Leaky interface phonons in $Al_xGa_{1-x}As/GaAs$ structures

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A dispersion equation for interface waves is derived for the interface of two cubic crystals in the plane perpendicular to [001]. A reasonable hypothesis is made about the total number of acoustic modes. According to this hypothesis the number is 64, but not all of the modes have the physical meaning of interface waves. Rules have been worked out to select physical branches among all 64 roots of the dispersion equation. The physical meaning of leaky interface waves is discussed. The calculations were made for the interface $Al_{0.3}Ga_{0.7}As/GaAs$. In this case all physical interface modes have been shown to be leaky. The velocities of the interface waves are calculated as functions of an angle in the plane of the interface. The results support a recent interpretation of weakfield magnetoresistance oscillations as a resonant scattering of a two-dimensional electron gas by the leaky interface phonons.

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I. INTRODUCTION

The propagation of acoustic surface and interface waves has attracted significant attention over recent decades. The concept of surface waves goes back to the famous paper by Lord Rayleigh.[1] The interface wave is a simple generalization of the surface wave, when the second medium is not vacuum, and the wave propagates along the boundary between two media. The theoretical study of interface waves was initiated by Stoneley[2] who considered the case of two isotropic solids.

In anisotropic materials the interface waves between hexagonal crystals[3,4] have been studied theoretically in sufficient detail. Relatively little is known about the effects of crystalline anisotropy when the interface is formed by cubic crystals. To the best of our knowledge the only numerical searches for true interface wave velocities for several combinations of materials so far have been carried out in Refs. 5 and 6.

Both surface and interface waves were initially studied in the context of seismological waves propagating in the Earth's crust.[7–10] Later on these waves were studied experimentally in semiconductors by light scattering.[11,12]

The earlier theoretical studies by Lord Rayleigh and Stoneley (see also Ref. 13) were restricted only to those roots of the secular equations that give an exponential decay of the surface wave in the medium under the surface and an exponential decay of the interface wave in both media away from the interface. Phinney[9] was probably the first to consider the so called leaky or pseudo waves that do not obey this prescription. Surface leaky waves have been widely studied theoretically for both isotropic and anisotropic crystalline materials (see the review by Maradudin[14] and references therein). To the best of our knowledge leaky interface waves have been studied only for the isotropic case[9,10] and for hexagonal crystals.[15]

The interest in leaky interface waves is stimulated by the fact that true interface waves exist inside a very narrow range of parameters. Therefore in the general case interface waves are leaky. This is not the case for surface waves where a true nonleaky mode always exists in a wide range of parameters.[16] However, the dispersion equation for surface waves also has several roots that give leaky solutions.

Structures with a two-dimensional electron gas (2DEG), such as heterostructures or quantum wells, provide another source of interest in interface waves. The interaction of a 2DEG with surface waves was investigated long ago.[17,18] If the 2DEG is far from the surface, the electrons may interact with interface waves. For example, the electrons may be scattered by thermally excited interface waves. This scattering should not be weaker than scattering by bulk phonons, since in the vicinity of the interface the three-dimensional densities of the bulk and interface phonons are of the same order. In Ref. 19 we explained the oscillations of magnetoresistance, observed in a high-mobility 2DEG in GaAs-$Al_xGa_{1-x}As$ heterostructure, by a magnetophonon resonance originating from the interaction of the 2DEG with thermally excited leaky interface acoustic phonon modes.

The primary goal of this paper is the calculation of the interface waves for an $Al_{0.3}Ga_{0.7}As/GaAs$ interface on the basal (001) face. This is exactly the interface used in the Ref. 19. We have shown that all interface waves in this case are leaky. To this end we have derived analytically the secular equation for the phase velocity v of the waves at the interface between two cubic crystals. We have discussed the selection rules for the modes and given a general qualitative picture of the leaky interface waves. In this picture we consider the conservation of energy and show that the amplitude of the wave never becomes infinite if the problem is properly formulated. We show that under some conditions leaky waves do not differ substantially from true waves. Finally, we have obtained numerical results, which were partially used in Ref. 19.

The paper is organized as follows. The basis of the method is outlined in Sec. II. In the third section we discuss general properties of the secular equation, the selection rules for its solutions, and the physical meaning of leaky waves. The numerical results and discussion are presented in Sec. IV. Finally, some auxiliary technical material regarding the calculations is given in the Appendix.

II. GENERAL FORMULATION

Within the framework of the linear theory of elasticity the equations of motion of an infinite medium are

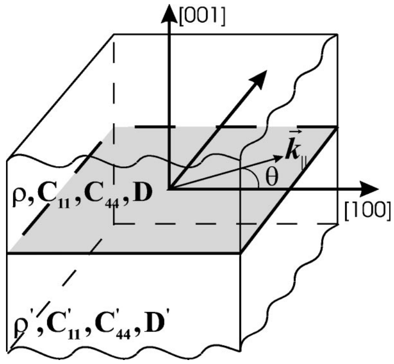

FIG. 1. Structure for the study of interface acoustic waves.

$$\rho \frac{\partial u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j}, \quad i=1,2,3, \tag{1}$$

where ρ is the mass density of the medium, $u_i(\mathbf{r},t)$ is a Cartesian component of the displacement of the medium at the point $\mathbf{r}$ at time t, and $\sigma_{ij}(\mathbf{r},t)$ is the stress tensor. This last is given by Hooke's law

$$\sigma_{ij} = \lambda_{ijkl} \frac{\partial u_k}{\partial x_l}, \tag{2}$$

where λ_{ijkl} is a symmetrical fourth-rank tensor. In a cubic crystal the stress tensor can be conveniently written as

$$\sigma_{ij} = C_{12}(\mathrm{div}\ \mathbf{u})\delta_{ij} + C_{44}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + D\frac{\partial u_i}{\partial x_j}\delta_{ij}, \tag{3}$$

where summation over i and j is not assumed in the last term. Here D is the anisotropy parameter:

$$D = C_{11} - C_{12} - 2C_{44}. \tag{4}$$

For an isotropic medium $D=0$.

In the following analysis we consider a system formed by two semi-infinite cubic crystals. The elastic moduli and density related to the lower part will be denoted by primed symbols (see Fig. 1). The interface coincides with the plane (001) and it is perpendicular to the x_3 axis. The coordinate axes x_1, x_2, and x_3 coincide with the [100], [010], and [001] directions, respectively, for both cubic media.

The equations of motion (1) have to be supplemented by the boundary conditions at the interface, expressing the continuity of the displacement and normal components of the stress tensor:

$$u_i = u_i'|_{x_3=0}, \quad i=1,2,3, \tag{5}$$

$$\sigma_{i3} = \sigma_{i3}'|_{x_3=0}, \quad i=1,2,3. \tag{6}$$

Homogeneous plane waves (bulk phonons) are the simplest solutions of the wave equation in one infinite medium. They are

$$\mathbf{u}^{(l)}(\mathbf{r},t) = \exp(i\mathbf{k}_\parallel\cdot\mathbf{x}_\parallel + ik_3x_3 - i\omega_{(l)}t) \tag{7}$$

for three different branches $l=1,2,3$, where $\mathbf{x}_\parallel$ and $\mathbf{k}_\parallel$ are two-dimensional vectors with components $(x_1,x_2,0)$ and $(k_1,k_2,0)\equiv k(\cos\theta,\sin\theta,0)$, respectively (the angle θ is measured from the [100] direction), and $\omega_{(l)} = s_{(l)}\sqrt{k^2+k_3^2}$ with the bulk sound velocity $s_{(l)} = s_{(l)}(\theta,\phi)$, where $\cos\phi = k_3/\sqrt{k^2+k_3^2}$.

The solution for the phase velocity can be determined by substituting the plane wave of Eq. (7) into the equations of motion (1). This yields a homogeneous set of linear equations. Setting the determinant of the coefficients equal to zero produces a cubic equation in v^2. The three roots of this equation are the squares of the velocities for three bulk phonons.

For propagation along the (001) plane one of the velocities $t_1 = \sqrt{C_{44}/\rho}$ is independent of θ and represents a transverse mode. Two others depend on the angle of propagation in the plane. They are neither longitudinal nor transverse, but we denote the upper branch by the letter "l" and the lower one by "t_2."

The interface between two semi-infinite media introduces an inhomogeneity in the x_3 direction. Therefore, we could expect that the plane waves will also become inhomogeneous in this direction. The frequency and wave vector $\mathbf{k}_\parallel$ are the same in both media, but the component k_3 of the wave vector may be complex and different in the upper and lower media. Moreover, since the boundary conditions Eqs. (5) and (6) consist of six equations, the simplest solution for an arbitrary direction of propagation should consist of a linear superposition of three terms described by Eq. (7) for each medium, with their own different complex components k_3.

The subsequent analysis is facilitated by performing a rotation of the coordinate frame in such a way that the direction of propagation of the acoustic wave in the plane of the interface is along the $\tilde{x}_1$ axis, i.e., $\tilde{\mathbf{k}}_\parallel = (k,0,0)$. Let

$$\hat{\mathbf{T}} = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{8}$$

be the transformation matrix that produces this rotation. Then the transformation law for the elements of the elastic modulus tensor under this rotation is

$$\tilde{\lambda}_{ijkl} = \sum_{i'j'k'l'} T_{ii'}T_{jj'}T_{kk'}T_{ll'}\lambda_{i'j'k'l'}. \tag{9}$$

At the first stage of the analysis we determine the possible values of k_3 for a given value of k. To this end, we define $k_3 \equiv ik\beta$, $\omega = kv$, and we suggest a solution for the interface waves in the rotated system in the form

$$u_i = A_i e^{-k\beta\tilde{x}_3}\exp[ik(\tilde{x}_1 - vt)] \quad \text{for} \quad \tilde{x}_3 > 0,$$

$$u_i' = A_i' e^{k\beta'\tilde{x}_3}\exp[ik(\tilde{x}_1 - vt)] \quad \text{for} \quad \tilde{x}_3 < 0. \tag{10}$$

The subsequent analysis is carried out in the rotated system only. Therefore we omit tildes for the sake of convenience. Conceptually, the x_3 dependence is a part of the "amplitude" (see Ref. 20) and the wavelike properties are described by a common propagation part $\exp[ik(x_1 - vt)]$. Thus, the propagation vector is always assumed to be parallel to the interface even though the exponent β may be complex.

If $\mathrm{Re}\beta,\beta'>0$, then such a form describes a wave that propagates in the x_1 direction, whose amplitude decays exponentially with increasing distance into each medium from the interface. The waves with (i) $\mathrm{Re}\beta<0$ and $\mathrm{Im}\beta<0$, (ii) $\mathrm{Re}\beta'<0$ and $\mathrm{Im}\beta'<0$, (iii) $\mathrm{Re}\beta,\beta'<0$, and $\mathrm{Im}\beta,\beta'<0$ are leaky waves that radiate energy outward from the interface.

Substituting Eqs. (9) and (10) into the equations of motion (1) yields a set of homogeneous equations for each medium,

$$L_{ij}(v,\beta)A_j=0,$$

$$L'_{ij}(v,\beta')'A'_j=0, \qquad (11)$$

where the matrix $\mathbf{L}$ (or $\mathbf{L}'$) has the form

$$\begin{bmatrix} -C_{44}\beta^2+C_{11}-\frac{1}{2}D\sin^2 2\theta-\rho v^2 & -\frac{1}{4}D\sin 4\theta & \pm i\beta(C_{11}-C_{44}-D) \\ -\frac{1}{4}D\sin 4\theta & -C_{44}\beta^2+C_{44}+\frac{1}{2}D\sin^2 2\theta-\rho v^2 & 0 \\ \pm i\beta(C_{11}-C_{44}-D) & 0 & C_{44}-C_{11}\beta^2-\rho v^2 \end{bmatrix}. \qquad (12)$$

The sign plus (minus) corresponds to the upper (lower) medium, and we omitted primes for the lower medium. In each medium Eqs. (11) have nontrivial solutions if the corresponding determinant of the coefficients vanishes:

$$\det(\mathbf{L})=0. \qquad (13)$$

This gives the secular equation for the unknown values of β with the phase velocity v as a parameter. The explicit form of Eq. (13) is given in the Appendix. The plane of the interface coincides with the plane (001) for both cubic crystals. This is a plane of mirror symmetry for both of them if they are considered separately. Because in our solution the vector $\mathbf{k}_\parallel$ is in this plane (see Fig. 1), the secular equation is bicubic in β and the roots have inversion symmetry with respect to the origin of the complex plane.[20]

One can also show that, if $\beta_l=\beta_{Rj}+i\beta_{Ij}$ for $j=1,\ldots,6$ are the roots of Eq. (13) with a complex velocity $v=v_R+iv_I$, then the roots $\beta_j=\beta_{Rj}-i\beta_{Ij}$ are the roots of the same equation with $v=v_R-iv_I$. Here the superscripts ''R'' and ''I'' denote the real and imaginary parts, respectively.

The amplitudes A_α (or A'_α) for any β_j (β'_j) are related by

$$\frac{A_1^{(j)}}{C_1^{(j)}}=\frac{A_2^{(j)}}{C_2^{(j)}}=\frac{A_3^{(j)}}{C_3^{(j)}}=K_j, \quad j=1,\ldots,6, \qquad (14)$$

where the K_j are constants and $C_\alpha^{(j)}(v,\beta_j)$ ($\alpha=1,2,3$) are the cofactors of the elements in the first row of the matrix $\mathbf{L}$:

$$C_1^{(j)}=L_{22}L_{33},$$

$$C_2^{(j)}=-L_{21}L_{33},$$

$$C_3^{(j)}=-L_{31}L_{22}.$$

The next step of our analysis is the construction of the general solution, that satisfies the boundary conditions Eqs. (5) and (6). To this end, we form linear combinations from the three terms (10) with undefined constants K_j and K'_j for each medium:

$$u_\alpha=\sum_{j=1}^{3}\frac{C_\alpha^{(j)}}{C_1^{(j)}}K_j\exp[ik(x_1-vt+i\beta_j(v)x_3)] \quad \text{for } x_3>0,$$

$$u'_\alpha=\sum_{j=1}^{3}\frac{C'^{(j)}_\alpha}{C'^{(j)}_1}K'_j\exp[ik(x_1-vt-i\beta'_j(v)x_3)], \quad \text{for } x_3>0. \qquad (15)$$

Substitution of this form for the displacement field into Eqs. (5) and (6) leads to a set of six (in the general case) homogeneous linear equations for K_j,K'_j. Nontrivial solutions exist if the corresponding determinant vanishes:

$$|D_{kl}^{(\gamma)}(v)|=0, \quad k,l=1,\ldots,6. \qquad (16)$$

Equation (16) is the dispersion relation for the phase velocity v of the interface acoustic wave. In general it has to be solved numerically. The left hand side function $D(v)\equiv|D_{kl}^{(\gamma)}|$ is some algebraic expression. Therefore, in general, the roots of Eq. (16) are complex. Moreover, since $D(v)$ contains six different decay constants $\beta_j(v),\beta'_j$, which involve square roots of some expressions of v^2, the function $D(v)$ is a multivalued analytical function of the complex variable v, defined on its associated Riemann sheets. The superscript γ enumerates these sheets. The number of Riemann sheets is determined by different combinations of β branches. However, not all of $6!/3!3!=20$ combinations of β_j are possible for each medium in the superpositions of Eq. (15). Each of the three decay constants must be taken from the different roots β^2 of the cubic equation $\det(\mathbf{L})=0$ for fixed v^2. Therefore, the total number of possible combinations is $2^3\times 2^3=64$. This is the number of Riemann sheets for our case. Since a simultaneous change of all signs of

β,β' in Eq. (16) does not change the form of determinant (see the Appendix), it is enough, in fact, to investigate 32 independent Riemann sheets in order to find all possible roots of the dispersion relation. In the isotropic case and for propagation along the directions of high symmetry the number of independent Riemann sheets reduces to eight.

The sign convention for the sheets is determined by the real part of β. It is denoted as follows:

$$(\mathrm{sgn}\,\mathrm{Re}(\beta_1),\mathrm{sgn}\,\mathrm{Re}(\beta_2),\mathrm{sgn}\,\mathrm{Re}(\beta_3),\mathrm{sgn}\,\mathrm{Re}(\beta_1'),\mathrm{sgn}\,\mathrm{Re}(\beta_2'),\mathrm{sgn}\,\mathrm{Re}(\beta_3')). \tag{17}$$

Let us assume that $\gamma=1$ corresponds to the case $(++++++)$. If a solution exists on this sheet, then it is a true interface wave, which is also called a Stoneley wave. All other γ correspond either to leaky waves or to nonphysical solutions. Some of them may also correspond to bulk phonons (see Sec. III). In the next section we formulate selection rules for physical solutions. The correct direction of the energy flux is the main principle for the selection. The explicit form of Eq. (16) and the method of enumerating its Riemann sheets are given in the Appendix.

III. SELECTION RULES FOR THE VELOCITY AND THE PHYSICAL MEANING OF LEAKY WAVES

The question of the total number of possible values of the velocity was investigated in the early 1970s theoretically[21] for the isotropic solid-liquid interface, and numerically for the case of two isotropic solids.[10] In the case of the liquid-solid interface there are *eight* Riemann sheets. It is shown[21] that the roots on all these sheets are the roots of an eighth-order polynomial in v^2 with real coefficients, and so there are *eight* complex roots which are either real or come in complex conjugate pairs. Numerical investigation of the Stoneley equation (A20) for an isotropic solid-solid interface[10] has shown that there are 16 independent roots on its 16 Riemann sheets.

Thus, we can put forward a simple hypothesis: The number of possible values of v^2 is equal to the number of Riemann sheets. However, some of them may be degenerate so we are speaking about the *maximum* number of different v^2. Note that this hypothesis is true for isotropic surface waves as well. It follows from it that the maximum number of modes in our interface is 64. To check this hypothesis we have calculated this number for one direction that does not have any special symmetry. The result is 64.

Let us turn now to the problem of classifying the roots for the case $\gamma>1$. First of all we discuss real roots for v of the dispersion equation Eq. (16). If all β are pure imaginary, this corresponds to the refraction of bulk phonons and has nothing in common with leaky waves. If at least one of the β on either side has a negative real part, such a solution should be considered as nonphysical. If it happens that some β are imaginary but some are complex with positive real part, then this relates to the problem of total internal reflection of bulk phonons. In our subsequent numerical analysis we discard such solutions, since they have a different nature.

Now we come to complex v. Let us assume that we have a real positive frequency $\omega>0$ and a complex root

$$v=v_R\mp iv_I \tag{18}$$

of Eq. (16). As follows from the Appendix all complex roots form such pairs. Then the wave vectors of propagation along the x_1 axis for these solutions will be complex and equal to

$$k=\omega/v=\omega/(v_R\mp iv_I)=k_R\pm ik_I. \tag{19}$$

If $k_R>0$, it corresponds to a running wave propagating from the left to the right with exponentially decreasing or increasing amplitude. Since both of these solutions always occur in pairs we will consider only the wave attenuated from the left to the right. Then we should chose only the root k_R+ik_I or v_R-iv_I, where $v_R,v_I,k_R,k_I>0$.

Since $\gamma>1$, one or several β have negative real part, i.e.,

$$\beta=-\beta_R-i\beta_I, \tag{20}$$

where $\beta_R>0$ and sgn β_I is not determined yet.

It is useful to introduce the following notations:

$$\tilde{v}_R=(v_R^2+v_I^2)/v_R, \tag{21}$$

$$\tilde{\beta}_R=\beta_R-\beta_I v_I/v_R, \tag{22}$$

$$\tilde{\beta}_I=\beta_I+\beta_R v_I/v_R. \tag{23}$$

After the substitution $k=\omega/v$ the term has the form of an inhomogeneous plane wave

$$e^{-i\omega(t-x/\tilde{v}_R-z\tilde{\beta}_I/\tilde{v}_R)}e^{-\omega/\tilde{v}_R(xv_I/v_R-z\tilde{\beta}_R)}. \tag{24}$$

In fact, the sign of β_I is not arbitrary, but is dictated by the radiation condition.[22,23] Indeed, since we consider here lossless media the only reason for the amplitude attenuation along the direction of propagation on the interface is the radiation of energy away from the interface into the bulk media. The total wave vector $\mathbf{q}=\omega/\tilde{v}_R(1,0,\tilde{\beta}_I)$ is no longer parallel to the boundary, but is inclined to it, which indicates the presence of a continuous flow of energy from the boundary to the bulk. Note that the direction of phase propagation $\mathbf{q}/q$ does not represent the direction of energy flow itself. The latter is determined by the time-averaged power flux

$$W_\alpha=-\mathrm{Re}\left\langle\frac{1}{2}\sigma_{\beta\alpha}\dot{u}_\beta^*\right\rangle,\quad \alpha,\beta=1,2,3. \tag{25}$$

One can show that for small v_I the sign of the component W_3 that determines the flow perpendicular to the interface coin-

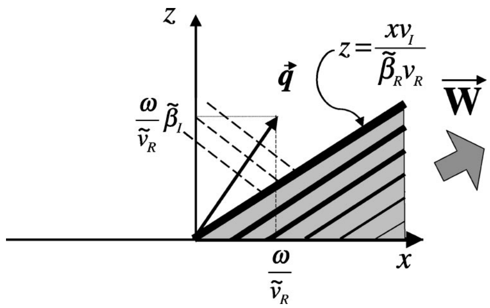

FIG. 2. Illustration of geometry of leaky interface wave term. Power flux **W** and wave vector **q** are shown. The full lines with different thicknesses are the lines of constant amplitude. The thickness of the line indicates schematically the absolute value of the amplitude. Dashed lines are the lines of constant phase. For visual clarity the angle of the constant amplitude lines has been exaggerated.

cides with the sign of $\tilde{\beta}_I$. Therefore, in the notations of Eq. (20) the sign $\tilde{\beta}_I$ must be positive to guarantee the proper radiation condition.

Now we come to the physical meaning of the leaky waves. Discussing Rayleigh waves, Landau and Lifshitz[13] prescribe dropping as nonphysical a solution that increases away from the surface. In the theory of leaky waves we take such a solution into consideration. The goal of this part is to give a physical explanation of leaky waves (see also the review by Maradudin[24]).

On both sides of the interface our solution consists of three inhomogeneous plane waves. At large values of x and z these waves can be considered as independent. So we concentrate on one of them, choosing the wave at $z>0$ with negative real part of β, i.e., a wave exponentially increasing with z. This wave has the form of Eq. (24):

$$e^{-i\omega(t-x/\tilde{v}_R-z\tilde{\beta}_I/\tilde{v}_R)}e^{-\omega/\tilde{v}_R(xv_I/v_R-z\tilde{\beta}_R)}, \tag{26}$$

where $\tilde{\beta}_R>0$ and $\tilde{\beta}_I>0$. This is an inhomogeneous bulk plane wave with wave vector $\mathbf{q}=\omega/\tilde{v}_R(1,0,\tilde{\beta}_I)$ propagating away from the interface. The lines of constant phase are determined by the equation $t-x/\tilde{c}_R-z\tilde{\beta}_I/\tilde{c}_R=C_1$, and the lines of constant amplitude are given by the equation $xv_I/v_R-z\tilde{\beta}_R=C_2$ (see Fig. 2). The latter expression shows that such modes attenuate when they move along the surface $z=0$.

The central point of our understanding of leaky waves is that one cannot consider these waves in the entire region of x values, since their amplitude becomes infinite when $x\to -\infty$. This happens because we have chosen the solution that propagates from the left to the right along the x axis. Thus, we should propose that the wave is created at some line, say $x=0$, in the plane of the interface. Our equations of motion do not include any dissipation; therefore the attenuation in the plane of the interface may be due only to radiation into the media. There is an important theorem[25] stating that for inhomogeneous plane waves the energy flux is parallel to the plane of constant amplitude. The cross sections of these planes with the plane zx are shown by full lines of different thickness. The uppermost line is thickest because the amplitude of the wave at the line $x=0$ is the largest, and it decreases with increasing x. That is why the amplitude at any point x increases with z for $z<xv_I/\tilde{\beta}v_R$. It follows from the above theorem that the energy flux cannot cross the planes of constant amplitude. It also cannot cross the plane of maximal amplitude. This means that the entire wave is within the wedge formed by the plane of the interface and the plane of maximal amplitude $z=xv_I/\widetilde{\beta_R v_R}$, at least in the sense that the entire energy of the wave is within this wedge. The amplitude of the wave is finite everywhere in this region.

One gets a severe contradiction on considering a stationary problem. Indeed, Eq. (26) gives a nonzero result outside the wedge as well. Moreover, the amplitude diverges when z tends to infinity. This is an artifact of the stationary consideration. The origin of the divergence is the infinite amplitude of the wave at the point $x=-\infty$. The increase of the amplitude at large z is an artifact originating from the flux coming from large negative x.

It is important to mention that the leaky wave does not differ substantially from a true interface wave only if $k_R \gg k_I$ in Eq. (18 or $v_R \gg v_I$. Since β_R is not small, this means that the angle between the plane, forming the wedge in Fig. 2 should be small. If this condition is not satisfied, the interface (or surface) wave cannot be considered as a wave since the wavelength is larger than the attenuation length.

The problem does not contain any small parameter that could cause this condition to be fulfilled. The numerics show, however, that the majority of modes have small attenuation. The roots of this phenomenon are not clear to us.

Thus, based on the discussion in this section we use the following selection rules for the values $v=v_R-iv_I$ that are solutions of Eq. (16). (1) $v_R>0$, $v_I\geqslant 0$. (2) If $v_I=0$, then Re β, Re $\beta'>0$. (3) If $v_I>0$ and Re $\beta<0$, then Im $\beta<0$. (4) If $v_I>0$ and Re $\beta'<0$, then Im $\beta'<0$.

IV. NUMERICAL RESULTS

To calculate velocities as a function of angle we use Eq. (A1) for β^2 and Eq. (A6). A numerical search for all the roots in the entire complex v plane is a very time-consuming process. Therefore we restrict our search to the rectangular region defined by the limits $2<v_R<7$ km/s, $0<v_I<0.6$ km/s. Our analysis have shown that almost all modes are located in this rectangle. Although some of the modes are outside the region, we have found that usually such modes either are nonphysical or have a very strong attenuation. Our choice of the particular interface $Al_{0.3}Ga_{0.7}As/GaAs$ was dictated by the experiment Ref. 19. In the first step we divide the complex plane v in the interval $2<v_R<7$ km/s, $0<v_I<0.6$ km/s into 400 squares. For a vertex of each square we find six values of β for the upper medium and six values of β' for the lower medium using Eq. (A1). For each value of v we find 32 different combinations of β (each of six values) and substitute them into Eq. (A6). For each Riemann sheet γ we find all minima of abs($|D_{ij}^{(\gamma)}(v)|$) with respect to v_R and v_I using a standard program. For those minima that are close to zero, we do an iterative search for roots. The parameters

TABLE I. Densities (g/cm^3), elastic constants (10^{10} N/m^2), and sound velocities (km/s) in the directions of high symmetry for bulk crystals (Ref. 26).

Crystal	ρ	C_{11}	C_{12}	C_{44}	$l_{[100]}$	t_1	$l_{[110]}$	$t_{2[110]}$
$Al_{0.3}Ga_{0.7}As$	4.794	12.24	5.65	5.90	5.05	3.51	5.56	2.62
GaAs	5.307	12.26	5.71	6.0	4.81	3.36	5.31	2.48

of the bulk lattices have been taken from Table I. To check the method some results were obtained using the completely different surface Green function matching method.[27,28,4] We have not found any differences between the results of the two methods.

For an additional check of the problem we have calculated true surface waves for both materials. The dispersion relation for surface waves on a (001) cut of cubic crystals can be obtained from the determinant of the truncated interface matrix Eq. (A5). For the upper (lower) medium we should take the lower left (right) 3×3 part of the matrix. We obtained 2.873 km/s (2.737 km/s) for GaAs ($Al_{0.3}Ga_{0.7}As$). These results may be compared with the results of Farnell.[20] Our results are slightly different because of the difference in the parameters of the bulk materials. Taking the parameters used by Farnell, we obtained his velocities with a very high accuracy.

The results for leaky interface waves are shown in Fig. 3 and Fig. 4. In plotting these figures we have taken into account all selection rules formulated at the end of Sec. III. The discontinuities appear because at some points these rules are not fulfilled and the corresponding modes become nonphysical. All the modes have different anisotropy, different attenuation, and different angular intervals in which they exist. In Fig. 3 we draw all the modes [note that the velocity scales in 3(a) and 3(b) are different]. One can see that there is an abundant number of leaky interface modes in the velocity range between 3 and 4 km/s. A thorough analysis shows, however, that a majority of these modes exists in a very restricted range of angles. It will probably be difficult to detect them experimentally. In Figure 4 we draw selected modes that exist in a large interval of the angles only. We left one mode (A) with a small angle range in the figure as a typical example of discarded modes. For further clarification of the picture we also discard all physical modes with a strong anisotropy of the real and/or imaginary parts of their velocity. One such mode with a strong anisotropy of the real part (B) is left in the figure as an example.

All numerical parameters for the modes presented in Fig. 4 are given in Table II. For classification of the modes we introduce the following parameters. (1) The real $\overline{v_R}$ and imaginary $\overline{v_I}$ parts of the velocity averaged over angles. (2) The angle range parameter $\delta_{an}=(\varphi_{\max}-\varphi_{\min})4/\pi$. It equals unity when a mode exists in the entire range of angles, and is smaller than unity otherwise. (3) Anisotropy parameters for the real and imaginary parts of the velocity,

$$\sigma_{v_R}=(v_{R\max}-v_{R\min})/\overline{v_R}, \quad \sigma_{v_I}=(v_{I\max}-v_{I\min})/\overline{v_I}. \tag{27}$$

Modes with smaller anisotropy have smaller σ.

Among the modes there are two (C and D in the figure) that are reminiscent of those in the surface acoustic problem. That is, for $Al_xGa_{1-x}As$ materials there are always[20] true surface acoustic waves (SAW's) (they are shown by dotted

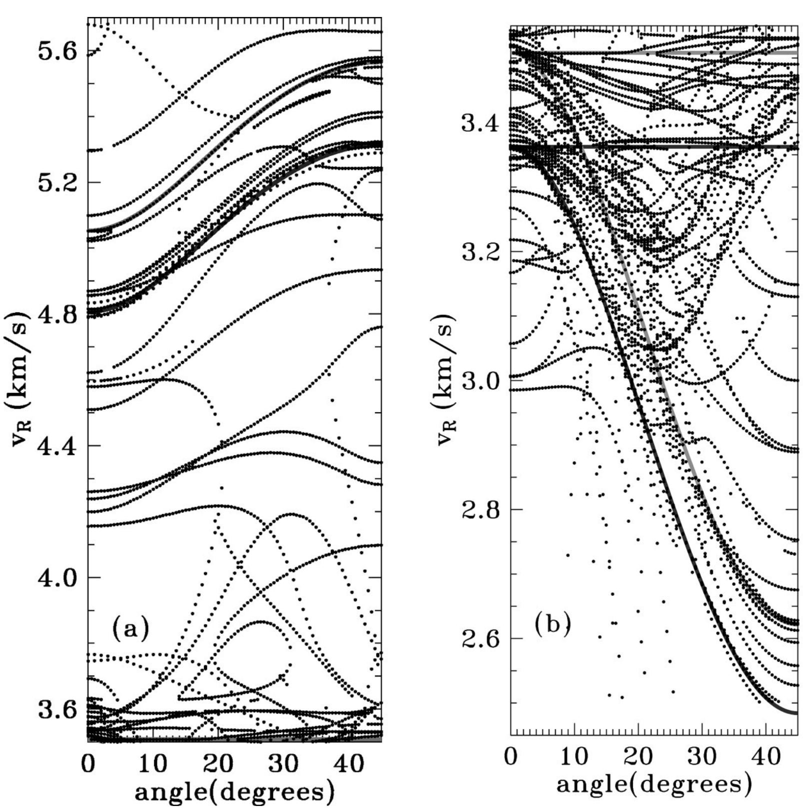

FIG. 3. The real parts of complex velocities for all leaky interface waves in the range $3.5 < v_R < 5.7$ km/s (a) and $2.4 < v_R < 3.5$ km/s (b). The solid lines represent velocities of bulk acoustic waves for both media.

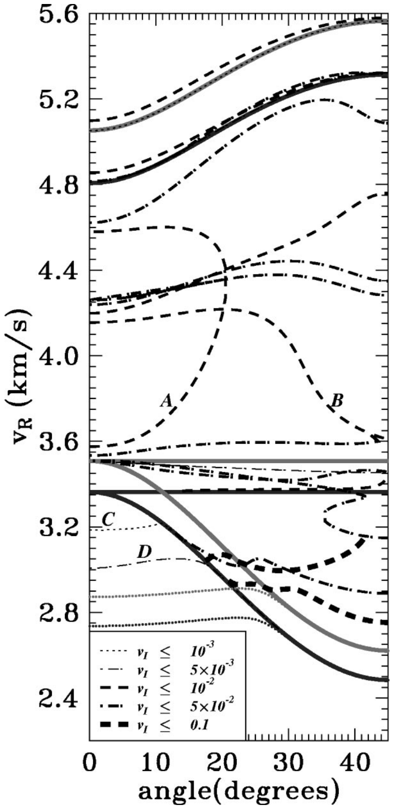

FIG. 4. The real parts of the complex velocities for selected modes in the range $2.4 < v_R < 5.7$ km/s. See explanation in the text. The numerical parameters for these modes are given in Table II. The value of the attenuation is determined by the imaginary part of the complex velocity. Different line styles and thicknesses correspond to different magnitudes of the average imaginary part $\overline{v_I}$ (km/s) of the velocity. The solid lines represent velocities of bulk acoustic waves, and the dotted lines are true surface acoustic waves for both media (Upper curves correspond to $Al_{0.3}Ga_{0.7}As$ and lower curves correspond to GaAs.)

lines in the figure), which change very little with angle until they meet the lowest bulk transverse velocity curves (they are shown by a solid line). After that point the true SAW's repeat the behavior of their bulk velocity curves up to the end—the 45° angle in the figure. Meanwhile, in the region between two transverse bulk velocity curves leaky surface acoustic waves appear with approximately the same real part of their velocity.

The situation for interface waves is different. As we mentioned, there are no true interface waves. However, there are leaky interface waves with a very small attenuation at small angles before they ''collide'' with the bulk transverse velocity curve. At larger angles the leaky modes acquire a larger imaginary part of the velocity and become more strongly attenuated (see Table II).

V. CONCLUSION

We have derived a dispersion equation for interface waves at the interface of two cubic crystals in the plane perpendicular to [001]. By analyzing different solutions for the interface waves we come to the conclusion that the maximum number of interface modes in each direction is equal to the number of its Riemann sheets. In our case this is 64. We have successfully checked this hypothesis by calculating the number of modes in one direction in the interface plane, that does not have any special symmetry.

The computations have been made for the interface $Al_{0.3}Ga_{0.7}As/GaAs$. We showed that in this case all interface modes that have physical meaning are leaky, but the majority of them have a small attenuation in the direction of propagation. We show that to understand the physical meaning of leaky waves one should consider not a stationary problem, but the problem starting with the creation of the wave at some line in the interface plane.

After that we are able to formulate how to separate these 64 modes into physical and nonphysical modes. This separation is mainly based upon some theorems on the energy flux and upon the assumption that, if a mode deviates from the interface in some medium, the energy flux should go into the same medium.

Using the elastic moduli of the bulk lattices we performed numerical calculations of the velocities of the interface waves as functions of an angle in the plane of the interface in a wide range of velocities. The results are shown in Fig. 3. One can see two close groups of modes within the intervals 3–3.5 km/s and 4.2–4.5 km/s, respectively. These groups may be responsible for the two periods of oscillations that have been observed in experiments with the two-dimensional electron gas in a magnetic field,[19] mentioned in the Introduction. Note that the velocities of the leaky interface waves may be sensitive to the difference of the bulk media parameters. This difference is not known well enough. This fact may be responsible for possible deviations of the results of our calculations from the experimental data.

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APPENDIX: EXPLICIT FORM OF THE DISPERSION RELATION IN GENERAL, SYMMETRY DIRECTIONS, AND ISOTROPIC CASES

From the determinant (13) we obtain the following equation for the unknown variable β with the phase velocity v as a parameter:

$$\beta^6-\beta^4\left[a+b+c-\frac{(\lambda^2-1-d)^2}{\lambda^2}\right] +\beta^2\left[ab+bc+ca-b\frac{(\lambda^2-1-d)^2}{\lambda^2}-\tau^2\right]+c(\tau^2-ab) =0, \tag{A1}$$

TABLE II. Parameters for the selected modes. The units for average velocities are km/s.

No.	δ_{an}	$\overline{v_R}$	$\overline{v_I}$	σ_{v_R}	σ_{v_I}	$v_{R\min}$	$v_{R\max}$	$v_{I\min}$	$v_{I\max}$
A	0.46	4.166	6.5×10^{-3}	0.25	0.39	3.58	4.60	5.2×10^{-3}	7.7×10^{-3}
B	0.99	4.022	9.5×10^{-3}	0.15	2.48	3.60	4.22	2.1×10^{-4}	2.4×10^{-2}
C_1	0.26	3.195	1.9×10^{-4}	0.01	2.65	3.18	3.22	1.8×10^{-11}	5.1×10^{-4}
C_2	0.73	3.000	3.3×10^{-2}	0.10	2.50	2.89	3.19	3.8×10^{-7}	8.4×10^{-2}
D_1	0.63	2.966	5.3×10^{-3}	0.11	1.00	2.72	3.05	1.9×10^{-3}	7.2×10^{-3}
D_2	0.53	2.856	6.6×10^{-2}	0.07	2.76	2.75	2.95	2.3×10^{-4}	0.18
1	1	5.369	7.9×10^{-3}	0.09	1.32	5.10	5.58	3.4×10^{-3}	1.4×10^{-2}
2	1	5.167	4.2×10^{-3}	0.1	0.31	4.83	5.32	3.7×10^{-3}	5.0×10^{-3}
3	1	5.330	2.1×10^{-4}	0.1	3.44	5.05	5.56	2.2×10^{-6}	7.1×10^{-4}
4	1	5.112	6.8×10^{-3}	0.09	0.79	4.86	5.32	4.1×10^{-3}	9.4×10^{-3}
5	1	5.115	4.0×10^{-3}	0.1	0.19	4.83	5.32	3.7×10^{-3}	4.5×10^{-3}
6	1	5.104	3.5×10^{-2}	0.1	1.41	4.81	5.32	9.5×10^{-3}	5.9×10^{-2}
7	1	4.960	3.5×10^{-2}	0.12	1.72	4.62	5.20	1.6×10^{-2}	7.7×10^{-2}
8	1	4.446	8.7×10^{-3}	0.13	1.75	4.20	4.76	2.6×10^{-3}	1.8×10^{-2}
9	1	4.360	2.1×10^{-2}	0.05	0.65	4.24	4.44	1.3×10^{-2}	2.7×10^{-2}
10	1	4.323	2.2×10^{-2}	0.03	0.58	4.26	4.38	1.4×10^{-2}	2.7×10^{-2}
11	0.94	3.578	2.0×10^{-2}	0.02	2.22	3.53	3.60	1.2×10^{-3}	4.6×10^{-2}
12	0.99	3.475	3.1×10^{-3}	0.02	1.27	3.45	3.51	2.0×10^{-4}	4.1×10^{-3}
13	0.99	3.452	3.1×10^{-2}	0.03	1.63	3.42	3.51	2.0×10^{-4}	5.1×10^{-2}
14	0.68	3.77	8.8×10^{-3}	0.01	1.35	3.37	3.42	8.6×10^{-4}	1.3×10^{-2}
15	0.99	3.79	4.1×10^{-2}	0.11	1.46	3.15	3.51	2.0×10^{-4}	5.9×10^{-2}
16	0.53	3.040	6.9×10^{-2}	0.05	1.69	3.00	3.15	1.0×10^{-3}	0.12

where

$$a=\lambda^2\left(1-\frac{v^2}{\lambda^2 t^2}\right)-\frac{d}{2}\sin^2 2\,\theta,$$

$$b=1-\frac{v^2}{t^2}+\frac{d}{2}\sin^2 2\,\theta,$$

$$c=\frac{1}{\lambda^2}\left(1-\frac{v^2}{t^2}\right),$$

$$\tau=\frac{d}{4}\sin 4\theta. \tag{A2}$$

The ''weight factors'' in Eq. (15) have the following forms:

$$\frac{C_\alpha^{(j)}}{C_1^{(j)}}=\begin{cases}1 & \text{for } \alpha=1\\ -\dfrac{L_{21}}{L_{22}}\equiv p_2^{(j)}(\beta_j^2)=\dfrac{D/4\sin 4\theta}{-C_{44}\beta_j^2+C_{44}+D/2\sin^2\theta-\rho v^2}, & \text{for } \alpha=2,\\ -\dfrac{L_{31}}{L_{33}}\equiv\mp i\beta_j p_3^{(j)}(\beta_j^2)=\mp i\beta_j\dfrac{C_{11}-C_{44}-D}{C_{44}-C_{11}\beta_j^2-\rho v^2}, & \text{for } \alpha=3,\end{cases} \tag{A3}$$

where the upper sign is for the upper medium, and for the sake of convenience we have omitted primes in formulas for the lower medium. Then, for each term in the sum (15) the condition (6) on the continuity of stress in the rotated frame can be written in the vector form:

$$\begin{bmatrix}\sigma_{13}^j\\ \sigma_{23}^j\\ \sigma_{33}^j\end{bmatrix}=i\begin{bmatrix}\pm i\beta_j C_{44} & 0 & C_{44}\\ 0 & \pm i\beta_j C_{44} & 0\\ C_{12} & 0 & \pm i\beta_j C_{11}\end{bmatrix}\begin{bmatrix}1\\ p_2^{(j)}\\ \mp i\beta_j p_3^{(j)}\end{bmatrix}. \tag{A4}$$

One can can see that the boundary conditions decouple for the sagittal plane $\{x_1x_3\}$ and the perpendicular direction x_2. With the help of Eq. (A4) and minor simplifications we obtain six homogeneous linear equations for the boundary conditions with the matrix $\mathbf{D}(v)$ equal to

$$\begin{bmatrix} 1 & 1 & 1 & -1 & -1 & -1 \\ p_2^{(1)} & p_2^{(2)} & p_2^{(3)} & -p_2'(1) & -p_2'^{(2)} & -p_2'^{(3)} \\ \beta_1 p_3^{(1)} & \beta_2 p_3^{(2)} & \beta_3 p_3^{(3)} & \beta_1' p_3'^{(1)} & \beta_2' p_3'^{(2)} & \beta_3' p_3'^{(3)} \\ C_{44}\beta_1 p_2^{(1)} & C_{44}\beta_2 p_2^{(2)} & C_{44}\beta_3 p_2^{(3)} & C_{44}'\beta_1' p_2'^{(1)} & C_{44}'\beta_2' p_2'^{(2)} & C_{44}'\beta_3' p_2'^{(3)} \\ C_{44}\beta_1(1-p_3^{(1)}) & C_{44}\beta_2(1-p_3^{(2)}) & C_{44}\beta_3(1-p_3^{(3)}) & C_{44}'\beta_1'(1-p_3'^{(1)}) & C_{44}'\beta_2'(1-p_3'^{(2)}) & C_{44}'\beta_3'(1-p_3'^{(3)}) \\ C_{12}+C_{11}\beta_1^2 p_3^{(1)} & C_{12}+C_{11}\beta_2^2 p_3^{(2)} & C_{12}+C_{11}\beta_3^2 p_3^{(3)} & -C_{12}'-C_{11}'\beta_1'^2 p_3'^{(1)} & -C_{12}'-C_{11}'\beta_2'^2 p_3'^{(2)} & -C_{12}'-C_{11}'\beta_3'^2 p_3'^{(3)} \end{bmatrix}. \tag{A5}$$

The condition for a nontrivial solution is that its determinant must vanish:

$$D^{(\gamma)}(v;\beta_1,\ldots,\beta_3')\equiv|D_{ij}^{(\gamma)}|=0. \tag{A6}$$

Since each β is a double-valued function of the complex variable v, this determinant has 64 Riemann sheets, which we denote by the superscript γ.

The sign convention for independent sheets is determined by the real part of β. It is given as follows:

$$\mathrm{sgn}(\mathrm{Re}(\beta_1),\mathrm{Re}(\beta_2),\mathrm{Re}(\beta_3),\mathrm{Re}(\beta_1'),\mathrm{Re}(\beta_2'),\mathrm{Re}(\beta_3')). \tag{A7}$$

That is, the Riemann sheet $(+\ +\ +\ -\ -\ -)$ corresponds to the case $\mathrm{Re}(\beta_j)>0$ and $\mathrm{Re}(\beta_j')<0$, where $j=1,2,3$.

The important property of the determinant is that its solutions are invariant against the simultaneous change of sign of all six decay constants. Indeed, the functions p_2 and p_3 are defined in such a way that they depend on β^2 only. Therefore, from the form of the matrix (A5) it follows that a simultaneous change of the sign of β leaves the secular equation unaltered. Thus, in order to find all the roots of Eq. (A6) it is enough to investigate only 32 independent Riemann sheets. To enumerate these sheets we first solve Eq. (A1) and sort the $\beta(v)$ obtained for each medium in the following order:

$$|\mathrm{Re}(\beta_1)|\leqslant|\mathrm{Re}(\beta_2)|\leqslant|\mathrm{Re}(\beta_3)|.$$

Second, we choose the notation that the sign of the real part β_1 is always positive. Then the uppermost Riemann sheet $\gamma=1$ corresponds to the case $(++++++)$ and the subsequent numbers for lower sheets are given in Table III.

Another feature of Eq. (A6) is the following. If $v=v_R+iv_I$ is the solution of the dispersion relation $D^{(\gamma)}(v)\equiv D_R^{(\gamma)}+iD_I^{(\gamma)}=0$, then $v=v_R-iv_I$ will also be a solution of Eq. (A6). Here we explicitly separated the real and imaginary parts of a complex function. This can be understood from the following consideration. Let $\beta_l=\beta_{R_l}+i\beta_{I_l}$ ($l=1,\ldots,6$) be solutions of Eqs. (13) for $v=v_R+iv_I$; then the solutions of Eqs. (13) for $v=v_R-iv_I$ are $\beta_l=\beta_{R_l}-i\beta_{I_l}$. Moreover, the simultaneous change $v\rightarrow v_R-iv_I$, $\beta_l\rightarrow\beta_{R_l}-i\beta_{I_l}$ in Eq. (A6) leads to a change of sign of the imaginary part of the determinant only:

$$D^{(\gamma)}(v_R-iv_I)=D_R^{(\gamma)}-iD_I^{(\gamma)}.$$

Thus $v=v_R-iv_I$ is also a solution.

If we suggest that the frequency of the interface acoustic wave is real, then $k=\omega/v$ will be complex. We will choose solutions with $v=v_R-iv_I$, which correspond to waves (for $\omega>0$) attenuated along their direction of propagation on the interface.

The dispersion relation simplifies considerably for propagation on the interface (001) along the directions of high symmetry ([100] and [110]) and in the isotropic case. For all these cases the matrix elements $L_{12}=L_{21}\equiv0$ [because $\sin 4\theta=0$ or $D=0$; see Eq. (12)]. Therefore, the system (11) for each medium breaks up into the pair

$$\begin{bmatrix} L_{11} & L_{13} \\ L_{13} & L_{33} \end{bmatrix}\begin{bmatrix} A_1 \\ A_3 \end{bmatrix}=0 \tag{A8}$$

and

TABLE III. Enumeration of Riemann sheets.

γ	Re β_1	Re β_2	Re β_3	Re β_1'	Re β_2'	Re β_3'
1	+	+	+	+	+	+
2	+	+	+	+	+	−
3	+	+	+	+	−	+
4	+	+	+	−	+	+
5	+	+	+	+	−	−
6	+	+	+	−	+	−
7	+	+	+	−	−	+
8	+	+	+	−	−	−
9	+	+	−	+	+	+
. . .	. . .	. . .	. . .	. . .	. . .	. . .
17	+	−	+	+	+	+
. . .	. . .	. . .	. . .	. . .	. . .	. . .
25	+	−	−	+	+	+
. . .	. . .	. . .	. . .	. . .	. . .	. . .
32	+	−	−	−	−	−

$$L_{22}A_2=0. \tag{A9}$$

The only nontrivial solution of the latter equation corresponds to a bulk transverse acoustic wave propagating parallel to the interface of the elastic media,[24] and therefore it is discarded. Thus, in these cases the interface waves are polarized in the sagittal plane and do not have a u_2 component.

For interface waves polarized in the sagittal plane the solvability condition for Eq. (A8) is the biquadratic equation

$$\lambda^2\beta^4-\beta^2[\gamma_1^2+\lambda^4\gamma_2^2-(\lambda^2-1-d)^2]+\lambda^2\gamma_1^2\gamma_2^2=0, \tag{A10}$$

where we have introduced the notation

$$\lambda^2=C_{11}/C_{44}, \tag{A11}$$

$$d=D/C_{44}, \tag{A12}$$

$$\gamma_1^2=1-v^2/t^2, \tag{A13}$$

$$t^2=C_{44}/\rho, \tag{A14}$$

and

$$\gamma_2^2=\begin{cases}1-v^2/(\lambda t)^2 & \text{for } \theta=0\\ 1-d/2\lambda^2-v^2/(\lambda t)^2 & \text{for } \theta=\pi/4.\end{cases} \tag{A15}$$

In the isotropic case ($d=0$) Eq. (A10) reduces to

$$\beta^4-\beta^2(\gamma_1^2+\gamma_2^2)-\gamma_1^2\gamma_2^2=0 \tag{A16}$$

with the obvious solutions

$$\beta_1=\pm\sqrt{1-v^2/t^2},$$

$$\beta_2=\pm\sqrt{1-v^2/(\lambda t)^2}. \tag{A17}$$

For all these cases the general solutions for the interface waves are linear combinations of two partial waves in both media:

$$u_1(\mathbf{r},t)=[K_1e^{-k\beta_1x_3}+K_2e^{-k\beta_2x_3}]e^{ik(x_1-vt)},$$

$$u_3(\mathbf{r},t)=[K_1p_3^{(1)}e^{-k\beta_1x_3}+K_2p_3^{(2)}e^{-k\beta_2x_3}]e^{ik(x_1-vt)},$$

$$u_1'(\mathbf{r},t)=[K_1'e^{k\beta_1'x_3}+K_2'e^{k\beta_2'x_3}]e^{ik(x_1-vt)},$$

$$u_3'(\mathbf{r},t)=[K_1'p_3'^{(1)}e^{k\beta_1'x_3}+K_2'p_3'^{(2)}e^{k\beta_2'x_3}]e^{ik(x_1-vt)}. \tag{A18}$$

After substituting solution (A18) into the boundary conditions (5) and (6) we obtain a set of four homogeneous linear equations with solvability condition

$$\begin{vmatrix} 1 & 1 & -1 & -1\\ \beta_1p_3^{(1)} & \beta_2p_3^{(2)} & \beta_1'p_3'^{(1)} & \beta_2'p_3'^{(2)}\\ C_{44}\beta_1(1-p_3^{(1)}) & C_{44}\beta_2(1-p_3^{(2)}) & C_{44}'\beta_1'(1-p_3'^{(1)}) & C_{44}'\beta_2'(1-p_3'^{(2)})\\ C_{12}+C_{11}\beta_1^2p_3^{(1)} & C_{12}+C_{11}\beta_2^2p_3^{(2)} & -C_{12}'-C_{11}'\beta_1'^2p_3'^{(1)} & -C_{12}'-C_{11}'\beta_2'^2p_3'^{(2)}\end{vmatrix}=0. \tag{A19}$$

For the isotropic case $p_3^{(1)}=-1/\beta_1^2$ and $p_3^{(2)}=-1$. Then the resulting dispersion relation reduces[2] to

$$\begin{aligned}&v^4[(\rho-\rho')^2-(\rho\beta_2'+\rho'\beta_2)(\rho\beta_1'+\rho'\beta_1)]\\&\quad+4Fv^2[\rho\beta_1'\beta_2'-\rho'\beta_1\beta_2-\rho+\rho']\\&\quad+4F^2(1-\beta_1\beta_2)(1-\beta_1'\beta_2')=0,\end{aligned} \tag{A20}$$

where

$$F=\rho t^2-\rho' t'^2. \tag{A21}$$

There are 16 independent roots on eight different Riemann sheets for the given equation. There is always a nonattenuated solution for $t=t'$, $\lambda=\lambda'$ and $\rho\neq\rho'$.

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