envelope of the slowness surface. In symmetry planes, there may be two types of characteristic points on concave slowness surface: inflectional point and parabolic point (see Fig. 1). These points will result in two types of points on the wave surface: cuspidal point and swallowtail point, respectively.

Because of the presence of concave regions on the slowness sheets, energy flow associated with a wave package will exhibit a focusing effect. Boundaries of the focusing pattern will be determined by the parabolic line. For cubic crystals, a set of critical conditions for various types of caustics in cubic crystals were formulated by calculating group velocities in the vicinity of symmetry directions [3]. The Gaussian curvature in the vicinity of symmetry axes in the crystals of various symmetries is also studied in order to formulate critical conditions for some caustics [4,5]. Numerically, extensive simulations have been done to illustrate focusing patterns and to determine size of focusing patterns in cubic crystals using the Monte-Carlo method [6]. However, an analytical scheme remains lacking for locating these points.

Main objective of this work is to establish a new scheme to elucidate these points analytically and explicitly based on the so-called Stroh formalism. The scheme is exemplified by examining cubic crystals.
The Stroh eigenvalue \( p_i \) can be determined by the characteristic equation \(|\Gamma| = 0\), a sextic equation:

\[
f(\tau) \equiv \sum_{i=0}^{5} a_i p_i^i = 0.\tag{3}
\]

When the velocity is sufficiently low, the eigenvalues appears as three pairs of complex conjugated numbers. At a so-called transonic state \([8]\) as shown in Fig. 2, the eigenvalues \( p_i \) will become degenerate pairwise

\[
p_1 = p_2 (= \tan \phi)\tag{4}
\]

where \( \phi \) defines the angle between \( k \) and \( m \). Note that the group velocity \( g \) is now parallel to \( m \), and \( \phi \) is actually the angle between \( k \) and \( g \). The degeneracy requires vanishing discriminant \( D[|\Gamma|] = 0 \)[9]. At an inflectional point, however, there will be a degeneracy with multiplicity of three (see Fig. 2b), implying

\[
p_1 = p_2 = p_3 (= \tan \phi)\tag{5}
\]

At a parabolic point, there will be a degeneracy with multiplicity of four (see Fig. 2c), requiring

\[
p_1 = p_2 = p_3 = p_4 (= \tan \phi)\tag{6}
\]

The geometric conditions above impose strong constraints on the Stroh eigenvalue equation, and this will enable us to find these points just by examining the characteristic equation (3) without actually solving it.

Let us consider a cuspidal point first. Such a point is always pertaining to a non-elliptic slowness branch \( S_0 \). By defining the reference plane \( (m, n) \) within a symmetry plane, the matrix \( \Gamma \) becomes diagonalized and the characteristic equation (3) becomes

\[
(a_4 p^4 + a_3 p^3 + a_2 p^2 + a_1 p + a_0) (b_2 p^2 + b_1 p + b_0) = 0\tag{7}
\]

and the Stroh eigenvalues can then be partitioned into \((p_1, p_2, p_3, p_4)\) and \((p_5, p_6)\) correspondingly.

The condition (5) will produce a set of restriction on the coefficients \( a_i \) in the quartic equation. Consider a monic quartic equation: \( x^4 + \beta x^3 + \gamma x^2 + \delta = 0 \). We can shown that a triple degeneracy requires \([10]\)

\[
\begin{align*}
\beta_1 &= \beta - 3 \alpha \gamma - 12 \delta = 0 \\
\beta_2 &= 9 \alpha^2 \gamma - \alpha \beta \gamma + 9 \gamma^2 + 32 \beta \delta^2 = 0.
\end{align*}\tag{8}
\]

By transforming (7) into monic equation, \( f_1 \) and \( f_2 \) can be expressed as two equations in \( \rho \nu^2 \) and \( \phi \). The variable \( \rho \nu^2 \) can be removed by calculating the resultant \([9]\) between \( f_1 \) and \( f_2 \):

\[
h \equiv \text{Res}(f_1, f_2)\tag{9}
\]

and \( h = 0 \) defines then the cuspidal point \( \phi \) explicitly.

In the \((001)\) plane, we define the reference plane \( (m, n) \) with \( m = \cos \phi e_x + \sin \phi e_y \) and \( n = \sin \phi e_x + \cos \phi e_y \). The matrix \( \Gamma \) is then given by the following elements:

\[
\begin{align*}
\Gamma_{11} &= p^2 (\cos^2 \phi + \sin^2 \phi) + p(1 - a) \sin^2 \phi + a \cos^2 \phi + s \sin^2 \phi + \rho \nu^2 \\
\Gamma_{12} &= (b + 1)(p^2 \sin 2\phi - 2 \cos 2\phi - \sin 2\phi) / 2 \\
\Gamma_{13} &= p^3 (\cos^3 \phi + a \sin^3 \phi) - p(1 - a) \sin^3 \phi + a \cos^3 \phi + s \sin^3 \phi + \rho \nu^2 \\
\Gamma_{33} &= p^3 - \rho \nu^2 + 1
\end{align*}\tag{10}
\]

Its characteristic equation (quartic part with \( a_4 \)) can be readily derived and they are simple polynomials in \( \nu \) and \( \rho \nu^2 \). By converting the quartic equation into monic form, we get \( f_1 \) and \( f_2 \) and \( h(\phi) = \text{Res}(f_1, f_2) \). The equation \( h = 0 \) is a simple third order equation in \( \cos 4\phi \).

Variation of its solution \( \phi_1 \), which define the cuspidal point, is illustrated in Fig. 3.

III. INFLECTIONAL POINT AND CUSPIDAL POINT IN (001) PLANE

The inflectional point is a point with zero in-plane curvature, and it can be determined by calculating curvature of slowness curve in a symmetry plane explicitly by setting \( k^4 \propto (s, s)(s, s) - (\bar{s}, \bar{s}) = 0 \) where \( s = \nu^{-1} \). However, because the condition (5) poses a strong constraint, one can determine the cuspidal point directly using the Stroh formalism.
IV. PARABOLIC POINT AND SWALLOWTAIL POINT IN (001) PLANE

The parabolic points are usually located in symmetry planes. Let the references plane \((\mathbf{m}, \mathbf{n})\) be defined in such a way with \(\mathbf{m}\) lying in a symmetry plane and \(\mathbf{n}\) parallel to the plane normal. The characteristic equation for (2), \(\|\Gamma\| = 0\), can always be written as a bicubic equation of \(p\):

\[
a_6 p^6 + a_4 p^4 + a_2 p^2 + a_0 = 0
\]

\(\text{(11)}\)

The condition \(p_1 = p_2 = p_3 = p_4\) can be rewritten as \(a_0 = a_2 = 0\). Again, since \(a_i\) are functions of \(\rho v^2\) and \(\theta\), we can locate the parabolic point \(\theta\) by removing \(\rho v^2\) by calculating resultant between \(a_0\) and \(a_2\):

\[
\text{Res}(a_0, a_2) = 0
\]

\(\text{(12)}\)

because the vanishing resultant guarantees a common root between the two polynomials \([9]\).

Let us consider (001) plane, with reference plane \((\mathbf{m}, \mathbf{n})\) defined by \(\mathbf{m} = \cos \theta \mathbf{e}_x + \sin \theta \mathbf{e}_y\), \(\mathbf{n} = -\mathbf{e}_z\). The matrix \(\Gamma\) becomes

\[
\begin{align*}
\Gamma_{11} &= p^2 - \rho v^2 + a \cos^2 \theta + \sin^2 \theta \\
\Gamma_{12} &= (b + 1) \sin \theta \cos \theta \\
\Gamma_{13} &= p (b + 1) \cos \theta \\
\Gamma_{22} &= [p^2(a - b) + (a + b) \sin^2 \theta - 2(\rho v^2 - 1)]/2 \\
\Gamma_{23} &= p (a - 1) \sin \theta \\
\Gamma_{33} &= [p^2(a + b + 2) + \Delta \sin^2 \theta - 2(\rho v^2 - 1)]/2.
\end{align*}
\]

\(\text{(13)}\)

The coefficients \(a_0\) and \(a_2\) and the resultant \(\text{Res}(a_0, a_2)\) can then be obtained. \(\text{Res}(a_0, a_2)\) turns out to be a third order equation in \(\cos 2\theta\) and position of the parabolic point \(\theta\) will be determined by the equation

\[
R \equiv \text{Res}(a_0, a_2) = 0
\]

\(\text{(14)}\)

The swallowtail caustic point is defined by the surface normal at the parabolic point. With the parabolic point \(\theta\) known, finding their surface normals within the symmetry plane poses a major challenge. Consider the surface normal at a parabolic point on \(S_a\) branch in GaAs.

The vector \(\mathbf{g}\) in Fig. 4 marks the surface normal at the parabolic point on \(S_a\) defined by angle \(\varphi\). Such a case refers to a transonic state pertaining to the point: in other word, the basis vector \(\mathbf{m}\) and \(\mathbf{n}\) must be defined in such a way that \(\mathbf{m}\) is parallel to \(\mathbf{g}\) and \(\mathbf{n}\) is parallel to the tangent \(L\), and the line \(L\) must have an appropriate velocity to form a tangent.

This construction implies that, (a) the inclination angle \(\phi\) must satisfy the relation \(\phi = \varphi - \varphi\); and (b) the angle \(\phi\) defines the degenerated Stroh eigenvalue \(\rho = \tan \phi\). These relations suggests that the characteristic equation \(\|\Gamma\| = 0\) must yield a degeneracy at the transonic velocity \(v\), which in turn requires vanishing discriminant \([9]\)

\[
D(\|\Gamma\|) = 0
\]

\(\text{(15)}\)

which is an equation in \(p\) and \(\varphi\). At the same time, the relation \(p = \tan \phi = \tan (\varphi - \varphi)\) can be reformulated into

\[
\rho = \rho^2(\cos 2\phi + \cos 2\varphi) + 2p \cdot \sin 2\varphi + (\cos 2\phi - \cos 2\varphi) = 0
\]

\(\text{(16)}\)

for the sake of later deduction.

Altogether, we have reached three conditions regarding the parabolic point: \(\rho = 0\) defines its location \(\theta\); \(\rho = 0\) secures degeneracy and gives a relation among \(p\) and \(\varphi\); and \(\rho = 0\) determines the velocity \(\theta\) and \(\varphi\). By eliminating \(\rho v^2, p\) and \(\theta\) from these three equations, one will obtain \(\varphi\) which describes direction of the surface normal at the parabolic point, namely, the swallowtail point. This is done by calculating resultants among these conditions successively \([9,11]\):

\[
g \equiv \text{Res}[\text{Res}(\rho, \rho, \rho), \rho, R].
\]

\(\text{(17)}\)

In the end, the angle \(\varphi\) will be given by
\[ g(\varphi) = 0, \]  

(18)

which defines position of the swallowtail point \( \hat{\varphi}_1 \) explicitly.

Now we continue the case in the (001) plane. Let \( m \) and \( n \) defined by \( m = \cos \varphi e_x + \sin \varphi e_y \), \( n = \sin \varphi e_x + \cos \varphi e_y \). The matrix \( \Gamma \) is still given by (10). From (10) one can formulate characteristic equation \( \| \Gamma \| = 0 \) and its discriminant \( D(\| \Gamma \|) = 0 \). From (14) and (16), the resultant \( g \) can be derived and it is given by

\[
g = (b+1)^2(2b^2+5b+a+2) \\
\left[ (b^2+2ab+3b+a+2)f_{\rho} + 2(b+1)^2(b^2+4b+a+2) \right]^2 \\
\left[ (b^2+4b^2+2ab^2+b^2+7ab+12b^2+3a+4) \right] f_{\rho} \\
+ 2(b^3+7b^2+ab+12b^2+3a+4)(b+1)^2 \Delta \cos^2 2\varphi = 0
\]

(19)

where \( f_{\rho} = (a-1)(a+b) + \Delta (b+1)^2 \) and \( \Delta = a - b - 2 \). Variation of its solution \( \hat{\varphi}_1 \), which define the swallowtail point, illustrated in Fig. 5.

\[ \text{Figure 5. Variation of the swallowtail point } \hat{\varphi}_1 \text{ on Sa.} \]

V. DISCUSSION AND EXAMPLES

For (0\(\bar{1}1\)) plane, similar analysis is carried out. There are two causpidal points (\( \varphi_{2a}, \varphi_{2b} \)) and two swallowtail points (\( \hat{\varphi}_{2a}, \hat{\varphi}_{2b} \)) in the plane. Table 1 and Fig. 6 show results for CaF\(_2\) and GaAs.

### Table 1: Numerical results for CaF\(_2\) and GaAs

<table>
<thead>
<tr>
<th></th>
<th>[001] plane</th>
<th>[110] plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \varphi_1/\hat{\varphi}_1 )</td>
<td>( \varphi_{2a}/\varphi_{2b} )</td>
<td>( \varphi_{2a}/\varphi_{2b} )</td>
</tr>
<tr>
<td>CaF(_2)</td>
<td>37.2 / -</td>
<td>42.2 / 49.8 / 42.6 / 72.3</td>
</tr>
<tr>
<td>GaAs</td>
<td>18.0 / 17.7</td>
<td>13.1 / 83.1 / - / 73.0</td>
</tr>
</tbody>
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VI. CONCLUDING REMARKS

In symmetry planes, the parabolic lines leave two types of signatures: inflectional/parabolic points. These signatures will result in cuspidal/swallowtail caustic points that define main characteristics of the phonon focusing pattern. By recognizing their connection to extraordinary degeneracies in the Stroh eigenvalue equation, we are able to determine explicitly the directions for all the caustic points in terms of simple expressions without solving either Christoffel equation or Stroh equation.