Due to rapid developments in nanotechnology and the importance of nanomaterial characterization, the study of the acoustic response of small structures is of significant current interest. Frequency domain techniques such as Raman scattering and direct time-resolved pump-probe experiments are nondestructive and complementary tools to detect and identify these acoustic vibrations. A possible application of these experimental works is the determination of the geometry of a nanostructure.

For this to be practical, one needs to find a way to go from a measurement of the set of frequencies of the normal modes to a determination of the values of whatever set of parameters are used to describe the shape. M. Kac drew attention to this general class of problem in a famous paper in 1966 entitled “Can one hear the shape of a drum?” However, in fact, the problem is more difficult than it appears because it turns out that the frequencies vary with the dimensions in a surprisingly complicated way as we will discuss in this thesis.

“Level repulsion” related mode localization is our primary interest. In 1956 Shaw observed a prominent vibration resonance localized at the edge of a thick barium titanate disk. It is known that for certain special values of Poisson’s ratio these modes are perfectly localized, are uncoupled to bulk modes, and thus do not lose energy by acoustic radiation. In this thesis we consider the conditions for mode localization in different structures, and show that regardless of the value of Poisson’s ratio it is often possible to
design a structure with an end shape such that a perfectly localized mode appears. This localization has interesting effects on the way that the vibrational patterns and frequencies of the normal modes of a structure are changed when the dimensions of the structure are altered.
Localized Modes and the Vibrations of Nanostructures

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A Dissertation Submitted in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy in the Department of Physics at Brown University

Providence, Rhode Island
May 2010
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This dissertation by Jing Ma is accepted in its present form by the Department of Physics as satisfying the dissertation requirement for the degree of Doctor of Philosophy.

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*Communications in Theoretical Physics, 43*: 341 - 348 (2005).


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Accepted by Journal of Applied Physics.

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Submitted to the 13th international conference on phonon scattering in condensed matter.

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Submitted to the 13th international conference on phonon scattering in condensed matter.
Acknowledgements

First and foremost, I would like to show my deep and sincere gratitude to my advisor Prof. H.J. Maris for his bright guidance and support over these years. His perfection on research and great intuition of physics give me a lot of inspiration. I also want to thank his patience and help when I had a difficult time. Even though I brought him a lot of trouble, he has never given me up.

My thanks go out to Prof. Ben Freund and Prof. Arto Nurmikko for taking time to read my thesis and provide me valuable suggestions. As a physics student, I am very lucky to have many opportunities to discuss my research with Prof. Freund. He always gave me insightful comments, which helps me understand the problem further from the solid mechanics. I have worked with Prof. Nurmikko on the acoustic microscopy project when I just began my Ph.D. study. His broad knowledge on laser and optics impresses me very much.

I wish to thank other people on the faculty and stuff of Brown who have encouraged me in various ways during my course studies, such as Prof. Allan Bower, Prof. Huajian Gao, Mr. Dean Hudek, and Mr. Ken Silva. I also wish to thank my labmates for working together and assisting on my research, especially Tom Grimsley who helps me on the sound and vibration experiments.
I am particularly thankful to the constant support from my best friends. No matter what happens, they always fully trust me and give me comforts. Without them, I won’t be happy at all.

Last, I want to show my deepest gratitude to my family - my dearest husband, my brother and our parents and grandparents. They are always besides me and experiencing the same feeling with me. This thesis cannot be written out without their support.
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Chapter 1

Introduction

In this thesis we will investigate the normal modes of elastic objects. This sounds like a simple thing but in fact it is surprisingly subtle. The study of the acoustic response of small structures is of current interest due to rapid developments in nanotechnology and the importance of nanomaterial characterization, for example, in memory devices [1], mechanical computation [2], molecular scale biological sensing [3] and ultrasensitive mass detection [4]. For these devices, the vibration frequency varies from a few gigahertz to hundreds of gigahertz for submicronic to nanometric sized metal particles and semiconductor quantum dots. Frequency domain technique such as Raman scattering and direct time-resolved pump-probe experiments are nondestructive and complementary tools to detect and identify these acoustic vibrations. The period and damping provides a wealth of information that can be used to understand the nanoobject geometry and structure attributes - size, shape, elastic constants and dielectric environment that they are locally interacting with.

When light encounters an obstacle or inhomogeneity, it will be scattered in all directions. An electromagnetic wave incident on matter induces the separation of charges, and these
dipole moments give a macroscopic polarization with the same frequency $\omega_i$ as the light. Owing to the thermal fluctuations at finite temperatures, the phonon normal modes with frequency $\omega_0$ are excited. These vibrations perturb the electrical susceptibility. Consequently sidebands on each side of the incident frequency of the polarization show up. To the first order in the vibration amplitude, this leads to three distinct frequencies of the scattered light $\omega_i$, $\omega_i + \omega_0$, and $\omega_i - \omega_0$. Scattered radiation with the frequency $\omega_i$ is elastic scattering, also named Mie or Rayleigh scattering. The shifted frequency $\omega_i \pm \omega_0$ is inelastic scattering, and is called Raman scattering. Thus, a measurement of the frequency difference between the scattered photon and the incident photon gives the value of the vibration frequency. If the resulting photon has a lower frequency, it is said to generate a Stokes line with a red shift; if it has a higher frequency, an anti-Stokes line with a blue shift.

Acoustical vibrational modes in nanocrystals were first observed by low-frequency Raman scattering measurements on MgCr$_2$O$_4$-MgAl$_2$O$_4$ material in 1986 [5]. The lowest eigenmodes of a spherical particle were measured and the Raman peak was found to have a linear dependence on the inverse diameter of the particle, agreeing with the Lamb theory of the modes of a homogeneous elastic body with a spherical shape. Later on, more experiments were conducted on quantum dots (QD’s) to study the coupling of vibrational modes to electronic states.

As another approach, ultrafast laser spectroscopy makes possible the direct time domain measurement of vibration frequencies and damping rates of metal nanoparticles and semiconductor QD’s. In experiments with metallic nanoparticles, energy is absorbed by the conduction electrons and quickly transferred to the thermal phonons. The abrupt
heating triggers the dilation and compression of each metal particle, just like a bell begins to ring under a sharp rap. Different elastic oscillations consistent with the symmetry of the initial heating are set into motion. The first investigation on the mechanical vibrations of nanostructures with picosecond ultrasonics was done by Lin et al. [6]. Frequencies and attenuation rates of the normal modes of patterned gold strips and dots on fused quartz substrates are measured. Excellent agreement is achieved between the experiment results and the finite element calculation. Usually modes with the lowest frequencies and with the minimum number of nodes of displacement are preferentially excited. This is because their vibration patterns are more likely to match with the approximately homogeneous heating that occurs if the light wavelength is much larger than the size of a metal particle. These excited modes periodically modulate the particle optical properties and hence may be detected by a time-delayed probe pulse.

Such ultrafast studies have been performed on samples with various shapes, including quantum dots, nanorods, nanoshells, nanocubes, and submicron spiral arrays [7]. This experimental work can be used to determine the geometry of a nanostructure. For this to work, one needs to find a way to go from a set of measured frequencies of normal modes to whatever parameters are used to describe the shape. M. Kac drew attention to this general class of problem in a famous paper in 1966 entitled “Can one hear the shape of a drum?” [8] Specifically, Kac considered the vibrations of a membrane under uniform tension and with a boundary at which the displacement is zero. He asked if knowledge of the frequencies of all the normal modes of a membrane is sufficient to determine the shape of the fixed boundary. It has been shown by example that, in fact, the shape cannot always be determined. First, Milnor was able to show that in 16 dimensions there could
be multiple shapes with the same frequencies (this was actually published before the paper by Kac) [9]. In 1998 Zelditch showed that in 2D if the shape is everywhere convex, the shape can be determined [10]. When the shape is not everywhere convex, he was able to give a specific example of two shapes which had all normal mode frequencies the same.

For practical applications, one is generally interested in a simpler problem. For example, one might be willing to assume that the structure under study is a rectangular prism with sides $a, b, c$. Then the problem would be to determine these parameters using the values of some set of measured normal mode frequencies $\{\omega_n\}$. At first sight, it would appear that this should be rather easy. However, in fact, the problem is more difficult than it appears because it turns out that the frequencies vary with the dimensions in a surprisingly complicated way as discussed in what follows. One can consider that these complications arise because for any particular values of the set of dimension parameters, the different normal modes may have very different characters. As a result, when one particular parameter $P$ is changed this may have a large effect on the frequency of some modes but a very small effect on the frequency of others. This leads to the frequency of adjacent modes approaching one another. And if the modes have the same symmetry, “level repulsion” occurs and there is a rapid change in the character of each of the original modes in some range of values of $P$. This effect has been studied in many papers, see, for example, the experimental work of Shaw [11] and the calculations of Gazis and Mindlin [12] for the modes of discs. This phenomenon of level repulsion is particularly interesting when one of the two modes is a vibration that is approximately localized in some part of the structure.
Based on the foregoing researches, this thesis is devoted to achieving a physical understanding of a change in the eigenmode frequencies that results from a change in shape or elastic properties of the sample. It is a very fundamental yet elusive question.

We are starting with a review of elastic wave propagation in an infinite plate in Chapter 2. Stress free boundary conditions give rise to a transcendental relation between angular frequency $\omega$ and propagation wave vector $k$. The dispersion curves can be continued from real space into complex space. In Chapter 3, the reflection of a Lamb wave incident on a straight edge of a semi-infinite plate is discussed. If the incident wave is the lowest symmetric Lamb wave carrying with an appropriate frequency, the edge resonance will be excited. For the particular values of Poisson’s ratio $\nu = 0$ and $\nu = 0.2248$, the vibrations are perfectly localized and not associated with acoustic radiation. Otherwise, the vibrations lose energy through the coupling to bulk modes. Chapter 4 invokes some numerical methods to calculate normal modes of a finite object with reference to the qualitative prediction by group theory. “Level repulsion” between frequency branches versus some parameter change is discussed in detail. Chapter 5 shows that for other values of $\nu$ it is possible to modify the shape of the end of a plate or bar in a way such that a perfectly localized edge mode is formed. We also extend the two dimensional discussion to three dimensional axisymmetric modes of a rod, which is more likely to be applicable to experiments. In Chapter 6 we give a brief investigation on algorithms that can be used to extract frequencies and damping rates from data obtained in ultra fast pump-probe experiments. This dynamic frequency analysis brings this thesis to a close.
Bibliography


Chapter 2

Theoretical Background

2.1 Rayleigh-Lamb Equation

The dispersion relation of a harmonic wave propagating through a bounded elastic medium is hard to obtain due to the complexity of the problem. Exact solutions are only available for an infinitely long rod by Pochhammer in 1876 [1] and Chree in 1889 [2] and for an infinitely long plate by Rayleigh [3] in 1888 and Lamb in 1889 [4, 5]. This section will briefly review the theoretical discussions of elastic wave motion in an infinite plate, which will serve as a basis for the later discussion of a finite rectangular one.

An infinite isotropic plate can support two independent kinds of stress wave motion consistent with the free surface boundary condition: SH modes and Lamb modes. SH modes are the pure horizontally polarized shear waves, and Lamb modes are the combination of vertically polarized shear (SV) waves and longitudinal (P) waves. The Rayleigh-Lamb theory is the theory describing the propagation of Lamb modes under plane strain conditions. We look for a solution for a wave propagating along the $x$ direction, and satisfying traction free boundary conditions at $y = \pm b/2$ where $b$ is the
width of an infinite plate. Such a solution cannot be constructed out of just P or SV waves; both waves have to be present in order to satisfy the traction free boundary conditions. However, either the P or the SV waves can be used to find solutions that satisfy the mixed boundary condition $\sigma_{xy} = 0$ and $u_x = 0$, or the mixed boundary condition $\sigma_{xy} = 0$ and $u_y = 0$, at $y = \pm b/2$ [6] as shown schematically in Figure 2.1 and Figure 2.2. Under these conditions, the P and/or SV waves have simple analytical dispersion relations similar to the SH modes.

![Figure 2.1: Partial wave pattern of the uncoupled P mode in an isotropic plate with mixed boundary conditions, $\sigma_{yy} = 0$ and $u_x = 0$ at $y = \pm b/2$.](image1)

![Figure 2.2: Partial wave pattern of uncoupled SV mode in an isotropic plate with mixed boundary conditions, $\sigma_{yy} = 0$ and $u_x = 0$ at $y = \pm b/2$.](image2)

The free surface condition makes it more complicated. To derive the Rayleigh-Lamb equation we have to consider the coupling of the P and SV waves at the boundary. To
guarantee the same propagating wave vector component $k$ along the $x$ axis, the P wave and SV wave have to propagate at different angles. Since plane strain holds in the $z$ direction, the nonzero potentials are the scalar potential $\Phi$ and the vector potential component $H_z$,

$$\Phi(x, y) = [A \cos(k_{d_l} y) + B \sin(k_{d_l} y)] \exp(-ikx), \quad (2.1)$$

$$H_z(x, y) = [C \cos(k_{s_l} y) + D \sin(k_{s_l} y)] \exp(-ikx), \quad (2.2)$$

with wave vector components in the $y$ direction given by

$$k_{d_l}^2 = \left( \frac{\omega}{v_l} \right)^2 - k^2 \quad (2.3)$$

and

$$k_{s_l}^2 = \left( \frac{\omega}{v_s} \right)^2 - k^2. \quad (2.4)$$

Here $v_l$ is the longitudinal sound velocity and $v_s$ is the shear sound velocity. These are related to the elastic constants $C_{11}$ and $C_{44}$ and the mass density $\rho$ by:

$$v_l = \sqrt{\frac{C_{11}}{\rho}} = \sqrt{\frac{\lambda + 2\mu}{\rho}}, \quad (2.5)$$

$$v_s = \sqrt{\frac{C_{44}}{\rho}} = \sqrt{\frac{\mu}{\rho}}. \quad (2.6)$$

Here $\lambda$ is the Lamé modulus and $\mu$ is the shear modulus. These, in turn, are related to the Young’s modulus $E$ and Poisson’s ratio $\nu$ for an isotropic linear elastic material by

$$\lambda = \frac{\nu E}{(1 + \nu)(1 - 2\nu)}, \quad (2.7)$$
\[ \mu = \frac{E}{2(1 + \nu)}. \]

The displacement field produced by the P wave is:

\[ u_x(x, y) = (-ik)[A \cos(k_{it}y) + B \sin(k_{it}y)] \exp(-ikx), \quad (2.9) \]

\[ u_y(x, y) = k_{it}[-A \sin(k_{it}y) + B \cos(k_{it}y)] \exp(-ikx). \quad (2.10) \]

The corresponding stress components are:

\[ \sigma_{yy}(x, y) = [C_{11}(-k_{it}^2) + C_{12}(-k_{it}^2)] [A \cos(k_{it}y) + B \sin(k_{it}y)] \exp(-ikx), \quad (2.11) \]

\[ \sigma_{xy}(x, y) = 2C_{44}(-ikk_{it}) [-A \sin(k_{it}y) + B \cos(k_{it}y)] \exp(-ikx). \quad (2.12) \]

The displacement field produced by the SV wave is:

\[ u_x(x, y) = (-k_{it})[-C \sin(k_{it}y) + D \cos(k_{it}y)] \exp(-ikx), \quad (2.13) \]

\[ u_y(x, y) = (-ik)[C \cos(k_{it}y) + D \sin(k_{it}y)] \exp(-ikx). \quad (2.14) \]

The corresponding stress components are:

\[ \sigma_{yy}(x, y) = (C_{11} - C_{12})(ikk_{it}) [C \sin(k_{is}y) - D \cos(k_{is}y)] \exp(-ikx), \quad (2.15) \]

\[ \sigma_{xy}(x, y) = C_{44}(k_{is}^2 - k_{it}^2) [C \cos(k_{is}y) + D \sin(k_{is}y)] \exp(-ikx). \quad (2.16) \]

With respect to the symmetry under y inversion, there are two types of parity in displacement fields. For the symmetric solutions, \( B = C = 0 \). At \( y = \pm b/2 \), one can combine the P and SV contributions to get \( \sigma_{yy} = 0 \) and \( \sigma_{xy} = 0 \),

\[ \begin{align*}
[C_{11}(-k_{it}^2) + C_{12}(-k_{it}^2)] \cos(k_{it}b/2)A & - [(C_{11} - C_{12})(ikk_{it}) \cos(k_{is}b/2)]D = 0, \quad (2.17) \\
2(ikk_{it}) \sin(k_{it}b/2)A & + [(k_{is}^2 - k_{it}^2) \sin(k_{is}b/2)]D = 0. \quad (2.18)
\end{align*} \]
The characteristic determinant of the above equations should be zero, and with the use of
the relation \( C_{11} = C_{12} + 2C_{44} \) which holds for an isotropic material, we have the Rayleigh-
Lamb equation for the symmetric solutions,

\[
\frac{\tan(k_a b / 2)}{\tan(k_d b / 2)} = - \frac{4k^2 k_t}{(k_t^2 - k^2)^2}.
\] (2.19)

In the same way, the antisymmetric solutions are given with \( A = D = 0 \),

\[
\frac{\tan(k_a b / 2)}{\tan(k_d b / 2)} = - \frac{(k_t^2 - k^2)^2}{4k^2 k_t k_s}.
\] (2.20)

The dependence of the angular frequency \( \omega \) on the propagating wave vector \( k \) can be
derived numerically from these transcendental equations. Figure 2.3 shows the dispersion
curves for an isotropic copper plate calculated from Eq. (2.19) and Eq. (2.20) by the
Newton-Raphson method. The lowest five antisymmetric branches are plotted as solid
curves, and the lowest four symmetric branches are plotted as dashed curves. Copper has
a Poisson’s ratio of \( \nu = 0.343 \), mass density \( \rho = 8.94 \text{g/cm}^3 \), and Young’s modulus
\( E = 129.4 \text{GPa} \). The longitudinal and shear sound velocities are calculated to be
\( v_l = 47.45 \text{A/ps} \) and \( v_s = 23.22 \text{A/ps} \).

From the Rayleigh-Lamb equations, the relation between the coefficients \( A \) and \( D \), or \( B \)
and \( C \) can be determined. The displacement fields are expressed in Eq. (2.21) for the
symmetric modes and Eq. (2.22) for the antisymmetric modes.
Figure 2.3: Lamb wave dispersion curves for the low order modes of an isotropic copper plate. Solid lines are for antisymmetric solutions; dashed lines are for symmetric solutions.
\[ u_x = \mp ik \left[ \cos(k_{it}, x) \cos(k_{ix}, b / 2) - \frac{k_i^2 - k_{ix}^2}{2k_{ix}^2} \cos(k_{it}, b / 2) \cos(k_{ix}, y) \right] e^{\mp ikx}, \]
\[ u_y = \left[ -k_{it} \sin(k_{it}, y) \cos(k_{ix}, b / 2) - \frac{k_i^2 - k_{ix}^2}{2k_{ix}^2} \cos(k_{it}, b / 2) \sin(k_{ix}, y) \right] e^{\mp ikx}, \]  
\[ u_x = \mp ik \left[ \sin(k_{it}, y) \sin(k_{ix}, b / 2) - \frac{k_i^2 - k_{ix}^2}{2k_{ix}^2} \sin(k_{it}, b / 2) \sin(k_{ix}, y) \right] e^{\mp ikx}, \]
\[ u_y = \left[ k_{it} \cos(k_{it}, y) \sin(k_{ix}, b / 2) + \frac{k_i^2 - k_{ix}^2}{2k_{ix}^2} \sin(k_{it}, b / 2) \cos(k_{ix}, y) \right] e^{\mp ikx}. \]  

The cutoff frequency at the limit of \( k = 0 \) is obtained by setting
\[
\frac{\tan(k_{ix}, b / 2)}{\tan(k_{it}, b / 2)} = 0
\]  
for the symmetric waves. Then the transverse wave vectors have
\[ k_{ix}, b = n \pi \ (n = 0, 2, 4, \ldots) \]  
(2.24)

or
\[ k_{it}, b = n \pi \ (n = 1, 3, 5, \ldots). \]  
(2.25)

\[
\frac{\tan(k_{ix}, b / 2)}{\tan(k_{it}, b / 2)} = -\infty
\]  
(2.26)

for the antisymmetric waves. Then the transverse wave vectors have
\[ k_{ix}, b = n \pi \ (n = 1, 3, 5, \ldots) \]  
(2.27)

or
\[ k_{it}, b = n \pi \ (n = 0, 2, 4, \ldots). \]  
(2.28)
Figure 2.4 and Figure 2.5 exhibit the displacement patterns for an isotropic copper plate in the nonpropagating limit \( k = 0 \). The alternation between independent pure shear and pure longitudinal appears in both symmetric and antisymmetric transverse standing waves. They are not coupled to each other by the stress free boundary condition.

Figure 2.4: Deformed vibration patterns for the lowest three symmetric modes at \( k = 0 \) for two phases. The figure shows just a section of the length of an infinite plate.

Figure 2.5: Deformed vibration patterns for the lowest three antisymmetric modes at \( k = 0 \) for two phases. The figure shows just a section of the length of an infinite plate.
Figure 2.6: Deformed vibration patterns at $kb = 1$ for the lowest three symmetric ($S_0$, $S_1$, $S_2$) and antisymmetric modes ($AS_0$, $AS_1$, $AS_2$). The figure shows a section of the length of an infinite plate.

When the wave number is non-zero, the coupling changes the vibration patterns strongly. When $kb$ is small, as shown by the example in Figure 2.6, the symmetric modes, often called dilatational, are expanding and contracting the boundary; the antisymmetric modes, often called flexural, are flexing the boundary. The vibration pattern changes drastically as $k$ keeps increasing [6]. When $\omega/k > v_l$, both the longitudinal and the shear parts vary with $y$ as sine and cosine functions. At $\omega/k = v_l$, the longitudinal part is uniform in the $y$ direction. When $v_l > \omega/k > v_s$, the longitudinal part decays exponentially into the
interior and so is concentrated at the surfaces of the plate. In the dispersion curves, there are only two modes below $\omega/k = v_r$: the lowest symmetric branch ($S_0$) and the lowest antisymmetric branch ($AS_0$). Both of them are approaching $\omega/k = v_R$ - the Rayleigh sound velocity in the limit of $kb \to \infty$ and then become degenerate with each other.

It is worthwhile to note that there is one special mode pattern happening at $\omega = \sqrt{2} k \nu$.

This is related to the perfectly localized edge mode for Poisson’s ratio $\nu = 0.2248$ which we will discuss later. Since $k = k_{ss}$, the Rayleigh-Lamb equation is reduced to

$$\text{Symmetric: } \tan(kb/2) \to \infty, \quad k = n\pi/b, \quad (n = 1, 3, 5...),$$

$$\text{Antisymmetric: } \tan(kb/2) = 0, \quad k = n\pi/b, \quad (n = 0, 2, 4...).$$

The SV wave is travelling at 45° to the $x$ direction and there is no coupling to the P wave. This Lamb wave is a pure SV wave, and is called the Lamé mode.

### 2.2 Some Features of the Rayleigh-Lamb Equation

The dispersion curves numerically calculated from the Rayleigh-Lamb equation have many interesting properties and have been discussed extensively. These features include the imaginary loop connecting the second and third symmetric branches in a certain range of Poisson’s ratio found by Aggarwal and Shaw [7], the frequency minimum between zero and the cutoff of the second symmetric branch studied by Mindlin [8], and the negative group velocity investigated by Tolstoy and Usdin [9].

Complex wave numbers and phase velocities associated with real frequencies are also an important feature. These branches were first found by Mindlin and Medick in an
approximate theory of extensional motion of an elastic plate [10-12]. They considered the coupling between extensional, symmetric thickness-stretch and symmetric thickness-shear deformations. To do this they replaced the displacements in the variational equations of motion by series expansions of Legendre polynomials in the thickness coordinate, and then integrated across the thickness to generate an infinite array of coupled two dimensional field equations. Truncations of this array, retaining zero-, first-, and second-order terms of the series expansions, led finally to the field equations of what is called the “second order theory”.

Since it is a third order algebraic equation, there should be three roots. Particularly for any given frequency less than the minimum on the second symmetric branch of dispersion curves, roots are one real and two complex conjugates. Mindlin and Medick found these roots and compared the results with the exact Lamb wave solution. Later on an infinite number of similar complex branches were found in the Rayleigh-Lamb and Pochhammer-Chree equations.

As an example, the frequency versus pure imaginary wave vector is plotted in Figure 2.7. The frequency is scaled by \( \omega = \pi v / b \), “AS” refers to the antisymmetric branch, and “S” refers to the symmetric branch. The thin solid lines are bounds [8] that can be derived by a method related to the two mixed boundary conditions mentioned earlier. Mindlin pointed out that through a simple calculation of the location and the slopes of the lines at intersection points between these bounds, dispersion curves can be sketched out directly without any numerical effort. He also mentioned that complex branches of the dispersion spectrum emanate from the points with a zero slope on the real or the imaginary arms. From Figure 2.7, we can imagine there should be a lot of branches extending to the
complex space originated from the local minimum and maximum on the imaginary branches. We will give an example of a three dimensional complex dispersion plot in the next section. These evanescent modes play a relevant role in the formation of edge modes.

Figure 2.7: Lamb wave dispersion curves for the pure imaginary wave vectors of an isotropic copper plate with $v_l/v_s = 2.043$. Thick solid lines are symmetric branches, thick dashed lines are antisymmetric branches. Thin lines are bounds of the branches calculated from mixed boundary conditions.
2.3 Root Determination from the Rayleigh-Lamb Equation

In Chapter 3, we will investigate the reflection of a Lamb wave that is incident on the free end of a plate. To do this using mode matching, we need to be able to efficiently find the real, imaginary, or complex propagation constants for a given arbitrary frequency. One way to do this would be to use Newton’s method. Since the solution is tractable at zero frequency, the iteration starts from $\omega = 0$, and gradually increases to the desired frequency value by taking $dk = -\left(\frac{\partial D}{\partial k}D\right)d\omega$ where $D(\omega,k) = 0$ is the Rayleigh-Lamb equation. However, one quickly finds that this evolution process is quite time consuming.

In 2001 a new matrix algorithm to directly determine the complex spectrum for any given frequency even in a high frequency range was proposed by Pagneux and Maurel [13]. This strategy does not need any initial guesses at all, so it is more convenient and applicable in calculations. The formulation is given in the following to correct some typos of the original paper. We took advantage of this method to determine all the partial modes for a frequency of an incident $S_0$ wave as part of the numerical results of Chapter 3.

The same coordinate system is used as in Figure 2.1. The $x$ direction extends to infinity, and the $y$ direction is restricted between $-b/2$ and $b/2$. $k$ is the propagating wave vector as before. The particle displacements can be written as:

$$
\begin{pmatrix}
  u_x \\
  u_y \\
\end{pmatrix} = \begin{pmatrix}
  u(y) \\
  v(y) \\
\end{pmatrix} \exp(ikx). \tag{2.31}
$$

From the equations of elasticity
\[- \rho \omega^2 u = (2 \mu + \lambda) \frac{\partial^2}{\partial x^2} u + \mu \frac{\partial^2}{\partial y^2} u + (\mu + \lambda) \frac{\partial^2}{\partial x \partial y} v, \quad (2.32) \]

\[- \rho \omega^2 v = (2 \mu + \lambda) \frac{\partial^2}{\partial y^2} v + \mu \frac{\partial^2}{\partial x^2} v + (\mu + \lambda) \frac{\partial^2}{\partial x \partial y} u. \quad (2.33) \]

Defining \( k_i = \omega \sqrt{\rho / (\lambda + 2 \mu)} \), \( k_s = \omega \sqrt{\rho / \mu} \), and \( \gamma = (\lambda + 2 \mu) / \mu \), the above equation is rewritten as:

\[ k^2 u - ik \frac{\gamma - 1}{\gamma} v - (k_i^2 u + \frac{1}{\gamma} u') = 0, \quad (2.34) \]

\[ k^2 v - ik (\gamma - 1) u' - (k_s^2 v + \gamma v') = 0. \quad (2.35) \]

The stress free boundary conditions \( \sigma_{xy} = 0 \) and \( \sigma_{yy} = 0 \) at \( y = \pm b / 2 \) are:

\[ \mu (u' (\pm b / 2) + ik v (\pm b / 2)) = 0, \quad (2.36) \]

\[ (2 \mu + \lambda) v' (\pm b / 2) + \lambda (ik) u (\pm b / 2) = 0. \quad (2.37) \]

The basic idea of the algorithm is to expand the displacement fields \( u \) and \( v \) in terms of a set of basis functions with the appropriate parity to give the symmetric and antisymmetric solutions, denoted by the superscript \( s \) and \( a \) respectively. Even basis functions \( \phi_n \) with respect to \( y \) are used for \( u^s, v^a \), and odd basis functions \( \psi_n \) with respect to \( y \) are used for \( u^a, v^s \). These basis functions satisfy

\[ \phi_n'' + \alpha_n^2 \phi_n = 0, \quad \phi_n' (0) = \phi_n' (b / 2) = 0, \quad (2.38) \]

\[ \psi_n'' + \chi_n^2 \psi_n = 0, \quad \psi_n' (0) = \psi_n' (b / 2) = 0. \quad (2.39) \]
ϕₙ(ψₙ) form a complete set to describe any even (odd) function, and their expressions are given as,

\[
\phi_n = \sqrt{\frac{2\varepsilon_n}{b}} \cos(\alpha_n y), \quad \begin{cases} 
\varepsilon_1 = 1, \varepsilon_n = 2, \text{ for } n \geq 2, \\
\alpha_n = \frac{2(n-1)\pi}{b}, 
\end{cases} \tag{2.40}
\]

\[
\psi_n = \sqrt{\frac{4}{b}} \sin(\chi_n y), \quad \chi_n = \frac{(2n-1)\pi}{b}. \tag{2.41}
\]

The displacement is then expressed in terms of the basis functions as

\[
u_s(y) = \sum_{n \geq 1} U_n^s \phi_n(y), \quad u^a(y) = \sum_{n \geq 1} U_n^a \psi_n(y), \tag{2.42a}
\]

\[
u_s(y) = \sum_{n \geq 1} V_n^s \psi_n(y), \quad v^a(y) = \sum_{n \geq 1} V_n^a \phi_n(y). \tag{2.42b}
\]

For the symmetric modes, apply the scalar product of \( \phi_n \) to both sides of Eq. (2.34). This gives

\[
\left( (\nu^s)' [\phi_n] \right) = \left( (v^s)' [\phi_n] \right)_0 - (v^s)' [\phi_n] = \sum_{m \geq 1} \left( \phi_n(h) \psi_m(h) - (\phi_n(h) \psi_m') \right) V_m^s, \tag{2.43}
\]

with \( v^s(0) = 0 \), and similarly

\[
((u^s)'') [\phi_n] = [(u^s)' [\phi_n] - u^s [\phi_n')]_0 + (u^s)' [\phi_n] = -ik \sum_{m \geq 1} \phi_n(h) \psi_m(h) V_m^s - \alpha_n^2 U_n^s, \tag{2.44}
\]

with \( u^s(0) = 0, \phi_n'(0) = 0, \phi_n'(b/2) = 0, \) and \( (u^s)'(b/2) = -ik v^s(b/2) \).

Let \( \mathbf{U}^s \) and \( \mathbf{V}^s \) be vectors composed by the coefficients \( U_n^s \) and \( V_n^s \), respectively. Then

\[
k^2 \mathbf{U}^s + kA^s \mathbf{V}^s + B^s \mathbf{U}^s = 0. \tag{2.45}
\]
In the above Eq. (2.45), the matrix $A^s$ and $B^s$ have the explicit expression,

$$A^s_{n,m} = i \left( \frac{\gamma - 1}{\gamma} \phi_m^a \psi^a_n + \frac{2 - \gamma}{\gamma} \phi_m^q(h) \psi^q_n(h) \right)$$

$$= \begin{cases} 
\frac{2\sqrt{2}i(2 - \gamma)}{b\gamma} (-1)^m, n = 1 \\
\frac{4i(-1)^{m+n}(\alpha^2_n + \chi^2_m(\gamma - 2))}{b\gamma(\alpha^2_n - \chi^2_m)}, n \geq 2,
\end{cases} \quad (2.46)$$

$$B^s_{n,m} = \left( \frac{\alpha^2_n}{\gamma} - k^2_s \right) \delta_{nm}. \quad (2.47)$$

Similarly, performing the scalar product by $\psi_n$ on both sides of Eq. (2.35), and combining with the boundary condition, the following relation is obtained

$$k^2 V^s + kC^s U^s + D^s V^s = 0, \quad (2.48)$$

where

$$C^s_{n,m} = -\gamma A^s_{m,n}, \quad (2.49)$$

$$D^s_{n,m} = (\chi^2 - k^2_s) \delta_{nm}. \quad (2.50)$$

The antisymmetric solution can be treated in the same way with result

$$k^2 U^a + kA^a V^a + B^a U^a = 0,$$

$$k^2 V^a + kC^a U^a + D^a V^a = 0,$$

$$A^a_{n,m} = i \left( \frac{\gamma - 1}{\gamma} \phi_m^a \psi^a_n + \frac{2 - \gamma}{\gamma} \phi_m^q(h) \psi^q_n(h) \right)$$

$$= \begin{cases} 
\frac{2\sqrt{2}i}{b\gamma} (-1)^m, n = 1 \\
\frac{4i(-1)^{m+n}(\chi^2_m + \alpha^2_n(\gamma - 2))}{b\gamma(\chi^2_m - \alpha^2_n)}, n \geq 2,
\end{cases} \quad (2.52)$$
We now have to solve the following nonlinear coupled eigenvalue equations to get the values of wave vector \( k \) for a given frequency \( \omega \):

\[
\begin{align*}
B_{n,m} &= \left( \frac{\alpha_n^2}{\gamma} - k_i^2 \right) \delta_{nm}, \\
C_{n,m} &= -\gamma A_{m,n}, \\
D_{n,m} &= \left( \alpha_n^2 \gamma - k_i^2 \right) \delta_{nm}.
\end{align*}
\]  

(2.53)  

(2.54)  

(2.55)

We now have to solve the following nonlinear coupled eigenvalue equations to get the values of wave vector \( k \) for a given frequency \( \omega \):

\[
k^2 U + k A V + B U = 0,
\]

(2.56a)

\[
k^2 V + k C U + D V = 0.
\]

(2.56b)

These equations can be transformed into a normal eigenvalue problem by the following change,

\[
k^2 X_1 + k F_1 X_1 + G_1 X_1 = 0,
\]

(2.57)

with

\[
X_1 = \begin{pmatrix} U \\ V \end{pmatrix}, \quad F_1 = \begin{pmatrix} 0 & A \\ C & 0 \end{pmatrix}, \quad G_1 = \begin{pmatrix} B & 0 \\ 0 & D \end{pmatrix}.
\]

(2.58)

Then, writing \( Y_1 = kX_1 \), and

\[
Z_1 = \begin{pmatrix} X_1 \\ Y_1 \end{pmatrix}, \quad M_1 = \begin{pmatrix} 0 & I_{2N} \\ -G_1 & -F_1 \end{pmatrix}
\]

(2.59)

where \( I_{2N} \) is the \( 2N \) by \( 2N \) identity matrix, the equation Eq. (2.57) is rewritten as

\[
M_1 Z_1 - k Z_1 = 0.
\]

(2.60)
In Eq. (2.60) the matrix dimension is $4N$, and the symmetry between $k \rightarrow -k$ is not taken into account. To reduce the efforts of solving matrix, we can calculate the eigenvalues for $k^2$, and the dimension is only half of Eq. (2.60). Express $V$ as a function of $U$ in Eq. (2.56b), and put it into Eq. (2.56a),

$$(k^2I_N - k^2A(k^2 + D)^{-1}C + B)U = 0. \quad (2.61)$$

The reduced problem for $K = k^2$ is

$$(K^2 + F_2K + G_2)X_2 = 0, \quad (2.62)$$

with $F_2 = (D - CA + A^{-1}BA)$, $G_2 = DA^{-1}BA$.

As the previous, introduce

$$Y_2 = KX_2, \ Z_2 = \begin{pmatrix} X_2 \\ Y_2 \end{pmatrix}, \ M_2 = \begin{pmatrix} 0 & I_N \\ -G_2 & -F_2 \end{pmatrix}. \quad (2.63)$$

The final formula is obtained:

$$M_2Z_2 - KZ_2 = 0. \quad (2.64)$$

To get very accurate solutions for the dispersion relation, it is better to choose the $k$ values from Eq. (2.64) as initial, and then implement Newton-Raphson iterations to reach convergence. To avoid spurious eigenvalues, the first $N$ values from Eq. (2.64) are selected according to the comparison with the exact values and the asymptotic values.

According to the Merkulov et al. [14] for large $k$, the asymptotic solutions are

$$k_n^b \frac{b}{2} = \frac{1}{2} \ln \left[ 2\pi(n + \frac{1}{2}) \right] - i \frac{1}{2} \left[ \pi(n + \frac{1}{2}) - \ln \left( \frac{2\pi(n+1/2)}{\pi(n+1/2)} \right) \right]. \quad (2.65)$$
We will give examples to show the power of this algorithm. According to our experience, the matrix dimension \( N = 100 \) is large enough to obtain an accurate solution.

Figure 2.8: Dimensionless complex Lamb wave spectrum at \( \omega = 2v_s / b \) for a copper plate. Open circles are matrix solution; Dots are asymptotic values.

Figure 2.8, Figure 2.9 and Figure 2.10 are the complex spectrum for increasing values of frequency for an infinite copper plate. Circles are the results directly from eigensolution of Eq. (2.64) without refinement. Dots are the asymptotic results from Eq. (2.65). It is very clear that with a higher and higher frequency, there are more and more propagating modes existing with \( \text{Im}(kb/2) = 0 \). With \( \omega b / v_s = 2 \) in Figure 2.8, there is only one propagating mode, and this fact turns out to be important for understanding the formation of edge modes.
Figure 2.9: Dimensionless complex Lamb wave spectrum at $\omega = 28v_s/b$ for a copper plate. Open circles are matrix solution; Dots are asymptotic values.

Figure 2.10: Dimensionless complex Lamb wave spectrum at $\omega = 56v_s/b$ for a copper plate. Open circles are matrix solution; Dots are asymptotic values.
Figure 2.11 is a three dimensional sketch of frequency versus the real and the imaginary parts of wave vectors. As mentioned before, there are complex branches emanating from zero slope points in real and imaginary space accordant with the Mindlin’s theory. As a specific example, one complex branch is associated with the lowest point on the second symmetric real branch.

Figure 2.11: Three dimensional representation of frequency versus the complex wave vectors for an infinite copper plate.
Bibliography


Chapter 3

Lamb Wave Reflection at the Free Edge of a Plate

3.1 Introduction

Usually when a propagating harmonic Lamb wave is incident on the free straight edge of a plate, mode conversion happens. The propagating wave is scattered into several propagating waves and decaying waves with the same symmetry. One special case occurs when the incident wave is the lowest symmetric mode $S_0$ and it has a frequency in the range where the propagating mode is only the $S_0$ mode. Under these conditions, there may be a resonance and a large but finite vibration localized to a narrow region around the free end is excited. The reflection coefficient of the mode $S_0$ exhibits an abrupt change near the resonance frequency.

The resonance occurs because there is a quasi-localized mode QLM with a weak acoustic radiation down the plate. This mode is a solution of the equations of elasticity that has a real frequency and with a displacement pattern that decays exponentially with distance from the end of the plate. It is called “quasi-localized” because except in special cases to be discussed below it does not exactly satisfy the boundary conditions at the end surface of the plate. Since it does not satisfy these conditions, it has a coupling to the propagating
$S_0$ mode and if the QLM is excited it will slowly lose energy by the mechanical radiation down the plate.

The QLM does satisfy the boundary conditions for two special values of Poisson’s ratios to become a really localized resonance. One value is $\nu = 0$ predicted mathematically by Roitberg [1] in 1998 and the other was numerically discovered to be $\nu = 0.2248$ by Pagneux [2] in 2006. For these two values, the propagating $S_0$ is decoupled from evanescent modes, and the resonant vibration is perfectly localized at the end.

Pagneux [2] uses the concept of complex resonance in acoustics to investigate the edge mode of a semi-infinite plate. He obtained the variation of the real and imaginary part of the dimensionless complex resonance frequency $\Omega_R = \omega b/(2\nu_s)$ versus Poisson’s ratio $\nu$ by numerical calculation. He found the approximate empirical formula

$$\text{Re}(\Omega_R) = 0.652\nu^2 + 0.898\nu + 1.9866,$$  \hspace{1cm} (3.1)

$$\text{Im}(\Omega_R) = -\frac{\nu^4(\nu - 0.2248)^2/0.0313}{1 + \left(\frac{\nu - 0.2062}{0.1696}\right)^2 + \left(\frac{\nu - 0.2062}{0.2606}\right)^4}.$$  \hspace{1cm} (3.2)

The real part of $\Omega_R$ is the frequency of the usual quasi-resonance of edge mode. From Figure 3.1, we can see that it increase almost linearly as $\nu$ increases. The imaginary part of $\Omega_R$ gives the rate of decay of the resonance. $\text{Im}(\Omega_R)$ shows a rather complicated behavior. Its magnitude increases rapidly when $\nu$ is larger than 0.3. With $\nu$ less than about 0.3, it is very small, on the scale of $10^{-4}$. From Figure 3.3 one sees that $\text{Im}(\Omega_R) = 0$ at two special values of Poisson’s ratios: $\nu = 0$ and $\nu = 0.2248$. For these two values, there is no time decay for the edge resonance.
Figure 3.1: Real part of the dimensionless complex resonance frequency versus Poisson’s ratio.

Figure 3.2: Imaginary part of the dimensionless complex resonance frequency versus Poisson’s ratio.
3.2 Collocation Method

In addition to the work of Pagneux by the acoustic scattering method, several other numerical efforts have been made to calculate the reflection of $S_0$ wave incidence at a free edge. Gazis and Mindlin got a crude solution by assuming only three modes reflected [3]. Torvik increased the number of modes to 21 and got a more accurate result [4]. Auld and Tsao applied a variational method to approach this problem based on the orthogonality of Lamb modes [5]. Later on, new experiments [6, 7] and calculations [8]...
illustrated the existence of a quasi-resonant edge mode at a beveled end with mode conversion now occurring between symmetric modes and antisymmetric modes.

Here we follow the “collocation method” used by Shen et al. [9] to study the reflection of an $S_0$ Lamb wave incident on a straight end. The phase change on reflection shows an interesting behavior of real resonance and quasi-resonance for different Poisson’s ratios. Though the completeness of the Lamb modes has not been proved mathematically, Lamb modes are orthogonal to each other and serve as basis functions to satisfy the stress free boundary condition at the end. In the discussion given here, the frequency is restricted to be lower than the minimum of the second symmetric branch of the dispersion spectrum. This means that there is only one propagating mode to consider, and so the numerical convergence criterion is simply that the amplitude of the reflected $S_0$ wave must be unity as follows from energy balance.

The structure geometry is illustrated in Figure 3.4. The incident wave is the left-going $S_0$ Lamb wave with wave vector $-k_0$, and the reflected waves include the right-going $S_0$ wave with the wave vector $k_0$ and complex waves with wave vectors $k_n$.

![Figure 3.4: Geometry of a semi-infinite plate extending along x direction.](image-url)
The total displacement and stress fields at \( x = 0 \) is written as:

\[
\begin{pmatrix}
    u_x \\
    u_y \\
    \sigma_{xx} \\
    \sigma_{xy}
\end{pmatrix} = e^{-ikx} \begin{pmatrix}
    u_x^{0-} \\
    u_y^{0-} \\
    \sigma_{xx}^{0-} \\
    \sigma_{xy}^{0-}
\end{pmatrix} + \sum_{n \geq 1} R_n e^{ik_n x} \begin{pmatrix}
    u_x^{n+} \\
    u_y^{n+} \\
    \sigma_{xx}^{n+} \\
    \sigma_{xy}^{n+}
\end{pmatrix},
\]

(3.3)

These are a linear summation of all partial wave contributions. The boundary conditions are explicitly written

\[
\sigma_{xx} = \sigma_{xy} = 0.
\]

(3.4)

Choose \( Q \) discrete points on the edge, and for each point \( i \),

\[
\sigma_{xx}^{0} (i) + \sum_{n \geq 1} \sigma_{xx}^{n} (i) R_n = 0,
\]

(3.5)

\[
\sigma_{xy}^{0} (i) + \sum_{n \geq 1} \sigma_{xy}^{n} (i) R_n = 0.
\]

Since both the stresses \( \sigma_{xx} \) and \( \sigma_{xy} \) and the reflection coefficients \( R_0, R_n \) are complex numbers, Eq. (3.5) is decomposed into the real parts and the imaginary parts

\[
\begin{align*}
\text{Re} \sigma_{xx}^{0} (i) + \text{Re} \sigma_{xx}^{n} (i) * \text{Re} R_n - \text{Im} \sigma_{xx}^{n} (i) * \text{Im} R_n &= 0, \\
\text{Im} \sigma_{xx}^{0} (i) + \text{Im} \sigma_{xx}^{n} (i) * \text{Re} R_n + \text{Re} \sigma_{xx}^{n} (i) * \text{Im} R_n &= 0, \\
\text{Re} \sigma_{xy}^{0} (i) + \text{Re} \sigma_{xy}^{n} (i) * \text{Re} R_n - \text{Im} \sigma_{xy}^{n} (i) * \text{Im} R_n &= 0, \\
\text{Im} \sigma_{xy}^{0} (i) + \text{Im} \sigma_{xy}^{n} (i) * \text{Re} R_n + \text{Re} \sigma_{xy}^{n} (i) * \text{Im} R_n &= 0.
\end{align*}
\]

(3.6)

At the end \( x = 0 \) stresses of the symmetric solution to Rayleigh-Lamb equation for any wave vector \( k \) along \( x \) direction are expressed as:

\[
\begin{align*}
\sigma_{xx} (y) &= \left[ C_{11} (-k_d^2) + C_{12} (-k_d^3) \right] \cos(k_d b/2) - (C_{11} - C_{12}) \frac{k^2 - k_d^2}{2} \cos(k_d b/2) \cos(k_{n_d} y), \\
\sigma_{xy} (y) &= C_{44} \left[ -2ikk_d \sin(k_d y) \cos(k_d b/2) - (k^2 - k_d^2) (\frac{ik}{2k_d} + \frac{k_n}{2ik}) \cos(k_d b/2) \sin(k_{n_d} y) \right].
\end{align*}
\]

(3.7)

To be consistent, consider a \( S_0 \) wave incident on \( x = 0 \) of a copper plate with the same aforementioned material parameters. It is worthy of emphasis that the accuracy of wave
vector $k_0$ and $k_n$ is critical to achieve the resonance position and the energy balance simultaneously. For each frequency, we add Newton–Raphson (NR) refinement to the eigenvalue calculation of the dispersion spectrum explained in Chapter 2. We found that without NR iteration, the values of $k$ found directly from the matrix eigenvalues are not precise enough to give the sensible results. In the following the total number of wave vectors is chosen to be 200. To avoid divergence, the imaginary part of complex $k$ is nonnegative, and the real part of complex $k$ could be positive or negative. Therefore the number of independent wave vectors is 100 having the form $(\pm k_R, ik_I)$ where $k_I \geq 0$.

![Figure 3.5: Reflection coefficients for the lowest partial waves versus incident frequency.](image)
In Figure 3.5 reflection amplitudes of partial waves are plotted as a function of the incident wave frequency. The number of modes \((A_0, A_1, A_3, A_5)\) is assigned with the increasing imaginary part of wave vector (see Table 3.1 as a reference). Note that a nonpropagating mode cannot transport the energy by itself – the Poynting vector is zero \([10]\). The energy balance is clearly maintained with \(A_0 = 1\). There is a distinct peak of \(A_1\) located at \(4.742v_s/\lambda\) for a semi-infinite copper plate; this is the edge mode resonance.

![Diagram](image.png)

Figure 3.6: Real and imaginary parts of partial wave vectors at the edge mode resonance \(\omega = 4.742v_s/\lambda\).

The partial wave vectors at the resonance frequency \(\omega = 4.742v_s/\lambda\) are shown in Figure 3.6 and their reflection coefficients are enumerated in Table 3.1 for the lowest 15 modes. From Table 3.1 we can see the largest contribution among the evanescent modes is from the one with the smallest imaginary part of wave vector (Mode 1 and 2). The amplitude is
about 6.5 times the amplitude of reflected $S_0$. The ratio between the largest amplitude of a complex mode and the largest amplitude of the reflected $S_0$ mode anywhere in the plate width is about 31; thus the evanescent mode makes a major contribution to the vibration pattern.

<table>
<thead>
<tr>
<th>Mode No.</th>
<th>Re(kb/2)</th>
<th>Im(kb/2)</th>
<th>Amplitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.804</td>
<td>0.000</td>
<td>0.99994</td>
</tr>
<tr>
<td>1</td>
<td>1.018</td>
<td>0.945</td>
<td>6.51815</td>
</tr>
<tr>
<td>2</td>
<td>-1.018</td>
<td>0.945</td>
<td>6.51815</td>
</tr>
<tr>
<td>3</td>
<td>1.574</td>
<td>5.016</td>
<td>0.14973</td>
</tr>
<tr>
<td>4</td>
<td>-1.574</td>
<td>5.016</td>
<td>0.14973</td>
</tr>
<tr>
<td>5</td>
<td>1.789</td>
<td>8.329</td>
<td>0.01938</td>
</tr>
<tr>
<td>6</td>
<td>-1.789</td>
<td>8.329</td>
<td>0.01938</td>
</tr>
<tr>
<td>7</td>
<td>1.938</td>
<td>11.549</td>
<td>0.00493</td>
</tr>
<tr>
<td>8</td>
<td>-1.938</td>
<td>11.549</td>
<td>0.00493</td>
</tr>
<tr>
<td>9</td>
<td>2.053</td>
<td>14.736</td>
<td>0.00178</td>
</tr>
<tr>
<td>10</td>
<td>-2.053</td>
<td>14.736</td>
<td>0.00178</td>
</tr>
<tr>
<td>11</td>
<td>2.147</td>
<td>17.908</td>
<td>8.22E-04</td>
</tr>
<tr>
<td>12</td>
<td>-2.147</td>
<td>17.908</td>
<td>8.22E-04</td>
</tr>
<tr>
<td>13</td>
<td>2.225</td>
<td>21.071</td>
<td>4.51E-04</td>
</tr>
<tr>
<td>14</td>
<td>-2.225</td>
<td>21.071</td>
<td>4.51E-04</td>
</tr>
</tbody>
</table>

Table 3.1: Reflection coefficients of the lowest partial modes at the resonance frequency $\omega = 4.742\nu_x / b$.

It is also interesting to study the $S_0$ mode phase change in the same frequency range of Figure 3.5. Figure 3.7 gives the real part and imaginary part of the $S_0$ reflection coefficient $R_0$ as a function of frequency. One can see the resonance clearly. The phase change and its derivative with respect to frequency are plotted in Figure 3.8 and Figure 3.9. The phase angle of the reflected $S_0$ jumps abruptly from $-\pi$ to $+\pi$ in a small region of frequency. The resonance width of the derivative of the phase is a direct measure of the attenuation of an edge mode.
Figure 3.7: Reflection coefficient $R_0$ of an incident $S_0$ wave versus frequency.

Figure 3.8: Phase change $\Phi$ of an incident $S_0$ wave versus frequency.
Figure 3.9: Derivative of phase change of an incident $S_0$ wave with respect to frequency.

Figure 3.10: Phase change of a $S_0$ wave incident on the edge of a plate with Poisson’s ratio $\nu = 0.2248$. 
As a comparison, the phase change of an incident $S_0$ wave and its derivative with respect to frequency for the special value of Poisson’s ratio $\nu = 0.2248$ are plotted in Figure 3.10 and Figure 3.11. The edge mode resonance happens at $\omega = 4.442\nu_s/b$. The resonance width of the phase derivative is essentially zero within the accuracy of the numerical computation meaning the edge mode is perfectly localized without attenuation.

Figure 3.11: Phase change derivative of a $S_0$ wave incident on the edge of a plate with Poisson’s ratio $\nu = 0.2248$.

3.3 Physical Explanation of Peculiar Poisson’s Ratios

Zernov et al. [11] interpreted the perfectly localized edge mode for two special Poisson’s ratios $\nu = 0$ and $\nu = 0.2248$ by the stress orthogonality between $S_0$ and the other modes in
these two cases. Let us explain their formation in our own way which may be more understandable.

From Eq. (3.7) we can see the stress components $\sigma_{xx}$ and $\sigma_{xy}$ of the Rayleigh-Lamb solution have different parities under wave vector $k$ inversion. $\sigma_{xx}$ is an even function of $k$ whereas $\sigma_{xy}$ is an odd function of $k$. Thus, it is not possible to make both of them vanish with a linear combination of the incident and reflected $S_0$ waves for arbitrary position $y$ at the end $x = 0$.

However for $\nu = 0$ and $\nu = 0.2248$, they accidentally have a common characteristic: for the symmetric $S_0$ mode, one stress component $\sigma_{xy}$ is equal to zero for any point along the end surface. So the stress free boundary condition at $x = 0$ can be easily satisfied by the incident and the reflected $S_0$ waves themselves. They won’t excite the evanescent modes and are fully decoupled to each other.

It is clearer to fully understand this if we start from the original expressions for the displacements of Lamb waves. Consider the displacement fields for the symmetric solution

$$u_x(x, y) = \left[(-ik)A\cos(k_n y) + (-k_n)D\cos(k_n y)\right]\exp(-ikx), \quad (3.8)$$

$$u_y(x, y) = [(-k_n)A\sin(k_n y) + (-ik)D\sin(k_n y)]\exp(-ikx). \quad (3.9)$$

The stress components at $x = 0$ are:

$$\sigma_{xx}(0, y) = C_{11}\left[(-k^2)A\cos(k_n y) + (ikk_n)D\cos(k_n y)\right]$$

$$\sigma_{xy}(0, y) = C_{12}\left[2ikk_n A\sin(k_n y) + (k_n^2 - k^2)D\sin(k_n y)\right] \quad (3.10)$$

$$\sigma_{yy}(0, y) = C_{11}\left[(-k^2)A\sin(k_n y) + (ikk_n)D\sin(k_n y)\right]$$

$$\sigma_{yz}(0, y) = C_{12}\left[2ik\cos(k_n y) + (k_n^2 - k^2)D\cos(k_n y)\right] \quad (3.11)$$
The first term is the P wave contribution; the second term is the SV wave contribution.

The boundary conditions at \( y = \pm \frac{b}{2} \) are

\[
\sigma_{yy} = \sigma_{xy} = 0. \tag{3.12}
\]

Explicitly, they are written as

\[
C_{11} \left[ (-k_{ii}^3) A \cos(k_{ii} b / 2) + (-ik_{ii} D) \cos(k_{ii} b / 2) \right] = 0, \tag{3.13}
\]

\[
C_{12} \left[ 2ik_{ii} A \sin(k_{ii} b / 2) + (k_{tt}^2 - k^2) D \sin(k_{tt} b / 2) \right] = 0, \tag{3.14}
\]

For \( \nu = 0 \), suppose there is no contribution from SV wave \( D = 0 \); then if \( k_{tt} = 0 \) the above two conditions Eq. (3.13) and Eq. (3.14) are satisfied. And since \( \nu_p / \nu_s = \sqrt{2} \), \( k^2 = k_{tt}^2 \), the associated stresses at the edge from Eq. (3.10) and Eq. (3.11) are:

\[
\begin{pmatrix}
\sigma_{xx}(0, y) \\
\sigma_{xy}(0, y)
\end{pmatrix} = C \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ C = \text{const.} \tag{3.15}
\]

So the incident \( S_0 \) wave stress minus the reflected wave \( S_0 \) stress can guarantee the total stress free at \( x = 0 \).

For \( \nu = 0.2248 \), suppose there is no contribution from the P wave (\( A = 0 \)). Then if \( k_{tt}^2 = k^2 \) and \( \cos(k_{tt} b / 2) = 0 \), Eq. (3.13) and (3.14) of the boundary condition at \( y = \pm b/2 \) are satisfied. The associate stresses at the end are:

\[
\begin{pmatrix}
\sigma_{xx}(0, y) \\
\sigma_{xy}(0, y)
\end{pmatrix} = C \begin{pmatrix} \cos\left(\frac{\pi}{2} y\right) \\ 0 \end{pmatrix}, \ C = \text{const.} \tag{3.16}
\]

Similarly, the total stress to be zero at the edge is possibly formed by the pure incident and reflected SV waves. This mode is usually called Lamé mode with frequencies
\[ \Omega = \frac{\omega b}{2 \nu_s} = \sqrt{2(n + \frac{1}{2})\pi}, n = 0,1... \] (3.17)

This solution is the SV partial wave traveling at 45° to the x axis mentioned in Chapter 2. If the eigenfrequency is coincidently equal to Lamé frequency, an undamped edge mode exists.


Chapter 4

Acoustic Vibrations for a Finite Plate

4.1 Introduction

A finite object usually has a very complicated variation of the frequency of the normal modes when the geometry is changed. We will start with an elementary example - a finite rectangular plate to illustrate this complexity. Many intriguing phenomena are involved, such as level repulsion and edge mode vibrations. For a bounded plate, the constraint of two adjacent free surfaces in the cross section makes the solution non-separable in the coordinates. There is no analytical solution available, except for the SH waves. We will focus our attention on a plate with in-plane deformation.

In the practical application to nanocharacterization mentioned earlier, the structures of interest are usually the interconnect metallic lines running from one transistor to another. These lines normally run for a distance which is much greater than the transverse dimensions. In addition, to a good approximation, the structure is excited uniformly over a distance $\zeta$ which is large compared to the transverse dimensions. Thus, as a simple first example, we can consider vibrations of a plate (see Figure 4.1a) restricting attention
to modes in which the displacement is in the $xy$-plane and is independent of the $z$-coordinate. The plate extends from $z = -\infty$ to $+\infty$, with dimensions in the $xy$-plane $a$ and $b$. For the subsequent discussion it is convenient to refer to $a$ as the length and $b$ as the width. The corresponding problem for a thin bar (see Figure 4.1b) with Poisson’s ratio $\sigma_{bar}$ is formally equivalent to the plate problem with a Poisson’s ratio of

$$
\sigma_{plate} = \frac{\sigma_{bar}}{1 + \sigma_{bar}}.
$$

(4.1)

In the following discussions, all the motions are restricted to a plane strain deformation. We can easily switch the results to a plane stress deformation by using Equation (4.1).

Figure 4.1: Sketch of a plate and a thin bar for plane strain and plane stress respectively.
4.2 Group Theory Prediction

To determine the natural vibrations of a finite structure, symmetry is always a primary factor to start with. Group theory is an appropriate tool to investigate the symmetry and qualitatively predict the vibration patterns. This is a big help to guide the numerical calculations.

First, let us think about a square. The cross section is plotted in Figure 4.2. From the symmetry point of view, the possible vibration patterns are predicted by the projection operators. A square has the symmetry group $C_4$, including five irreducible representations. Since one representation is two dimensional, there are six kinds of vibration modes and two of them are degenerate. We follow Kynch [1] and Fraser [2] to name the modes: longitudinal, first screw, torsional, second screw, bending-$x$ and bending-$y$ modes. The two bending modes are degenerate.

The character table is a convenient way to display the properties of any given group in the various representations. The columns are labeled by the classes, preceded by the number $N_k$ of elements in each class. The rows are labeled by the irreducible representations. The entries in the table are the trace of one element in every class in
every irreducible representation, due to the fact that all elements in the same class have the same trace. We denote $\chi^{(i)}(C_k)$ for the $k$-th class $C_k$ in the $i$-th representation. The character table is constructed using the basic principles of group theory as follows [3, 4]:

1. The number of irreducible representations equals the number of classes of group elements.
2. The dimensionality $l_i$ of each $i$-th irreducible representation is determined by $\sum l_i^2 = h$. $h$ is the total number of elements in the group. Since the identity element always exists and is represented by a unit matrix, the first column of the table is $\chi^{(i)}(E) = l_i$. There is always a one dimensional representation in which every group element is unity, so the first row of the table is $\chi^{(i)}(C_k) = 1$.
3. The rows of the table must be orthogonal and normalized to $h$, with weighting factor $N_k$ the number of elements in the class $C_k$.

$$\sum_k \chi^{(i)}(C_k)^* \chi^{(j)}(C_k) N_k = h\delta_{ij}. \tag{4.2}$$

4. The columns of the table must be orthogonal and normalized to $h/N_k$.

$$\sum_i \chi^{(i)}(C_k)^* \chi^{(i)}(C_i) = h/N_k \delta_{kl}. \tag{4.3}$$

5. Elements in the $i$-th row are related by

$$N_j \chi^{(i)}(C_j) N_k \chi^{(i)}(C_k) = l_i \sum c_{jkl} N_l \chi^{(i)}(C_l), \tag{4.4}$$

where the $c_{jkl}$ are the constants defined by the equation governing class multiplication.
$$C_j C_k = \sum_l c_{jl} C_l. \quad (4.5)$$

For the square in Figure 4.2, the symmetric operations are: Identity operation \((E)\), rotation \(\pi \) about \(z\) axis \((C_2)\), rotation \(\pi/2\) and \(3\pi/2\) about \(z\) axis \((2C_4)\), reflection about \(x\)-axis and \(y\)-axis \((2\sigma_v)\), and reflection about the two dashed diagonals \((2\sigma_d)\). These symmetry operations constitute the \(C_{4v}\) group, and the character table is built by the above rules.

<table>
<thead>
<tr>
<th></th>
<th>(E)</th>
<th>(C_2)</th>
<th>(2C_4)</th>
<th>(2\sigma_v)</th>
<th>(2\sigma_d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A_{1g})</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(A_{2g})</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>(B_{1g})</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>(B_{2g})</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>(E_u)</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 4.1: Character table of \(C_{4v}\) group.

There are 8 elements in this group. \(1^2+1^2+1^2+1^2+2^2=8\) is the only available combination to make the second rule valid. Five classes produce five irreducible representations, four of them \(A_{1g}, A_{2g}, B_{1g}, B_{2g}\) are one dimensional and one of them \(E_u\) is two dimensional. To assess the vibration pattern according to each irreducible representation, we define the projection operator as

$$\hat{P}_\alpha^{(i)}(R) = \frac{1}{\hbar} \sum_R \Gamma^{(i)}(R)_{\alpha\alpha} \hat{P}_R,$$  \hspace{1cm} (4.6)$$

where \(R\) is an arbitrary operator in this group, and \(\Gamma^{(i)}(R)\) is the matrix expression of \(R\) in the \(i\)-th irreducible representation. For example, consider the projection operator of \(A_{1g}\) on a unit displacement along positive \(x\)- and positive \(y\)-direction. Define operations \(A, B,\)
and $C$ as rotations of $\pi$, $\pi/2$ and $3\pi/2$ around $z$-axis respectively. $X$, $Y$ are reflections along the $x$- and $y$-axes, and $D$, $E$ reflections along the diagonal directions. Then

$$\hat{P}^{(A_c)} = \frac{1}{8}(\hat{P}_E + \hat{P}_A + \hat{P}_b + \hat{P}_c + \hat{P}_x + \hat{P}_y + \hat{P}_D + \hat{P}_E)$$

(4.7)

Figure 4.3: The effect of the projection operator $A_{1g}$ on unit displacements along the $x$ and $y$ directions.

In Figure 4.3 $A_{1g}$ produces a longitudinal mode also called as “breathing mode”. The boundary of a square expands and shrinks every half a period. The displacement vector on the corner is always inclined at 45 degrees to the $x$ and $y$ direction. Through similar procedures, Figure 4.4 gives the result of using the projection operator for each irreducible representation of the $C_{4v}$ group acting on the unit positive $i$ or positive $j$ at one corner of the square. $A_{1g}$ is longitudinal mode, $B_{1g}$ is first screw mode, $A_{2g}$ is
torsional mode, $B_{2g}$ is second screw mode, $E_u$ is bending mode. We will confirm these vibration patterns later by numerical calculations.

Figure 4.4: $C_{4v}$ group projection operator actions on unit positive $x$ or $y$ displacement.
In the same way, the above projector method is extended to apply to a rectangle like Figure 4.5. The symmetry group of a rectangle is the Vierergruppe. This is the only group of order four apart from the cyclic group \((A, A^2, A^3, A^4=E)\). The Vierergruppe contains the elements: identity operation \((E)\), rotation \(\pi\) around z axis \((C_2)\), reflection about x axis \((\sigma_x)\), and reflection about y axis \((\sigma_y)\). The character table is listed in Table 4.2.

There are four modes existing in a rectangular geometry: longitudinal, torsional, and two bending modes. None of these modes are degenerate with the other since the four irreducible representations are all one dimensional. The longitudinal \((A_{1g})\) and first screw \((B_{1g})\) modes which are distinguishable in a square couple to give only a longitudinal mode \((L)\). Similarly, the torsional \((A_{2g})\) and second screw \((B_{2g})\) modes couple to give a torsional mode \((T)\). The degeneracy of the two bending modes in a square is broken in a
rectangle and two bending modes \((X, Y)\) are distinguishable from each other [1, 2, 5]. Applying the projection operator for the four irreducible presentations, the possible eigenmode vibration patterns are as shown in Figure 4.6. In contrast to the patterns for a square, the angle of the displacements on the corners in Figure 4.6 with respect to the \(x\) or \(y\) axis is not fixed at 45 degrees anymore and can have any value according to the ratio between length \(a\) and width \(b\), the elastic properties of the material, and the particular mode.

![Vibration patterns for a rectangle](image)

**Figure 4.6:** The vibration patterns for a rectangle.

### 4.3 Rayleigh – Ritz Method

The lack of an analytical solution for the vibration eigenmodes of a finite rectangular plate has led to the development of various numerical methods, including the collocation method [2], the mode-matching method [6], and the crosswise superposition of single series method [7]. All these schemes are using a series of analytical functions to construct the displacement fields and determine their coefficients to satisfy the boundary conditions. The other methods are based on the variational principle, such as the Ritz method [8]. For example, the trial functions are chosen to be products of sines and cosines of the coordinates [9], or products of Legendre polynomials of the coordinates [10]. In 1991 Visscher, Migliori and Bell expanded the displacements in terms of basis functions which
were simple products of the Cartesian coordinates [11]. The mode frequencies can
conveniently be obtained by solving a generalized eigenvalue equation. This method has
led to the development of “acoustic spectroscopy”. In this technique the frequencies of
the normal modes of an object of known dimensions are measured and these frequencies
are used to determine the elastic constants [12, 13].

We now describe the numerical method in detail. We need to solve the equation

$$\rho \frac{\partial^2 u_\alpha}{\partial t^2} = \frac{\partial}{\partial x_\beta} \sigma_{\alpha \beta} = C_{\alpha \beta \gamma \delta} \frac{\partial^2 u_\gamma}{\partial x_\rho \partial x_\delta}$$ \hspace{1cm} (4.8)$$

with the boundary condition that everywhere on the surface, the traction is zero, i.e.,
$$\sigma_{\alpha \beta} n_\beta = 0.$$ \hspace{1cm} $\rho$ is the material mass density, and $C_{\alpha \beta \gamma \delta}$ are the elastic constants. $u_\alpha$ is the
displacement along the $\alpha$ direction, and $\sigma_{\alpha \beta}$ is the stress tensor.

The procedure is to form the matrices

$$E_{n, m, \alpha} = \omega^2 \delta_{n, m} \int \rho \phi_n \phi_m dV,$$ \hspace{1cm} (4.9)

$$\Gamma_{n, m, \alpha} = \int C_{\alpha \beta \gamma \delta} \frac{\partial \phi_n}{\partial x_\beta} \frac{\partial \phi_m}{\partial x_\delta} dV,$$ \hspace{1cm} (4.10)

where $\{\phi_n\}$ are, in principle, a complete set of functions. The normal mode frequencies
are obtained from the eigenvalue equation

$$\omega^2 \sum_n E_{n, m} A_n = \sum_n \Gamma_{n, m} A_n$$ \hspace{1cm} (4.11)

and the displacement pattern of the mode is $u_\alpha = \sum_m A_{\alpha m} \phi_m$.

To prove that this is indeed a solution, we insert Eq. (4.9) and Eq. (4.10) into Eq. (4.11),
This can be written as

$$\sum_m \omega^2 \delta u_\alpha \rho \phi_m A_{\gamma\alpha} dV = \sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \frac{\partial \phi_m}{\partial x_\beta} A_{\gamma\delta} \frac{\partial \phi_n}{\partial x_\delta} dV.$$  \hspace{1cm} (4.12)

Now multiply both sides of the equation by the variation $\delta A_{\alpha m}$ and sum over $m$. Then

$$\omega^2 \int \rho \delta u_\alpha u_\alpha dV = \sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \frac{\partial \delta u_\alpha}{\partial x_\beta} \frac{\partial u_\gamma}{\partial x_\delta} dV = 0,$$  \hspace{1cm} (4.13)

where we are defining $\delta u_\alpha = \sum_m \delta A_{\alpha m} \phi_m$. We can integrate by parts the second term of this equation to get

$$\sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \frac{\partial \delta u_\alpha}{\partial x_\beta} \frac{\partial u_\gamma}{\partial x_\delta} dV = -\sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \delta u_\alpha \frac{\partial^2 u_\gamma}{\partial x_\beta \partial x_\delta} dV + \sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \delta u_\alpha \frac{\partial u_\gamma}{\partial x_\delta} n_\beta dS.$$  \hspace{1cm} (4.15)

Putting this into Eq. (4.14) gives

$$\left[ \int \rho \omega^2 u_\alpha + \sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \frac{\partial^2 u_\gamma}{\partial x_\beta \partial x_\delta} \right] \delta u_\alpha dV - \left[ \sum_{\beta\gamma\delta} C_{\alpha\beta\gamma\delta} \frac{\partial u_\gamma}{\partial x_\delta} n_\beta \right] \delta u_\alpha dS = 0,$$

which can be simplified to

$$\left[ \int \rho \omega^2 u_\alpha + \sum_{\beta} \frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta} \right] \delta u_\alpha dV - \left[ \sum_{\beta} \sigma_{\alpha\beta} n_\beta \delta u_\alpha dS \right] = 0.$$  \hspace{1cm} (4.16)

Since $\{\phi_m\}$ is a complete set of functions, $\delta u_\alpha$ can have an arbitrary value, and therefore both of the integrands must vanish. Therefore at all points in the interior,
\[ \rho \omega^2 u_a + \sum_{\beta} \frac{\partial \sigma_{a\beta}}{\partial x_\beta} = 0, \]  
(4.17)

and everywhere on the surface

\[ \sum_{\beta} \sigma_{a\beta} n_\beta = 0. \]  
(4.18)

Then the generalized eigenvalue equation for the natural vibration frequencies is

\[ \omega^2 E a = \Gamma a. \]  
(4.19)

The above equation can be solved by a subroutine called RSG in EISPACK [14, 15]. From the expressions of the matrix \(E\) and \(\Gamma\), it is apparent that the mass density and the elastic constant could be space dependent and the shape of the studied object could be irregular. Convergence of the higher frequency modes is always a concern in this numerical calculation. Since the basis functions are truncated to a certain maximum order and do not form a complete set, the high frequencies are difficult to be calculated and are sometimes sensitive to the basis function choice. Of course, more basis functions will give a more precise result, but there is an upper limit to dimension of matrices that can be solved using the RSG subroutine [16]. Many of the results that we present below were checked against the Finite Element Software ABAQUS. Agreement was obtained up to three significant figures.

We choose the same basis functions as Nishiguchi et al. [17] – the powers of the Cartesian coordinates normalized by the transverse dimensions of a plate (Figure 4.1a). In a two dimensional Cartesian coordinates with origin at the center of a rectangle with length \(a\) and width \(b\), the basis functions are written as
\[ \Phi_\lambda(x, y) = \left( \frac{2x}{a} \right)^M \left( \frac{2y}{b} \right)^N, \]

where the index of function is \( \lambda = (M, N) \). The matrix elements are calculated by integration from \(-a/2\) to \(a/2\) in the \(x\) direction and from \(-b/2\) to \(b/2\) in the \(y\) direction.

\[ E_{\lambda \lambda'} = \delta_{\lambda \lambda'} \rho a b f (M + M', N + N'), \quad (4.20) \]

\[ \Gamma_{\lambda \lambda' 1} = C_{11} \frac{4b}{a} MM' f (M + M' - 2, N + N') + C_{44} \frac{4a}{b} NN' f (M + M', N + N' - 2), \]

\[ \Gamma_{\lambda \lambda' 2} = C_{44} \frac{4b}{a} MM' f (M + M' - 2, N + N') + C_{11} \frac{4a}{b} NN' f (M + M' N + N' - 2), \]

\[ \Gamma_{\lambda \lambda' 1} = 4(C_{44} NM' + C_{12} MN') f (M + M' - 1, N + N' - 1), \]

\[ \Gamma_{\lambda \lambda' 2} = 4(C_{44} MN' + C_{12} NM') f (M + M' - 1, N + N' - 1). \quad (4.21) \]

Here \( f(M, N) = \delta_{M, \text{even}} \delta_{N, \text{even}} \frac{1}{(M + 1)(N + 1)}. \) \( C_{11}, C_{12} \) and \( C_{44} \) are the linear elastic constants. For an isotropic material, \( C_{11} = C_{12} = 2C_{44}. \) It is important to note that Eq. (4.21) is valid for a plate in plane strain deformation and all the following calculations are based on this. To fully utilize the symmetry property of a rectangle to simplify the procedure and fully exploit the ability of RSG to solve large matrices, we calculate the eigenfrequencies separately for each kind of symmetry. This means the exponents of \( x/a \) or \( y/b \) in the basis functions are chosen accordingly. The basis functions have even (+) or odd (-) parity under sign inversion of the \(x\) or \(y\) coordinate. As an example, for a longitudinal (L) mode, the exponent of \( x/a \) should be odd and the exponent of \( y/b \) should be even in the \( u_x \) displacement expansion.
Table 4.3: Parities of displacement components for different symmetries of a rectangle.

<table>
<thead>
<tr>
<th>mode</th>
<th>$u_x$</th>
<th>$u_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>longitudinal</td>
<td>$(-,+)$</td>
<td>$(+,-)$</td>
</tr>
<tr>
<td>torsional</td>
<td>$(+,-)$</td>
<td>$(-,+)$</td>
</tr>
<tr>
<td>bending_x</td>
<td>$(-,-)$</td>
<td>$(+,+)$</td>
</tr>
<tr>
<td>bending_y</td>
<td>$(+,+)$</td>
<td>$(-,-)$</td>
</tr>
</tbody>
</table>

The vibration patterns of the eigenmodes of a copper square with width 2500Å are shown in Figure 4.7. Contour plots of the displacement magnitude $\sqrt{u_x^2 + u_y^2}$ are shown for the lowest eigenmodes of non-zero frequency with each symmetry. Comparing Figure 4.7 with Figure 4.4, the deformed shapes are exactly those predicted by the group theory. There are three zero frequencies representing rigid body motion along the x or y direction and rotation about the z-axis. These are the lowest frequency modes of bending-x, bending-y, and torsional symmetry, respectively. In Figure 4.7 the modes are arranged with the increasing frequency value and are named according to their symmetry. In the graph the largest displacement magnitude is normalized to one.
Next we change the geometry from square to rectangle. The width of the plate is kept fixed at 2500Å in the y direction, and the length of the plate is varied from 2500Å to 25000 Å in the x direction. The eigenfrequencies as a function of the ratio of length to width are plotted in Figures 4.8, 4.9, 4.10 and 4.11 for longitudinal (L), torsional (T), bending-x (X) and bending-y (Y), respectively. Seven nonzero branches are plotted in each figure.
Figure 4.8: Longitudinal modes as a function of length over width.

Figure 4.9: Torsional modes as a function of length over width.
The eigenmode frequencies decrease monotonically as the length increases. Two peculiar plateaus appear in Figures 4.8 and 4.11 for the longitudinal (L) and bending-y (Y) modes. The lower one around 2.37 is associated with the edge mode that was discussed in
Chapter 2, a mode with a pronounced amplitude at the end edges and a weak propagating wave along the length of the plate. As pointed out previously, this localized mode is weakly coupled with the propagating wave. This coupling is zero when the Poisson’s ratio equal to 0 or 0.2248. The higher plateau around 2.92 in Figures 4.8 and 4.11 is related to the width stretch resonance. If Poisson’s ratio were zero, this is a mode for which the particle displacement is in the $y$-direction, and the frequency is $\nu/\sqrt{2b}$ and the frequency of this mode would not change with changes in the length of the plate. If Poisson’s ratio is not zero, this mode for $a/b \to \infty$ is associated with the lowest point on the second symmetric branch of dispersion spectrum [18].

4.4 Level Repulsion Phenomena

Another interesting phenomenon is the level repulsion between two close branches having the same symmetry. This can be seen in Figures 4.8 through 4.11. If all the curves on these figures are plotted in one graph, the curves belonging to different symmetries are seen to cross one another while the modes of the same symmetry do not cross. In different physics or engineering problems this general phenomenon is referred to as “anticrossing” or “level repelling” or “mode veering”. When two curves approach as the length of the plate is changed, the vibration patterns of the modes change by a large amount. After the level repulsion has been completed, the vibration patterns of the two modes have been interchanged. This occurrence has been described nicely by Leissa [19], as “figuratively speaking, a dragonfly one instant, a butterfly the next, and something indescribable in between.” To illustrate this in the present context, we plot in Figure 4.12
the mode pattern of longitudinal modes in the third and fourth branches when the ratio of length to width ratio is increased from 3 to 5. The deformation shapes are almost interchanged between these two branches.

Figure 4.12: Vibration mode patterns for the 3rd and the 4th branches with L symmetry.
Bibliography


Chapter 5

Edge Mode Vibration

5.1 Introduction

Edge mode vibration was first found in an experiment performed by Shaw. In 1956 he studied the vibrations of a series of thick circular disks made of barium titanate by employing an optical interference technique [1] that was first developed by Osterberg and Dye in the study of quartz crystals. The purpose of his research was to gain insight into the modes of transducers operating in thickness resonance and to find the optimal value of the ratio of radius $a$ to semithickness $l$.

In the experiment, only normal modes with axial symmetry were excited. Measurements were made on a single disk of barium titanate. Initially, this disk had $a/l \approx 6.6$; the radius was then continuously reduced until $a/l \approx 1.0$. Shaw observed a particular mode whose resonant frequency was almost independent of the ratio $a/l$ and was far below the lowest frequency associated with the real wave vector of the second branch for an infinite plate. This mode of vibration had maximum motion occurring at the edge and decreasing rapidly toward the center.
This mode was not able to be recognized in earlier work due to the high requirement of accurate disk shape; small perturbations to the shape cause the mode to break into several non-axially symmetric modes which are only weakly excited by application of the driving electric field.

Unfortunately Shaw erroneously interpreted the mode as a surface wave resonance and tried to explain the fact that the frequency does not match with the surface wave velocity by suggesting that the boundary condition at the flat plane surfaces increases the effective length of the cylindrical surface to become larger than its physical length.

5.2 Vibration Patterns of Edge Mode in a Rectangular Plate

We now return to discuss the modes of a rectangular plate in plane strain deformation. In Chapter 4, we plotted the normal mode frequency versus length \(a\) to width \(b\) ratio for each of the four different symmetries. Both the longitudinal mode (L) and the bending-\(y\) mode (Y) have a plateau located at 2.37 that is attributed to the edge mode. To be clearer, displacement fields of an edge mode in L and Y symmetry are separately shown in Figure 5.1 and Figure 5.2 for \(a/b = 6\) for a copper plate.

The above fields (\(U\) magnitude, \(U_x, U_y\)) are all normalized by the maximum displacement amplitude within the plate. To magnify the interior motion, we show the displacement fields using a color plot in which the range of colors represents the range of \(U_x\) and \(U_y\) between -0.1 and 0.1. The actual range of \(U_x\) and \(U_y\) is still -1 to 1, but the displacements are large only near to the ends.
Figure 5.1: Longitudinal displacement fields of an edge mode with $a/b = 6$ for a copper plate.

Figure 5.2: Bending-$\gamma$ displacement fields of an edge mode with $a/b = 6$ for a copper plate.

We now compare these results with what happens for the special Poisson’s ratio $\nu = 0.2248$ in Figures 5.3 and 5.4. These graphs confirm that for this particular case the
coupling of the edge mode to the propagating $S_0$ wave becomes zero. There is no vibration in the middle of the plate far enough away from the ends.

Figure 5.3: Longitudinal displacement fields of an edge mode with $a/b = 6$ for a plate with $\nu = 0.2248$.

Figure 5.4: Bending-$y$ displacement fields of an edge mode with $a/b = 6$ for a plate with $\nu = 0.2248$. 
5.3 Related Physical Model for Edge Resonance

In the Section 1 of Chapter 3, we have described a physical picture of the edge resonance. At each end of the plate there is a localized mode “solution” which satisfies the equations of elasticity and approximately satisfies the boundary conditions at the surface of the plate. We called this a quasi-localized mode QLM. Suppose now that one sets up an initial displacement having the form of a QLM at the left hand end \((x=0)\). Because the solution is only approximate, this will result in a vibration localized at the end of the plate plus sound radiation along the plate. Due to the radiation of sound along the plate in the positive \(x\) direction, the amplitude of the vibration localized at the left hand end of the plate will decrease with time. For a semi-infinite plate, i.e., a plate extending from \(x=0\) to \(\infty\), the amplitude would decrease as \(\exp(-\Gamma t)\) where \(\Gamma\) is a measure of how strongly the QLM is coupled to the radiation. For a plate of finite length \(a\) the physics will be different since there will also be a QLM of the same frequency at the right hand end of the plate. The radiation coming from the left hand end will resonantly excite the mode at the right hand end which can then reradiate back to the left.

One can construct a simple model (Figure 5.5) to describe some of the physics of the edge mode. Two masses \(M\) are connected to an elastic rod by springs of stiffness \(K\). The length of the rod is \(a\) and the springs are attached to points at distance \(c\) from each end.

![Figure 5.5: One dimensional simple model for edge mode.](image-url)
Only symmetric motion with respect to the origin is considered here. For a rod with effective Young’s modulus $E$, and mass density $\rho$, the displacement satisfies the equation of motion

$$\rho \ddot{u}(x,t) = E \frac{\partial^2 u(x,t)}{\partial x^2}. \quad (5.1)$$

Due to the discontinuity at $x = a/2 - c$, the solution to this problem is separated into two regions. In the region $0 \leq x \leq a/2 - c$, the displacement $u_1$ is

$$u_1(x,t) = \sin(\beta x)e^{\beta t} \quad (5.2)$$

in order to satisfy the requirement that the displacement be zero at the center of the rod.

The wave number is $\beta = \omega / v_p$ and the sound velocity is $v_p = \sqrt{E / \rho}$.

In the region $a/2 - c \leq x \leq a/2$, the displacement is

$$u_2(x,t) = [\gamma_0 \sin(\beta x) + \gamma_1 \cos(\beta x)]e^{\beta t}, \quad (5.3)$$

with the coefficients $\gamma_0$ and $\gamma_1$ to be determined by two boundary conditions: zero traction at $x = a/2$ and displacement continuity at $x = a/2 - c$. Then

$$0 = \gamma_0 \cos(\beta a/2) - \gamma_1 \sin(\beta a/2), \quad (5.4)$$

$$\sin[\beta(a/2 - c)] = \gamma_0 \sin[\beta(a/2 - c)] + \gamma_1 \cos[\beta(a/2 - c)]. \quad (5.5)$$

Then we can get

$$\gamma_0 = 1/[1 + \cot(\beta a/2)\cot[\beta(a/2 - c)]], \quad (5.6)$$

$$\gamma_1 = 1/[\tan(\beta a/2) + \cot[\beta(a/2 - c)]].$$

The equation of motion of the mass point $M$ on the right hand side is

$$M \ddot{u}_M(t) = -K[u_M(t) - u_1(a/2 - c)], \quad (5.7)$$

and the force balance equation is
\[
[\sigma_1(x,t) - \sigma_2(x,t)]_{x=a/2-c} = E \left( \frac{\partial u_1}{\partial x} - \frac{\partial u_2}{\partial x} \right) = K[u_M(t) - u_1(x,t)]_{x=a/2-c}, \quad (5.8)
\]

Since the mass point has the same vibration frequency as the wave propagating down the rod, we can write \( u_M(t) = \alpha e^{i\omega t} \) where \( \alpha \) is a constant. Combining Eq. (5.6), (5.7) and (5.8) together, the final transcendental equation for the mode frequency is

\[
(K - M\omega^2) \left[ K \sin \beta(a/2 - c) + \frac{E\beta \cos \beta a/2}{\cos \beta c} \right] = K^2 \sin \beta(a/2 - c). \quad (5.9)
\]

We now try to match the result of this 1D simple model to a real 2D copper plate. In Figure 4.8, the localized mode frequency is \( \tilde{\omega}_{loc} = 2.37 \) in units of \( 2\nu_s/b \). Furthermore, from Figure 2.3, we know that the related phase velocity on the first branch of the symmetric modes is \( v_p/v_s \approx 1.314 \). In the limit in which \( E/K \) is very large there are two types of solution which correspond to vibrations which are only weakly coupled. Modes of frequency approximately \( \sqrt{K/M} \) involve vibrations of the masses \( M \). Modes of frequency \( n\pi v_p/a \) with \( n = 1, 3, 5,... \) are primarily vibrations of the rod. If \( E/K \) is infinite, then as \( a \) is increased the frequencies of these modes can cross. A finite value of \( E/K \) results in hybridization as the mode frequencies approach each other. By choosing \( E/K = 160b \) and \( \sqrt{K/M} = 4.74 \) and for simplicity taking \( c = 0 \), we obtain a good fit to the variation of the dimensionless mode frequency \( \omega b/\nu_s \) with the length \( a \) as calculated numerically using basis functions. This fit is shown in Figure 5.6. The fit to the detailed numerical calculations is good except in the region of the first plateau. It is not surprising that the model cannot describe the first plateau since this is for a plate of length only about twice the width.
Figure 5.6: Comparison between frequencies of 1D simple model (solid curve) and numerical result of 2D copper plate from Figure 4.8 (dotted curve).

5.4 Change the End Shapes of a Plate

It would be of interest to observe the perfectly localized modes experimentally, i.e., the localized modes in a material that has the required value of $\nu$. A compendium of values of Poisson’s ratio has been prepared by Anderson [2]. One material with $\nu$ close to 0.2248 is silicon ($\nu = 0.223$) and materials with $\nu$ close to 0.290 include iron (0.285), nickel (0.288) and zinc (0.287). It should also be possible to prepare an alloy with the desired value.

But since Poisson’s ratio is hard to adjust precisely to a desired value, here we consider an alternative approach in which the shape of the end of the plate is changed [3, 4]. We first investigate the end shape shown in Figure 5.7. The numerical method is as follows.
We choose a value for the parameter $c$ together with a value for Poisson’s ratio. We then use the basis function method to find the normal modes of $L$ symmetry for a plate with the same shape at each end. The length $a$ of the plate is chosen to be large compared to the width $b$, typically $a/b$ is 10. This has the consequence that at the center of the plate the displacement due to a QLM at the end of the plate (approximately or exactly localized) will be small. Therefore the displacement at the midpoint of the length of the plate comes primarily from the propagating waves radiated by the localized vibrations at the ends.

If the value of Poisson’s ratio is such that the localization is perfect (i.e., no propagating waves are produced), the displacement at the center of the plate will be zero (apart from the exponential tails of the localized modes). Using this simple method we are then able to determine the value of $c$ required for localization for a sequence of different values of $\nu$ (Figure 5.8). This calculation shows that by modifying the shape of the end of the plate it is possible to create a localized mode at the end regardless of the value of Poisson’s ratio provided it lies in the normal range between 0 and 0.5. The frequency of the localized modes is shown in Figure 5.9.

![Figure 5.7: The change in the shape of the end of the plate needed to result in a localized mode.](image)
Figure 5.8: Geometry parameter $c$ in Figure 5.7 for producing a localized mode as a function of Poisson’s ratio.

Figure 5.9: The dimensionless frequency of the localized modes for the structure shown in Figure 5.7 as a function of Poisson’s ratio.
Results obtained by changing the shape of the end of a plate in a different way are shown in Figure 5.10. Again, it is found that there is always a shape that gives a completely localized mode in Figure 5.11.

Figure 5.10: The change in the shape of the end of the plate needed to result in a localized mode.

Figure 5.11: Geometry parameter $c$ in Figure 5.10 for producing a localized mode as a function of Poisson’s ratio.
As already noted, there is only one propagating mode that has the correct symmetry and frequency to be excited by the localized mode. By changing the shape of the end of the plate and, at the same time, the pattern of vibration of the localized mode it is possible to make the amplitude of this wave to become zero and to give complete localization. It is interesting to note that the simple model (Figure 5.5) can also give a non-radiating localized mode if the parameters are suitably chosen. The condition is that the length $c$ have the value

$$c = \frac{n \pi v_p}{2} \sqrt{\frac{M}{K}},$$  \hspace{1cm} (5.10)$$

where $n = 1, 3, 5, ...$ When this condition is satisfied the mass $M$ vibrates and a standing wave is set up in the part of the rod between the end and the point at which the spring is attached. The displacement within this section of rod is $\pi$ out of phase relative to the vibration of the mass. The amplitudes of vibration of the mass and of the end section of the rod are such that the total oscillatory force acting on the center section of the rod adds to zero and thus no disturbance is propagated down the rod. Investigation of the family of shapes shown in Figure 5.12 leads to an interesting result in Figure 5.13. First, we find that unless $\nu$ lies in the range between about 0.15 and the special value 0.2248, there is no value of $c/b$ that leads to a localized mode uncoupled to propagating modes. Second, the plot of $c/b$ versus $\nu$ ends at a critical value where $c/b = 0.252$ and $\nu = 0.205$. We have investigated the reason for this. We find that as $c/b$ increases, the frequency of the localized mode increases (see Figure 5.14) and at the critical value just given becomes larger than the frequency of the second symmetric propagating mode. When this happens, the frequency of the localized mode is such that there are two distinct extended
modes that can propagate along the plate. Consequently, for the mode to be completely localized, i.e., to not lose energy by radiation, it is necessary for the shape of the end of the plate to be such that the coupling to both propagating modes be zero. Clearly, this is unlikely to happen if only one geometrical parameter is varied.

Figure 5.12: The change in the shape of the end of the plate needed to result in a localized mode.

Figure 5.13: Geometry parameter $c$ in Figure 5.12 for producing a localized mode as a function of Poisson’s ratio.
5.5 Axisymmetric Edge Mode in a Rod

It is also interesting to consider the three dimensional problem of a rod. It may be more practical to perform experiments on a rod than on a plate or bar. Here we consider the axisymmetric vibrations in which the particle displacement lies in a plane that contains the axis. The analytical solution of the equation of motion is generally impossible to achieve for a finite rod. The stress free boundary conditions have to be satisfied at the circular surface and two flat ends [5, 6].

To find the normal modes, we have used the Rayleigh-Ritz method as described previously. The nonzero displacements are only $u_r$ and $u_\theta$, and these are expanded in terms of the normalized basis functions.
\[ \Phi_{\lambda}(r, z) = \left( \frac{r}{R} \right)^n \left( \frac{2z}{H} \right)^m. \] (5.11)

where \( R \) is the radius and \( H \) is the length. The normalized eigenfrequency versus the length for a copper rod with the same radius all along its length is plotted in Figure 5.15. The edge mode is located at \( \omega = 3.03R/v_s \).

Figure 5.15: Eigenmode frequency versus length for a copper rod with a fixed radius.

Besides \( \nu = 0 \), there is another Poisson’s ratio \( \nu = 0.158 \) which gives a perfectly localized mode for a straight rod. We now investigate the effect on the localized mode of a change in the shape of the ends (Figure 5.16). The resulting relation between \( c \) and the value of Poisson’s ratio that is required to produce a purely localized edge mode is shown in Figure 5.17. When a flat circular disk is attached to the end of the rod (disk thickness \( c \).
equal to the difference between the radius of the disk and the radius of the rod $R$), the value of $\nu$ required to produce a localized mode decreases, and becomes zero for $c \approx 0.11R$.

![Diagram of a rod with a disk attached](image)

Figure 5.16: The change in the shape of the end of the rod needed to result in a localized mode.

![Graph of $\nu$ vs. $\frac{c}{R}$](image)

Figure 5.17: Geometry parameter $c$ in Figure 5.16 for producing a localized mode as a function of Poisson’s ratio.

We have also considered the related problem (Figure 5.18) of a rod of radius $R$ with a disk of smaller radius and thickness $c$ attached to the end. In Figure 5.19 the critical value of $\nu$ first increases to a maximum value of 0.21 then decreases. The curve stops when the
frequency of the localized mode has increased to reach the lowest frequency of the second propagating mode from the Pochhammer equation [7], at which point it is impossible find a localized mode for the same reason that was given in the discussion of a 2D plate. It is clear that for the geometry shown in Figure 5.18 we should find that when $c$ is increased so that it approaches the value of $a$ there should again be a localized mode with $\nu = 0.158$.

Figure 5.18: The change in the shape of the end of the rod needed to result in a localized mode.

Figure 5.19: Geometry parameter $c$ in Figure 5.18 for producing a localized mode as a function of Poisson’s ratio.
5.6 Structures with Different End Dimensions

We now consider the modes in plates that have a different shape at the two ends, specifically the isosceles trapezoid shown in Figure 5.20. Because of the lowered symmetry, there will now be a mixing between the longitudinal (L) and bending-Y (Y) modes, and so there will be normal modes (LY) with displacements that are linear combinations of these two symmetries. It is now of interest to understand how these modes vary with three parameters, i.e., Poisson’s ratio, the ratio \( a/b \) and the fractional difference \( \frac{\Delta b}{b} \) in the width of the plates at the two ends.

![Figure 5.20: Sketch of an isosceles trapezoid plate in plane strain deformation.](image)

In Figure 5.21 we show the frequencies of the LY modes as a function of \( a/b \) for copper with \( \frac{\Delta b}{b} = 0.05 \). There are now two series of plateaus at the dimensionless frequencies of 4.63 and 4.86. The length of each plateau is close to one half of the length of the plateaus for the rectangular plate RP (see Figure 4.8). Inspection of the vibration patterns for these modes reveals that in the range of the upper plateaus the vibration is a QLM localized at the narrow end of the plate (frequency \( \Omega_{\text{narrow}} \)) and the lower plateau is a QLM at the wide end (frequency \( \Omega_{\text{wide}} \)).
These results are straightforward to understand in terms of an extended version of the simplified model already discussed. The frequencies for the RP shown in Figure 4.8 are for modes with pure L symmetry. The approximate localized modes with this symmetry can only hybridize with L symmetry extended modes. When the plate is a trapezoid the localized modes can hybridize with both L and bending-Y symmetry extended modes. Thus the number of extended modes which can hybridize with the localized modes is doubled and so the length of each plateau is reduced by a factor of two compared to the plateaus for the RP.

Figure 5.21: The frequency of modes of LY symmetry in an isosceles copper trapezoid. The calculations are for $\Delta b/b = 0.05$. 
The difference between the frequencies $\Omega_{\text{narrow}}$ and $\Omega_{\text{wide}}$ of the QLM at the two ends of the plate is primarily due to the difference in the width. However, careful examination of the results in Figure 5.21 reveals that these frequencies (taken, for example, at the center of each plateau) also depend weakly on the length $a$ of the plate. The variation with change in $a$ is in the opposite direction for the QLM at the two ends, and becomes less rapid as $a$ increases. This variation arises because the frequency depends not just on the width of the plate but also on the angle $\theta$ (see figure 5.20). As the length $a$ increases this angle decreases toward the limiting value of $\pi/2$ at the right hand end while the corresponding angle at the left hand increases towards $\pi/2$.

Figure 5.22: Ratio of the magnitude of the mode displacement at the two ends of a trapezoid as a function of the parameter $\Delta b/b$ for different values of Poisson’s ratio.
For the rectangular plate the magnitude of the displacement of a localized mode is the same at each end since the mode has either even or odd symmetry (L or bending-Y). For trapezoidal plates, the mode pattern changes such that for sufficiently large $Δb/b$ the mode amplitude becomes much larger at one end than the other. Figure 5.22 shows the ratio of the mode amplitudes at the two ends of a plate as a function of $Δb/b$ for a series of values of $ν$. The plate length is sufficiently long ($a/b = 8$) for there to be no significant effect of the length on the results. For $ν$ close to the critical value $ν_c$ of 0.2248, even a very small difference in the widths of the ends of the plate results in the mode becoming localized at one end. One can understand the results as follows. When $ν$ is close to $ν_c$ one can find a QLM at the end of the plate that is coupled very weakly to the extended modes. Consequently, this mode is very sharp and can only be excited by incoming waves that have a frequency lying in a very narrow range. Thus, as soon as there is a small difference in the frequency of the QLM at the two ends of the plate, (due to a difference in plate width), the propagating radiation emitted by the QLM at one end does not significantly excite the QLM at the other end.

Similarly, we consider a specific example of the effect of localization consider the modes of a rod that has a radius varying along its length from $R + \Delta R/2$ to $R - \Delta R/2$ as shown in Figure 5.23. In this example, the length of the rod is taken to be eight times the radius. If both ends of the rod have the same radius ($\Delta R = 0$), the vibrational amplitudes at each end will be the same and there will be modes that have even and odd parity along the rod (Figure 5.23a and b). In Figure 5.23c and d, we show how these modes change when $\Delta R/R$ equals 0.01 in the case that $ν = 0.35$. For this value of $ν$, the QLM are strongly coupled to the propagating mode and so even though the QLM at opposite ends of the rod
have slightly different frequencies, they are still coupled together through the propagating mode. Consequently the modes of the structure have a vibration pattern that has close to even or odd parity. For \( \nu = 0.14 \) close to the particular \( \nu = 0.158 \), on the other hand (Figure 5.23e and f), the coupling to the propagating mode is much weaker and a difference between the end radii of \( 0.01R \) results in the mode pattern changing so that the vibration is localized almost completely at one end of the rod or at the other.

Figure 5.23: The effect of making the radii at the two ends of the rod different. a) and b) show the mode patterns for modes symmetric and anti-symmetric along the length when the radii at the two ends are equal, and Poisson’s ratio is 0.35. The patterns of these modes when \( \Delta R/R = 0.01 \) are shown in c) and d) for \( \nu = 0.35 \), and in e) and f) for \( \nu = 0.14 \).


Chapter 6

Dynamic Mode Frequency Analysis

6.1 Introduction

In Chapter 1, we mentioned experimental studies of the normal modes of nanostructures. Raman scattering can give the frequencies directly, but the pump-probe experiments measure the response of the sample in the time domain and do not directly give the resonance frequencies. Since the nanostructures are usually embedded in a substrate, the frequencies are normally complex. The imaginary part depends strongly on the nanostructure and substrate interaction. In this chapter, we will describe some numerical methods for finding frequencies from this type of experimental data, and show some specific examples and applications.

6.2 Damped MUSIC (DMUSIC) Algorithm

The difficulty of extracting the complex frequencies from the damped sinusoidal signal is that the signal is nonstationary and the correlation matrix cannot be found. The data extends over a limited time range and this makes it difficult to determine accurately the
mode frequencies by taking a Fourier transform. A large number of algorithms have been devised to solve this problem. One such algorithm was first proposed by Tufts and Kumaresan [1], and extended by Cadzow [2] and Van Huffel [3]. Later on Y. Li et al. devised an improved parameter estimation – damped MUSIC (multiple signal classification) algorithm using both the Hankel and the rank-deficiency properties of the prediction matrix [4]. This algorithm has been called DMUSIC.

In these approaches it is assumed that the time dependent signal consists of $K$ damped sinusoidal components. Suppose that the data of this signal is taken at a set of $N$ times with a uniform time interval $\tau$, so that

$$y(n) = \sum_{k=1}^{K} C_k e^{s_k n} + w(n), \quad (6.1)$$

where $C_k$ is the complex linear amplitude of each oscillation $k$, and $s_k = (-\alpha_k + i\omega_k)\tau$ with $\alpha_k$ and $\omega_k$ the damping factor and the angular frequency respectively. $w(n)$ is the high frequency portion, such as white noise. The data runs from $n = 0$ to $n = N - 1$.

To derive the algorithm of DMUSIC, we first construct a prediction matrix $A$ with elements

$$A_{ij} = y(i + j - 2). \quad (6.2)$$

From (6.1) it is clear that we must have $N \geq 2K$. A standard choice of the matrix $A$ is to make it have the dimension $N/2$ by $N/2$.

$$A = \begin{pmatrix} y(0) & y(1) & \cdots & y(N/2 - 1) \\ y(1) & y(2) & \cdots & y(N/2) \\ \vdots & \vdots & \ddots & \vdots \\ y(N/2 - 1) & y(N/2) & \cdots & y(N - 1) \end{pmatrix} \quad (6.3)$$

Combining (6.1) and (6.2), any element of $A$ is
\[ A_{ij} = \sum_{k=1}^{K} C_k r_i^k r_j^k + w_{ij} \] with \( r_i^k = \exp[(i-1)s_k] \). \hspace{1cm} (6.4)

Written in a matrix form, A is transformed to

\[ A = \sum_{k=1}^{K} C_k r(s_k) r^T(s_k) + W = SCS^T + W. \] \hspace{1cm} (6.5)

Here

\[
\begin{pmatrix}
1 \\
e^{s_1} \\
\vdots \\
e^{(N/2-1)s_K}
\end{pmatrix},
\]

\[
S = [r(s_1), r(s_2), \ldots, r(s_K)],
\]

\[
C = \begin{pmatrix}
C_1 & 0 & \ldots & 0 \\
0 & C_2 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & C_K
\end{pmatrix},
\]

If the \( s_k \)'s are distinct from each other, then \( r(s_k) \) for \( k = 1 \cdots K \) are linear independent, so \( S \) is of full column rank. Since the rank of \( C \) is \( K \), the rank of \( A \) is equal to \( K \) if there is no measurable noise. First, assume that there is no noise so that \( W = 0 \). The matrix \( A \) can be written as the product of three \( N/2 \) by \( N/2 \) matrices by singular value decomposition (SVD),

\[ A = UXV^T \] \hspace{1cm} (6.9)

Here \( U, V \) are unitary matrices, so that \( UU^T = 1 \) and \( VV^T = 1 \). \( X \) is a diagonal matrix which has the elements from \( K + 1 \) to \( N/2 \) all zero. Then,

\[ AV = UX \] \hspace{1cm} (6.10)

Since \( X_{kk} = 0 \) for \( k = K + 1, \cdots N/2 \), we can get the orthogonality relations
\[ A v_k = 0, \quad (6.11) \]

where \( v_k \) is the \( k \)-th column of \( V \). So from (6.5) and (6.11)

\[ \text{SCS}^T v_k = 0 \quad \text{for} \quad k = K + 1, \ldots, N/2. \quad (6.12) \]

Due to the fact that both \( S \) and \( C \) are of full rank, \( S^T v_k = 0 \), equivalently \( r^T (s_n) v_k = 0 \), for \( k = K + 1, \ldots, N/2 \) and \( n = 1, 2, \cdots K \). When noise is present, the orthogonality relations (6.11) are no longer available. In this case, the criterion of searching for the best value of \( s_n \) is to make it most closely satisfy the relation (6.11), so \( \left| r^T (s_n) v_k \right| \) should be minimized for every \( n \). In summary, we list the recipe for implementing the DMUSIC algorithm.

- **Step 1**: set up the prediction matrix \( A \) from the experiment data.
- **Step 2**: perform SVD of \( A \) to find matrix \( V \).
- **Step 3**: choose a value of the parameter \( s \equiv (−\alpha + i\omega)\tau \) and adjust it until the maximum of the “peak function” is obtained

\[
p(s) = \frac{1}{\sum_{k=K+1}^{N/2} \sum_{j=1}^{N/2} r_j V_{jk}^2}, \quad \text{here} \quad r_j = \exp[(j - 1)s]. \quad (6.13)
\]

After getting the frequencies and damping factors from DMUSIC, a general linear least squares method is applied to obtain the coefficients \( C_k, k = 1, \cdots, K \). To exhibit the power of this algorithm, some examples are given below. Figure 6.1 is a sequence of experimental data from the pump-probe setup in our lab. Figure 6.2 is a sequence of experimental data from the MetaPULSE system of Rudolph Technologies, Inc. These data were taken for samples of metal lines embedded in some soft material. In both of
these two graphs, there are three contributions: the decaying sinusoidal oscillations, a slowly varying background, and high frequency noise particularly evident in Figure 6.2. The background and the high frequency noise can be removed by fast Fourier transform (FFT) filtering. The remaining signal is analyzed by the DMUSIC algorithm.

Figure 6.1: Pump-probe experimental data from the setup in our lab.

Figure 6.2: Pump-probe experimental data from the MetaPULSE tool.
Figure 6.3: DMUSIC fitting of the signal in Figure 6.1 without the background.

Figure 6.4: Signal in Figure 6.1 is compared to the DMUSIC fitting added with the background.
First, we deal with the data in Figure 6.1. We use only the data after time 218 ps; before this time the “background” is too rapidly varying for us to make a reliable subtraction. To determine the background, the FFT of the data is taken. This FFT is then multiplied by the function

\[ F(f) = \begin{cases} 
1 - f^2 / f_{cutoff}^2, & f < f_{cutoff} \\
0, & f > f_{cutoff} 
\end{cases} \]

where \( f_{cutoff} = 0.87 \) GHz determined by the total number of data and time interval, and the inverse transform is taken to determine the background in the time domain. After subtracting the background from the original data, we use DMUSIC to extract the mode frequencies. The DMUSIC result and the signal without background are compared in
Figure 6.3, and also the DMUSIC result plus the background is compared to the original data in Figure 6.4.

In the same way, we analyzed the data in Figure 6.2; these data are considerably noisier. In Figure 6.5, we directly show the final DMUSIC fitting plus the background compared to the original data in Figure 6.2. We can see the peak positions are caught fairly well.

To improve the accuracy and reliability, we can add Levenberg-Marquardt (LM) iterations to polish the outcomes [5]. LM method is the standard of nonlinear least-squares routines. It combines the extremes of the inverse-Hessain method and the steepest descent method. The latter is used far from the minimum and switches smoothly to the former as the minimum is approached. Since it treats all the parameters including linear and nonlinear in the same way, in many applications it is hard to give each parameter a proper initial input. But here we can put the values of all the parameters found from DMUSIC and the linear least squares as the initial values to the LM method, and look for the minimum value of the fitting error.

About the DMUSIC algorithm, it is worth mentioning that one has to make an initial guess at the number $K$ of sinusoids that make a major contribution to the signal. This is a significant problem. Criteria proposed by Akaike (AIC) [6] and by Schwartz [7] and Rissanen (MDL) [8] have been used to detect the number for signals received by a sensor array [9]. Fuchs developed a perturbation based criterion of the data auto-correlation matrix for detecting the number of frequencies [10]. Information theoretic criteria built on SVD were proposed for the detection of damped/undamped sinusoids number [11] to maximize the likelihood function. We have implemented this algorithm to determine the frequency number $K$ but did not find it effective.
6.3 RELAX Algorithm

Li and Stoica proposed a relaxation based estimator, called the RELAX algorithm to estimate the frequencies and complex amplitudes for the undamped sinusoids with unknown colored noise [12]. Later, an extended RELAX algorithm appeared to calculate the parameters of exponentially damped sinusoidal signals [13]. It has been claimed that this has a better performance than the DMUSIC algorithms.

We developed a similar algorithm to the extended RELAX method. The recipe for implementing this algorithm is quite straightforward.

- Step 1: remove the background and noise from the experimental data to get the signal.
- Step 2: take the FFT of the signal and determine the first angular frequency \( \omega_1 \) with the highest amplitude.
- Step 3: make a best fit to the signal with the function
  \[
  e^{-\alpha t} \left[ A_1 \cos(\omega_1 t) + B_1 \sin(\omega_1 t) \right]
  \]
  by Levenberg-Marquardt (LM). In making this best fit the first angular frequency \( \omega_1 \) and the damping \( \alpha_1 \) are adjusted.
- Step 4: subtract the first frequency’s contribution from the signal, take the FFT of the remaining and determine the second frequency \( \omega_2 \) with the highest amplitude.
- Step 5: make a best fit to the signal with the following function
  \[
  e^{-\alpha_1 t} \left[ A_1 \cos(\omega_1 t) + B_1 \sin(\omega_1 t) \right] + e^{-\alpha_2 t} \left[ A_2 \cos(\omega_2 t) + B_2 \sin(\omega_2 t) \right]
  \]
  by LM to adjust the first and second frequencies \( \omega_{1,2} \) and dampings \( \alpha_{1,2} \).
- Step 6: subtract the first and second frequencies from the signal, and take FFT to get the third frequency, and then use LM to adjust the first three frequencies and
dampings to fit the signal.

- Step 7: keep adding more frequencies, and repeat the above procedure until some convergence condition is satisfied.

As mentioned in the discussion of DMUSIC, the determination of the number $K$ of frequencies is difficult. Here we can choose the value of $K$ based upon how much improvement in the fit results from the addition of each frequency.


