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RESONANT ULTRASOUND SPECTROSCOPY AND

SOLID HELIUM RESEARCH

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ABSTRACT

Recent experiments have indicated some interesting phenomena in solid helium. We have been adapting resonant ultrasound spectroscopy (RUS), which can be used to measure all of a solid's elastic moduli, for use with solid helium. In the RUS technique, a cell with known geometry is attached with ultrasound drive and receive transducers so that a number (10-30) of the cell's natural frequencies may be measured; by analyzing the natural frequencies, valuable information about elastic moduli of the cell’s content (solid helium) can be gained. For RUS to work, it is essential that the normal modes of the cell be well understood. We developed a cell which will maintain robust normal modes when the cell is cycled in temperature and pressure. Normal modes of the vibration of the can fall into two distinct classes: In one class, nearly all energy is in the steel can, and the modes and natural frequencies of this group are almost the same as the empty can. However, helium inside does move with the can and slightly shifts the natural frequency. The second class only show up when there is helium inside the cell and they depend mostly on the helium properties. It was anticipated that the transducers, being outside of the can, would not be sensitive to the second class of normal modes. The plan was to determine elastic properties of helium by analyzing the small frequency shifts of the first class of normal modes. It turns out that transducers are able to determine the natural frequencies of some of the second class modes, which are much more sensitive to helium properties. A finite element method is used to track how resonance frequencies change as $^4$He (elastic) properties change. This is achieved by comparing the similarity of the resonance modes. We find that resonance frequencies that are sensitive to solid $^4$He increase by ~2% from 1 K to 2 K in our experiment. According to our calculation, this corresponds to a ~4% increase in solid $^4$He shear modulus. This shear modulus change could be explained using dislocation theory with appropriate parameters.
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Chapter 1 Introduction

Purpose of the thesis

For a new material, one of the first properties people want to know about is its elastic properties. In engineering science, elastic properties of a new material could determine its appropriateness in various applications. In material science, elastic properties give hints about the microscopic structure of the material. Positions of the atoms are determined by the minima of the potential energy field. The curvature of the potential energy at the minima would be given by the elastic constants. Thermodynamic changes are reflected in the behavior of the elastic constants. The elastic constants are a sensitive probe of various solid-state physics phenomena, including phase transitions. Their accurate and precise measurement is very important.

For many years, there has been considerable interest in a possible new state of matter called supersolid. This is a remarkable state, since it has a property, flow without viscosity, which is counterintuitive for a solid. In 2004, Kim and Chan found some probable experimental evidence for this new state of matter in torsional oscillator (TO) experiments on solid $^4$He samples [1, 2]. The study reveals that the resonant frequency of the oscillator increases below ~250 mK and below a rim velocity of ~10$^{-4}$ m/s. Using conventional analysis, it is assumed that the natural frequency changes when part of the mass becomes superfluid and decouples from rotation at critical temperature and velocity. Several groups have reproduced the results of Kim and Chan [3-7]. There is no doubt about the existence of such an exotic phenomenon, but the physical interpretation is far from clear now. Recent results [8-11] have shown that the elastic properties play a crucial role in the supersolid phenomenon. Measurements of the elastic properties which do not involve a TO show behavior of the shear elastic constant and attenuation which has the same temperature, dislocation density and helium 3 impurity dependence as the
torsional oscillator, but with magnitudes which may be too small to explain the TO result [12]. The purpose of this research is to perform experiments to help understand the possible supersolid state of helium 4. The experiments involve the development of resonant ultrasound spectroscopy (RUS) [13], a relatively new method for measuring the elastic properties of solid helium. A significant advantage of our RUS measurements is that they can detect various types of resonance modes over a wide range of frequency. They can also be made in a cell similar to those used in torsional oscillator measurements. In this thesis, resonant ultrasound spectroscopy and finite element modeling for application to supersolid research will be described.

**Helium, the quantum solid**

The mass of a helium 4 atom is relatively small compared to other atoms or molecules. This means that a helium atom has a relatively large thermal de Broglie wavelength at low temperature and quantum effects play an important role in helium properties. Liquid helium 4 does not solidify at all under its saturated vapor pressure, even at absolute zero. This is a direct effect of quantum mechanics, as the zero point energy is too high to allow freezing. Helium 4 solidifies only under great pressure; it was first solidified in 1926 [14]. The zero point energy is also responsible for a large molar volume. Solid helium 4 is very compressible because atoms are widely spaced and moderate pressure produces relatively large change in volume and other properties. The bulk modulus of solid helium is approximately $5 \times 10^7$ Pa, while the bulk modulus of water is about 40 times larger.

Superfluidity was first noticed in liquid helium 4 in 1938 [15]. When liquid becomes superfluid at low temperatures, it can flow without viscosity and has an effectively infinite thermal conductivity. Superfluidity is related to Bose-Einstein Condensation (BEC), where in the condensed state, particles all move together in a coherent way, reducing energy dissipation significantly. In 1969 Andreev and Lifshitz [16] proposed that vacancies (lattice sites where
atoms are missing) in a quantum solid such as helium 4 could undergo BEC; such an effect would produce a supersolid analogous to superfluid helium. Other theories for a supersolid by Chester (involving atomic quantum exchange) [17] and by Leggett [involving “non-classical rotational inertia” (NCRI)] [18] soon followed. Inspired by the early theoretical predictions, a number of experimental searches were undertaken [19-22] to observe supersolid helium, but none were convincing. Kim and Chan reported the first probable observation of supersolid helium phase in 2004.

In the vacancy picture, vacancies could behave like real quantum particles: they can move via quantum tunneling with neighboring atoms. If the atoms are bosons, then so are the vacancies and at low temperatures vacancies could undergo BEC. The flow of vacancies is an inverse flow of mass. It is possible to observe the coexistence of solid and superflow without friction. However, the creation of vacancies costs more than 10 K [23], far above the supersolid transition temperature observed in the experiment. Quantum Monte Carlo simulation also show that vacancies in a $^4$He crystal phase separate instead of forming a supersolid [24]. It is also difficult to explain the large range of NCRI fractions (~1% in [1] to ~20% in [25]) using the vacancy theory.

Defects may play a crucial role in the supersolid observation. It is found that annealing suppresses the rotational anomaly [3]. Mass flow through solid helium is detected in crystals containing grain boundaries (interface between two grains in a polycrystalline material), but not for crystals without grain boundaries [26]; the effect may be due to a superfluid flow at the grain boundaries. Theoretical studies indeed show that mass inside defects (dislocation defects [27] and grain boundaries [28]) can become superfluid. These may give the appearance of supersolid behavior.

The shear modulus of solid $^4$He increases below 200 mK [8], and has the same dependence on strain amplitude, $^3$He impurities and annealing as the NCRI in torsional oscillator experiments. The stiffening is interpreted as a pinning of dislocation lines at $^3$He impurities. The
elastic property measurement raises the question of the relation between the elastic anomaly and NCRI. Helium 3 also shows a similar elastic anomaly but does not have an NCRI signal [29]. This supports the supersolid idea since helium 3 are fermions and cannot form BEC. There has also been an experiment showing that NCRI of solid helium 4 is not affected under elastic modulus variation [30].

A blocked annulus experiment [2, 25] is the most convincing support for the existence of supersolid state. In the blocked annulus setup, NCRI is not found. This shows that the rotational anomaly in the free annulus experiment may be due to a macroscopic mass flow and it might be a non-local effect. Heat capacity measurements [31, 32] also show the signature of a phase transition. The interplay of rotational, relaxational and shear dynamics in solid \(^4\)He was investigated recently [33], showing no indication of a supersolid phase transition. At this stage, the relations between mechanical properties, supersolidity, and the role of defects in supersolidity are not clear.

**Organization of the thesis**

In this research, we try to study solid helium using the RUS technique, a method different from all other methods employed in all solid helium research so far. A basic introduction of elasticity theory is presented in Chapter 2. This includes some basic concepts and theoretical calculation methods. A significant part of the project involves the development of the calculation tools used to analyze the resonance modes. The finite element method was used to do the simulation and this is presented in Chapter 3. Approximation errors of this method and comparisons with other analysis methods are also discussed in this Chapter.

The experiment setup is discussed in Chapter 4. This includes the low temperature setup, frequency calibration and measurement. A primary goal was to design a cell that can be used repeatedly giving consistent results. The detail of the cell design is presented in Chapter 4.
We discuss the experiment results in Chapter 5. A surprise in the experiment is that the spectrum is not as simple as conjectured and it requires some novel methods to analyze the data. It is necessary to compare the spectrum in different conditions, find ways to reduce the effect of calculation approximations and identify specific modes in the resonance spectrum. Such operations cannot be easily done with commercial finite element software. A unique program was written to do all the calculations. All the programs used in this research are presented in the Appendix.

In the final chapter, we compare the experiment results with other experiments and try to use dislocation theory to explain the elastic properties. Possible improvements of the setup are also discussed.
Chapter 2 Theory of elasticity

A brief review of the theory of elasticity is provided here to give the background information for the resonant ultrasound spectroscopy (RUS) method used in our experimental research.

**Basic concepts**

Two quantities are related with elasticity: a load applied to an object and the deformation of the object, or more accurately, stress and strain (Figure 2.1). The simplest case is a spring. Consider two nearby points \(x\) and \(x + dx\) marked on the spring (we are considering small deformation and linear elasticity), under some tensile force \(F\), their new positions are \(x + u(x)\) and \((x + dx) + u(x + dx)\), where \(u(x)\) is the displacement field. Deformation is reflected in the difference between \(u(x + dx) - u(x)\) and \((x + dx) - x\). The ratio

\[
\epsilon = \frac{u(x + dx) - u(x)}{(x + dx) - x} = \frac{u(x + dx) - u(x)}{dx} = \frac{du}{dx}, \tag{2.1}
\]

which tells us whether the spring is stretched, compressed or not, is defined as strain. It is the fractional change of the distance between the two nearby points and hence dimensionless. Hooke’s law says that force is proportional to the strain

\[
F = C \frac{du}{dx}. \tag{2.2}
\]

If the spring has length \(l\), total stretch would be

\[
\Delta x = l \frac{du}{dx}, \tag{2.3}
\]

with spring constant \(K\), we get the familiar equation
\[ F = K \Delta x = Kl \frac{du}{dx}. \] (2.4)

Comparing with Eq. (2.2), we see that \( K = C/l \).

![Figure 2.1 Strain of a spring.](image)

The above formula can be generalized to higher dimension. Configuration change now is measured by

\[
\frac{\partial u_i}{\partial x_j} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right)
\]

\[ = \epsilon_{ij} + O_{ij} \] (2.5a)

It can be shown that \( O_{ij} \) corresponds to a local rigid rotation, where no deformation is involved [34]. \( \epsilon_{ij} \) describes the elastic property of the material and is defined as the elastic strain tensor. From the above definition it is clear \( \epsilon_{ji} = \epsilon_{ij} \). \( \epsilon_{ii} \) is tensile strain, it describes fractional change in length in the same direction: \( x' = x(1 + \epsilon_{11}) \). \( \epsilon_{ij} \) \((i \neq j)\) is shear strain. It describes shear deformation.

The load on an object is described by the stress tensor \( \sigma_{ij} \), which corresponds to the idea of pressure. \( \sigma_{ij} \) is the directional force in the \( i \)th coordinate direction per unit area acting on a surface with an outward normal direction \( j \). It has the same dimension as pressure. The traction is defined as

\[
\frac{dF_i}{dA} = \sigma_{ij} n_j
\] (2.6)
where \( n_j \) is the unit normal direction vector of surface area element \( A \). Figure 2.2 shows that if the small volume element is in an angular momentum equilibrium state, it is required that \( \sigma_{23} = \sigma_{32} \) (otherwise it would rotate), and similarly we can get \( \sigma_{ij} = \sigma_{ji} \) for other \((ij)\) pairs.

The fundamental assumption of linear elasticity theory is that for small deformation, an elastic medium obeys Hooke’s law: local stress is proportional to elastic strain:

\[
\sigma_{ij} = c_{ijkl} \epsilon_{kl}.
\] (2.7)

\( c_{ijkl} \) is the elastic tensor. Due to the symmetry of \( \sigma_{ij} \) and \( \epsilon_{ij} \), \( c_{ijkl} = c_{jikl} = c_{ijlk} \), in three dimensions, this reduces the independent components from 81 to 36. As a result of the symmetry in the pairs of indices, a convenient contraction of the index pairs may be used, as follows: (11→1, 22→2, 33→3, 23→4, 31→5, 12→6, these are the only 6 combinations for symmetric \((ij)\)). The elastic (strain) energy density is

\[
U = \frac{1}{2} \epsilon_{ij} c_{ijkl} \epsilon_{kl} .
\] (2.8)

This shows \( c_{ijkl} = c_{klij} \), and there are only 21 independent components in the most general case. Intrinsic symmetry of the solid can further reduce the number of independent components. There are cases where other notions are convenient. I will list them here without showing the mathematical details as excellent explanations can be found in the literature [34, 35].

![Figure 2.2 Stress of an infinitesimal element.](image)
Lamé coefficients, bulk modulus

In the isotropic case, we can change the format of stress-strain relations by separating the trace and traceless part of the tensor:

$$\sigma_{ij} = -\lambda \delta_{ij} \text{Tr} \varepsilon - 2\mu \varepsilon_{ij} \quad (2.9a)$$

$$= -K \delta_{ij} \text{Tr} \varepsilon - 2\mu (\varepsilon_{ij} - \frac{1}{3} \delta_{ij} \text{Tr} \varepsilon) \quad (2.9b)$$

$$= -K \delta_{ij} \nabla \cdot \mathbf{u} - \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{u} \right) \quad (2.9c)$$

$\lambda$ and $\mu$ are known as Lamé coefficients. $K = \lambda + \frac{2}{3} \mu$ is the bulk modulus, $\text{Tr} \sigma = 3K \text{Tr} \varepsilon$ is the trace of the strain tensor. To see how $K$ is related with volume, consider the volume of deformed cubic element under the pressure change $dp$ (In this case, the diagonal elements of the strain tensor are all $-dp$, so $\text{Tr} \sigma = -3dp$):

$$V' = a'^3 = a^3(1 + \varepsilon_{11})(1 + \varepsilon_{22})(1 + \varepsilon_{33}) \equiv a^3(1 + \text{Tr} \varepsilon)$$

$$= V(1 + \text{Tr} \varepsilon) \quad (2.10)$$

$$\frac{dV}{V} = \text{Tr} \varepsilon = \frac{\text{Tr} \sigma}{3K} = -\frac{dp}{K} \quad (2.11)$$

$$K = -V \frac{dp}{\partial V} \quad (2.12)$$

This shows the physical meaning of $K$. The bulk modulus, like other elastic quantities, is a thermodynamic quantity whose value depends on the thermodynamic process involved in the deformation.

Young’s modulus and Poisson’s ratio

If a rod with free sides is elongated (compressed) by a uniform stress $\sigma_{zz}$ along the axial direction, transverse compression (expansion) will accompany the axial movement. In this case:

$$\sigma_{zz} = -\frac{9K\mu}{3K + \mu} \varepsilon_{zz} \equiv -E \varepsilon_{zz} \quad (2.13)$$
\[ \epsilon_{xx} = \epsilon_{yy} = \left( \frac{1}{6\mu} - \frac{1}{9K} \right) \sigma_{zz} \equiv -\nu \epsilon_{zz} \]  

(2.14)

where

\[ \nu = \frac{1}{2} \left( \frac{3K - 2\mu}{3K + \mu} \right) \]  

(2.15)

\( E \) and \( \nu \) are known as Young’s modulus and Poisson’s ratio. Most materials have Poisson’s ratio value ranging between 0 and 0.5. With the advance of material engineering, some novel materials with negative Poisson’s ratio value have been synthesized [36, 37]. Their cross sections will expand when stretched in the axial direction, opposite to the behavior of ordinary materials.

Shear modulus.

One key difference between solid and liquid is that a solid can have shear motion. To get an intuitive picture of shear modulus, we can think of the ideal case of a rod with infinite length and square cross section with \( \sigma_{xy} = \sigma_{yx} = f \) and all the other stress components zero (Figure 2.3). Change in angle is \( 2\epsilon_{xy} = \frac{f}{G} \). \( G \) is called shear modulus.

![Figure 2.3 Shear modulus](image)

In the above analysis, we are considering static equilibrium configurations. There are equilibrium equations governing the stress tensor field distribution. It is not that every stress tensor field satisfying the basic symmetric conditions is a realistic solution to the problem.
In viscous fluids, shear stress comes from velocity gradient instead of shear deformation as for an elastic solid medium. The form of the stress tensor in viscous fluids and elastic solid reflects their physical differences. Energy dissipates in liquid because of viscosity, but for solid, there is no energy dissipation due to the shear elasticity.

The elastic constant tensor can be calculated from interatomic potentials \([38-41]\). The elastic energy of crystal as a function of strain can be written in the form:

\[
U(\varepsilon) = U_0 + \frac{1}{2}U_0''\varepsilon^2 + \frac{1}{6}U_0'''\varepsilon^3 + \cdots
\]  

(2.16)

In a harmonic approximation, elastic constants may be written as the second derivatives of the lattice energy:

\[
c_{ijkl} = \left( \frac{\partial^2 U}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \right)_0
\]

(2.17)

Higher order terms in Eq. (2.16) reflect the dependence of elastic constant on strain. By measuring the values of elastic constants, we can gain some information about the interatomic potential.

Symmetry of materials can further reduce the number of independent elastic tensor components. Under coordinate transformation, elastic tensor transforms as a four rank tensor:

\[
c'_{ijkl} = a_ipaqkrats_{pqrs}
\]

(2.18)

For example, with the mirror reflection matrix:

\[
(a_{ij}) = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -1
\end{pmatrix}
\]

(2.19)

c_{ijkl} is invariant under this transformation, so

\[
c'_{ijkl} = a_{ip}aqkrats_{pqrs}
\]

\[
= a_ia_ja_kra_\ell c_{ijkl} = c_{ijkl}.
\]

(2.20)

If \(a_{33}\) shows up once or three times in the subscript, then this term is zero. For example, incorporating the contracted index scheme we have \(c_{1333} = c_{3133} = c_{3313} = c_{3331} = c_{35} = 0\).
Likewise, $c_{1113} = c_{15} = 0$, $c_{2333} = c_{45} = 0$, $c_{2223} = c_{24} = 0$, $c_{1123} = c_{14} = 0$, $c_{2213} = c_{25} = 0$, $c_{3323} = c_{34} = 0$, $c_{1312} = c_{56} = 0$, $c_{2312} = c_{46} = 0$.

For monoclinic crystal, the elastic tensor is in the form:

$$
\begin{pmatrix}
  c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\
  c_{12} & c_{22} & c_{23} & 0 & 0 & c_{26} \\
  c_{13} & c_{23} & c_{33} & 0 & 0 & c_{36} \\
  0 & 0 & 0 & c_{44} & c_{45} & 0 \\
  0 & 0 & 0 & c_{45} & c_{55} & 0 \\
  c_{16} & c_{26} & c_{36} & 0 & 0 & c_{66}
\end{pmatrix}
$$

monoclinic (2.21)

Independent components are reduced from 21 to 13 in this symmetry. Cubic symmetry has 3 independent components:

$$
\begin{pmatrix}
  c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\
  c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
  c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\
  0 & 0 & 0 & c_{44} & 0 & 0 \\
  0 & 0 & 0 & 0 & c_{44} & 0 \\
  0 & 0 & 0 & 0 & 0 & c_{44}
\end{pmatrix}
$$
cubic (2.22)

Isotropic materials (property is the same in every direction) have two independent components: there is a relation $2c_{44} = c_{11} - c_{12}$ added to the cubic case. Using Lamé coefficients, the elastic tensor is in the format:

$$
\begin{pmatrix}
  \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\
  \lambda & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\
  \lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\
  0 & 0 & 0 & \mu & 0 & 0 \\
  0 & 0 & 0 & 0 & \mu & 0 \\
  0 & 0 & 0 & 0 & 0 & \mu
\end{pmatrix}
$$
isotropic (2.23)

**Dynamics**

Considering the force in the $i$th direction on a small volume element, Newton’s second law can be written as (we are using Einstein’s summation rule here):

$$
\rho \ddot{u}_i = -\frac{\partial \sigma_{ij}}{\partial x_j},
$$

(2.24)
assuming there is no external force. In the following discussion, we assume the elastic tensor is constant across the isotropic medium. Using Eq. (2.9c), the equation of motion written in the vector form is:

\[
\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \mu \nabla^2 \mathbf{u} + \left( K + \frac{1}{3} \mu \right) \nabla (\nabla \cdot \mathbf{u}).
\]  
(2.25)

We need to compare the analytical solution of an isotropic sphere with finite element calculation later, so we give one analytical solution here. Under proper conditions, the displacement field can be decomposed into a curl free longitudinal component and a divergence free transverse component [34] (Helmholtz decomposition):

\[
\mathbf{u} = \mathbf{u}_l + \mathbf{u}_t, \quad \nabla \times \mathbf{u}_l = 0; \quad \nabla \cdot \mathbf{u}_t = 0.
\]  
(2.26, 2.27)

Analytical solutions only exist in special cases. We consider a special case for an isotropic sphere with a free surface executing radial oscillations in the form:

\[
\mathbf{u}(x, t) = \Re u(r)e^{-i\omega t} \hat{r}.
\]  
(2.28)

It is easy to check that \(\nabla \times \mathbf{u}(x, t) = 0\), so this is longitudinal motion. Substituting the above equation into Eq. (2.25), we get (being careful about the vector Laplacian operator \(\nabla^2\)):

\[
u'' + \frac{2}{r} u' + \left( \frac{\rho \omega^2}{\lambda + 2\mu} - \frac{2}{r^2} \right) u = 0
\]  
(2.29a)

\[
\sigma_{rr} = -\frac{1}{r^2} (r^2 u')' - 2\mu u' = 0
\]  
(2.29b)

Eq. (2.29b) is a boundary condition, which will yield an equation determining the eigenfrequencies. The non-singular solution at the origin to Eq. (2.29a) is the spherical Bessel function \(j_1(\omega r/c_l)\), \(c_l = \left( \frac{\lambda + 2\mu}{\rho} \right)^{\frac{1}{2}}\). We get an equation for the eigenfrequency using the boundary conditions:

\[
\frac{\omega}{c_l} a * \frac{(\lambda + 2\mu)}{4\mu} * j_0 \left( \frac{\omega}{c_l} a \right) = j_1 \left( \frac{\omega}{c_l} a \right)
\]  
(2.30)

This is one type of resonance mode for an elastic isotropic sphere.
Measurement techniques

Due to the importance of material elastic properties in engineering and science, a number of techniques have been developed to measure them. Generally, these methods can be divided into two groups: static and dynamical methods. In static methods, a force or torque is applied to the object and the resulting static deformation is measured. The elastic tensor elements can be calculated directly from their definitions. The material of interest can be compressed, bended or twisted under uniform or non-uniform loading. These methods are useful for isotropic, regularly shaped objects, but for anisotropic materials, it could be quite complex [42].

Resonance frequency and sound propagation speeds depend on the elastic properties of the constituent materials [43, 44]. This is the idea of measuring the elastic tensor using dynamical methods. It is hard to give the various techniques a general name since their specific realizations depends on the situation. A comparison of different experimental techniques for determining elastic properties of solids is explained in the literature [45]. The high precision of dynamic methods is evident. The difference between dynamic and static measurement of Young’s moduli is investigated in [46]. The author suggests when seeking useful physical property information, both dynamic and static values should be considered.

Sound propagation speed in crystals depends on the propagation and polarization directions. For a cubic crystal, the longitudinal wave propagating in the [100] direction has velocity \( v[100]_{\text{cubic}} = \sqrt{\frac{c_{11}}{\rho}} \). Two transverse modes propagating in the [110] direction have velocity \( v[110]_{\text{cubic1}} = \sqrt{\frac{c_{44}}{\rho}} \), \( v[110]_{\text{cubic2}} = \sqrt{\frac{(c_{11} - c_{12})}{2\rho}} \). If we can get accurate sound speed measurements in these three directions, we can get all the elastic constants for cubic materials. In the ultrasonic pulse echo method, a transducer generates a short ultrasound pulse and receives its echo as it is reflected. Sound velocity can be calculated from the transit time and geometry and then the corresponding elastic constants can be calculated [48]. It is important to get uncoupled propagation modes, since coupling/conversion between different modes would
make velocity measurement less accurate. A sample should be prepared in a way that it has uniform, parallel and finely polished surfaces. Another issue in the pulse echo method is the coupling between transducer and sample that influences the transit time. It is difficult to measure elastic constants of crystals with lower symmetries using this method: it requires more measurements of sound propagation in different directions that could reduce overall accuracy. To solve this problem, more complex modes are analyzed and elastic constants can be calculated from group velocity measurements [49, 50].

In summary, resonance frequencies of a sample depend on the elastic constants, sample geometry and boundary conditions, and it is not difficult to excite the resonance. We can get information about elastic constants from resonance frequencies, and if we have enough resonance frequencies we can get the value of all elastic constants. The obstacle to this problem is that it requires large amount of computation except for a simple special sample geometry. In essence, this is a second order partial differential equation with complex domain and boundary conditions. There is no analytical solution in general. A historical development of the normal mode problem can be found in the literature [51].

**Resonant ultrasound spectroscopy**

Many references have talked about the historical development, formulation and application of resonant ultrasound spectroscopy [13, 43, 51-54]. The resonant Ultrasound Spectroscopy technique is used to measure various kinds of materials under different environments. These include thin films [55-57], quasicrystals [58, 59], thermoelectric materials [60] and so on. A typical configuration is shown in Figure 2.4. There are two transducers attached to the sample, one is the driver used to generate vibration and the other is the receiver used to measure the mechanical response of the sample to different drive frequencies. The process proceeds in small frequency steps over a previously determined frequency region of interest.
Later we will give a detailed explanation about choosing the starting and ending frequencies used in our setup. During a frequency sweep, if the excitation frequency is not matched by any resonance frequency, then there would be little vibration, and the receiver gets a very small signal. On the other hand, at resonance, the energy delivered to the sample is increased by a factor equal to $Q$ ($Q$ is the quality factor reflecting dissipation process in the sample) and the samples act like a natural amplifier. The receiver measures a relatively large signal at resonance.

![Figure 2.4 RUS setup.](image)

The following is a short review about the most basic principles.

**Hamilton’s principle**

Hamilton’s principle states that for all the paths between the fixed endpoints, the real dynamical trajectory makes the action of the system stationary. In mathematical formula it is:

$$\delta \int_{t_1}^{t_2} L \, dt = 0 \; ; \text{with fixed endpoints in time.} \quad (2.31)$$

$L$ is the Lagrangian of the system. For an elastic object we are interested in, the Lagrangian is:

$$L = T - V$$
\[
\frac{1}{2} \rho \frac{\partial u_i}{\partial t} \frac{\partial u_i}{\partial t} = \frac{1}{2} c_{ijkl} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} dV. \tag{2.32}
\]

Substituting the equation into Eq. (2.31), we get:

\[
0 = \int \int \rho \frac{\partial \delta u_i}{\partial t} \frac{\partial u_i}{\partial t} - c_{ijkl} \frac{\partial \delta u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} dtdV
\]

\[
= \int \rho \frac{\partial u_i}{\partial t} \delta u_i|_t dV - \int \int \rho \frac{\partial^2 u_i}{\partial t^2} \delta u_i dtdV - \int \int c_{ijkl} \frac{\partial u_k}{\partial x_l} \delta u_i dA_j
\]

+ \int \int c_{ijkl} \frac{\partial^2 u_k}{\partial x_l \partial x_j} \delta u_i dt dV. \tag{2.33}
\]

\(dA_j\) is the boundary surface element. The first term is zero because of the fixed endpoints in time, the third term is spatial boundary condition and it would vanish for both fixed and free boundary conditions (for fixed boundaries, \(\delta u_i = 0\); for free surface boundary conditions, surface traction \(c_{ijkl} \frac{\partial u_k}{\partial x_l} dA_j = 0\)). In our experiment, we have free surface boundary. We are interested in resonance solutions in the form: \(u_i(x, t) = u_{0i}(x) \cos(\omega t + \phi)\). Solutions to the problem are \(u_i\) that make \(\int \rho \omega^2 u_i u_i - c_{ijkl} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} dV\) stationary and satisfy the boundary condition of the problem.

**Variation principle**

Solutions to the problem can also be formulated in another way. Solutions are those that make the following functional stationary and satisfy the appropriate boundary conditions:

\[
\omega^2 (u) = \frac{\int c_{ijkl} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} dV}{\int \rho u_i u_i dV} \equiv \frac{L_1}{L_2}. \tag{2.34}
\]

The proof is as follows:

\[\delta \omega^2 (u) = \delta \left( \frac{L_1}{L_2} \right) = \frac{\delta L_1}{L_2} - \frac{L_1 \delta L_2}{L_2^2}\]
\[
\frac{\delta I_1}{I_2} - \frac{\delta I_2}{I_2} = \frac{1}{I_2} (\delta I_1 - \omega^2 \delta I_2)
\] (2.35)

The remaining parts are the same as in Eq. (2.33).

**Ritz method**

The solutions are those that make the action a minimum among the whole function space satisfying the boundary conditions. Unfortunately, if we do not have analytical solutions we have no way to search the whole function space and find the solution. What we can do is to find a set of trajectories that minimize the action in a smaller function space. We choose an \( m \) dimension basis function set \( \{ \phi_m, m = 1, \cdots, 3N \} \) and write the trial function in terms of these basis functions:

\[
u_i = a_{i,m} \phi_m, \quad i, j, k, l = 1, 2, 3.
\] (2.36)

\( u_i \) is the \( i \)th component of the solution function \( \nu \). For each component \( \{x, y, z\} \) the basis set has \( N \) (could be different) functions. Now the Lagrangian can be written as:

\[
L = \frac{1}{2} \int \rho \omega^2 a_{i,m} \phi_m a_{i,n} \phi_n - c_{ijkl} a_{i,m} \frac{\partial \phi_m}{\partial x_j} \frac{\partial \phi_n}{\partial x_l} a_{k,n} dV.
\] (2.37)

In the equation, summation is over all the repeated indices. \( a_{i,m} \) can be formulated as a row or column vector with \( 3N \) components. If \( a_{i,m} \) is taken as a column vector:

\[
[a_{1,1}, a_{1,2}, \cdots, a_{1,N}, a_{2,N+1}, \cdots, a_{2,2N}, a_{3,2N+1}, \cdots, a_{3,3N}]^T,
\] (2.38)

Eq. (2.37) can be written as:

\[
L = \frac{1}{2} \int A^T \rho \omega^2 \phi_m A - A^T c_{ijkl} \frac{\partial \phi_m}{\partial x_j} \frac{\partial \phi_n}{\partial x_l} A^T dV
= \frac{1}{2} A^T (\omega^2 M - K) A.
\] (2.39)

\( M \) (called the mass matrix) is a \( 3N \times 3N \) matrix:
\[ M = \int \rho \begin{bmatrix} \phi_1 & \cdots & \phi_1 \\ \vdots & \ddots & \vdots \\ \phi_{3N} & \cdots & \phi_{3N} \end{bmatrix} \ast \begin{bmatrix} \phi_1 & \cdots & \phi_{3N} \\ \vdots & \ddots & \vdots \\ \phi_1 & \cdots & \phi_{3N} \end{bmatrix} dV. \] (2.40)

\( K \) (called the stiffness matrix) is a \( 3N \times 3N \) matrix with element:

\[ (K)_{mn} = \int c_{\left\lfloor \frac{m}{N} \right\rfloor j \left\lfloor \frac{n}{N} \right\rfloor k} \frac{\partial \phi_m}{\partial x_j} \frac{\partial \phi_n}{\partial x_l} dV; \quad \text{with summation over } j, k = 1, 2, 3. \] (2.41)

\[ m, n = 1, \ldots, 3L; \left\lfloor \frac{m}{N} \right\rfloor \text{is the smallest integer equal or greater than} \frac{m}{N}. \]

Setting \( \delta L = 0 \), we get the equation:

\[ (\omega^2 M - K)A = 0, \] (2.42)

where \( M \) and \( K \) are matrices whose values can be calculated from the trial functions. This is a generalized eigenvalue problem. Eigenvalues and eigenvectors give us resonance frequencies and the corresponding modes of the system respectively. Two important criteria for choosing basis functions are:

1.) Completeness: any Eigen-functions can be built up from them.

2.) Ease of computation.

Approximation error of Ritz method

We now analyze the approximation error in the Ritz method. For convenience, in the following, a generalized, non-rigorous format will be used. The problem is to find functions and corresponding eigenvalues that make the functional extremum:

\[ L = u \ast K \ast u - \lambda \ast M \ast u \] (2.43)

\( K \) and \( M \) are integral and differential operators in the elastic dynamics problem. Taking a variation with the displacement vector \( u \), we need to solve the eigenvalue problem:

\[ (K - \lambda M)u = 0 \] (2.44)
This is the generalized eigenvalue problem in linear algebra. Many physics problems, when written in differential equations, are also of this format. If $K$ and $M$ are operators, $u$ is a function. We can think of a function as a column vector with infinite elements, each element is the value of the function at a point in the domain. Depending on the property of the operators and boundary conditions, the solution space (i.e. independent functions), could have infinite dimensions $\{u_1, u_2, u_3, \ldots \}$. 

$$(K - \lambda M) \begin{pmatrix} \vdots \\ \vdots \\ \vdots \end{pmatrix} = 0 \quad (2.45)$$

If $K$ and $M$ are $n \times n$ matrices, the solution would be $n$ independent $n$ dimensional vectors $\{u_1, u_2, u_3, \ldots, u_n\}$. 

$$(K - \lambda M) \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} = 0 \quad (2.46)$$

The Ritz method uses a finite dimension space to approximate the whole solution space in both cases. Suppose a trial function/vector is written as a combination of exact orthonormal solutions basis:

$$u_k = a_{ki} \phi_i \quad (2.47)$$

Using Eq. (2.44) and orthonormal relations, the trial eigenvalue is:

$$\lambda'_k = \frac{\sum_i \lambda_i * a_{ki}^2}{\sum_i a_{ki}^2} \quad (2.48)$$

The approximated eigenvalue is a weighted average of the exact eigenvalues that are contained in the trial vector. If it is a good approximation, $a_{kk} = 1$, $|a_{ik}| = |\epsilon_i| \ll 1$, then

$$\lambda'_k \cong \lambda_k + \sum \epsilon_i^2 (\lambda_i - \lambda_k) + o(\epsilon_i^4). \quad (2.49)$$

Or it can be written in the format:

$$\frac{\lambda'_k}{\lambda_k} \cong 1 + \sum \epsilon_i^2 \left( \frac{\lambda_i}{\lambda_k} - 1 \right). \quad (2.50)$$
The eigenvalue approximation error is of second order in the small quantities $\epsilon_i$. In the special case of lowest eigenvalue, the approximated value provides an upper bound for the exact lowest eigenvalue. Several issues need to be considered in the approximation:

1.) We cannot find a complete basis compatible with boundary conditions: if we could, we actually have found the exact solution, assuming $(K - \lambda M) \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} = 0$ has been satisfied to sufficient accuracy.

2.) In Eq. (2.47), it is assumed that we know which one we are approximating. Except for simple cases, in reality, it is not always easy to have a good guess about a specific solution.

3.) $\lambda_i/\lambda_k$ can be very large. In this case, a tiny mixture from a large eigenvalue can increase the error a lot.

To test the Ritz method, we consider the case of a uniform, free-free end string with length, density and strength all one. We first approximate the continuous (functional) case with trial function basis $\{ \phi_m = x^{m-1}, m = 1 \ldots 20. | 1, x, x^2, x^3, \ldots x^{19} \}$. Exact eigenvalues are $\{0, 1, 4, 9, \ldots n^2 \ldots \} \pi^2$.

For this simple 1-D problem, it is easy to calculate the mass and stiffness matrices. The stiffness matrix in the Rayleigh-Ritz method is:

$$K_{mn} = \int c * \frac{\partial \phi_m}{\partial x} \frac{\partial \phi_n}{\partial x} \, dx = \frac{(m - 1)(n - 1)}{m + n - 3}. \quad (2.51)$$

The mass matrix is:

$$M_{mn} = \int \rho \phi_m \phi_n \, dx = \frac{1}{m + n - 1}. \quad (2.52)$$
The calculated $\frac{\omega^2}{\pi^2}$ of the lowest resonance modes of a string using the Ritz method is listed in Table 2-1. The resonance modes from the Ritz approximation is compared with exact solution in Figure 2.5.

Table 2-1 Calculated $\frac{\omega^2}{\pi^2}$ of the lowest resonance modes of a string using Ritz method.

<table>
<thead>
<tr>
<th>mode</th>
<th>Exact solution</th>
<th>Ritz method</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>-62.4863</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0071</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>8.4432</td>
</tr>
<tr>
<td>3</td>
<td>9</td>
<td>9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>12.8597</td>
</tr>
<tr>
<td>4</td>
<td>16</td>
<td>16</td>
</tr>
<tr>
<td>5</td>
<td>25</td>
<td>25.0001</td>
</tr>
</tbody>
</table>

Figure 2.5 Approximated modes from Ritz method for a free-free end string, eigenvalue is shown in Table 2-1.
This result shows that:

1.) The lowest eigenvalue is negative and there are eigenvalues that do not have corresponding exact solutions. This is because trial functions do not meet the free-free end boundary conditions. Some trial functions lower the Lagrangian but do not belong to the solution space.

2.) Due to the mixture, some eigenvalues can be very close. This is not a problem for a simple geometry, but for a complex geometry, it can be misleading. We cannot tell if it is a degenerate mode or a wrong result just from the eigenvalue.

An interesting question is how the approximation results depend on the trial solution. However, it is difficult to test in a function space since the function space is of infinite dimension. To test the robustness of the approximation method we use the finite element method to solve the string problem again (calculated by a Matlab program RitzFEM.m, code and explanation are in the Appendix). For the lowest eigenvalue solutions, the Finite element approximation is very close to the exact solution. We “simulate” the full solution space by the finite element method results and thus reduce it to finite dimension and we can do the test in the finite space. Trial vectors are chosen in three different ways:

1.) Trial vectors are randomly generated.

2.) Random vectors are improved so that lower eigenvalue solutions have a relatively larger weight in the trial vectors. This is achieved by multiplying random vectors from the left side with $K^{-1}$.

3.) Trial vectors are generated in the format $\{1, x, x^2, \ldots x^{WT}\}$ (say we have six nodes in the unit length string finite element meshing $[0, 0.2, 0.4, 0.6, 0.8, 1]$, the first three trial vectors would be $\{[1, 1, 1, 1, 1, 1]; [0, 0.2, 0.4, 0.6, 0.8, 1]; [0^2, 0.2^2, 0.4^2, 0.6^2,}$
0.8², 1²}], we try to “simulate” the polynomial basis function). \(NT + 1\) is the dimension of the trial space.

Results for case 1) and 2) are not exactly repeatable since the random vectors cannot be repeated exactly. However, the patterns of the result are consistent upon different trial random vectors. In real applications using the Ritz method, the trial functions can never be as random as a random vector used in 1.). The random vector “simulating” the random trial function is much more random than any continuous functions we can think of. This is not likely at all in the Ritz approximation when we choose trial solutions. Here we just use it to show the influence of trial basis on the approximation results. The approximated value of \(\omega²/\pi²\) of the several lowest resonant modes for the simple string problem with a different basis is shown in Table 2-2. And the resonance modes from different basis are shown in Figure 2.6 (using a random vector as trial solutions), Figure 2.7 (using \(K^{-1}\times\) (random vector) as the trial vector), and Figure 2.8 (using vectors generated in the format \{1, x, x², …\} as the trial basis).

This shows that the approximation accuracy of the Ritz method depends strongly on how close the trial vectors are to the exact solutions. The trial basis of \{1, x, x², …\} is much better. It is not an easy task to find some good guesses for a complex geometry.

<table>
<thead>
<tr>
<th>FEM</th>
<th>random</th>
<th>(K^{-1}\times)random</th>
<th>{1, x, x², …}</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.0000</td>
<td>-91.2314</td>
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<td>2.7712E+07</td>
<td>1.0038</td>
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<td>3.0164E+07</td>
<td>100.2013</td>
<td>36.2407</td>
</tr>
</tbody>
</table>
Figure 2.6  Ritz approximation of the lowest eigenmodes of a string using random trial vectors

Figure 2.7 Ritz approximation results using $K^{-1} \times$ (random vector) as the trial vector.
Figure 2.8 Ritz approximation results using vectors generated in the format \{1, x, x^2, \ldots\} as the trial basis.
Chapter 3 Modal analysis using the finite element method

The finite element method can be used to analyze the resonance modes of a complex geometry. There is a significant number of branches of science using the Finite Element Method. Here we will focus on the Finite Element Method used for modal analysis in a variation formula. As shown in Chapter 2, there are two ‘infinite dimensions’ in the partial differential equation problem. One is the ‘infinite dimension’ of the functional space \( \{ f_1(x), f_2(x), \ldots, f_n(x), \ldots \} \). The other ‘infinite dimension’ is that of each function \( f(x), a < x < b \). We can consider there are infinite points in the domain \([a, b]\). The Ritz method approximates the infinite solution space \( \{ f_1(x), f_2(x), \ldots, f_n(x), \ldots \} \) with a finite dimensional trial function space \( \{ f_1(x), f_2(x), \ldots, f_n(x) \} \). This transforms parts of the analysis problem to an algebra problem that can be handled well with modern computers. The Finite element method simplifies the ‘infinite’ dimension from the other perspective. The FEM approximates \( \{ f(x), a < x < b \} \) with \( \{ f(x_1), f(x_2), \ldots, f(x_n) \} \), where \([x_1, x_2, \ldots, x_n]\) are called nodes, using a mesh with domain \([a, b]\) and reduces the problem to finite dimension. In this approximation, all the other points are interpolated with values at the nodes. The problem is to find configurations at \([x_1, x_2, \ldots, x_n]\) that satisfy boundary conditions and make the Lagrangian extremum.

A typical finite element approximation has three procedures:

1.) Preprocessing. In preprocessing, the data and structure of the problem are defined. The object is discretized (meshing). Material properties and solution parameters are set.

2.) Processing. The problem is formulated in this procedure. This includes calculation of the element stiffness matrix, mass matrix, assembly of the element matrices to get a global stiffness and mass matrix. Boundary conditions may be applied to the
problem. We usually get a generalized eigenvalue problem and then proceed to get a solution of the eigenvalue problem.

3.) Postprocessing. The results from the processing section are visualized and analyzed for further consideration.

Now with the broad application of the finite element method in different areas, there are many kinds of commercial FEM software developed with different emphasis. Initially we used COMSOL for modeling and simulation. We find it is not always convenient to calculate certain quantities in which we are interested using COMSOL. Our calculation is very specific, and a specialized finite element program was written using Matlab. A simple example, a uniform string used in Chapter 2, will be shown below to illustrate the procedure. Then we will consider more complex, three-dimensional problems mostly used for calculation in our project. The formula and notations follow those in [61].

A simple one-dimension problem

We consider the resonance modes of a one-dimension string with density \( \rho \) and tension \( \tau \). The Lagrangian of the problem is:

\[
L = \frac{1}{2} \left( \rho \left( \frac{\partial u}{\partial t} \right)^2 - \tau \left( \frac{\partial u}{\partial x} \right)^2 \right) dt dx. \tag{3.1}
\]

For resonance modes, we try to find \( u(x, t) = A \cos(\omega t + \varphi) \cdot u(x) \) with \( u(x) \) minimizing functional:

\[
L = \int \frac{1}{2} \left( \rho \omega^2 u^2 - \tau \left( \frac{\partial u}{\partial x} \right)^2 \right) dx. \tag{3.2}
\]

In FEM method we use a set \( \{u_0, u_1, u_2, ..., u_n\} \) to approximate an exact solution \( u(x) \). This set can be considered as ‘degrees of freedom’ of the problem.
A uniform string can be divided into \( n \) parts with equal length \( d = \frac{1}{n} \). For simplicity, we just assume density and tension are both unity. They can be some function of the position and the format used in the finite element calculation will be similar. The displacement vector \( u(x), (0 < x < d) \) is approximated by:

\[
u(x) = \frac{d - x}{d} u_0 + \frac{x}{d} u_1, \quad (0 < x < d).
\] (3.3)

This is just linear interpolation. We approximate \( u(x) \) along the whole string in the same way.

Now we need to find \( \{u_0, u_1, u_2, \ldots u_n\} \) that makes the following extremum:

\[
L = \sum_{i=1}^{n} \int \frac{1}{2} \left( \omega^2 u^2 - \left( \frac{\partial u}{\partial x} \right)^2 \right) dx,
\] (3.4)

where \( u(x) \) is given by Eq. (3.3). Summation is over all the finite elements. Integration is over each element of length \( d \). We will just do the first element calculation:

\[
\int_0^d \left\{ \omega^2 \times [u_0 \ u_1] \times \left[ \frac{1 - x}{d} \right] \times \left[ \frac{1 - x}{d} \right] \times \left[ u_0 \ u_1 \right] - [u_0 \ u_1] \times \left[ \frac{1}{d} \right] \times \left[ \frac{1}{d} \right] \times \left[ u_0 \ u_1 \right] \right\} dx
\]

\[
= [u_0 \ u_1] \times \omega^2 \times \left[ \frac{d/3}{d/6} \right] \times \left[ u_0 \ u_1 \right] - [u_0 \ u_1] \times \left[ \frac{1}{d} \right] \times \left[ \frac{1}{d} \right] \times \left[ u_0 \ u_1 \right].
\] (3.5)

Adding all the elements together, we would get the Lagrangian in the following form:

\[
L = [u_0 \ u_1 \ldots u_n] \times (\omega^2 \times M - K) \times \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_n \end{bmatrix}.
\] (3.6)

Take variation with respect to \( [u_0 \ u_1 \ldots u_n] \), we get the generalized eigenvalue problem:

\[
\omega^2 M U = K U,
\] (3.7)

with
\[ M_{n \times n} = \frac{d}{6} \times \begin{bmatrix} 2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 4 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 4 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 4 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 4 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 2 \end{bmatrix}, \quad (3.8) \]

and

\[ K_{n \times n} = \frac{1}{d} \times \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}, \quad (3.9) \]

The solution to this problem is given in Chapter 2.

**Linear tetrahedron element for the 3-dimension problem**

In finite element meshing, we get a large number of the same type of element, say linear tetrahedrons; we want a “standard” way to deal with all the elements so that calculations can be easily done in a computer program. A one-to-one map between the mesh element and a standard simplex (linear tetrahedron in this section) is established for this purpose. The coordinates of the standard simplex are referred to as natural coordinates. In finite element modeling, the field value (can be coordinates, displacement, stress, etc.) at the nodes are the “degree of freedom”. The physical field value at any points other than the nodes is interpolated with a set of basis functions, called shape functions, \( N_i \). The fitting coefficients are determined by the value of the field at the nodes: \( \psi \approx \sum_i N_i \cdot \psi_i = \mathbf{N} \cdot \mathbf{\psi} \). The shape function has a property that it has a value of one at its paired node and zero at other nodes: \( N_i(\mathbf{r}_j) = \delta_{ij} \). The shape functions also satisfy: \( \sum_i N_i = 1 \). If the shape functions are used to represent both the element geometry and the problem unknowns, like displacement of the structure, they are called isoparametric shape functions.
In the linear tetrahedron case (Figure 3.1), the coordinate transformation is:

\[
\begin{bmatrix}
1 \\
x \\
y \\
z
\end{bmatrix}
= \begin{bmatrix}
1 & 1 & 1 & 1 \\
x_1 & x_2 & x_3 & x_4 \\
y_1 & y_2 & y_3 & y_4 \\
z_1 & z_2 & z_3 & z_4
\end{bmatrix}
\begin{bmatrix}
N_1 \\
N_2 \\
N_3 \\
N_4
\end{bmatrix}
= \begin{bmatrix}
1 & 1 & 1 & 1 \\
N_1 \\
N_2 \\
N_3 \\
N_4
\end{bmatrix}
\begin{bmatrix}
\zeta_1 \\
\zeta_2 \\
\zeta_3 \\
\zeta_4
\end{bmatrix}
\]

(3.10)

Shape function \(N_i\) is just the natural coordinate (function) \(\zeta_i\). There are only three independent variables, so \(\zeta_4 = 1 - \zeta_1 - \zeta_2 - \zeta_3\). For convenience, we write the inverse transformation here (In a real calculation, we have the coordinates data at the nodes, so this inverse can be easily done. \(a_i, b_i, c_i, V_i, i = 1 - 4\), all can be expressed in terms of the known coordinate data. They are used in later calculations and the matrix format is very convenient in writing Matlab programs.):

\[
\begin{bmatrix}
\zeta_1 \\
\zeta_2 \\
\zeta_3 \\
\zeta_4
\end{bmatrix}
= 6V \begin{bmatrix}
V_1 & a_1 & b_1 & c_1 \\
V_2 & a_2 & b_2 & c_2 \\
V_3 & a_3 & b_3 & c_3 \\
V_4 & a_4 & b_4 & c_4
\end{bmatrix}
\begin{bmatrix}
1 \\
x \\
y \\
z
\end{bmatrix}
\]

(3.11)

\[
V = \frac{1}{6} \text{det} \begin{bmatrix}
1 & 1 & 1 & 1 \\
x_1 & x_2 & x_3 & x_4 \\
y_1 & y_2 & y_3 & y_4 \\
z_1 & z_2 & z_3 & z_4
\end{bmatrix}
\]

(3.12)
is the volume of the tetrahedron element. The displacement vector is transformed using the same shape functions as for the coordinate vector: \( X = X_0 \cdot N \), \( U = U_0 \cdot N \). This is called an isoparametric transformation.

\[
\begin{bmatrix}
  u_x \\
  u_y \\
  u_z
\end{bmatrix} =
\begin{bmatrix}
  u_{x1} & u_{x2} & u_{x3} & u_{x4} \\
  u_{y1} & u_{y2} & u_{y3} & u_{y4} \\
  u_{z1} & u_{z2} & u_{z3} & u_{z4}
\end{bmatrix}
\begin{bmatrix}
  \zeta_1 \\
  \zeta_2 \\
  \zeta_3 \\
  \zeta_4
\end{bmatrix}
\tag{3.13a}
\]

For convenience in calculation, it can be written in the form:

\[
\begin{bmatrix}
  u_x \\
  u_y \\
  u_z
\end{bmatrix} =
\begin{bmatrix}
  \zeta_1 & \zeta_2 & \zeta_3 & \zeta_4 & 0 & 0 \\
  0 & \zeta_1 & \zeta_2 & \zeta_3 & \zeta_4 & 0 \\
  0 & 0 & \zeta_1 & \zeta_2 & \zeta_3 & \zeta_4
\end{bmatrix}
\begin{bmatrix}
  u_e \\
  \partial u_e / \partial \zeta_1 \\
  \partial u_e / \partial \zeta_2 \\
  \partial u_e / \partial \zeta_3 \\
  \partial u_e / \partial \zeta_4
\end{bmatrix}
\tag{3.13b}
\]

\( u^e \) is the displacement vector at all the nodes in each element. Their configuration defines resonance modes. We are looking for configurations of \( u^e \) that make the Lagrangian extremum.

Writing the strain \( \epsilon_{ij} = \frac{1}{2} ( \partial u_i / \partial x_j + \partial u_j / \partial x_i ) \) in a column vector (the coefficient 2 in \( \epsilon_{xx} \) in the column vector in Eq. (3.15) is related with the definition of the strain tensor) one has:

\[
\epsilon =
\begin{bmatrix}
  \epsilon_{xx} & \epsilon_{xy} \\
  \epsilon_{yx} & \epsilon_{yy} \\
  \epsilon_{zx} & \epsilon_{zy} \\
  2 \epsilon_{xz} & 2 \epsilon_{xy}
\end{bmatrix}
\begin{bmatrix}
  \frac{\partial}{\partial x} & 0 & 0 \\
  0 & \frac{\partial}{\partial y} & 0 \\
  0 & 0 & \frac{\partial}{\partial z} \\
  \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \\
  \frac{\partial}{\partial z} & \frac{\partial}{\partial x} & 0
\end{bmatrix}
\begin{bmatrix}
  u_x \\
  u_y \\
  u_z
\end{bmatrix}
\tag{3.15}
\]

\[
\epsilon = \frac{\partial U}{\partial X} = \frac{\partial N}{\partial Z} \frac{\partial Z}{\partial X} u^e = \frac{\partial N}{\partial \Pi} * J^{-1} * u^e = B * u^e.
\tag{3.16}
\]

\( Z \) is the natural coordinate, \( N \) is the shape function, \( U \) is the displacement field, \( u^e \) is the displacement field value at the nodes of an element and \( J \) is the Jacobian coordinate transformation matrix.
The elastic energy for a specific element is:

\[ e = \frac{1}{2} \int (B \ast U_0)^T \ast E \ast (B \ast U_0) dV. \]  \hspace{1cm} (3.17)

If the displacement vector is written in the form of Eq. (3.14), matrix \( B \) for the element is:

\[
B = \frac{1}{6V} \begin{bmatrix}
a_1 & a_2 & a_3 & a_4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & b_1 & b_2 & b_3 & b_4 & 0 & 0 & 0 & 0 & c_1 & c_2 & c_3 & c_4 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & c_1 & c_2 & c_3 & c_4 & b_1 & b_2 & b_3 & b_4 \\
c_1 & c_2 & c_3 & c_4 & 0 & 0 & 0 & 0 & a_1 & a_2 & a_3 & a_4
\end{bmatrix}. \] \hspace{1cm} (3.18)

This can be verified by calculating, for example:

\[
\varepsilon_{xx} = \frac{\partial u_x}{\partial x} = \frac{\partial \zeta_i}{\partial x} u_{xi} = \frac{\partial \zeta_i}{\partial x} \frac{\partial \zeta_j}{\partial x} u_{xj} = \frac{1}{6V} \delta_{ij} a_j u_{xj} = \frac{1}{6V} a_j u_{xj} \] \hspace{1cm} (3.19)

The stiffness matrix is \( K^e = \int B^T E B dV \). Since \( B \) is constant in each linear tetrahedron element, integration is just multiplying by volume \( V \). In case \( B \) is not constant, like in the case of a quadratic tetrahedron element, the integration can be approximated by numerical Gauss quadrature with \( n_g \) points:

\[
K^e = \sum_{k=1}^{n_g} w_k J_k B_k^T E B_k. \] Subscript \( k \) means evaluation at the \( k \)th Gauss quadrature points. \( J_k \) is the value of the determinant of the Jacobian Matrix at the \( k \)th Gauss points. The kinetic energy is:

\[
ke = \frac{1}{2} \int \rho \omega^2 u_i u_i dV. \] \hspace{1cm} (3.20)

Using Eq. (3.13b), and

\[
\int \zeta_i dV = \frac{1}{4} V, \hspace{1cm} (3.21a)
\]

\[
\int \zeta_i \zeta_j dV = \begin{cases} 
\frac{1}{10} V, & i = j \\
\frac{1}{20} V, & i \neq j
\end{cases} \hspace{1cm} (3.21b)
\]

and if the displacement vector is written as in Eq. (3.14), the mass matrix for a linear tetrahedron is:
The next step is to assemble the element matrices to get a global matrix. This is a matter of indexing. In the linear tetrahedron case, the stiffness and mass matrix are of size (4*3)*(4*3): 4 nodes, 3 dimensions. Suppose we are considering the jth element with 4 nodes \( n = \{ n_1, n_2, n_3, n_4 \} \), the 12*12 matrix will be distributed to rows and columns: \( \{3(n_1 - 1) + 1, ..., 3(n_4 - 1) + 1, 3(n_1 - 1) + 2, ..., 3(n_4 - 1) + 2, 3(n_1 - 1) + 3, ..., 3(n_4 - 1) + 3 \} \). For example, if element 37 has nodes in the order [3 1 2 5], then the 12*12 matrix is distributed with row and column indices [7 1 4 13 8 2 5 14 9 3 6 15] in the global matrix. This assembly (distributing local mass/stiffness matrix into global matrix value) is shown in Figure 3.2. \((ij)\) is the row/column index. A general pattern showing the assembly is explained with graphic detail in [62].

Figure 3.2 Linear tetrahedron assembling.
Quadratic tetrahedron element for the 3-dimension problem

Instead of just using 4 nodes and linear shape functions in linear tetrahedron element, a quadratic tetrahedron has 10 nodes and uses quadratic shape functions (Figure 3.3).

The isoparametric relations are:

\[
\begin{bmatrix}
1 \\
r_1 \\
r_2 \\
\vdots \\
r_{10}
\end{bmatrix}
= 
\begin{bmatrix}
1 & \ldots & 1 \\
r_1 & \ldots & r_{10}
\end{bmatrix}
\begin{bmatrix}
N_1 \\
\vdots \\
N_{10}
\end{bmatrix},
\]

(3.23)

with coordinate and displacement vector:

\[
\begin{bmatrix}
X \\
Y \\
Z
\end{bmatrix}, \quad
\begin{bmatrix}
U_x \\
U_y \\
U_z
\end{bmatrix}.
\]

(3.24)

The shape functions \( \{N_i, \ i = 1 \ldots 10\} \) are:

\[
N_1 = \zeta_1(2\zeta_1 - 1), \quad
N_2 = \zeta_2(2\zeta_2 - 1),
\]

\[
N_3 = \zeta_3(2\zeta_3 - 1), \quad
N_4 = \zeta_4(2\zeta_4 - 1),
\]

\[
N_5 = 4\zeta_1\zeta_2, \quad
N_6 = 4\zeta_2\zeta_3,
\]

\[
N_7 = 4\zeta_1\zeta_3, \quad
N_8 = 4\zeta_1\zeta_4,
\]

\[
N_9 = 4\zeta_2\zeta_4, \quad
N_{10} = 4\zeta_3\zeta_4.
\]
\[ \zeta_4 = 1 - \zeta_1 - \zeta_2 - \zeta_3. \] (3.25)

Let \( ND_{ij} = \frac{\partial N_i}{\partial \xi_j}, i = 1 \ldots 10, j = 1 \ldots 3 \) be the derivative matrix, then the coordinate transformation matrix is \( J_3 = X \ast ND \). As in the linear tetrahedron case, the strain now is:

\[ \epsilon = \frac{\partial U}{\partial X} = \frac{\partial N}{\partial E} \frac{\partial E}{\partial X} u^e = \frac{\partial N}{\partial E} \ast J_3^{-1} \ast u^e = B \ast u^e. \] (3.26)

If we write

\[ Q_{10 \times 3} = ND \ast J_3^{-1} = [Q_1 \quad Q_2 \quad Q_3], \] (3.27)

matrix \( B \) is:

\[
B_{6 \times 30} = \begin{bmatrix}
Q_1^T & 0 & 0 \\
0 & Q_2^T & 0 \\
0 & 0 & Q_3^T \\
Q_2^T & Q_1^T & 0 \\
0 & Q_3^T & Q_2^T \\
Q_3^T & 0 & Q_1^T
\end{bmatrix};
\] (3.28)

the stiffness matrix is:

\[ K = B^T \ast E \ast B \ast \text{det}(J_3); \] (3.29)

the mass matrix is

\[
M = \begin{bmatrix}
M_2 \\
M_2 \\
M_2
\end{bmatrix}, \quad M_2 = N^T \ast N \ast \text{det}(J_3). \] (3.30)

Displacement field is aligned as in the linear tetrahedron case (Eq. (3.14)). One difference is that matrix \( B \) is not constant over an element anymore. We need to use numerical approximation to do the integration. The assembly process to get the global stiffness and mass matrix is also similar to the linear tetrahedron case. Details are provided in the corresponding Matlab programs.
Approximation error

We consider two types of error here: discretization error and numerical calculation error. The finite element method approximates a continuous variable using discrete values and interpolation. In the harmonic mode analysis we are considering, this involves the spatial discretization of the object we are interested in, although no time discretization is involved here. For the numerical error, one example is the Gauss integration of the element stiffness matrix in the quadratic tetrahedron element case. The calculation of the final eigenvalue problem also involves numerical approximation. The eigenvalue problem is solved by Matlab’s built-in function. We will not talk about this error.

In the string example and the following eigenmode calculations, the approximation results are all approximations to the lowest eigenvalues. We are considering different ‘waves’ of different resonance modes. Spatial discretization of the object cuts off those modes with smaller wavelengths, i.e. those with large energies. Only those modes with the largest wavelengths or smallest energies are included in the approximation results.

We do some numerical analysis of rectangular parallelepiped geometry analyzed in [51]. The properties are listed in Table 3-1. \( l_x \) is the half edge length.

**Table 3-1 Properties of rectangular parallelepiped geometry used in the numerical analysis.**

| \( c_{11} \) = 1.1 Mbar      | \( 2l_x = 0.4221 \text{ mm} \) |
| \( c_{12} \) = 0.3 Mbar      | \( 2l_y = 0.4221 \text{ mm} \), \( \rho = 2.359 \text{ g/cc} \) |
| \( c_{44} \) = 0.4 Mbar      | \( 2l_z = 0.5761 \text{ mm} \) |

Influence of meshing size

In this calculation, we used quadratic tetrahedron elements. We first check the influence of the number of elements in the meshing. Intuitively, we should get more accurate result as we
decrease the element size. As we increase the number of elements, the computation costs more time.

Figure 3.4 Accuracy and calculation time vs. number of nodes. $f_0$ is the frequency calculated using 1777 quadratic elements nodes meshing.
Discussion:

1.) As the number of elements increases (element size decreases), calculated eigenvalues decrease. We conjecture without proof here that the approximated eigenvalue is always larger than the exact results, and as we further decrease element size (at least in this specific type of finite element calculation here), the calculated values move closer to exact solutions. For all the numerical calculations done with different geometry, this is always true: as element size decreases, eigenvalues decrease.

2.) The lowest eigenvalue calculation does not have highest accuracy.

3.) The finite element calculation program QuadTetraModeT1.m performs the following tasks: importing mesh data, calculating element stiffness and mass matrix, assembling these matrices, and solving the eigenvalue problem. As the number of elements increases, the calculation time and memory required increase rapidly.

**Linear tetrahedron vs. quadratic tetrahedron**

A linear tetrahedron element has four nodes, while a quadratic tetrahedron has 10 nodes. To compare the accuracy and efficiency between linear and quadratic meshing, we perform two tests:

1.) To avoid the influence of element size on both situations, the first comparison is done on the same mesh data. The original mesh is obtained using quadratic tetrahedron element meshing. To get the linear data, we divided each quadratic element into 8 small linear tetrahedron elements (8 is the largest division number, as one cannot get more than 8 small tetrahedrons). In this way, both calculations are using the same coordinate data, i.e. the same mesh. The only difference comes from the finite element formulation. We can see how the accuracy compares with each other.
2.) We compare one linear mesh data with another quadratic mesh data calculation that costs about the same amount of time.

In Figure 3.5 $f_0$ is the calculated result from quadratic mesh data. We compared the lowest 14 (x axis in Figure 3.5 is resonance mode number) resonance frequencies calculated using linear tetrahedron with $f_0$. The series with the number of nodes are compared following idea 1) above. The fifth one is comparing one linear (12130 nodes, ~80 seconds) with one quadratic element calculation (9046 nodes, ~60 seconds).

![Figure 3.5 Linear vs. quadratic tetrahedron element approximation.](image-url)
Discussion:

1.) The above numerical calculation shows that linear element calculation results are always larger than the corresponding quadratic element calculation (for the same mesh data or same amount of calculation time). Linear tetrahedron element calculation is less accurate.

2.) As the elements size decrease, both linear and quadratic calculation moves closer to the exact result. In this process, their difference decreases too (compare the 52170 nodes case with the 1777 nodes case in Figure 3.5).

One major difference between linear tetrahedron and quadratic tetrahedron is that for the quadratic mesh, the element surfaces and edges can be curved instead of just a flat surface or a straight line as in the linear tetrahedron case. Curved edges and surfaces can better approximate the real object, especially when the model involves curved surfaces, like a cylinder or sphere and so on.

Integration with different Gauss points

When definite integral of a function cannot be solved exactly, we can approximate the integral by a weighted sum of the function values at specified points within the domain. An n-point Gaussian quadrature rule is constructed in a way to give an exact result of definite integrals of polynomials of degree 2n-1 or less by suitably choosing the integration points and weights at these points. We compare two different Gauss integration rules. One has 14 integration points, and the other has 27 points. The 14 points data is from [63], and the 27 points data is from [64]. For convenience, these two sets of integration points and weights are listed here. There is no special reason for choosing these two specific sets of data. Numerical calculation is done mainly to check the influence of integration rules.
Table 3-2 14 points Gauss integration from [63].

<table>
<thead>
<tr>
<th>Gauss 1</th>
<th>$\zeta_1$</th>
<th>$\zeta_2$</th>
<th>$\zeta_3$</th>
<th>$w_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.000000000</td>
<td>0.333333333</td>
<td>0.333333333</td>
<td>0.008501593</td>
</tr>
<tr>
<td>2</td>
<td>0.333333333</td>
<td>0.000000000</td>
<td>0.333333333</td>
<td>0.008501593</td>
</tr>
<tr>
<td>3</td>
<td>0.333333333</td>
<td>0.333333333</td>
<td>0.000000000</td>
<td>0.008501593</td>
</tr>
<tr>
<td>4</td>
<td>0.333333333</td>
<td>0.333333333</td>
<td>0.333333333</td>
<td>0.008501593</td>
</tr>
<tr>
<td>5</td>
<td>0.771145474</td>
<td>0.076284842</td>
<td>0.076284842</td>
<td>0.050615550</td>
</tr>
<tr>
<td>6</td>
<td>0.076284842</td>
<td>0.771145474</td>
<td>0.076284842</td>
<td>0.050615550</td>
</tr>
<tr>
<td>7</td>
<td>0.076284842</td>
<td>0.076284842</td>
<td>0.771145474</td>
<td>0.050615550</td>
</tr>
<tr>
<td>8</td>
<td>0.076284842</td>
<td>0.076284842</td>
<td>0.076284842</td>
<td>0.050615550</td>
</tr>
<tr>
<td>9</td>
<td>0.405500313</td>
<td>0.405500313</td>
<td>0.094499687</td>
<td>0.127255238</td>
</tr>
<tr>
<td>10</td>
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<td>0.405500313</td>
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<td>14</td>
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<td>0.094499687</td>
<td>0.405500313</td>
<td>0.127255238</td>
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</tbody>
</table>
Table 3-3 27 points Gauss integration from [64].

<table>
<thead>
<tr>
<th>Gauss 2</th>
<th>$\zeta_1$</th>
<th>$\zeta_2$</th>
<th>$\zeta_3$</th>
<th>$w_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.705002210</td>
<td>0.232357801</td>
<td>0.007059631</td>
<td>0.000580935</td>
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<tr>
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<td>0.031319995</td>
<td>0.000929497</td>
</tr>
<tr>
<td>3</td>
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<td>0.232357801</td>
<td>0.055580358</td>
<td>0.000580935</td>
</tr>
<tr>
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<td>0.019633303</td>
<td>0.001907203</td>
</tr>
<tr>
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<td>0.120791820</td>
<td>0.087102985</td>
<td>0.003051525</td>
</tr>
<tr>
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</tr>
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<td>0.514338662</td>
<td>0.015626939</td>
<td>0.002836649</td>
</tr>
<tr>
<td>11</td>
<td>0.347003766</td>
<td>0.514338662</td>
<td>0.069328786</td>
<td>0.004538638</td>
</tr>
<tr>
<td>12</td>
<td>0.347003766</td>
<td>0.514338662</td>
<td>0.123030633</td>
<td>0.002836649</td>
</tr>
<tr>
<td>13</td>
<td>0.347003766</td>
<td>0.267380320</td>
<td>0.043459556</td>
<td>0.009312682</td>
</tr>
<tr>
<td>14</td>
<td>0.347003766</td>
<td>0.267380320</td>
<td>0.192807957</td>
<td>0.014900292</td>
</tr>
<tr>
<td>15</td>
<td>0.347003766</td>
<td>0.267380320</td>
<td>0.342156358</td>
<td>0.009312682</td>
</tr>
<tr>
<td>16</td>
<td>0.347003766</td>
<td>0.057847604</td>
<td>0.067074242</td>
<td>0.008162651</td>
</tr>
<tr>
<td>17</td>
<td>0.347003766</td>
<td>0.057847604</td>
<td>0.287850335</td>
<td>0.003060241</td>
</tr>
<tr>
<td>18</td>
<td>0.347003766</td>
<td>0.057847604</td>
<td>0.528743888</td>
<td>0.008162651</td>
</tr>
<tr>
<td>19</td>
<td>0.072994024</td>
<td>0.730165028</td>
<td>0.022184303</td>
<td>0.003047877</td>
</tr>
<tr>
<td>20</td>
<td>0.072994024</td>
<td>0.730165028</td>
<td>0.098240474</td>
<td>0.004876603</td>
</tr>
<tr>
<td>21</td>
<td>0.072994024</td>
<td>0.730165028</td>
<td>0.174656645</td>
<td>0.003047877</td>
</tr>
<tr>
<td>22</td>
<td>0.072994024</td>
<td>0.379578230</td>
<td>0.061696019</td>
<td>0.001000614</td>
</tr>
<tr>
<td>23</td>
<td>0.072994024</td>
<td>0.379578230</td>
<td>0.273713873</td>
<td>0.006009828</td>
</tr>
<tr>
<td>24</td>
<td>0.072994024</td>
<td>0.379578230</td>
<td>0.485731727</td>
<td>0.001000614</td>
</tr>
<tr>
<td>25</td>
<td>0.072994024</td>
<td>0.082121568</td>
<td>0.095219880</td>
<td>0.008770475</td>
</tr>
<tr>
<td>26</td>
<td>0.072994024</td>
<td>0.082121568</td>
<td>0.422442204</td>
<td>0.014032760</td>
</tr>
<tr>
<td>27</td>
<td>0.072994024</td>
<td>0.082121568</td>
<td>0.749664528</td>
<td>0.008770475</td>
</tr>
</tbody>
</table>

Table 3-4 shows the percentage difference between the calculated resonance frequencies using two different sets of Gauss integration points for the same geometry and meshing. Their difference is negligible compared with errors caused by other factors, like element size. This may be related with the way the two sets of integration point are derived. The four mesh data sets in Figure 3.6 have 5519, 22759, 33214 and 52170 nodes respectively. f1 is the result got using 14 points, and f2 is the result got using 27 integration points.
Table 3-4 Calculated resonance frequencies difference from two integration rules.

<table>
<thead>
<tr>
<th># Node</th>
<th>5519</th>
<th>33214</th>
</tr>
</thead>
<tbody>
<tr>
<td># Element</td>
<td>3612</td>
<td>22986</td>
</tr>
<tr>
<td>Time gauss1</td>
<td>30.29</td>
<td>531.39</td>
</tr>
<tr>
<td>Time gauss2</td>
<td>59.90</td>
<td>677.06</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mode</th>
<th>$\Delta f$ (%)</th>
<th>$\Delta f$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.25E-09</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>2</td>
<td>6.50E-09</td>
<td>-2.37E-10</td>
</tr>
<tr>
<td>3</td>
<td>7.83E-09</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>4</td>
<td>5.54E-09</td>
<td>-4.16E-10</td>
</tr>
<tr>
<td>5</td>
<td>5.47E-09</td>
<td>-3.82E-10</td>
</tr>
<tr>
<td>6</td>
<td>9.11E-09</td>
<td>-1.91E-10</td>
</tr>
<tr>
<td>7</td>
<td>2.20E-08</td>
<td>0.00E+00</td>
</tr>
<tr>
<td>8</td>
<td>3.67E-09</td>
<td>-5.11E-10</td>
</tr>
<tr>
<td>9</td>
<td>1.32E-08</td>
<td>-4.88E-10</td>
</tr>
<tr>
<td>10</td>
<td>4.66E-09</td>
<td>-1.59E-10</td>
</tr>
</tbody>
</table>

Figure 3.6 Percentage difference of calculated eigenfrequencies using two different sets of Gauss integration points.
As in the comparison between linear and quadratic elements, when element size decreases, percentage difference between these two Gauss integration rules also decreases. Since the difference is negligible and the 27 points rule costs more calculation time, we use the 14 points in our calculation.
Comparison of analytic, Rayleigh-Ritz and FEM methods

We next compare the accuracy between the Rayleigh-Ritz method and the finite element method used in our calculation. One example is the isotropic parallelepiped mentioned before and the other is an isotropic sphere. The Rayleigh-Ritz results are from [51](Table VII page 19) with basis order $R=12$. The finite element results are calculated with 52170 nodes quadratic mesh data, using the 14-point Gauss integration rule. As can be seen from Table 3-5 where the Rayleigh-Ritz method gives a smaller result, we think it is more accurate. One possible reason might be that this geometry has a ‘good shape’ that is suitable to use ‘xyz’ style basis functions.

Table 3-5 Rayleigh-Ritz vs. FEM approximation.

<table>
<thead>
<tr>
<th>Mode</th>
<th>R-R</th>
<th>FEM</th>
<th>$\Delta f$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.2686</td>
<td>3.2686</td>
<td>0.001</td>
</tr>
<tr>
<td>2</td>
<td>4.2131</td>
<td>4.2131</td>
<td>0.000</td>
</tr>
<tr>
<td>3</td>
<td>4.2131</td>
<td>4.2131</td>
<td>0.000</td>
</tr>
<tr>
<td>4</td>
<td>4.8050</td>
<td>4.8051</td>
<td>0.002</td>
</tr>
<tr>
<td>5</td>
<td>5.2344</td>
<td>5.2344</td>
<td>0.000</td>
</tr>
<tr>
<td>6</td>
<td>5.2344</td>
<td>5.2344</td>
<td>0.000</td>
</tr>
<tr>
<td>7</td>
<td>5.3891</td>
<td>5.3891</td>
<td>-0.001</td>
</tr>
<tr>
<td>8</td>
<td>5.8762</td>
<td>5.8763</td>
<td>0.001</td>
</tr>
<tr>
<td>9</td>
<td>6.1454</td>
<td>6.1455</td>
<td>0.001</td>
</tr>
<tr>
<td>10</td>
<td>6.2699</td>
<td>6.2700</td>
<td>0.002</td>
</tr>
<tr>
<td>11</td>
<td>6.3215</td>
<td>6.3216</td>
<td>0.001</td>
</tr>
<tr>
<td>12</td>
<td>6.3813</td>
<td>6.3814</td>
<td>0.001</td>
</tr>
<tr>
<td>13</td>
<td>6.3813</td>
<td>6.3814</td>
<td>0.001</td>
</tr>
<tr>
<td>14</td>
<td>6.4486</td>
<td>6.4486</td>
<td>0.000</td>
</tr>
<tr>
<td>15</td>
<td>6.8982</td>
<td>6.8982</td>
<td>0.000</td>
</tr>
<tr>
<td>16</td>
<td>6.9171</td>
<td>6.9171</td>
<td>0.000</td>
</tr>
<tr>
<td>17</td>
<td>6.9171</td>
<td>6.9171</td>
<td>0.000</td>
</tr>
<tr>
<td>18</td>
<td>7.1199</td>
<td>7.1200</td>
<td>0.001</td>
</tr>
<tr>
<td>19</td>
<td>7.2246</td>
<td>7.2247</td>
<td>0.001</td>
</tr>
<tr>
<td>20</td>
<td>7.6621</td>
<td>7.6622</td>
<td>0.002</td>
</tr>
</tbody>
</table>
For the parallelepiped geometry used in the numerical calculation, there are exact solutions called Lame modes. One such result is listed in Table 3-6. The data is from [51] (Table X page 21). Again, the Rayleigh-Ritz method gives a smaller result.

Table 3-6 Analytic vs. approximation.

<table>
<thead>
<tr>
<th>Analytic solution</th>
<th>Rayleigh-Ritz</th>
<th>FEM</th>
<th>Δf_{RA} (%)</th>
<th>Δf_{FA} (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.898198</td>
<td>6.898198</td>
<td>6.898229</td>
<td>0.000</td>
<td>0.0004</td>
</tr>
</tbody>
</table>

The eigenvalue problem of an isotropic homogenous elastic sphere can also be solved analytically. There are two classes of normal modes: torsional oscillations that are pure shear motions with no compression or extension and spheroidal oscillations that involve mixed shear and dilatational displacement [34]. In Chapter 2, we derived the analytical solution for a special spheroidal oscillation, whose displacement field is in the form of \(\mathbf{Re}u(r) e^{-i\omega t}\hat{r}\). The displacement field of this special case only depends on radial coordinates, and only has components in the radial direction. The sphere maintains the spherical shape in this resonance motion.

For an isotropic elastic sphere with radius \(a\), the longitudinal wave speed and shear wave speed are:

\[
c_l = \sqrt{\frac{\lambda + 2\mu}{\rho}}, \quad c_s = \sqrt{\frac{\mu}{\rho}}.
\]  

(3.31)

with two dimensionless frequencies:

\[
\eta = \frac{\omega * a}{c_s}, \quad \xi = \frac{\omega * a}{c_l}.
\]

(3.32)

The characteristic equation for the special spheroidal solution derived in Chapter 2 is (Eq. 2.30):

\[
C = \xi * \frac{(\lambda + 2\mu)}{4\mu} * \frac{J_1(\xi)}{\frac{\xi}{2}} - \frac{J_3(\xi)}{\frac{\xi}{2}} = 0.
\]

(3.33)

The characteristic equation for the general spheroidal oscillation is given by [65]:

\[ 0 = C = \frac{2\xi}{\eta} \left[ \frac{1}{\eta} + \frac{(n-1)(n+2)}{\eta^2} \left( \frac{J_{n+3/2}(\eta)}{J_{n+1/2}(\eta)} - \frac{n+1}{\eta} \right) \right] \times J_{n+3/2}(\xi) + \]
\[ \left[ -\frac{1}{2} + \frac{(n-1)(2n+1)}{\eta^2} + \frac{1}{\eta} \left( 1 - \frac{2n(n-1)(n+2)}{\eta^2} \right) \frac{J_{n+3/2}(\eta)}{J_{n+1/2}(\eta)} \right] J_{n+1/2}(\xi), \]  
(3.34)

while for torsional oscillations, the equation is
\[ (n-1)J_{n+1/2}(\eta) - \eta J_{n+3/2}(\eta) = 0. \]  
(3.35)

Numerical solution to these equations can be found using Matlab (program spheremode.m).

Table 3-7 Parameters of the sphere.

<table>
<thead>
<tr>
<th>( c_{11} = 1.1 \text{ Mbar} )</th>
<th>( c_{12} = 0.3 \text{ Mbar} )</th>
<th>( c_{44} = 0.4 \text{ Mbar} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho = 2.359 \text{ g/cc} )</td>
<td>( r = 1 \text{ cm} )</td>
<td>( \mu = c_{44} = 0.4 \text{ Mbar} )</td>
</tr>
<tr>
<td>( \lambda = c_{12} = 0.3 \text{ Mbar} )</td>
<td>( c_s = \sqrt{\mu/\rho} = 4117.81 \text{ m/s} )</td>
<td>( c_t = \sqrt{((2\mu+\lambda)/\rho)} = 6828.61 \text{ m/s} )</td>
</tr>
</tbody>
</table>

One can label these two groups of modes by \( T_{n,m} \) and \( S_{n,m} \). \( n \) is the Bessel function half integer. \( m \) labels the subgroup for each \( n \) (the roots of the characteristic equation). Table 3-8 gives the analytical and the Rayleigh-Ritz (RR) approximation results from [51]. \( \eta_0 \) is the analytic solution of the variable \( \eta \) in the above characteristic equations. The mode number is different because the RR method gives some ‘fake’ mode solutions.

Table 3-8 Dimensionless resonance frequencies of isotropic sphere.

<table>
<thead>
<tr>
<th>Analytic solution [51]</th>
<th>Rayleigh-Ritz [51]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mode</td>
<td>( \eta_0 )</td>
</tr>
<tr>
<td>1 ( T_{2,0} )</td>
<td>2.5011326</td>
</tr>
<tr>
<td>2 ( S_{2,0} )</td>
<td>2.6398693</td>
</tr>
<tr>
<td>4 ( T_{3,0} )</td>
<td>3.8646998</td>
</tr>
<tr>
<td>6 ( S_{0,1} )</td>
<td>4.4399982</td>
</tr>
<tr>
<td>9 ( T_{4,0} )</td>
<td>5.0946156</td>
</tr>
<tr>
<td>13 ( S_{3,1} )</td>
<td>6.4543693</td>
</tr>
<tr>
<td>16 ( T_{2,1} )</td>
<td>7.1360096</td>
</tr>
<tr>
<td>26 ( T_{8,0} )</td>
<td>9.6209991</td>
</tr>
<tr>
<td>32 ( S_{0,2} )</td>
<td>10.4939244</td>
</tr>
<tr>
<td>37 ( S_{4,2} )</td>
<td>11.0390581</td>
</tr>
</tbody>
</table>
The calculated results ($\eta_0$) using the program are given in Table 3-9. The calculated spheroidal mode frequencies are different from those given by [51].

Table 3-9 Analytical modes of an isotropic elastic sphere.

<table>
<thead>
<tr>
<th>Spheroidal</th>
<th>$S_{0,m}$</th>
<th>$S_{1,m}$</th>
<th>$S_{2,m}$</th>
<th>$S_{3,m}$</th>
<th>$S_{4,m}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.12846333</td>
<td>3.34498638</td>
<td>2.63484123</td>
<td>3.89972502</td>
<td>4.98080733</td>
</tr>
<tr>
<td>1</td>
<td>10.01176677</td>
<td>4.49340946</td>
<td>4.75993391</td>
<td>6.33897760</td>
<td>7.94424622</td>
</tr>
<tr>
<td>2</td>
<td>15.36665332</td>
<td>6.51697660</td>
<td>5.76345920</td>
<td>9.56164382</td>
<td>8.18256145</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Torsional</th>
<th>$T_{1,m}$</th>
<th>$T_{2,m}$</th>
<th>$T_{3,m}$</th>
<th>$T_{4,m}$</th>
<th>$T_{8,m}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>5.76345920</td>
<td>2.50113262</td>
<td>3.86469978</td>
<td>5.09461563</td>
<td>9.62099907</td>
</tr>
</tbody>
</table>

All the torsional modes agree well with [51], while none of the spheroidal modes agree with [51](and $S_{0,1}$ in [51] probably should be labeled $S_{0,0}$, some of the other $S_{n,m}$’s labeling is also problematic). The finite element calculation supports our results. Table 3-10 compares the lowest 15 resonance frequencies given by analytical solution and finite element calculation. For the degenerate modes, the value is calculated using the lowest frequency.

Discussion:

1.) For all the results that are comparable with each other (all the torsional modes), the Rayleigh-Ritz method is more accurate.

2.) As in the simple string example, Rayleigh-Ritz method produces modes that do not really exist (Mode number 300 in the Rayleigh-Ritz versus Mode number 37 in analytical solution).

3.) For all the modes shown here, eigenfrequencies given by FEM are all larger than the analytical solutions, consistent with all observations so far.
Table 3-10 Analytical vs. FEM results.

<table>
<thead>
<tr>
<th>Mode</th>
<th>( \eta_0 )</th>
<th>( \eta_{FEM} )</th>
<th>( \Delta \eta ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.50113262</td>
<td>2.50114090</td>
<td>0.000</td>
</tr>
<tr>
<td>2</td>
<td>2.63484123</td>
<td>2.63485041</td>
<td>0.000</td>
</tr>
<tr>
<td>3</td>
<td>3.34498638</td>
<td>3.34501269</td>
<td>0.001</td>
</tr>
<tr>
<td>4</td>
<td>3.86469978</td>
<td>3.86477287</td>
<td>0.002</td>
</tr>
<tr>
<td>5</td>
<td>3.89972502</td>
<td>3.89983222</td>
<td>0.003</td>
</tr>
<tr>
<td>6</td>
<td>4.12846333</td>
<td>4.12846833</td>
<td>0.000</td>
</tr>
<tr>
<td>7</td>
<td>4.75993391</td>
<td>4.76007591</td>
<td>0.003</td>
</tr>
<tr>
<td>8</td>
<td>4.98080733</td>
<td>4.98125860</td>
<td>0.009</td>
</tr>
<tr>
<td>9</td>
<td>5.09461563</td>
<td>5.09487838</td>
<td>0.005</td>
</tr>
<tr>
<td>10</td>
<td>5.76345920</td>
<td>5.76383480</td>
<td>0.007</td>
</tr>
<tr>
<td>11</td>
<td>5.99358697</td>
<td>5.99488047</td>
<td>0.022</td>
</tr>
<tr>
<td>12</td>
<td>6.26576785</td>
<td>6.26646825</td>
<td>0.011</td>
</tr>
<tr>
<td>13</td>
<td>6.33897760</td>
<td>6.33941087</td>
<td>0.007</td>
</tr>
<tr>
<td>14</td>
<td>6.51697660</td>
<td>6.51728802</td>
<td>0.005</td>
</tr>
<tr>
<td>15</td>
<td>6.97435279</td>
<td>6.97735883</td>
<td>0.043</td>
</tr>
</tbody>
</table>

Post processing

We can use the calculated eigenvector to show the resonant shape. This can help to check whether the method and solution are correct or not. This can be done in the GID software [66] used to generate the mesh. For convenience and flexibility, we used Matlab to draw the resonance modes here.

The shape is reflected in the movement of the surface elements and the surface is the only part we can see. To reduce the computation cost, we only show surface node movement in the Matlab program. Even in quadratic meshing, only 3 points are used for each element surface. The boundary nodes can be found using union and set difference functions in Matlab. Details can be found in the Matlab program. Figure 3.7 shows the lowest 15 resonance modes of the parallelepiped geometry with size and elastic tensors specified in Table 3-1. Due to shape and elastic tensor symmetry, some modes are degenerate.
Figure 3.7 Lowest 15 resonance modes of the parallelepiped geometry.

**Backward calculation**

The finite element method discussed so far constitutes the forward calculation. In real applications, we need to solve the inverse problem, i.e., using the forward calculation program to adjust the elastic constants to fit the calculated resonance frequencies to the measured ones.
The resonance frequency depends on geometry, elastic tensor, and mass density. If the geometry is quite complex, we need many parameters to describe the geometry. The fitting problem gets more difficult as the number of parameters increases. To get an idea about each factor’s influence on natural frequency, we calculate the frequency derivative with respect to these different factors using the finite difference method. The geometry of the object in Table 3-11 is similar to the real cell used in our experiment. The material property in Table 3-12 is used in the calculation. Table 3-13 gives the resonance frequency dependence on cell geometry and material parameters. There is a slight, but not substantial, difference if different finite difference (say a 5% vs. 3% increase in the parameter, we used a 5% increase here) is used to do the calculation.

Table 3-11 Geometry of the cell.

<table>
<thead>
<tr>
<th>/cm</th>
<th>Height</th>
<th>Radius</th>
<th>Inside height</th>
<th>Inside radius</th>
<th>Bottom thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0th</td>
<td>1.1684</td>
<td>0.55118</td>
<td>0.79248</td>
<td>0.47498</td>
<td>0.16002</td>
</tr>
<tr>
<td>H'</td>
<td>1.2260</td>
<td>0.55118</td>
<td>0.79248</td>
<td>0.47498</td>
<td>0.16002</td>
</tr>
<tr>
<td>R'</td>
<td>1.1684</td>
<td>0.57900</td>
<td>0.79248</td>
<td>0.47498</td>
<td>0.16002</td>
</tr>
</tbody>
</table>

Table 3-12 Material of the cell.

<table>
<thead>
<tr>
<th>Rho</th>
<th>C11</th>
<th>C22</th>
<th>C33</th>
<th>C44</th>
<th>C55</th>
<th>C66</th>
<th>C23</th>
<th>C31</th>
<th>C12</th>
<th>[g/cc, 100GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.0</td>
<td>2.874</td>
<td>2.874</td>
<td>2.874</td>
<td>0.85</td>
<td>0.85</td>
<td>0.85</td>
<td>1.174</td>
<td>1.174</td>
<td>1.174</td>
<td></td>
</tr>
</tbody>
</table>
Table 3-13 Resonance frequency dependence on geometry and elastic tensor.

<table>
<thead>
<tr>
<th>0°/kHz</th>
<th>$\frac{df}{dh}/h$</th>
<th>$\frac{df}{dr}/r$</th>
<th>$\frac{df}{d\rho}/\rho$</th>
<th>$\frac{df}{dc_{11}}/c_{11}$</th>
<th>$\frac{df}{c_{66}}/c_{66}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.079914</td>
<td>0.005</td>
<td>1.051</td>
<td>-0.482</td>
<td>0.148</td>
</tr>
<tr>
<td>2</td>
<td>0.080847</td>
<td>0.007</td>
<td>1.130</td>
<td>-0.482</td>
<td>0.115</td>
</tr>
<tr>
<td>3</td>
<td>0.080853</td>
<td>0.006</td>
<td>1.130</td>
<td>-0.482</td>
<td>0.115</td>
</tr>
<tr>
<td>4</td>
<td>0.091969</td>
<td>-0.462</td>
<td>0.736</td>
<td>-0.482</td>
<td>0.033</td>
</tr>
<tr>
<td>5</td>
<td>0.091973</td>
<td>-0.462</td>
<td>0.736</td>
<td>-0.482</td>
<td>0.033</td>
</tr>
<tr>
<td>6</td>
<td>0.094047</td>
<td>0.098</td>
<td>2.790</td>
<td>-0.482</td>
<td>0.151</td>
</tr>
<tr>
<td>7</td>
<td>0.094072</td>
<td>0.097</td>
<td>2.786</td>
<td>-0.482</td>
<td>0.151</td>
</tr>
<tr>
<td>8</td>
<td>0.105868</td>
<td>-1.024</td>
<td>1.151</td>
<td>-0.482</td>
<td>0.000</td>
</tr>
<tr>
<td>9</td>
<td>0.113723</td>
<td>1.327</td>
<td>0.000</td>
<td>-0.482</td>
<td>0.176</td>
</tr>
<tr>
<td>10</td>
<td>0.123932</td>
<td>-0.450</td>
<td>0.810</td>
<td>-0.482</td>
<td>0.104</td>
</tr>
<tr>
<td>11</td>
<td>0.123941</td>
<td>-0.065</td>
<td>0.809</td>
<td>-0.482</td>
<td>0.104</td>
</tr>
<tr>
<td>12</td>
<td>0.132032</td>
<td>0.046</td>
<td>2.454</td>
<td>-0.482</td>
<td>0.168</td>
</tr>
<tr>
<td>13</td>
<td>0.132088</td>
<td>0.047</td>
<td>2.447</td>
<td>-0.482</td>
<td>0.168</td>
</tr>
<tr>
<td>14</td>
<td>0.145359</td>
<td>-0.354</td>
<td>1.238</td>
<td>-0.482</td>
<td>0.080</td>
</tr>
<tr>
<td>15</td>
<td>0.145362</td>
<td>-0.355</td>
<td>1.238</td>
<td>-0.482</td>
<td>0.080</td>
</tr>
</tbody>
</table>

The numbers in Table 3-13 give the corresponding approximate percentage change in resonance frequency when there is a 1 percent change in the parameter. For example for the 1st mode, when there is a 1 percent change in height, the frequency of the 1st mode will change by -0.003 percent. There is only one material in this setup, so all the resonance frequencies are shifted by the same amount in respond to a change in density. This can be easily seen from the eigenvalue equation $\omega^2MU = KU$. Some modes should be degenerate because of the symmetry of elastic tensor and geometry. However, meshing breaks the symmetry and there is a slight difference between the degenerate frequencies.
In the backward calculation, we try to find a set of parameters such that calculation results based on these parameters agree best with the experiment result. This is a function minimization problem. However, due to the large number of parameters (geometry, density and elastic tensor) and the fact that geometry has a relatively large effect on resonance frequencies, it is very difficult to fit all the parameters so that the experiment results agree with finite element calculation. The dependence on the number of elements also makes it less meaningful to do least square fitting. We wrote a program to do the minimization but the result is not satisfying. The fitting often gets lost in the parameter space. The program is listed in the appendix.
Chapter 4 Experiment setup

The low temperature of the experiment is realized in Dewar stations [67]. A vacuum pumping system is used to reduce $^4$He vapor pressure in the Dewar and achieve low temperatures. A cryostat insert provides an interface between room temperature and the low temperature environment. These parts will be explained separately.

Low temperature setup

Dewar station

Figure 4.1 shows the design of the Dewar system. The Dewar station consists of two Dewar vessels: a $^4$He Dewar sitting coaxially inside of a liquid nitrogen Dewar. The top annular space between the two Dewar vessels are packed with cotton and partially wrapped with tape. This limits water vapor from being cryo-pumped into the liquid nitrogen Dewar. The liquid nitrogen is used to precool the system and shield the $^4$He Dewar from thermal radiation from the ambient room temperature outside. Both Dewars are double walled glass and silvered. The vacuum between the double walls of a Dewar vessel reduces heat conduction and silvering reduces thermal radiation. The liquid nitrogen Dewar is permanently sealed. However, the Dewar we are using is so old that some gas has diffused into the vacuum jacket. We had it pumped by the manufacturer before doing the experiment. The $^4$He Dewar has a glass to stainless steel tube connection that can be connected to a pump. It also has a pressure relieve valve and a thermocouple pressure gauge. Helium gas can diffuse through glass walls. Each time before we transfer liquid helium we pump out helium that may have diffused into the vacuum jacket to reduce the heat conduction between the helium Dewar and nitrogen Dewar. On each side of the
Dewar, a one-centimeter strip is left uncoated by silver so that it is easy to check levels of $^4$He and liquid nitrogen left inside while doing the experiment.

The Dewar vessels are mounted inside a support structure made of slotted aluminum angle. We made a wall for the supporting structure using 4 pieces of transparent Plexiglas plate to protect the Dewar. At about two thirds of the height, two pieces of foam, each with a half circle cut, support the Dewar. The supporting structure is anchored on the floor.

There are two filling tubes for the liquid nitrogen Dewar. One goes all the way down to the bottom of the Dewar and the other stops at about ten cm below the top. The top end of the longer tube can be connected to a vacuum pump to pump out any possible water condensed at the bottom of the Dewar. The shorter one is used to transfer liquid nitrogen into the Dewar. To prevent ice from accumulating at the top of the Dewar station, we installed a short tube that can be connected to compressed air. During the experiment, we blow air towards the top part of the Dewar to prevent ice buildup.
Without pumping the helium vapor gas inside the helium Dewar, we can get liquid $^4$He temperature at one atm (4.2 K). Lower temperatures can be achieved by pumping the vapor above the liquid helium bath. We have some valves close to the Dewar system used to regulate the pumping speed as shown in Figure 4.2. The 1 inch valve is for fine tuning. A dial gauge close to the small valve is used to measure vapor pressure inside the helium Dewar. It is not very accurate. In the normal liquid state, there is a temperature gradient from the surface of liquid helium to the bottom of liquid helium where our experiment cell is located. The temperature converted from the pressure reading is not exactly the same as the temperature at the bottom. We relied on this dial
gauge during the first experiment. In the following experiments, we used a separate pressure tube to measure the pressure and converted it to get the temperature at the cell. This pressure tube is explained in a later section.

There are three vacuum pumps in total at the end of the pumping line: a Kinney KS-47 rotatory pump (22lit/sec), a water-cooled Edwards 9B3 diffusion-type booster pump (850 liters/sec) and an Alcatel 2020A pump. They are arranged as shown in Figure 4.3.

![Figure 4.2 Pumping speed regulator valves.](image-url)
When we are not running the experiment, valve 2 and valve 3 are closed. Valve 1 and valve 4 are open and only the Alcatel 2020A pump is running. To get lower temperatures, we close valve 1, valve 3, open valve 2 and run the Kinney KS-47 pump. To get even lower temperatures, we close valve 4, valve 2, open valve 1, valve 3 and run the Edwards 9B3 booster pump and Kinney KS-47 pump.

Although the pumps are located in a separate room, the big vibration noise still can affect the experiment measurements. To reduce this noise, we put several lead bricks on top of the Dewar station and several places along the vacuum pumping tube. From the experiment result, it can be seen that this indeed reduces the noise.

**Cryostat insert**

The cryostat insert is an interface between the room temperature measurement equipment and the low temperature environment where the experiments take place. It has two main parts,
one is the mechanical and vacuum connections and the other is electrical connections. The electrical connections are composed of transducer circuits and the temperature regulation circuits.

Figure 4.4 Cryostat insert.

The insert is shown in Figure 4.4. A hexagonal piece at the top part of the cryostat insert has three valves: for vacuum pumping the long stainless steel tube and experiment cell, admitting helium and pressure relief. Below the hexagonal piece is a big brass flange. It sits on an O-ring to seal the Dewar system. Several interface connections are made through the top flange as shown in Figure 4.5. These include the helium filling tube to the Dewar, helium capillary to the stainless steel tube.
steel cell (used to transfer helium to the cell), temperature regulator and pressure gauge. The long stainless steel tube can be pumped separately. It is separated from the outside Dewar system and the inside $^4$He growing space. The bottom end of the 1 inch stainless steel tube is connected to the bottom flange, shown in Figure 4.6.

Figure 4.5 Top flange feed through.

Figure 4.6 Bottom flange.
To detect possible leaking of the stainless steel cell, we fill the stainless steel cell with high-pressure gas. Any leak from the cell will go to the surrounding 1-inch stainless steel tube. This can be easily detected by a helium mass spectrometer leak detector connected to the 1-inch SS tube.

**High pressure panel**

The high pressure panel is used to control the growth of solid helium. The connections are shown in Figure 4.7.

![High pressure panel diagram](image)

Figure 4.7 High pressure panel.

Before doing any experiment, we filled all the tubes with high-pressure helium gas and leak detected all parts. Each time we run the experiment; we fill the whole helium path with helium gas, pump everything out, fill helium gas and then pump again for several times. In this way, we cleaned all the helium paths so there won’t be any pollution to the helium and no
condensed water/ice formed inside the capillary which would block the helium path. After filling the helium Dewar in each experiment, we open valve V1 to let some helium gas flow into the pressure tube submerged inside the liquid helium. The helium gas will condense inside the pressure tube, then we close valve V1. From now on, the high purity helium gas will be transferred from the tank to the ‘bomb’ and then to the stainless steel cell where solid helium forms.

**Temperature regulation and pressure measurement**

The temperature is regulated using an a.c. bridge circuit with a feedback heater. The setup is the one used in [68]. The temperature sensor is a germanium resistance temperature detector (RTD), Lake Shore Cryotronics GR-200A-100. The regulator design is described in [68]. The temperature controlling is a dynamical process. As the temperature fluctuates (pumping cools the liquid/heater heats up the liquid), the resistance of the Germanium RTD fluctuates (Germanium has negative temperature coefficient/NTC), and the lock in amplifier will detect the imbalance and adjust the heating current.

There is a one-to-one correspondence between the helium vapor pressure and temperature [69]. If we can get an accurate measurement of the vapor pressure, we can look up the corresponding temperature. This is how the temperature is determined in this experiment. The temperature controller can stabilize temperature at a fixed temperature. This is achieved by adjusting the Gertsch RT20R ratio transformer (Figure 4.8) to the correct value. The vapor pressure, temperature and corresponding ratio setup data is listed in Table 4-1. The temperature regulator data are not exactly repeatable; it is only a guide in adjusting the temperature.

The measurement range of the Kurt Lesker piezo gauge is 1-1000 torr. Below 1 torr, the pressure reading is not reliable. Instead we used the observed temperature-resistance data fit
(square data points and black power fit line) to get the corresponding resistance data for the several lowest temperatures (triangle data points in Figure 4.9).

Table 4-1 Helium vapor pressure, temperature and temperature regulator resistance.

<table>
<thead>
<tr>
<th>P/torr</th>
<th>T/K</th>
<th>R/KΩ</th>
</tr>
</thead>
<tbody>
<tr>
<td>154.75</td>
<td>2.9</td>
<td></td>
</tr>
<tr>
<td>31.06</td>
<td>2.1</td>
<td>0.3930</td>
</tr>
<tr>
<td>17.25</td>
<td>1.9</td>
<td>0.4607</td>
</tr>
<tr>
<td>12.29</td>
<td>1.8</td>
<td>0.5019</td>
</tr>
<tr>
<td>8.46</td>
<td>1.7</td>
<td>0.5496</td>
</tr>
<tr>
<td>5.60</td>
<td>1.6</td>
<td>0.6123</td>
</tr>
<tr>
<td>3.54</td>
<td>1.5</td>
<td>0.6846</td>
</tr>
<tr>
<td>2.12</td>
<td>1.4</td>
<td>0.7855</td>
</tr>
<tr>
<td>1.18</td>
<td>1.3</td>
<td>0.8864</td>
</tr>
<tr>
<td>1.2</td>
<td>1.2</td>
<td>1.0100</td>
</tr>
<tr>
<td>1.1</td>
<td>1.1</td>
<td>1.1720</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>1.3798</td>
</tr>
<tr>
<td>0.92</td>
<td>1.5</td>
<td>1.5870</td>
</tr>
</tbody>
</table>
The “refluxing” tube line is designed as shown in Figure 4.8 to eliminate the problem of superfluid film flow [68]. A small amount of liquid is formed at the bottom of the pressure tube and superfluid film flow is only restricted to the bottom part. There is no direct contact between the film and the inner tube. The vapor pressure of the small volume liquid helium is correctly measured by the piezo gauge located outside the Dewar. The temperature regulation instruments are similar to the one in [68].

Response time of the piezo gauge is 50 ms. In one experiment, when the inside liquid helium surface is at certain level, there is thermal oscillation (Taconis oscillation [70, 71]) in the pressure tube just like what is happening when using a “dipstick” to measure helium level in a vessel. We saw this when transferring helium into the Dewar and just after transferring. As helium level goes down, this oscillation disappears. The Kurt Lesker vacuum controller cannot
get a stable reading when there is thermal oscillation. We connected the analog output signal to a Keithley 2010 multimeter to get a stable reading.

We list the major procedures of the experiment here.

1.) Leak detect every part of the setup.

2.) Fill the helium path with helium, pump out the gas and repeat this several times.

   Pump out the helium Dewar vacuum jacket.

3.) Install vapor pressure measurement tube inside the helium Dewar.

4.) Fill the nitrogen Dewar the night before doing the experiment.

5.) Pressurize the vapor pressure measurement tube to several atm.

6.) Let some helium gas into the helium Dewar to reach pressure of about 650 torr (smaller than 1 atm, so helium gas would not lift the top brass flange). When the helium Dewar is vacuum, there is little heat conduction between the outside liquid temperature and the inside experiment space. The whole experiment space inside the helium Dewar is still at high temperature. The helium gas added would increase heat conduction, lowering the temperature of the experiment space.

7.) Let whole inside system reach liquid nitrogen temperature overnight.

8.) Increase the helium gas pressure inside the Dewar to 1 atm (so no air would fill in while transferring helium). Put in the transfer tube and transfer helium.

9.) Take out transfer tube and install temperature controller (they are using the same feed through on the top flange).

10.) Increase pressure inside the pressure tube to 1 atm. Liquid forms at the bottom of refluxing tube.

11.) Fill helium gas into the cell. Liquid forms inside the cell. Pressurize to above 1 atm. to avoid bubbles.
12.) Lower temperature by adjusting pumping rate. Control the pressure inside the cell through valves on the high-pressure panel. Grow solid helium using blocked capillary method. Follow the melting line in P-T phase diagram. We see superfluid transition in the helium Dewar when the pressure tube reading is ~40 torr.

13.) Capillary blocked at 2.1 K. Pressure gauge reading is not the stainless steel cell (helium) pressure anymore.

14.) Turn on the booster pump after taking 1.3 K data. Pressure in the pressure tube is below 1 torr, beyond piezo gauge scale. Regulate the temperature using the resistance-temperature fit data. Lowest temperature is ~0.9 K.

**Cell design**

The initial design of the cell used to grow solid helium is illustrated in Figure 4.10. First a stainless steel (ss304) cylinder is drilled through. Held in a lathe, the cylinder is hollowed out with a small boring tool, leaving a relatively thin wall (but still thick enough to withstand the high pressure needed for growing solid helium) and relatively thick top/bottom surfaces (so there is enough contact to hold scaling plugs tightly). The top and bottom side surfaces are then machined with a tapered pipe thread (1/16-27 NPT) as shown in Figure 4.10. Stainless steel plugs are machined with matching tapered thread and faced off so that a cylindrical cavity is formed when they are screwed in tightly. The length should be matched as closely as possible. Then we drill a hole at the top for the 0.020 inch o.d., 0.016 inch i.d. CuNi capillary and hard soldered the capillary. The plug threads are given a light coating of Stycast 2850 FT epoxy prior to being screwed in tightly. The tight fit provided by tapered threads guaranteed mechanical integrity and the epoxy insures the can is leak tight. The outside parts of the plugs are machined off later by cutting a tiny layer each time so that torque will not be large enough to crack the epoxy. A cold finger at the bottom is hard soldered to the bottom plug before the bottom plug is screwed in. One
of the epoxy seals was leaking for our first cell. We changed the design of the new cell a little bit to decrease the chance of leaking.

![Initial design of cell](image)

**Figure 4.10 Initial design of cell.**

The new cell, shown in Figure 4.11, has only one plug at the top. The bottom threaded seals is eliminated to lower the chance of leaking. The cold finger is hard soldered to the stainless steel cell directly instead of to the plug as in the original design. The other steps are similar to the original one.

![New cell design](image)

**Figure 4.11 New cell design.**

After the cell is finished, we used Dynaloy 320 epoxy silver “solder” to attach two piezoelectric transducers diagonally at the top and bottom surfaces of the stainless steel cell. One
provides the driving signal and the other receives the response. Another way is to attach the transducers very weakly and the loading is small enough to be ignored in the calculation, i.e. in the model we only consider the cell, an object with free boundary condition. This makes the model building and calculation easier. In our room temperature RUS experiment, we find the loading has some effect and it is not easy to get loadings that are consistent each time we do the measurement. The loading is consistent among all the runs if the transducers are strongly attached to the cell, though it makes the geometry a bit complex. The transducers are manufactured by Boston-Piezo-Optics, Inc. It is a 10 deg. Rotated Y lithium niobate crystal, 3 mm diameter and 0.025 inch thick. It can generate both longitudinal and shear waves [72]. There is a 4 inch long soft copper alloy wire at the center. For our experiment, the original copper wire is still too rigid and it influences the spectrum of the cell. We removed these wires and replaced them with even thinner and less rigid copper wires. The final cell configuration is shown in Figure 4.12.

![Cell configuration](image)

Copper base:
- Radius: 0.87 cm;
- Height: 1.3 cm.

Copper neck:
- Radius: ~0.15 cm;
- Height: ~0.88 cm.

Cold copper finger:
- 0.020 inch o.d. CuNi large capillary and 0.016 inch i.d. thin capillary.

Stainless steel cell:
- Inside radius: ~0.47 cm;
- Inside height: ~0.8 cm;
- Cell radius: ~0.56 cm;
- Cell height: ~1.2 cm;
- Bottom thickness: ~0.16 cm.

Transducer:
- 10 deg. Rotated Y lithium niobate crystal, 3 mm diameter and 0.025 inch thick.
Frequency measurement

The resonance spectrum is measured using an instrument and software (not in production any more) produced by Dynamical Resonance Systems (DRS) Inc. It can generate a sinusoidal signal used to drive the transducer and process the response signal from the receiver transducer. It can also do calculations for Rectangular Parallelepiped Resonance (RPR). We did not use this function in our experiment. The drive signal creates mechanical deformation in the transducer crystal (converse piezoelectric effect). If the excitation frequency is not matched to any natural frequencies of the system, little energy is dissipated to the system. The receiver transducer crystal has little deformation and there is little or no signal out from the receiver. At resonance, energy is delivered to the object and the object acts like a natural amplifier generating much larger vibrations. These vibrations will cause the receiver transducer to deform and generates a voltage signal that is captured by the DRS instrument. As we sweep the frequency range we are interested in, we get all the resonance frequencies of the object.

The resonance signal has the following mathematical form [51]:

\[
\psi(f) = A \frac{\left(\frac{f}{f_0}\right) \cos \phi + \left(1 - \left(\frac{f}{f_0}\right)^2\right) Q \sin \phi}{\left(\frac{f}{f_0}\right)^2 + \left(1 - \left(\frac{f}{f_0}\right)^2\right)^2 Q^2}
\]  

(4.1)

If we include a background noise due to crosstalk:

\[
\psi(f) = a_0 + a_1 f + a_2 f^2 + a_3 f^3 + \cdots + A \frac{\left(\frac{f}{f_0}\right) \cos \phi + \left(1 - \left(\frac{f}{f_0}\right)^2\right) Q \sin \phi}{\left(\frac{f}{f_0}\right)^2 + \left(1 - \left(\frac{f}{f_0}\right)^2\right)^2 Q^2}
\]

(4.2)

In our fitting, we used, at most, the quadratic term together with Eq. (4.1). \(A\) is a dimensionless constant, \(f\) is frequency, \(f_0\) is the resonance frequency, \(Q\) is quality factor and \(\phi\) is a phase angle of electronic and acoustic origin. A typical fitting is shown in Figure 4.13 and Table 4-2.
Figure 4.13 Resonance peak fitting.

Table 4-2 A typical resonance fitting result.

<table>
<thead>
<tr>
<th>curve number</th>
<th>$A$</th>
<th>$f_0$</th>
<th>$Q$</th>
<th>$\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$0.0225\pm2.8651e-4$</td>
<td>$88.0786\pm2.1344e-4$</td>
<td>$2196.1913\pm20.9523$</td>
<td>$3.0076\pm0.019$</td>
</tr>
<tr>
<td>2</td>
<td>$0.0362\pm2.3729e-4$</td>
<td>$88.106\pm1.116e-4$</td>
<td>$2539.9507\pm15.4843$</td>
<td>$3.2366\pm0.013$</td>
</tr>
<tr>
<td>parabola 3</td>
<td>$a_0 = -1.6632 \pm 30.9862$</td>
<td>$a_1 = 0.0375 \pm 0.7034$</td>
<td>$a_2 = -2.1279e - 4 \pm 0.004$</td>
<td></td>
</tr>
</tbody>
</table>

The fitting scheme works very well for simple resonance peaks, typically when there are only one or two peaks and they do not mix much. However, for complex combination of resonance peaks, the fitting results are not always satisfying. As the number of peaks in an interested range increase (sometimes we cannot just divide them into smaller ranges), the number of unknown parameters increases. The fitting algorithm can get stuck in a region that is not the real destination [73]. Factors that may affect the results include: the initial guessing of the parameters, the range included in the fitting (how much tail to be included on both sides). If we miss one small peak, this might change the quality factor or the phase or both for the other peaks’ fitting results. In this kind of situation, the result is we miss some peaks and the missing of one peak causes the error to increase in the other peak fitting. Unfortunately, we are never sure what
the real peaks should be like. We do not get consistent fitting results all the time. In our experiment there are more than 100 peaks for each run and the resonance pattern is quite complex, so we find the peak by visual fitting most of the time.

**DRS calibration**

In our experiment, we found a disturbing performance of the DRS system. Each time we give different input parameters, we get a different spectrum: the center frequency can shift by as much as 40 Hz, which is about the same order as shift due to elastic constant change in some cases. We indeed get consistent spectrum if the input scan parameters are the same. Still the natural resonance frequency of the object should not depend on how we measure them. An example of shifting is shown in Figure 4.14: $f_1 = 77.7205$ kHz, $Q_1 = 2741$, $f_2 = 77.7646$ kHz, $Q_2 = 2093$, $\Delta f = 44.1$ Hz.

![Figure 4.14 Scanned resonance peak with different input parameters.](image_url)
Inside the DRS system is a CMOS AD9850 frequency synthesizer (the Direct Digital Synthesizer core provides a 32-bit frequency tuning word). The clock frequency in the DRS system is 128 MHz. Resolution of the DRS system is:

\[ \delta f = \frac{128 \text{ MHz}}{2^{32}} = 0.02980232239 \text{ Hz} \quad (4.3) \]

The scan input parameters that are relevant to this are the starting frequency, ending frequency and the number of points for the scan. For neighboring points, the frequency change is given by

\[ \Delta f = \frac{f_{\text{end}} - f_{\text{start}}}{\text{# of points}} \quad (4.4) \]

If \( \Delta f/\delta f \) is not an integer, there could be a large rounding off error in the measured resonance frequency. For the case shown in Figure 4.14:

<table>
<thead>
<tr>
<th>starting/kHz</th>
<th>ending/kHz</th>
<th># of points</th>
<th>( \Delta f/\text{Hz} )</th>
<th>( \Delta f/\delta f )</th>
<th>( [\Delta f/\delta f] )</th>
<th>peak data#</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>77.5</td>
<td>77.9</td>
<td>4000</td>
<td>0.1</td>
<td>3.355443</td>
<td>3</td>
<td>2205</td>
</tr>
<tr>
<td>2</td>
<td>77.55</td>
<td>77.9</td>
<td>4000</td>
<td>0.0875</td>
<td>2.936013</td>
<td>3</td>
<td>2453</td>
</tr>
</tbody>
</table>

The first error is calculated by: \( \Delta_1 f = 2205 \times (\Delta f - 3\delta f) = 23.4 \text{ Hz} \). This error is on the same order as the difference we observed in the experiment. To solve this problem we change the starting frequency, ending frequency and number of points in such a way that the starting frequency, ending frequency and frequency increase \( \Delta f \) are all equal to an integer multiplying the resolution \( \delta f \) of the system. We write down the formulas in an excel file. Each time we start a new scan we will use the ‘modified’ input parameters in the scanning:

1.) New starting frequency = \( \delta f \times (\text{integer part (old starting frequency/} \delta f)) \).

2.) New \( \Delta f = \text{integer part (old } \Delta f / \delta f +0.5) \times \delta f \).
3.) New # points = integer part ((old ending frequency – new starting frequency)/new $\Delta f$ + 1).

4.) New ending frequency = new starting frequency + new # points*new $\Delta f$.

This guarantees that the starting frequency, ending frequency and frequency increase are all integer numbers multiplying the resolution of the system and eliminates round off error in the experiment. For the same setup as the above two trial runs, we get much better results using the modified input parameters as shown in Figure 4.15 (One peak is shifted vertically a little bit).

Table 4-4 New scan input parameters with small approximation error.

<table>
<thead>
<tr>
<th>starting/kHz</th>
<th>ending/kHz</th>
<th># of points</th>
<th>$\Delta f/\delta f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1b</td>
<td>77.499986</td>
<td>77.900082</td>
<td>4475</td>
</tr>
<tr>
<td>2b</td>
<td>77.549994</td>
<td>77.900022</td>
<td>3915</td>
</tr>
</tbody>
</table>

$f_{1b} = 77.699 \text{ kHz}$,  
$Q_{1b} = 3072$  
$f_{2b} = 77.699 \text{ kHz}$,  
$Q_{2b} = 3064$  
$\Delta f = 0 \text{ Hz}$

Figure 4.15 Scanned peak with new input parameters.
Chapter 5 Experiment results and data analysis

We first measured the resonance spectrum of the empty cell from room temperature to 4.2K to test our transducers and frequency measurements. We then had liquid helium filled the cell and took the spectrum measurements.

Empty cell

We measured the resonance spectrum of the empty cell from room temperature down to 4.2K. This data set was taken without ‘calibrating’ the DRS frequency measurement. The frequency measurements are not as accurate as later measurements. We would like to see if the elastic constant change (lowering the temperature) could be reflected on the resonance frequency measurement, and if so, how the frequency is going to change and how this is compared with calculation. It is not easy to identify all the normal frequencies. Some new frequencies may show up while some existing ones may disappear during the experiment. Instead of identifying frequencies at different temperatures one by one, we scatter plot all the peaks that are easy to recognize in the same graph in Figure 5.1. This can show how the frequencies change and can help us identify some of the peaks. For better viewing, we also plot the graph in a smaller vertical range in Figure 5.2.
Figure 5.1 Empty cell resonance frequency vs. temperature.
Figure 5.2 Empty cell resonance frequency vs. temperature. Lines are those calculated using ss304 and ss316 data. Vertical scales are different in these graphs.
We computed the resonance frequency of the top stainless steel part excluding the copper neck and copper base in Figure 5.3. Reasons for using this simplified geometry are:

1.) In our later calculation, we are interested in modes in which helium has a relatively big influence. These modes mainly involve motion of the top stainless steel cell.

2.) The copper base has a large volume and in finite element meshing the copper base accounts for a large portion of the total number of elements. This increases the computation cost significantly.

3.) We are not able to do the inverse calculation/fitting efficiently and correctly due to a large number of parameters involved in the physical process. Including the copper base will not give us a better result.

![Figure 5.3 Cell used in experiment (left) and calculation (right).](image)

The stainless steel elastic constant and density data are from [74, 75]. We assume the steel material is isotropic (so it is not exactly the same as in [74, 75]).
Table 5-1 Stainless steel property.

<table>
<thead>
<tr>
<th>T/ K</th>
<th>$\rho$/ g/cc</th>
<th>$c_{11}$/ 100GPa</th>
<th>$c_{44}$/ 100GPa</th>
<th>$\rho$/ g/cc</th>
<th>$c_{11}$/ 100GPa</th>
<th>$c_{44}$/ 100GPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>295</td>
<td>7.88</td>
<td>2.614</td>
<td>0.774</td>
<td>7.92</td>
<td>2.578</td>
<td>0.752</td>
</tr>
<tr>
<td>280</td>
<td>7.88</td>
<td>2.622</td>
<td>0.779</td>
<td>7.92</td>
<td>2.589</td>
<td>0.757</td>
</tr>
<tr>
<td>260</td>
<td>7.88</td>
<td>2.637</td>
<td>0.787</td>
<td>7.92</td>
<td>2.602</td>
<td>0.764</td>
</tr>
<tr>
<td>240</td>
<td>7.88</td>
<td>2.651</td>
<td>0.793</td>
<td>7.92</td>
<td>2.615</td>
<td>0.770</td>
</tr>
<tr>
<td>220</td>
<td>7.88</td>
<td>2.664</td>
<td>0.800</td>
<td>7.92</td>
<td>2.627</td>
<td>0.777</td>
</tr>
<tr>
<td>200</td>
<td>7.88</td>
<td>2.675</td>
<td>0.806</td>
<td>7.92</td>
<td>2.639</td>
<td>0.783</td>
</tr>
<tr>
<td>180</td>
<td>7.88</td>
<td>2.688</td>
<td>0.813</td>
<td>7.92</td>
<td>2.649</td>
<td>0.789</td>
</tr>
<tr>
<td>160</td>
<td>7.88</td>
<td>2.698</td>
<td>0.819</td>
<td>7.92</td>
<td>2.660</td>
<td>0.795</td>
</tr>
<tr>
<td>140</td>
<td>7.88</td>
<td>2.710</td>
<td>0.825</td>
<td>7.92</td>
<td>2.671</td>
<td>0.801</td>
</tr>
<tr>
<td>120</td>
<td>7.88</td>
<td>2.719</td>
<td>0.831</td>
<td>7.92</td>
<td>2.680</td>
<td>0.806</td>
</tr>
<tr>
<td>100</td>
<td>7.88</td>
<td>2.724</td>
<td>0.835</td>
<td>7.92</td>
<td>2.687</td>
<td>0.811</td>
</tr>
<tr>
<td>80</td>
<td>7.88</td>
<td>2.729</td>
<td>0.838</td>
<td>7.92</td>
<td>2.690</td>
<td>0.814</td>
</tr>
<tr>
<td>60</td>
<td>7.88</td>
<td>2.724</td>
<td>0.839</td>
<td>7.92</td>
<td>2.691</td>
<td>0.817</td>
</tr>
<tr>
<td>40</td>
<td>7.88</td>
<td>2.691</td>
<td>0.825</td>
<td>7.92</td>
<td>2.685</td>
<td>0.817</td>
</tr>
<tr>
<td>20</td>
<td>7.88</td>
<td>2.679</td>
<td>0.821</td>
<td>7.92</td>
<td>2.671</td>
<td>0.811</td>
</tr>
<tr>
<td>5</td>
<td>7.88</td>
<td>2.678</td>
<td>0.821</td>
<td>7.92</td>
<td>2.669</td>
<td>0.810</td>
</tr>
</tbody>
</table>

The cell is made of stainless steel 304. However, the ss304 calculation does not fit better than ss316 calculation. The experiment and calculation do not agree well with each other. We are using an over simplified model for the calculation:

1.) The geometry is different. The copper base has effect on the calculation, and there is error on the size of the stainless steel cell, which has a large effect according to finite element calculation.

2.) Rolled stainless steel rod is not isotropic and the density is not constant as we assumed in the calculation.

3.) Parts of the cell are epoxy and copper.

Despite all of these, the general trend is correct. The change in elastic constant has a recognizable effect on the spectrum. The overall percentage change in experimental resonance frequency is close to the calculated change. It is difficult to say which elastic constant, $c_{11}$ or shear modulus has a larger effect, since both of them are changing. A typical calculated and experiment frequency change is shown in Figure 5.2. We plot $c_{11}(T)/c_{11}(295\ K)$, $c_{44}(T)/$
\(c_{44}(295\,\text{K})\), the calculated eighth mode \(f_8(T)/f_8(295\,\text{K})\) using SS304 data, and one experiment \(f_{\text{exp}}(T)/f_{\text{exp}}(287\,\text{K})\) versus temperature. The calculated frequency at low temperature goes down as the elastic constant value decreases. Generally, when the elastic constant increases, resonance frequency increases. The experiment resonance frequency has a flatter end at the low temperature end (below 50 K) than the calculated results (these low-temperature elastic constant anomalies arise from magnetic phase transitions [75]). The flatter end in our results may be related with annealing and the effects of machining.

![Graph showing the relationship between pressure, temperature, and frequency](image)

Figure 5.4 The elastic constant, calculated normal frequency and experiment frequency versus temperature. The experiment reference frequency is the one measured at 287 K, different from the 300 K of the other variables.
All the normal frequencies change in a similar pattern, both for experimental and calculated results. For a small cell with a complex geometry as in our case, deformation involves both shear and longitudinal strain. Shear and longitudinal motions are strongly coupled. This might be the reason why we cannot tell whether a normal mode is mainly squeezing or doing torsional motion just from its frequency change.

![Normalization of normalized resonance frequencies vs. temperature.](image)

**Figure 5.5 Experiment and calculated normalized resonance frequencies vs. temperature.**

**Experiment data Run #1**

We grow solid helium using the blocked capillary method (constant volume growth). The helium grown in this method is of lower crystalline order (polycrystalline) compared with those grown at constant pressure or constant temperature [76, 77]. Polycrystalline makes our finite element calculation easier. We assume helium in our cell is isotropic with only two independent
elastic constant, $c_{11}$ and $c_{44}$. The amount of helium inside the cell is constant, so the average density is constant. Mass density affects resonance frequencies and constant density means one less varying parameter. In this way, we can focus our calculation on the effect of the helium elastic tensor on resonance frequencies. We used commercially ultra-high purity (99.999%) helium in our experiment.

We fill the cell with liquid helium at high pressure (1040 psi) at 4.2 K in our experiment. The cell is inside a vacuum space and the helium filling capillary goes through the liquid Helium bath and then the bottom flange as show in Figure 4.4. In the experiment, when we lower the temperature, the filling capillary gets cooler earlier than the cell inside the vacuum space. The capillary will be blocked somewhere at the anchoring point on the flange or along the line in the liquid helium bath first. In either case, the amount of helium inside the cell is constant after the capillary is blocked. We wait at 2.9 K until the pressure is stable. In this run, we cooled down slowly, taking data along the way. $^{4}$He inside the cell solidifies along the melting line and the pressure drops. This continues until all helium becomes solid inside the cell at about 2.1 K in our experiment.

Figure 5.6 $^{4}$He phase diagram and growth process.
After the filling capillary is blocked, reading of the pressure gauge is not equal to the pressure inside the cell any more. We do not have any pressure gauge inside the cell to measure the pressure directly in our design. The data in [78] shows an approximate 10% drop of solid Helium pressure from 2.1 K to 1.7 K.

In this experiment, we did not anneal the solid ^4He. We took the frequency scan when we reached the temperature point of interest. The resonant frequency dependence on temperature is shown in Figure 5.7 and Figure 5.8. We show part of the whole spectrum in Figure 5.9 that has all the typical features of the spectrum change.

![Figure 5.7 Resonance peak frequency of the empty cell and the cell filled with helium. The empty cell peaks measured at 4.2 K are shifted to 4.3 K for better viewing.](image-url)
Figure 5.8 Second half resonance peak frequency of the empty cell and the cell filled with helium. The empty cell peaks measured at 4.2 K are shifted to 4.3 K for better viewing.
Figure 5.9 Typical resonance spectrum. The amplitude is in arbitrary unit. Spectrum at different temperatures is shifted vertically a little bit for clarity. The vertical shift is not proportional to temperature change.

- **Cell filled with liquid $^4$He**
- **Empty cell**
- **Old peaks that exist when cell is empty do not shift much**
- **New peaks show up after $^4$He filled in**
- **In the liquid range, these peaks do not change much.**
- **Frequency shifts big at solidification.**
- **Below 1.9K, many peaks disappear.**
We see from this spectrum:

1.) There are some peaks that exist in all three states: empty cell, cell with liquid helium and cell with solid helium. Most of these peaks shift little in the whole process.

2.) The liquid to solid phase transition has an observable effect on the spectrum. Some peak frequencies decreases faster beginning from somewhere between 2.8 K and 2.9 K. This is consistent with the experimental procedure. We grow solid helium beginning at about 1040 psi (70.8 atm).

3.) For some reason, many peaks (peaks that show up when helium is filled inside the cell) disappeared beginning at 1.9 K. The overall spectrum below 1.9 K is very different from those above 1.9 K.

It is not enough just to be able to calculate the resonance modes. We need to analyze how the resonance frequency changes when the properties of the materials, stainless steel or $^4$He change. The analysis method is explained in the next section.

**Calculation methods**

It is not necessary to fit the elastic tensor accurately from the spectrum for our complex configuration. We are interested in the elastic property of solid $^4$He, which is grown inside the cell. $^4$He will cause the spectrum to change. The main problem is how to get information about solid helium from the change in the spectrum.

Growing solid $^4$He inside the cell will not just shift each resonance peak of the empty cell a little bit. A stainless steel cell filled with liquid or solid $^4$He has ‘more’ normal modes than an empty stainless steel cell. This is because the mechanical properties of $^4$He differ so much from that of stainless steel. Solid $^4$He is much lighter and more compressible. For a bulk sample of
solid helium, its ‘fundamental’ normal frequencies are much smaller than that of stainless steel with the same geometry and the difference between two neighboring normal frequencies is much smaller for $^4$He than for stainless steel. The ‘density’ of the normal modes is much larger for a cell with solid $^4$He inside than for an empty stainless steel cell as shown in Figure 5.10. We give an estimate about the frequency here. The data used in the estimation and following calculation is listed in Table 5-2. The stainless steel data is from [74, 75] and the helium data is estimated from [76, 79-84].

Sound velocity: $v = \sqrt{\frac{c}{\rho}} = \lambda f$. $\lambda$ is wavelength. Our cell is about 1 cm in size. Taking the cell size as wavelength, the characteristic frequency (shear wave) for stainless steel cell is:

$$f = \frac{1}{\lambda} \sqrt{\frac{c}{\rho}} \approx 300 \text{ kHz.} \quad (5.1)$$

For solid $^4$He, the frequency is:

$$f = \frac{1}{\lambda} \sqrt{\frac{c}{\rho}} \approx 30 \text{ kHz.} \quad (5.2)$$

Table 5-2 Material parameters used in calculation.

<table>
<thead>
<tr>
<th></th>
<th>Density/ g/cm$^3$</th>
<th>c11/100 GPa</th>
<th>c44/100 GPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>stainless steel</td>
<td>7.880</td>
<td>2.678</td>
<td>0.821</td>
</tr>
<tr>
<td>solid $^4$He</td>
<td>0.210</td>
<td>0.00077</td>
<td>0.00022</td>
</tr>
<tr>
<td>liquid $^4$He</td>
<td>0.210</td>
<td>0.00055</td>
<td>0.00000</td>
</tr>
</tbody>
</table>
Figure 5.10 ‘Density’ of normal states of an empty stainless steel cell and the same stainless steel cell filled with solid $^4$He.

The transducer cannot detect all the normal modes of the new system because many modes generate too small a signal for the transducer to pick up. We need to find a way to identify the peaks in the experiment spectrum. The transducer can pick up modes that involve large deformations of the stainless steel cell. These modes have similar shapes to those of the empty cell. A program is written to find the similarity between the modes in these two cases. If two modes are similar, the dot product of the two eigenvectors from the eigenvalue solution should be relatively large. This is the idea of a “similarity matrix” in the program. To calculate the similarity matrix, the dimensions of the two eigenvectors must be the same. We calculate both the empty cell and cell filled with $^4$He using the same mesh file.

Using the same mesh file:
1.) Reduces finite element approximation error (The finite element calculation results depend on the number of mesh elements.).

2.) Makes it possible to calculate the similarity between eigenmodes in the empty and filled case (We are comparing the motion of the same group of nodes.). If the mesh file is different, the nodes are not the same. Then it is impossible to compare ‘similarity’ between the two modes.

To calculate the empty cell natural frequencies, we use zero values for the solid $^4\text{He}$ density and elastic tensor. This makes the global stiffness and mass matrix singular. The Matlab built-in sparse eigenvalue solver cannot handle a singular mass matrix. We rearrange the matrix index so the ‘zero’ inside nodes (corresponding to the helium nodes) are all moved to the lower right corner of the new matrix and this part is excluded in the new eigenvalue equation. In the program QuadTetra2Mode.m or QT2ModeParal.m the material 2 property input parameters must have zero values. It cannot correctly calculate spectrum of a cell filled with real solid $^4\text{He}$. This should be calculated using the programs QuadTetraModeT1.m or QuadTetraModeT1Parallel.m.

Procedure for comparing the modes:

1.) Use GID software to build the geometry similar to the experiment. This includes geometry and material assignment. Assign solid $^4\text{He}$ to material 2 in the model.

2.) In the material property file, assign all parameters of helium (material 2) as zero. Use QT2ModeParal.m to calculate the resonance modes of a pseudo-empty cell and export the modes (eigenvector) file, and a ‘normalized’ eigenvector file (In the generalized eigenvalue problem, eigenvectors are normalized using the mass matrix $M$: $\omega^2 MU = KU$, $u_iMu_j = \delta_{ij}$.).
3.) Assign solid $^4$He its real parameters and use the QuadTetraModeT1Paralle.m program to calculate the resonance modes for a cell filled with solid $^4$He. This will also produce the eigenvector $v_i$ file.

4.) Use the program vdot.m to calculate the similarity $v_iM_{ij}$ between these two groups of modes.

An example of a calculation is shown in Table 5-3 and Table 5-4 to check the idea of the similarity matrix. We calculated 20 normal frequencies of the cell filled with solid $^4$He around one normal frequency (113 kHz) of an empty cell.

Table 5-3 Resonance frequencies of an empty cell (red number at the right) and the same cell filled with solid $^4$He (blue number on the left).

<table>
<thead>
<tr>
<th>Resonance Frequency /kHz</th>
<th>Solid $^4$He</th>
<th>Mode</th>
<th>Empty</th>
</tr>
</thead>
<tbody>
<tr>
<td>110.588</td>
<td>1</td>
<td>79.029</td>
<td></td>
</tr>
<tr>
<td>110.641</td>
<td>2</td>
<td>80.194</td>
<td></td>
</tr>
<tr>
<td>110.683</td>
<td>3</td>
<td>80.218</td>
<td></td>
</tr>
<tr>
<td>110.984</td>
<td>4</td>
<td>91.046</td>
<td></td>
</tr>
<tr>
<td>110.996</td>
<td>5</td>
<td>91.049</td>
<td></td>
</tr>
<tr>
<td>111.120</td>
<td>6</td>
<td>93.366</td>
<td></td>
</tr>
<tr>
<td>111.201</td>
<td>7</td>
<td>93.412</td>
<td></td>
</tr>
<tr>
<td>111.203</td>
<td>8</td>
<td>104.887</td>
<td></td>
</tr>
<tr>
<td>111.996</td>
<td>9</td>
<td>112.276</td>
<td></td>
</tr>
<tr>
<td>112.012</td>
<td>10</td>
<td>122.640</td>
<td></td>
</tr>
<tr>
<td>112.202</td>
<td>11</td>
<td>122.680</td>
<td></td>
</tr>
<tr>
<td>112.241</td>
<td>12</td>
<td>131.209</td>
<td></td>
</tr>
<tr>
<td>112.426</td>
<td>13</td>
<td>131.279</td>
<td></td>
</tr>
<tr>
<td>112.615</td>
<td>14</td>
<td>143.685</td>
<td></td>
</tr>
<tr>
<td>113.103</td>
<td>15</td>
<td>143.688</td>
<td></td>
</tr>
<tr>
<td>114.033</td>
<td>16</td>
<td>157.177</td>
<td></td>
</tr>
<tr>
<td>114.041</td>
<td>17</td>
<td>157.183</td>
<td></td>
</tr>
<tr>
<td>114.639</td>
<td>18</td>
<td>167.886</td>
<td></td>
</tr>
<tr>
<td>114.664</td>
<td>19</td>
<td>168.296</td>
<td></td>
</tr>
<tr>
<td>115.370</td>
<td>20</td>
<td>168.346</td>
<td></td>
</tr>
</tbody>
</table>
Table 5-4 'Similarity' between normal modes of an empty cell (red column index) and the same cell filled with solid \(^4\)He (blue row index).

<table>
<thead>
<tr>
<th>Similarity Matrix</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0.0006</td>
<td>-0.0002</td>
<td>-0.0006</td>
<td>-0.0017</td>
<td>-0.0003</td>
<td>0.0006</td>
</tr>
<tr>
<td>9</td>
<td>0.0002</td>
<td>-0.0037</td>
<td>-0.0032</td>
<td>-0.0039</td>
<td>-0.0494</td>
<td>0.0007</td>
</tr>
<tr>
<td>10</td>
<td>0.0005</td>
<td>-0.0015</td>
<td>0.0009</td>
<td>-0.0503</td>
<td>0.0041</td>
<td>-0.0006</td>
</tr>
<tr>
<td>11</td>
<td>-0.0001</td>
<td>-0.0005</td>
<td>0.0228</td>
<td>-0.0144</td>
<td>-0.0007</td>
<td>-0.0007</td>
</tr>
<tr>
<td>12</td>
<td>-0.0001</td>
<td>-0.0008</td>
<td>-0.0157</td>
<td>0.0011</td>
<td>-0.0165</td>
<td>0.0004</td>
</tr>
<tr>
<td>13</td>
<td>0.0002</td>
<td>0.0001</td>
<td>-0.9369</td>
<td>-0.0001</td>
<td>0.0006</td>
<td>0.0000</td>
</tr>
<tr>
<td>14</td>
<td>-0.0001</td>
<td>-0.0980</td>
<td>-0.0008</td>
<td>0.0009</td>
<td>0.0008</td>
<td>0.0001</td>
</tr>
<tr>
<td>15</td>
<td>0.0003</td>
<td>0.0311</td>
<td>-0.0011</td>
<td>-0.0006</td>
<td>0.0007</td>
<td>0.0003</td>
</tr>
<tr>
<td>16</td>
<td>-0.0001</td>
<td>0.0001</td>
<td>0.0000</td>
<td>0.0005</td>
<td>0.0040</td>
<td>0.0022</td>
</tr>
<tr>
<td>17</td>
<td>0.0000</td>
<td>-0.0014</td>
<td>-0.0009</td>
<td>0.0034</td>
<td>-0.0015</td>
<td>0.0003</td>
</tr>
</tbody>
</table>

Table 5-4 shows that the 13\(^{th}\) (relative index) normal mode (112.426 kHz) of the cell filled with solid \(^4\)He is very similar to the 9\(^{th}\) normal mode (112.276 kHz) of the empty cell. Their difference is only 150 Hz (~0.13%). It can be smaller than the difference between calculations using different numbers of mesh elements. It is also on the same order as error from a DRS frequency measurement (we explained how to fix DRS error in Chapter 4).

The 9\(^{th}\) and the 13\(^{th}\) resonance modes are shown in Figure 5.11. It can be seen that pairs having a large similarity number indeed resonant in a similar way and have close resonance frequencies. This way of identifying modes works.
Figure 5.11 Mode of an empty cell (l.h.s) and the corresponding mode of the same cell filled with solid $^4$He (r.h.s).

**Stable peaks**

There are peaks that do not shift much when the cell is filled with $^4$He. One question is whether these peaks change in different ways, and if so, how they are related with material property changes. We analyze three groups of peaks (104 kHz, 121 kHz and 148 kHz) that have good resonance shapes over the whole temperature range. Due to the complex geometry, we cannot align the experiment resonance frequencies with the calculated resonant frequencies even for the empty cell. However, these three groups of peaks are relatively isolated both in experiment and in the calculation.

Using the similarity matrix discussed above, in theory, we can calculate how these ‘stable’ peaks (modes that have a similar deformation to the corresponding modes of the empty cell) should change. The lowest 20 modes of the empty cell, their corresponding normal frequencies of the cell filled with solid $^4$He, and their similarity index are shown in Table 5-5. Modes 2, 3, 18 and 19 have two corresponding solid $^4$He cell modes with the similarity indices shown in the extra columns. The similarity index alone cannot tell for sure how the peaks are going to move. We can check resonance animation in this case.
Table 5-5 Resonance frequencies of the empty cell and \(^4\)He cell.

<table>
<thead>
<tr>
<th>Mode</th>
<th>empty freq/kHz</th>
<th>Solid (^4)He cell freq/kHz</th>
<th>similarity</th>
<th>Solid (^4)He cell freq (extra)</th>
<th>Similarity (extra)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>79.029</td>
<td>77.700</td>
<td>-0.8629</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>80.194</td>
<td>83.615</td>
<td>-0.6890</td>
<td>76.688</td>
<td>-0.6309</td>
</tr>
<tr>
<td>3</td>
<td>80.218</td>
<td>83.626</td>
<td>0.6899</td>
<td>76.697</td>
<td>0.6294</td>
</tr>
<tr>
<td>4</td>
<td>91.046</td>
<td>91.719</td>
<td>-0.8817</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>91.049</td>
<td>91.723</td>
<td>-0.8817</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>93.366</td>
<td>90.976</td>
<td>-0.7752</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>93.412</td>
<td>91.002</td>
<td>-0.7735</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>104.887</td>
<td>104.777</td>
<td>0.9813</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>112.276</td>
<td>112.426</td>
<td>-0.9369</td>
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</tr>
<tr>
<td>10</td>
<td>122.640</td>
<td>123.191</td>
<td>0.8658</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>122.680</td>
<td>123.220</td>
<td>0.8563</td>
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</tr>
<tr>
<td>12</td>
<td>131.209</td>
<td>132.460</td>
<td>0.8650</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>131.279</td>
<td>132.520</td>
<td>0.8635</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>143.685</td>
<td>143.264</td>
<td>-0.8213</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>143.688</td>
<td>143.293</td>
<td>-0.7745</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>157.177</td>
<td>157.121</td>
<td>0.6175</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>157.183</td>
<td>157.128</td>
<td>-0.7460</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>167.886</td>
<td>168.171</td>
<td>0.5298</td>
<td>168.191</td>
<td>0.4535</td>
</tr>
<tr>
<td>19</td>
<td>168.296</td>
<td>167.584</td>
<td>-0.3113</td>
<td>167.465</td>
<td>-0.3055</td>
</tr>
<tr>
<td>20</td>
<td>168.346</td>
<td>167.584</td>
<td>-0.3262</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The experimental resonance frequency around 104 kHz changes little. In the calculation, this mode is not degenerate and it is relatively far away from the neighboring peaks. Nevertheless, we find three nearby peaks around 104 kHz and they have nice resonance shapes over the whole temperature range. We think these three may correspond to the calculated 8\(^{th}\) normal mode.
Table 5-6 Frequency and quality factor of the mode around 104 kHz.

<table>
<thead>
<tr>
<th></th>
<th>T/K</th>
<th>f/kHz</th>
<th>Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empty</td>
<td>4.2</td>
<td>102.7269</td>
<td>2440</td>
</tr>
<tr>
<td>Liquid</td>
<td>4.2</td>
<td>102.7217</td>
<td>2459</td>
</tr>
<tr>
<td></td>
<td>3.5</td>
<td>102.7265</td>
<td>2484</td>
</tr>
<tr>
<td></td>
<td>2.9</td>
<td>102.7317</td>
<td>2513</td>
</tr>
<tr>
<td>Solid</td>
<td>2.2</td>
<td>102.7316</td>
<td>2521</td>
</tr>
<tr>
<td></td>
<td>1.7</td>
<td>102.7329</td>
<td>2511</td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td>102.7323</td>
<td>2521</td>
</tr>
</tbody>
</table>

Figure 5.12 Resonance spectrum of the peaks around 104 kHz. ‘4.2Ke/4.2Kl’ is spectrum of empty/liquid Helium cell at 4.2 K.

According to calculation, there is one mode around 122 kHz that shifts little. We experimentally find one peak in the experiment measurement around 121 kHz, which has a nice shape over all the range and shifts little (compared with the 104 kHz mode, the shift is large, but the shift is actually very small as shown in the graph containing all the peaks). We think this one may correspond to the 10th and 11th calculated normal modes. Despite the fact that the shift is very small (less than 0.5%), we still can find hints indicating the change from empty to liquid to solid.
Figure 5.13 Resonance peak around 121 kHz.

There is a set of peaks around 148.5 kHz in the experiment with good shapes and small shift. We think this one may correspond to the 14th calculated normal mode.

Figure 5.14 Stable resonance peaks around 148 kHz.
Figure 5.15 Reduced frequency of two stable peaks. $f_0$ is the one around 121 kHz.

Figure 5.16 Reduced quality factor of two stable peaks around 104 kHz and 121 kHz.
The 121 kHz mode shifts more, and its quality factor has a bigger change compared with
the other two stable peaks. Around 1.8–1.9 K, the spectrum changes a lot and so does the quality
factor of the 121 kHz mode. It is not clear why for this run the quality factor for this mode
decreases at this temperature and why the spectrum changes drastically.

The similarity is defined by: \( u_{s,i} \cdot M_e \cdot u_{e,j} \), with \( u_{s,i} \cdot M_s \cdot u_{s,j} = \delta_{ij} \) and \( u_{e,i} \cdot M_e \cdot u_{e,j} = \delta_{ij} \). \( u_{s,i} / u_{e,j} \) is the \( i^{th} / j^{th} \) calculated mode of the cell filled with solid \(^4\)He /empty cell. \( M_e / M_s \) is the mass matrix of the empty cell/cell filled with solid \(^4\)He. Larger similarity index means
that the solid \(^4\)He motion plays a minor part. The stainless steel cell accounts for most of the
mechanical energy in these modes: \( E = \frac{1}{2} \omega^2 u_{s,i} \cdot M_s \cdot u_{s,j} \). This also suggests that these modes
may depend mostly/ little on the property of stainless steel/ solid \(^4\)He. To check this idea, we
computed the derivative matrix (derivative of frequency with respect to density and elastic tensor:
\( \frac{df}{dp} / \frac{df}{p} \)) of these modes. The result is shown in Table 5.7-5.9. For some frequencies, the calculation
may be wrong, since when we change the parameter in the calculation, the order of the resonance
frequencies of different modes may change. This is different from the calculation of the empty
stainless steel cell. In that case, the frequency interval is large enough to prevent this from
happening. To do it precisely we would need to check all the modes and compare them with
modes before parameter change. We just use these numbers for comparisons here. We compared
all the modes using a similarity matrix in our latter calculation.
Table 5-7 Calculated derivative matrix of the normal mode around 105 kHz. The frequency in blue is the one we are interested in. It is similar to the 8th mode of the empty cell.

<table>
<thead>
<tr>
<th>Freq/105 kHz</th>
<th>(df/df)/(dp/p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freq/kHz</td>
<td>rho ss</td>
</tr>
<tr>
<td>102.843</td>
<td>-0.098</td>
</tr>
<tr>
<td>102.856</td>
<td>-0.071</td>
</tr>
<tr>
<td>102.980</td>
<td>-0.093</td>
</tr>
<tr>
<td>103.010</td>
<td>-0.006</td>
</tr>
<tr>
<td>104.777</td>
<td>-0.337</td>
</tr>
<tr>
<td>104.963</td>
<td>0.000</td>
</tr>
<tr>
<td>104.974</td>
<td>0.000</td>
</tr>
<tr>
<td>105.216</td>
<td>0.000</td>
</tr>
<tr>
<td>105.230</td>
<td>0.000</td>
</tr>
<tr>
<td>105.529</td>
<td>-0.002</td>
</tr>
<tr>
<td>105.543</td>
<td>-0.002</td>
</tr>
<tr>
<td>105.953</td>
<td>-0.001</td>
</tr>
<tr>
<td>105.976</td>
<td>-0.001</td>
</tr>
</tbody>
</table>

Table 5-8 Calculated derivative matrix of the normal mode around 123 kHz. The frequency in blue is the one we are interested in. It is similar to the 10th and 11th modes of the empty cell.

<table>
<thead>
<tr>
<th>Freq/123 kHz</th>
<th>(df/df)/(dp/p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freq/kHz</td>
<td>rho ss</td>
</tr>
<tr>
<td>121.883</td>
<td>-0.014</td>
</tr>
<tr>
<td>122.793</td>
<td>0.000</td>
</tr>
<tr>
<td>122.835</td>
<td>0.000</td>
</tr>
<tr>
<td>122.862</td>
<td>0.000</td>
</tr>
<tr>
<td>123.123</td>
<td>0.000</td>
</tr>
<tr>
<td>123.164</td>
<td>0.000</td>
</tr>
<tr>
<td>123.191</td>
<td>0.029</td>
</tr>
<tr>
<td>123.220</td>
<td>0.033</td>
</tr>
<tr>
<td>123.371</td>
<td>0.076</td>
</tr>
<tr>
<td>123.425</td>
<td>0.079</td>
</tr>
<tr>
<td>123.838</td>
<td>0.161</td>
</tr>
<tr>
<td>123.910</td>
<td>0.154</td>
</tr>
<tr>
<td>124.837</td>
<td>0.052</td>
</tr>
<tr>
<td>124.867</td>
<td>0.052</td>
</tr>
</tbody>
</table>
Table 5-9 Calculated derivative matrix of the normal mode around 144 kHz. The frequency in blue is the one we are interested in. It is similar to the 14th mode of the empty cell.

<table>
<thead>
<tr>
<th>Freq/144 kHz</th>
<th>(df/f)/(dp/p)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>rho ss</td>
</tr>
<tr>
<td>141.844</td>
<td>-0.009</td>
</tr>
<tr>
<td>142.014</td>
<td>-0.027</td>
</tr>
<tr>
<td>142.047</td>
<td>-0.029</td>
</tr>
<tr>
<td>143.067</td>
<td>-0.147</td>
</tr>
<tr>
<td>143.094</td>
<td>-0.147</td>
</tr>
<tr>
<td>143.264</td>
<td>-0.028</td>
</tr>
<tr>
<td>143.293</td>
<td>-0.028</td>
</tr>
<tr>
<td>143.736</td>
<td>-0.012</td>
</tr>
<tr>
<td>143.875</td>
<td>-0.009</td>
</tr>
<tr>
<td>143.980</td>
<td>-0.014</td>
</tr>
<tr>
<td>144.196</td>
<td>-0.020</td>
</tr>
<tr>
<td>144.282</td>
<td>-0.020</td>
</tr>
<tr>
<td>144.497</td>
<td>-0.001</td>
</tr>
<tr>
<td>144.542</td>
<td>-0.002</td>
</tr>
</tbody>
</table>

The one mode we are interested in around 105 kHz depends strongly on the density of stainless steel. This may be the reason why the peak frequency shifts so little since the density is unlikely to change significantly in this small temperature range. The peaks around 122 kHz and 144 kHz have a relatively large dependence on the stainless steel elastic tensor and there is no special dependence on the solid $^4$He elastic tensor. Nevertheless, they indeed depend on the $^4$He parameter and this can explain their frequency shift. As to why we cannot see any hints of change from empty to liquid to solid from the 144 kHz resonance mode, this may be related with the specific mode’s deformation.

Although the one mode around 121 kHz indicates transition from empty to liquid to solid, the frequency shifts of these modes are too small to get any reliable information about the solid $^4$He elastic tensor. The derivative matrix shows that for some modes the frequency depends more on the elastic property of solid $^4$He than on stainless steel. This is counterintuitive considering the very small values of the density and elastic constants of solid $^4$He. The small
frequency shift of the mode around 104 kHz shows that the stainless steel property stays more or less the same over the experiment temperature range. In the following calculations, we will assume the stainless steel parameters are all constants.

**Shifted peaks**

We observe significantly more peaks when there is liquid or solid $^4$He inside the cell. This is consistent with the calculation, although we do not have as many as predicted by calculation. The signals of some peaks are probably too small to be picked up. We see a clear shift in the resonance frequencies for many peaks. A group of typical shift peaks’ frequency, quality factor, and spectrum are shown in Figure 5.17-5.18.

![Figure 5.17 Center frequencies and reduced frequencies $f(T)/f(4.2 \text{ K})$ of the peaks around 115 kHz.](image-url)
We fit the peaks using Eq. (4.2) to get the center frequency and quality factor. Some degenerate peaks get separated like the one in Figure 5.19 (the 3rd peak/peaks). In this case we just used one peak to fit that part to get consistent data (only at the several lowest temperatures can we see a clear separation of that peak). The fitted center frequency and quality factor are listed in Table 5-10. The fit result has little variance (The variance of the quality factor can be large, if there are several peaks together and it is difficult to separate them. We usually fit it with one peak to get the center frequency. The quality factor has little meaning in this situation.)
ignored the variance in the fitting results and did not draw an error bar here. We used three peaks to fit the spectrum in this frequency range. These three peaks do not exist in the empty cell. Starting from 1.9 K, these peaks are not observable in the spectrum any more. It is not clear why the whole spectrum changes at this temperature.

<table>
<thead>
<tr>
<th>T/K</th>
<th>f1/kHz</th>
<th>Q1</th>
<th>f2</th>
<th>Q2</th>
<th>f3</th>
<th>Q3</th>
</tr>
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<tbody>
<tr>
<td>liquid</td>
<td>4.2</td>
<td>115.9942</td>
<td>4507.1452</td>
<td>116.0988</td>
<td>2421.1461</td>
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<tr>
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<td>116.2081</td>
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<td>116.2786</td>
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<td>4815.6249</td>
<td>113.1196</td>
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<td>1027.6971</td>
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<td>1.7</td>
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</tr>
<tr>
<td>1.6</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

For this group of shifted peaks, the center peak frequencies fluctuate in the liquid case. There is no apparent increase or decrease trend in the liquid range. When the solidification begins at about 2.8~2.9 K, they drop quickly. These three peaks also shift in a similar pattern and their
percentage changes are about the same. Unlike the center frequencies, the quality factor change is more complex. Their difference could be due to the error in fitting.

Some other shifted peaks that exist over all the temperature range above 1.9 K are shown in Figure 5.20. The reference data is the frequency at 4.2 K, of the cell filled with liquid $^4$He. The shift is about the same except the one around 79 kHz. The quality factor of the one around 79 kHz is also different from the others. We did not draw all the modes’ quality factor. Some fitting results for the quality factor have big variances. The sudden drop in quality factor occurs at the same temperature when many resonance peaks disappear. A larger dissipation may cause this.

![Graph showing reduced resonance frequencies and quality factor of the shifted peaks.](image)

**Figure 5.20 Reduced resonance frequencies and quality factor of the shifted peaks.**

**Experiment data Run #2**

We got little resonance peak data below 1.9 K for Run #1. The reason is not clear. Most of the peaks that show up when $^4$He is filled in the cell disappear when the temperature is below 2
K. To investigate this possible change, we took Run #2. This time we grew $^4$He in the same way as the previous run. The pressure starts with 1040 psi. We collect the data of the cell filled with liquid starting at 4.2 K. The next data is taken at 2.9 K, then 2.1 K (the change from 2.9 K to 2.1 K is faster than Run #1), then we collected the data with 0.1 K steps until the lowest temperature we can achieve, 0.9 K. As in the Run #1, we did not wait for $^4$He to anneal in the experiment. We took the measurement whenever the temperature arrives at the desired temperature point.

**Experiment results**

The resonance frequency change is shown in Figure 5.21. At T=4.2 K and 2.9 K, we do not have as many resonance peaks as in the last run, or as many as the spectrum at and below 2.1 K. These effects may be related to the fact that in this run we lowered the temperature from 4.2 K to 2.9 K to 2.1 K very fast. The solidified $^4$He is not stable yet. Many new peaks show up beginning from 2.1 K and they exist in all spectra taken over the 2.1-0.9K temperature range. The spectrum is not exactly the same as that of the last run, but the stable peaks are the same in both runs. For those peaks that show up as $^4$He is filled in, some peaks show up in both runs, but there are also some different resonance peaks. We believe this is because the solid $^4$He we grow is not the same, and this is reflected in the spectrum detail.
Figure 5.21 Resonance peaks of experiment Run #2.
Figure 5.22 Stable peaks are reproducible (4.2Ke/l is empty/liquid cell at 4.2 K).

Figure 5.23 Shifted peaks are not exactly reproducible.
The shifted resonance peaks change in a similar way as in Run #1. The reduced resonance frequencies are shown in Figure 5.24. The reference data point for 62 kHz data is the resonance frequency at 2.0 K since the 62 kHz peak data at 2.1 K is missing. The quality factor stays more or less the same as shown in Figure 5.24. We do not have as many quality factor data because some quality factor data fitting is not precise.

Figure 5.24 Reduced resonance frequency and quality factor of experiment Run #2.

Analysis

The key question here is why the normal frequencies decrease. The filling capillary is blocked so the amount of $^4$He inside the cell is constant so the density of $^4$He is constant.

For a liquid, the shear modulus is zero. In our calculation, we set $c_{44} = 0$, and $c_{11} = c_{12} = 55$ MPa. There are significantly more peaks in a small frequency range than in the
spectrum of the empty cell or cell filled with solid $^4$He. This makes it difficult to align the frequencies (In each calculation, we can get a large number of eigenfrequencies, but they are very close, if the parameter changes a lot, the frequency of the mode we are interested in will go out of the calculation range). We only get the results for 4 different $c_{11}$ values in the liquid $^4$He case. This already shows the trend.

We calculate the resonance frequencies with different solid $^4$He parameters:

1.) Decrease $c_{11}$ from 77 MPa by 0.385 MPa ($77*0.005$) each step for a total of 20 steps while keeping all other parameters constant.

2.) Decrease $c_{44}$ from 22 MPa by 0.11 MPa ($22*0.005$) each step for a total of 20 steps while keeping all other parameters constant.

The resonance frequency dependence on $c_{11}$ and $c_{44}$ is shown in Figure 5.25. ‘C44 solid~85 kHz’ is the normal frequency change of a peak around 85 kHz, as a function of $c_{44}$, with $c_{11}$ fixed. Elastic constants decrease from right to left in the horizontal axis (decrease step, with 20 the original data, 15 means decrease (20-15=5) steps from the original data), in order to get a pattern similar to the experiment result.

Figure 5.25 Calculated resonance frequency dependence on elastic constant.
We next focus on the effect of $c_{44}$ on the resonance frequencies. There are two reasons for this:

1.) Liquids have zero shear modulus while a solid can support shear strain. This is one key difference between solids and liquid material.

2.) In the supersolid transition range, the shear modulus increases a lot. Our experiment is done at far above the supersolid temperature. Nevertheless, we can do a simulation to see how the shear modulus change can influence the resonance spectrum.

Even for the stable peaks, their behaviors are different. The stable peak around 121 kHz in Run #1 has a very small shift but still is large enough to see the effect of liquid-solid transition. Some other peaks shift little and we cannot tell from their change the transition from liquid to solid, like the one around 104 kHz (Figure 5.26). We would like to do a calculation to see if there is any difference in calculation for these two peaks assuming only $c_{44}$ is changing.

Figure 5.26 Stable peak around 104 kHz and 123 kHz.
The frequencies of some modes change faster. An initially larger one could become a smaller one as the $^4$He parameter changes. We cannot just order the frequencies from small values to large values and align them according to this order. This will mix the frequencies of different modes. We solve this problem using the similarity matrix technique. The procedure is:

1.) Using the initial $^4$He parameter value, we calculate a number of modes (say 10) around the mode we are interested in (in this case, it is the one that has a small shift, i.e. the one that already exists even when the cell is empty), and get the eigenfrequencies and eigenvectors.

2.) For each new set of parameter values, we calculate the normal frequencies (say 30 or 40 if there is a big change in the parameter value) and the similarity matrix between this group of normal modes and the original group of normal modes.

3.) Using the similarity matrix, we realign the normal frequencies. This guarantees that the frequencies in a group correspond to the ‘same’ mode.

Our results show the similarity matrix idea works fine. We can align the frequencies with some certainty. The calculated resonance frequencies of the stable peak around 104/123 kHz and nearby peaks that have a larger shift are shown in Figure 5.27. From 115.690 kHz to 125.191 kHz there are 45 peaks. We only draw three of the representative shifted peaks. The others shift a similar amount. We can also see a ‘crossover’ of the resonance frequencies. The calculated reduced resonance frequencies of the two stable peaks around 104/123 kHz and nearby shifted peaks are shown in Figure 5.28. In the calculation, the stable peak around 104 kHz shift much less than the one around 123 kHz. This agrees with the experiment result shown in Figure 5.26.
Figure 5.27 Calculated shifted vs. stable peaks.

Figure 5.28 Calculated reduced frequencies of different peaks.
Experiment data Run #3

The previous experiments show a decrease in resonance frequency as temperature decreases and our analysis shows that a decrease in solid $^4$He shear modulus can cause this. There are other possibilities that need to be considered.

1.) The decrease may be due to a property change of the stainless steel rather than the change in solid $^4$He. The fact that there are ‘stable’ peaks that shift little in our experiment does not support this idea. Nevertheless, we still went on to do the measurement of an empty cell.

2.) We did not wait long enough for solid $^4$He to anneal in our previous runs. The decrease in resonance frequency may be the result of annealing, or it is indeed related to temperature decrease.

To check these ideas, we measured the resonance spectrum of the empty stainless steel cell in the same temperature range. We grew solid $^4$He over a longer period to check for a $^4$He annealing effect.

Empty cell

There are only ‘stable’ peaks for the empty cell. We analyzed two special peaks as for a previous calculation. One is around 104 kHz and one around 121 kHz. We analyzed the same two peaks of the empty cell (unlike those ‘shifted’ peaks, these ‘stable’ peaks are repeatable; they show up in every run). The calculation in Table 5-5 shows that the original peaks change little when helium is filled into the cell.

We did not wait for the stainless steel to anneal. We took the measurement whenever the temperature is stable at the point we are interested in. We started from 3.42 K and took the
measurements as the temperature goes down. The 4.1 K data was taken about 12 hours later than the other data. It takes a very long time for the helium in the Dewar to warm up from below superfluid temperature 1.2 K to 4.1 K.

Table 5-11 Center frequency and quality factor of resonance peaks of an empty cell.

<table>
<thead>
<tr>
<th>Day</th>
<th>T/K</th>
<th>f</th>
<th>Q</th>
<th>f</th>
<th>Q</th>
<th>f</th>
<th>Q</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>104 kHz</td>
<td></td>
<td>121 kHz</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Day 1</td>
<td>3.42</td>
<td>103.8574</td>
<td>3084.955</td>
<td>103.9553</td>
<td>3323.593</td>
<td>120.8942</td>
<td>2281.418</td>
</tr>
<tr>
<td></td>
<td>3.1</td>
<td>103.8652</td>
<td>3853.917</td>
<td>103.9671</td>
<td>2947.363</td>
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<td>2391.995</td>
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<td></td>
<td>2.9</td>
<td>103.8670</td>
<td>3933.021</td>
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<td>2904.268</td>
<td>120.8973</td>
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</tr>
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<td></td>
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<td></td>
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<td>103.9759</td>
<td>2835.894</td>
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<tr>
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<td>103.8629</td>
<td>3515.937</td>
<td>103.9623</td>
<td>2973.347</td>
<td>120.8932</td>
<td>2618.772</td>
</tr>
</tbody>
</table>

Figure 5.29 Resonance spectrum of the peaks around 104/121 kHz.

The empty cell and helium cell frequency dependence on temperature is compared in Figure 5.30. The resonance frequency of the empty cell increases slightly as we lower the temperature. This is opposite to what we see for a cell filled with solid $^4$He. In that case, the resonance frequencies decrease as we lower the temperature. We know from the empty cell
calculation that if $c_{11}$ and/or the shear modulus increase, the resonance frequency will increase. We did not find any data about the elastic constants of stainless steel below 5 K. From our experiment results, $c_{11}$ and/or the shear modulus of stainless steel 304 should increase below 4.1 K as the temperature lowers. The shift is only about 0.01%, this is much smaller than the 2% frequency decrease of the cell filled with solid $^4$He. This much smaller increase of resonance frequencies of the empty stainless steel shows that the frequency decrease we observed in our previous runs is not likely due to the change of a stainless steel property.

![Figure 5.30 Resonance frequency dependence on temperature of an empty cell vs. helium cell.](image)

**Annealing of the empty cell and cell filled with solid $^4$He**

$^4$He is grown the same way as before. This time we waited a long time at 2.0 K (solid $^4$He) and took measurements every hour for a total of 10 measurements at 2.0 K (we achieved 2.0 K from a higher temperature point). We checked the ‘shifted’ peaks here as analyzed before, since the ‘stable’ peaks have only a small dependence on helium inside the cell.
Table 5-12 Annealing effect on resonance frequency.

<table>
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<tr>
<th>T/ K</th>
<th>time elapsed/ min</th>
<th>f1/kHz</th>
<th>Q1</th>
<th>f2</th>
<th>Q2</th>
<th>f3</th>
<th>Q3</th>
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<td>63.9355</td>
<td>589</td>
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</tr>
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<td>63.8893</td>
<td>586</td>
</tr>
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<td>70.1277</td>
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<td>63.8692</td>
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</tr>
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<td>2596</td>
<td>70.1276</td>
<td>2121</td>
<td>63.8678</td>
<td>587</td>
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<td>69.9028</td>
<td>2584</td>
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<td>2142</td>
<td>63.8741</td>
<td>589</td>
</tr>
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<td>2.0</td>
<td>295</td>
<td>69.9142</td>
<td>2608</td>
<td>70.1467</td>
<td>2159</td>
<td>63.8856</td>
<td>588</td>
</tr>
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<td>69.9247</td>
<td>2641</td>
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<td>2135</td>
<td>63.8939</td>
<td>589</td>
</tr>
<tr>
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<td>415</td>
<td>69.9302</td>
<td>2568</td>
<td>70.1618</td>
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<td>63.8987</td>
<td>588</td>
</tr>
<tr>
<td>2.0</td>
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<td>69.9391</td>
<td>2665</td>
<td>70.1720</td>
<td>2155</td>
<td>63.9071</td>
<td>587</td>
</tr>
<tr>
<td>2.0</td>
<td>535</td>
<td>69.9426</td>
<td>2585</td>
<td>70.1757</td>
<td>2190</td>
<td>63.9109</td>
<td>585</td>
</tr>
</tbody>
</table>

Figure 5.31 Reduced resonance frequency during annealing. Horizontal axis is time in minutes.

The interesting thing here is that the frequency moves down first and then moves up instead of just changing in one direction. One good fit equation is (the red line in the Figure 5.31):

$$y = 0.9999 + 0.3472 \times \exp\left(-\frac{x}{143.7566}\right) - 0.3471 \times \exp\left(-\frac{x}{144.8473}\right)$$  (5.3)

One guess is since we got to 2.0 K from a higher temperature point, during the annealing, the stainless steel becomes harder (bulk/shear modulus increases) while solid $^4$He becomes softer.
(shear modulus decreases). Solid $^4$He and stainless steel are relaxing in different manners. This would be consistent with the experiment and calculation. We cannot check helium relaxation alone but we are able to check the relaxation process of stainless steel cell alone. The annealing data of an empty cell (Figure 5.32, from Run #4, the time=0 data is taken at 4.2 K, all the other data is taken at 2.0 K) does not support this idea. We did not replicate the annealing result of the filled cell (Figure 5.33). The annealing may depend on the thermal history.

![Figure 5.32 Annealing of an empty cell.](image)

![Figure 5.33 Annealing of the helium cell in two different runs.](image)
Even though we did not get the same annealing behavior, we can still compare the effect of annealing with the effect of temperature change. The annealing effect is much smaller than that of the temperature change (Figure 5.34, 0.1% change over 10 hours compared with 0.8% change from 1.92 K \(\rightarrow\) 1.73 K). The resonance frequency decrease of the ‘shifted’ peaks is not due to annealing. The annealing effect is too small for the frequency shift.

Figure 5.34 Annealing effect vs. temperature change effect.

The frequency shift of the shifted peaks observed in this run (~1% decrease from 2 K to 1.7 K) is consistent with our previous results. The spectrum changes a lot as in Run #1. Many peaks disappear below ~1.8 K. Even as we warm up the cell up a bit and then cool it down, these peaks still do not show up.
Experiment data Run #4

The purpose of this experiment is:

1.) Double check the annealing behavior of the cell filled with solid $^4$He.
2.) Check the annealing behavior of an empty stainless steel.
3.) Try to get a good spectrum down to 0.9 K, as for Run #2.
4.) Measure the resonance spectrum of the cell filled with superfluid liquid $^4$He, keeping temperature constant at 1.5 K and increasing the pressure from 75 psi to 375 psi with a 75 psi step size.
5.) Try a faster cool-down from 2.9 K to 2.1 K, with pressure held more constant.

Resonance frequency change

We did not get the same annealing results, but both results show that frequency change during annealing is much smaller than the frequency decrease as we lower the temperature. Many of the peaks we are interested in disappeared at some point. The quality factor of these peaks became very small (Figure 5.36). We got some of the resonance peak data, but peak fitting is not as accurate. The frequencies decrease is by about the same magnitude as before. However, the peaks do not change exactly like those in previous experiments. Some peaks have a much larger decrease than others have, see Figure 5.35.
Cell filled with superfluid $^4$He

For this experiment, the cell was filled with liquid helium at a relatively low pressure of 75 psi. We kept the temperature stable at 1.5 K and then changed the pressure from 75 psi to 375
psi with a step size of 75 psi. The resonance spectrum for the cell filled with superfluid \(^4\)He has more peaks than all the other cases. The viscosity of superfluid \(^4\)He is essentially zero. There is less ‘damping’, so less resonances have low quality factors. This may be the reason for more observable peaks. Both the liquid sound speed and density do change when we increase the liquid \(^4\)He pressure. Combined with the fact that an increase of 75 psi causes the frequencies to shift a lot, this makes it difficult to align the peaks. We fitted two groups of peaks that we believe belong to the ‘same’ modes.

Table 5-13 Resonance frequency and quality factor of superfluid helium cell at different pressure.

<table>
<thead>
<tr>
<th>Pressure (psi)</th>
<th>Frequency (kHz)</th>
<th>Quality Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>75</td>
<td>77.129</td>
<td>6654</td>
</tr>
<tr>
<td>150</td>
<td>61.5428</td>
<td>3334</td>
</tr>
<tr>
<td>225</td>
<td>67.2464</td>
<td>3409</td>
</tr>
<tr>
<td>300</td>
<td>71.4803</td>
<td>3305</td>
</tr>
<tr>
<td>375</td>
<td>75.4462</td>
<td>3263</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pressure (psi)</th>
<th>Frequency (kHz)</th>
<th>Quality Factor</th>
</tr>
</thead>
<tbody>
<tr>
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<td>375</td>
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</table>

<table>
<thead>
<tr>
<th>Pressure (psi)</th>
<th>Frequency (kHz)</th>
<th>Quality Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>86.2618</td>
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</tr>
<tr>
<td>225</td>
<td>93.8956</td>
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<td>300</td>
<td>99.4911</td>
<td>6615</td>
</tr>
<tr>
<td>375</td>
<td>105.6959</td>
<td>5005</td>
</tr>
</tbody>
</table>
We compared this data with normal sound velocity at the same temperature from [85]. They change in a similar way. Then normal sound velocity in liquid is: \( v = \sqrt{\frac{B}{\rho}} \) (I use B for bulk modulus here to avoid confusion with the stiffness matrix below). In a finite element calculation of resonance frequency: \( Ku = \omega^2 Mu \). The stiffness matrix \( K \) is ‘linear’ in elastic constants (bulk
modulus $B$ for liquid $^4\text{He}$). Mass matrix $M$ is ‘linear’ in terms of density. Accordingly resonance frequency is ‘linear’ in $\sqrt{\frac{B}{\rho}}$ and so the shift is ‘proportional’ to $\frac{B}{\sqrt{\rho}}$. The resonance frequency will change in a similar pattern like the velocity change.

![Figure 5.38 Reduced resonance frequencies of the cell filled with superfluid $^4\text{He}$. Reference data of freq2 is the frequency at 175 psi. The sound velocity vs. $P$ data is from [85].](image)
Chapter 6 Interpretation in terms of dislocation theory

Dislocation defects affect elastic properties of solid samples. Using dislocation theory, we find that the shear modulus could increase with temperature as indicated by our experimental results in our setup. Comparison with other experimental results is also discussed.

Dislocation theory

Dislocations are one-dimensional defects in crystals. They can affect the elastic properties of solids significantly and may be caused by different mechanisms. Some anomalous behavior in sound velocity and attenuation measurements of solid $^4$He samples are explained using dislocation theory, as reported in the literature [86]. Recent shear modulus measurements are also explained with dislocation theory [8, 10]; although measurements were made at much lower temperatures. We do not have enough data to quantitatively evaluate all the parameters in dislocation theory; we will just check prediction by dislocation theory qualitatively. We will use Granato-Lücke theory [87] for the analysis and check the formula used in the calculation with results in the literature [88-91] whenever possible.

In solids with dislocations, the strain is made up of two kinds, the elastic strain and a dislocation strain caused by motion of dislocations under an applied stress field [87, 88]. The apparent modulus change comes from the interaction of the dislocation line and the stress field (as in a sound wave). The interaction between the dislocation and the applied stress is related to a resonance frequency of the dislocation line (related to the length of the dislocation line) and frequency of the applied stress. The two important parameters are dislocation line length $l$ (this is the length that can bow out; if there is an impurity and the impurity can pin down dislocation lines, this would change the effective dislocation line length) and resonance frequency $\omega$. 
Depending on the length of a dislocation line, it may increase or decrease the shear modulus. The total shear modulus change is an integral of the individual contributions, considering the dislocation line distribution function. The shear modulus thus could decrease or increase from the dislocation influence. The magnitude of the change also depends on the dislocation density; a larger dislocation density would cause a larger change. Dislocation-phonon interaction depends on temperature, so modulus change also depends on temperature.

According to dislocation theory [87, 88, 91], the sound attenuation and change in elastic modulus related with one dislocation line from an applied stress is given by:

\[
(\alpha)_l = -\left(\frac{2\Lambda \rho c_0^2 b^2 l^2}{\pi^3 T}\right) \left[\frac{(1 - f_r^2)}{1 - f_r^2 + \left(\frac{f_r}{Q}\right)^2}\right], \quad (6.1)
\]

\[
(\delta)_l = \left(\frac{\Delta G}{G}\right)_l = \frac{f}{c_0} \left(\frac{2\Lambda \rho c_0^2 b^2 l^2}{\pi^2 T}\right) \left(\frac{f_r/Q}{1 - f_r^2 + \left(\frac{f_r}{Q}\right)^2}\right). \quad (6.2)
\]

\[f_r = \frac{\omega}{2\pi f_l} = f/f_i\] is a reduced frequency and \(Q = 2\pi f_i \rho_L/R_L\) is the quality factor for the damped fundamental mode for the line dislocation. \(\rho_L = \rho b^2 \frac{1}{1-\sigma}\) is the mass per unit length for a line dislocation; \(\rho\) is the mass density of the material; \(b\) is burger’s vector (\(b=0.32\) nm for solid helium in literature [92]); \(\sigma\) is Poisson’s ratio; \(T = c_{44} b^2 \frac{1}{4\pi} \left(ln\frac{2l}{b} - \frac{1}{4(1-\sigma)} - ln4 - 1\right)\) is the tension for line dislocation; \(f_l = \frac{1}{2i} \sqrt{\frac{T}{\rho_L}}\) is the fundamental natural frequency of a line dislocation of length \(l\).

\(c_0\) is the longitudinal sound velocity; \(R_L\) is the damping constant for dislocation motion and the temperature dependence of \(R_L \propto T^3\) is assumed [88]. \(\Lambda\) is the total dislocation line length per unit volume (the total dislocation line length in cm per cubic cm volume).

We assume the dislocation line is exponentially distributed with an average dislocation line length \(L\) and let
\[ P(l) = \frac{\Lambda}{L^2} \exp\left[-\frac{l}{L}\right], \quad (6.3) \]

\( P(l)dl \) is the number of dislocation loops with length between \( l \) and \( l + dl \). The total decrement and total change of elastic modulus are:

\[ \alpha = \Theta \int_0^\infty \left( \frac{\alpha_l}{\Lambda} \right) lP(l)dl; \quad (6.4) \]

\[ \delta = \frac{\Delta G}{G} = \Theta \int_0^\infty \left( \frac{\delta_l}{\Lambda} \right) lP(l)dl. \quad (6.5) \]

\( \Theta \) is an orientation factor (taken to be a constant, can be integrated into the parameter \( \Lambda \)). There is no closed form for this integration. It can be numerically integrated in a computer program. Besides the dislocation length and frequency of applied stress, another important parameter is the damping constant \( R_L \). We will assume \( R_L \propto T^3 \) following [88]. This is origin of the temperature dependence. Our experimental results will be compared with other results first in order to find the right parameters that can be used to explain our results.

**Comparison with other measurements**

Because of interest in supersolid behavior, most of recent studies of elastic phenomena in solid 4He have been undertaken in the \(~100\) mK region [7, 8, 11, 33, 93-96] on samples of low disorder, grown slowly and annealed well. Earlier sound velocity/elastic measurements [86, 88, 89, 91, 97] show the elastic modulus change of a few tenths of a percent. There has been one experiment performed on a highly disordered sample (blocked capillary method) [89]. In this experiment, the elastic modulus changed by 30%, but in the opposite direction. Our samples have high disorder and are formed in a cell with suitable dimension (~1 cm) (different from the confined geometry of other experimental setups).

We try to use dislocation theory to show that shear modulus in our setup should increase with temperature. In the fitting, there are several considerations:
1.) An attempt was made to get $G_{eff}(T = 1 \text{ K})/G_{eff}(T = 2.1 \text{ K}) \sim 0.96$ when adjusting the parameters.

2.) When modeling $\Delta G/G$, a much larger value than those in the reference [88, 91, 98] was assumed. In these references, it is used to fit just the dislocation part change, which is much smaller than the phonon part change.

3.) In the above formula, the average dislocation line length is assumed to be constant over the whole temperature range. At lower temperatures, impurities can pin down the dislocation line and thus reduces the average dislocation line length, while at higher temperatures, impurities become mobile and they no longer pin the dislocation lines. This is a temperature dependence not included in the formula. Temperature only enters the equation through $R_L \ast T^3$, which describes damping from dislocation-phonon interaction.

The fitting is done using the program dislocation.m with parameters shown in Table 6-1.

<table>
<thead>
<tr>
<th>ref.</th>
<th>disorder</th>
<th>f / kHz</th>
<th>L / µm</th>
<th>$\Theta A$ $10^9 \text{ m}^2$</th>
<th>$R_L 10^8 \text{ N s/m}^2$</th>
<th>T1 K</th>
<th>T2 K</th>
<th>$\Delta \delta$</th>
<th>$\Delta \delta_{\exp}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beamish [91]</td>
<td>low</td>
<td>3000</td>
<td>3.8</td>
<td>0.36</td>
<td>2.24$T^3$</td>
<td>0.3</td>
<td>2.5</td>
<td>0.12</td>
<td>0.13</td>
</tr>
<tr>
<td>Tsymbalenko [90]</td>
<td>low</td>
<td>80</td>
<td>100</td>
<td>0.05</td>
<td>1.1$T^1$</td>
<td>0.4</td>
<td>1.6</td>
<td>5</td>
<td>8</td>
</tr>
<tr>
<td>Iwasa [88]</td>
<td>low</td>
<td>10000</td>
<td>3.9</td>
<td>1.18</td>
<td>2.48$T^3$</td>
<td>0.7</td>
<td>1.5</td>
<td>0.14</td>
<td>0.12</td>
</tr>
<tr>
<td>Paalanen [89]</td>
<td>high</td>
<td>0.33</td>
<td>8</td>
<td>15.6</td>
<td>2.0$T^2$</td>
<td>0.04</td>
<td>1.7</td>
<td>0</td>
<td>-30</td>
</tr>
<tr>
<td>This work</td>
<td>high</td>
<td>63</td>
<td>6</td>
<td>4</td>
<td>0.6$T^3$</td>
<td>0.9</td>
<td>2.1</td>
<td>3.71</td>
<td>3.66</td>
</tr>
</tbody>
</table>

At low temperatures, helium3 impurities can pin to dislocation lines. This introduces a time lag, with a temperature dependent delay time $\tau$, and the fractional shift in modulus must be multiplied by Debye relaxation factor $[1 + (2\pi f \tau)^2]^{-1}$ [33, 94]. Low temperature measurements
[33] indicate that $\tau = \tau_0 T^{-2.75}$ with $\tau_0$ an adjustable parameter. The expression in Eq. (6.5) multiplied by this factor with $\tau_0 = 40 \text{ ns}$, was evaluated as a function of temperature for two different frequencies 8 kHz and 63 kHz. The fitting Figure 6.1 shows that the shear modulus should increase from $T=0.9 \text{ K}$ to $T=2.1 \text{ K}$ in the frequency range in our experiment.

![Figure 6.1 Reduced shear modulus vs. temperature.](image)

To summarize, we see the clear resonance frequency shift as we change the temperature. These shifted modes are affected by solid helium and they reflect the property of the solid helium inside because: 1.) These peaks do not exist when the cell is empty; 2.) These peaks are shifting in comparison to the stable empty cell peaks. Solid helium is very compliant compared with steel. However, the pressure inside the cell to maintain a solid $^4\text{He}$ state is very high (~4 MPa for solid helium inside), and deformation of the helium inside has a measurable effect on the stainless steel.
Summary

As discussed in the introduction, the possible observation of a supersolid state in 4He is one of the most exciting events in condensed matter physics. After considerable research, it has become clear that the effect involves disorder in the solid (which could be in the form of vacancies, grain boundaries, glassy regions or dislocations), involves the relation between disorder and the elastic properties of the solid, and furthermore involves the interaction of 3He impurities with the disorder. The goal of this thesis has been to add further knowledge concerning the elastic behavior of hcp solid 4He. Some particular goals include:

1.) Use resonant ultrasound spectroscopy to determine hcp solid helium elastic constants in a cell which is essentially the same as cells used in torsional oscillator measurements on supersolid helium. Indeed, the cell could be used to make simultaneous RUS and TO measurements.

2.) Develop a cell which could be cycled in temperature (between room temperature and helium temperatures) and in pressure (from saturated liquid pressures to solid helium pressures) with minimal changes in its basic RUS spectrum.

3.) Try to make a connection between the temperature dependence of the solid helium elastic behavior and the dislocation model of solid helium.

As discussed in the thesis, the RUS method actually exceeded expectations, in that the transducers external to the cell were able to detect normal modes for which most of the motion were confined to the solid helium inside the stainless steel cell. Other modes which involved mostly motion of the stainless steel cell were very robust, virtually the same in every experimental run; and these modes also reflected the influence of the solid helium inside the cell. Finally, the basic temperature dependence of the elastic behavior of the solid helium was found to
support the dislocation model, with parameters which were consistent with those found in lower temperature measurements.

To summarize the results of this experimental thesis research, all of the goals of the project were met with some success.
Appendix

Calculation programs

The programs used for calculation are listed here. Some parameters need to be changed for specific situations.

1. RitzString.m

This is the program used in Chapter 1 to calculate the resonance of a string using Raleigh-Ritz method. This is a script, not a function.

clear all;
clc;
clf;
N=20;       % trial and error shows (N,A) working pair (20,1)
A=1;        % for N=20, M is not too small, A can be chosen value 1
K=zeros(N,N);  % (30,10e11) (50,10e12) (100,10e14) (230,10e15)
M=zeros(N,N);  % pre-allocation
% density*w^2*M*u=tension*K*u
for n=1:N
    for m=1:N
        K(m,n)=(m-1)*(n-1)/(m+n-3); % basis function {1,x,x^2, ... x^(N-1)}
        M(m,n)=A/(m+n-1); % basis function {1,x,x^2, ... x^(N-1)}
    end
    % for basis function {x,x^2, ... x^N}
end
    % (m->m+1) (n->n+1) in the formula;
d=det(M);                 % as N increase, det(M) decreases fast,
K(1,2)=0;                 % use A to modify the number, so Matlab
K(2,1)=0;                 % can handle with right precision.
[V,D]=eig(K,M);

[lambda,ix]=sort(A*(diag(D))/pi^2); % sort eigenvalue in ascending order
V(:,ix)=V(:,ix);
% rearrange eigenvectors to match up with sorted eigenvalues
%V=V./repmat(V(1,:),N,1);
x=0:0.01:1;   % plot approximate eigenvectors
for mm=1:10
    p=polyval(fliplr(V(:,mm)),x);
    p=p/max(abs(p)); % normalize amplitude
    subplot(5,2,mm);
    plot(x,p,'r+','MarkerSize',2);
    hold on
    plot(x,sign(p(1))*cos(round(sqrt(abs(lambda(mm))))*pi*x));
text(1,0.85, ['$\omega^2/\pi^2=', num2str(lambda(mm))],'FontSize',8,...
    'HorizontalAlignment','right'); %'Color','r');
plot([0,1],[0,0],'k');
%xlabel('x');
ylabel('Amplitude');
%axis([-0.1,1.1,-1.1,1.1]);

end
legend('Ritz approximation','exact solution with closest eigenvalue',...'Location','NorthEastOutside');
This program checks the approximation error of Ritz method depending on different trial vectors.

clear all;
clc;
N=10000;  % # of elements, unit length is divided to N parts
A=0.27;   % (N,A)=(10000,0.27)
NM=10;   % # of modes to calculate
NT=20;   % # of trial vectors, must be larger than NM
a=vertcat((1:N)',(1:(N-1))',(2:N)');
% row index for mass/stiffness(sparse) matrix
b=vertcat((1:N)',(2:N)',(1:(N-1))'); % column index for sparse matrix
%
% M in the format(open end case)
% (for fixed end Boundary Conditions delete first/last row/column):
% [ 2 1 0 0 0 0 ... 0 0 0
% 1 4 1 0 0 ... 0 0 0 0 0
% 0 1 4 1 0 ... 0 0 0 0 0
% 0 0 1 4 1 0 ... 0 0 0 0
% ... ... ... ... ......
% 0 0 ... 0 1 4 1 0 0
% 0 0 ... 0 0 0 1 4 1
% 0 0 ... 0 0 0 0 1 2]

K: same as above format, change (2->1) (1->-1) (4->2)
%
K=6*N^2*K;   % normalize string length to 1;
M=A*M;
dM=det(M);
[v,d]=eigs(K+M,M,NM,2); % shift eigen value by 1; since K is singular
[f,ix]=sort(A*(diag(d)-1)/pi^2); % sort eigenvalue in ascending order
% and shift eigenvalue to
v(:,:)=v(:,ix);
% rearrange eigenvectors to match up with sorted eigenvalues
v=v./repmat(max(v(:,:,)),N,1);
sv=sign(v(1,:));
v=v.*repmat(sv,N,1);
%
% following codes test influence of choice of trial vectors on small
% eigenvalue approximation. Ritz method, matrix size reduction
switch choice
    case 1

c = rand(N, NT);  % choice 1: random trial vectors

case 2
  c = rand(N, NT);
  c = (K + M) \ c;
  % choice 2: improved trial vectors, no problem for
  % fixed end BC, since 0 is not eigenvalue, but for free
  % open end BC, K is singular, cannot get inverse.

case 3
  x = linspace(0, 1, N)';
  % choice 3: trial vectors chosen as [1, x, x^2 ... x^(N-1)]
  c = zeros(N, NT);
  for clm = 1:NT
    c(:, clm) = 20e1 * x.(clm - 1);
    % 20e1 is used to modify c'*M*c, so all the value are in the
    % range Matlab can handle
  end

otherwise
  disp('error, choice not 1, 2 or 3');
end

[v2, d2] = eig(c'*(K+M)*c, c'*M*c);
% c'*M*c is not sparse anymore and for whatever the reason the result of
% eigs is not stable.

dm2 = det(c'*M*c);
dkm2 = det(c'*(K+M)*c);

[ff, ix2] = sort(((d2-1) * A / pi^2);

v2(:, :) = v2(:, ix2);

v2 = c'*v2;
% transform back to eigenvector of original problem
v2 = v2./repmat(max(abs(v2(:, :))), N, 1);  % normalize eigenvector

sv2 = sign(v2(1, :));
v2 = v2.*repmat(sv2, N, 1);

clf;

% following is drawing graphs for different cases.
for mm = 1:10
  subplot(5, 2, mm);
  if (choice == 1)
    plot(linspace(0, 1, N), v2(:, mm), 'r+', 'MarkerSize', 0.8);
  else
    plot(linspace(0, 1, N), v2(:, mm), 'r+', 'MarkerSize', 1.2);
  end;

  hold on
  if (choice == 3)
    if (round(sqrt(abs(ff(mm)))) < 10)
      plot(linspace(0, 1, N), v(:, 1 + round(sqrt(abs(ff(mm)))));
    end;
  else if (choice == 1)
    plot(linspace(0, 1, N), v(:, mm));
  end;
end;

plot([0, 1], [0, 0], 'k');
ylabel('Amplitude');

if ((mm == 1) || (mm == 2))
  axis([0, 1, -1, 1.1]);
else
    axis([0,1,-1,1]);
end;
switch choice
    case 1
        legend('Ritz approximation, random trial vector', ...
               'Location','NorthEastOutside');
    case 2
        legend('Ritz approximation, \(\mathbf{K}^{-1}\)\*random trial vector', ...
               'exact solution with closest eigenvalue', ...
               'Location','NorthEastOutside');
    case 3
        legend('Ritz approximation, \(1,x,x^2,...\) trial vector', ...
               'exact solution with closest eigenvalue', ...
               'Location','NorthEastOutside');
end
This program is used to get analytical solution of some special resonance modes of isotropic sphere.

```matlab
format long
mu=0.4;
lambda=0.3;
k=sqrt(mu/(mu*2+lambda));
n=1;
fs0=@(x) x*besselj(0.5,x)*(lambda+2*mu)/(4*mu)-besselj(1.5,x);

fsn=@(x) 2*k*(1/x + ((n-1)*(n+2)/x^2)*(besselj(n+1.5,x)/... 
    besselj(n+0.5,x)-(n+1)/x))*besselj(n+1.5,k*x)...
    +(-0.5+(n-1)*(2*n+1)/x^2 + (1/x)*(1-2*n*(n-1)*(n+2)/x^2)...
    *besselj(n+1.5,x)/besselj(n+0.5,x))*besselj(n+0.5,k*x); 
ftn=@(x) (n-1)*besselj(n+0.5,x)-x*besselj(n+1.5,x);

rs0=zeros(5,1);
rsn=zeros(5,1);
rtn=zeros(5,1);

for ii=1:5
    rs0(ii)=fzero(fs0,0.5*ii+2)*sqrt((lambda+2*mu)/mu);
    rsn(ii)=fzero(fsn,0.5*ii+6);
    rtn(ii)=fzero(ftn,ii+3);
end
disp(n);
disp(rsn);
disp(rtn);
```
4. QuadTetraModeT1.m

This program is used to calculate resonance modes, using quadratic tetrahedron element mesh, calling subfunction KM.m which itself calls subfunction elementKM.m.

```matlab
function [freq,v] = QuadTetraModeT1(femdata,n0,k0,smode)
% ----------------------------------------------------------------------
% calculate resonance modes of an object.
% input:
% files needed: mesh data file and the material data file.
% femdata is the file name of the mesh data file without extension
% of the file.
% if smode==1, emports mode file (used for animation), otherwise not.
% n0 is the number of modes to calculate, default value is 20.
% k0 is the frequency close to the frequency of interested modes, in kHz.
% default value is 20 (kHz).
% For a femtest.txt mesh data file calculate 25 eigenfrequency around 30
% kHz and export the mode file, command is:
% QuadTetraModeT1('femtest',25,30,1);
% This function calls function 'KM' which itself calls function
% 'elementKM', these two function needs to be in the same file folder or
% the codes is listed in this file.
% the femdata.txt file is generated in by GID
% software, or as long as the mesh data file is in format:
%=======================================================================
% Coordinates
% 1 0.29489 -0.45886 3.41225
% 2 0.28003 -0.46807 3.37962
% end coordinates
% Elements
% 1 19528 19586 19458 18518 19549 19523 19501 18993 19016 18960
% 2 7973 7408 8083 7133 7677 7723 8026 7539 7270 7579
% end elements
%=======================================================================
% The first line is ignored in importing the data, like 'Coordinates' in
% the file generated by GID is ignored. From the second line, they are
% nodes number followed by coordinates of the nodes. Two lines following
% the ends of the nodes coordinates list are ignored. Then there are the
% connectivity table, containing elements number, nodes in the element,
% and material of the element, index of the material follows the order in
% the material property file below. When calculating the stiffness/mass
% matrix, first column (nodes # or element #) is deleted first.
% There must be a file containing the material property with file name
% femdata_material.txt in the format:
%=======================================================================
% Rho C11 C22 C33 C44 C55 C66 C23 C31 C12 [g/cm^3, 100GPa]
% 8.000 2.613 2.613 2.613 0.773 0.773 0.773 1.067 1.067 1.067
% 8.940 2.027 2.027 2.027 0.479 0.479 0.479 1.069 1.069 1.069
%=======================================================================
% output: [freq,v], v is the eigenmodes vector, freq is the eigenfrequency.
% two text files containing v and freq are written out separately with file
```
tic; % time counting
if nargin == 1
    n0 = 20;
    k0 = 20;
    smode = 0;
end
if nargin == 2
    k0 = 20;
    smode = 0;
end

% set default values

M = importdata(fullfile(femdata, '.txt'),' ',1);
% import mesh data file, CO is coordinate data. CN is connectivity table.
CO = M.data;
CO(:,1) = [];
% delete first column, nodes #.
M = importdata(fullfile(femdata, '_material.txt'),' ',size(CO,1)+3);
CN = M.data;
CN(:,1) = [];
% delete first column, element #.

M = importdata(fullfile(femdata, '_material.txt'),' ',l);
% import material property file
El = M.data;
density = 1000*El(:,1);
clear M;

E = cell(size(density,1),1);
for nm = 1:size(density,1)
    E{nm} = 10^11*blkdiag([El(nm,2) El(nm,10) El(nm,9);
                          El(nm,10) El(nm,3) El(nm,8);
                          El(nm,9) El(nm,8) El(nm,4)],...
                          El(nm,5),El(nm,6),El(nm,7));
end
% elastic tensor.
clear El;

load Gausspoints.txt;
% Guass integral points
CO(:, :) = CO(:, :)/100;
% change size of object, meter or centimeter.

Row = zeros(900*size(CN,1),1);
Col = zeros(900*size(CN,1),1);
% creat row/column index for the assembly (global) matrix, for each element
% it is a 30*30 matrix, 900 elements in total, using a column vector.
MAD = zeros(900*size(CN,1),1);
MBD = zeros(900*size(CN,1),1);
% MAD: matrix A(stiffness) data; MBD: matrix B(mass) data.

NN = size(CO,1);
% # of nodes
L = size(CN,2)-1;
% # nodes of each tetrahedron element
for j = 1:size(CN,1)
% loop over tetra elements; j is not complex number j.
    [K,M] = KM(CO(CN(j,1:L),:),Gausspoints,E{CN(j,L+1)},
               density(CN(j,L+1))); 
    Row(900*(j-1)+1:900*j) = kron([3*(CN(j,1:L)-1)+1,3*(CN(j,1:L)-1)+2,...
                                    3*(CN(j,1:L)-1)+3],ones(1,30));
    Col(900*(j-1)+1:900*j) = repmat([3*(CN(j,1:L)-1)+1,...
                                    3*(CN(j,1:L)-1)+2,3*(CN(j,1:L)-1)+3],1,30);
    MAD(900*(j-1)+1:900*j) = reshape(K,1,900);
    MBD(900*(j-1)+1:900*j) = reshape(blkdiag(M,M,M),1,900);
end
A = sparse(Row,Col,MAD,3*NN,3*NN);
BM = sparse(Row,Col,MBD,3*NN,3*NN);
[v2 d] = eigs(A,BM,n0,(2*pi*k0*1000)^2);
freq = sqrt(sort(diag(d)))/(2*pi);
 [~, IX] = sort(diag(d));
% order frequency and get the order index: IX.
inum = 0;
im = 1;
while abs(freq(im))<10
    im = im+1;
    inum = inum+1;
end
% find the rigid modes, rigid modes' eigenvector is close to 0.
v = v2(:,IX);
% reording the eigenvector using order index IX.
v(:,1:inum) = [];
v = v./repmat(sqrt(diag(v'*BM*v')),3*NN,1);
% normalize eigenvector with respect to mass matrix BM;
disp(freq);
% display freqs in matlab command window, this includes the 6 rigid mode,
% if the 6 modes is among the calculated results.
dlmwrite([femdata '_freqAround' num2str(k0) 'KHz.txt'],freq(inum+1:n0),...
    'delimiter', ' ', 'precision', '%.6f');
% export freqs data to text file, does not include the 6 rigid mode.
if(smode == 1)
    dlmwrite([femdata '_modeAround' num2str(k0) 'KHz.txt'],v,' ');
% export mode data to text file, this is used for animation.
end
toc;
function [K,M] = KM(X,P,El,rho)
% calculates element stiffness and mass matrix,
% X is coordinates of the 10 nodes of the tetrahedron,
% size is 10*3, in format [x1-x10,y1-y10,z1-z10];
% P is Gauss integral points data, size 4*10, the first three data
% are coordinates of integral points, the fourth is weight, 10 Gauss
% points in total; E is elastic tensor, size 6*6.
% output: [K,M], K/M is element stiffness/mass matrix.
% This function calls function 'elementKM', which calculates contribution
% to the element matrix at each Gauss point.
K = zeros(30,30); % element stiffness matrix
M = zeros(10,10); % element mass matrix
for i = 1:size(P,1)
% loop over Gauss integral points
[K2, M2] = elementKM(X,P(i,1:3),El);
K = K+K2*P(i,4);
M = M+M2*P(i,4)*rho;
enend
function [K2,M2] = elementKM(X,zt,El)
% calculates stiffness and mass matrix contribution at one Gauss points,
% X same as above explanation, zt is Gauss points data (natural
% coordinates), in format: [zt(1), zt(2), zt(3)]; E is 6*6 elastic tensor.
% ND is derivative of shape function w.r.t natural coordinates
% [zt(1), zt(2), zt(3)], ND = DN/Dzt, 10 shape functions: [N1, ..., N10]',
% ND(ij) = dN(i)/dzt(j), ND size 10*3.
ND = [4*zt(1) - 1, 0, 0;...
      0, 4*zt(2) - 1, 0;...
      0, 0, 4*zt(3) - 1;...
      4*zt(1) + 4*zt(2) + 4*zt(3) - 3, 4*zt(1) + 4*zt(2) + 4*zt(3) - 3,...
      4*zt(1) + 4*zt(2) + 4*zt(3) - 3;...
      4*zt(1), 4*zt(2) - 1, 0;...
      0, 4*zt(3), 4*zt(2);...
      4*zt(3), 0, 4*zt(1);...
      4 - 4*zt(2) - 4*zt(3) - 8*zt(1), -4*zt(1), -4*zt(1);...
      -4*zt(2), 4 - 8*zt(2) - 4*zt(3) - 4*zt(1), -4*zt(2);...
      -4*zt(3), -4*zt(3), 4 - 4*zt(2) - 8*zt(3) - 4*zt(1)];

J3 = X' * ND;
% J3 is jacobian matrix: DX/Dz = D(X0'*N)/Dzt = X0'*DN/Dzt = X0'*ND;
Q = ND / J3;
B = zeros(6,30);

B(1,1:10) = Q(:,1);'
B(2,11:20) = Q(:,2);'
B(3,21:30) = Q(:,3);'
B(4,1:10) = Q(:,2);'
B(4,11:20) = Q(:,1);'
B(5,11:20) = Q(:,3);'
B(5,21:30) = Q(:,2);'
B(6,1:10) = Q(:,3);'
B(6,21:30) = Q(:,1);'

K2 = B' * El * B * abs(det(J3));
% absolute value is necessary, the jacobian matrix is not always positive;
N = [ zt(1)*(2*zt(1) - 1), zt(2)*(2*zt(2) - 1), zt(3)*(2*zt(3) - 1),...
      (zt(1) + zt(2) + zt(3) - 1)*(2*zt(1) + 2*zt(2) + 2*zt(3) - 1), ...
      4*zt(1)*zt(2), 4*zt(2)*zt(3), 4*zt(1)*zt(3), ...
      -4*zt(1)*(zt(1)+zt(2)+zt(3) - 1), ...]
      -4*zt(2)*(zt(1)+zt(2)+zt(3) - 1), ...]
      -4*zt(3)*(zt(1)+zt(2)+zt(3) - 1)];

M2 = N.' * N * abs(det(J3));
This program calculates resonance modes using linear tetrahedron element. If the input mesh file is 10-node quadratic tetrahedron, this program converts it to linear tetrahedron. If the input mesh file is already linear tetrahedron, then do the calculation using linear tetrahedron directly. This function calls subfunction KMlinearTetra.m.

```matlab
function [freq,v] = linearorQTetraT2(femdata,n0,k0, smode)
% This program is used to compare accuracy of quadratic and linear
tetrahedron element.
% if mesh data is quadratic tetrahedron, changes it to linear tetrahedron,
each quadratic element is divided into 8 small linear tetrahedron
% elements, if it is already linear tetrahedron, then no change to mesh
data.
% mesh data file: femdat.dat
% material file: femdat_material.dat
% command format:
% linearorQTetraT2('femdat',20,20,0);
% smode = 1 exports eigenvector.
% output femdata_freqL2QAroundk0KHz.txt, femdata_modeL2QAroundk0KHz.txt

tic;                        % time counting begins
if nargin == 1
    n0 = 20;
    k0 = 20;
    smode = 0;
end
if nargin == 2
    k0 = 20;
    smode = 0;
end

M = importdata([femdata '.txt'],',',1);
% import mesh data file
COlt = M.data;
COlt(:,1) = [];
% delete first column, node index.
M = importdata([femdata '.txt'],',',size(COlt,1)+3);
CN1 = M.data;
CN1(:,1) = [];
% delete first column, element index.
if size(CN1,2) == 11
    CN1t = [CN1(:,1) CN1(:,5) CN1(:,7) CN1(:,8) CN1(:,11);
            CN1(:,2) CN1(:,6) CN1(:,5) CN1(:,9) CN1(:,11);
            CN1(:,3) CN1(:,7) CN1(:,6) CN1(:,10) CN1(:,11);
            CN1(:,8) CN1(:,9) CN1(:,10) CN1(:,4) CN1(:,11);
            CN1(:,5) CN1(:,6) CN1(:,8) CN1(:,9) CN1(:,11);
            CN1(:,6) CN1(:,10) CN1(:,8) CN1(:,9) CN1(:,11);
            CN1(:,6) CN1(:,7) CN1(:,5) CN1(:,8) CN1(:,11)];
    % above is a different of of dividing a quadratic tetrahedron element
```

5. linearorQTetraT2.m
% to linear tetrahedron element.
CNlt = [CN1(:,1) CN1(:,5) CN1(:,7) CN1(:,8) CN1(:,11); 
CN1(:,2) CN1(:,6) CN1(:,5) CN1(:,9) CN1(:,11); 
CN1(:,3) CN1(:,7) CN1(:,6) CN1(:,10) CN1(:,11); 
CN1(:,8) CN1(:,9) CN1(:,10) CN1(:,4) CN1(:,11); 
CN1(:,5) CN1(:,6) CN1(:,7) CN1(:,9) CN1(:,11); 
CN1(:,6) CN1(:,10) CN1(:,7) CN1(:,9) CN1(:,11); 
CN1(:,10) CN1(:,8) CN1(:,7) CN1(:,9) CN1(:,11); 
CN1(:,5) CN1(:,7) CN1(:,8) CN1(:,9) CN1(:,11)];
else
CNlt = CN1;
end

M = importdata([femdata ' _material.txt' ],',1);
% import material property file
El = M.data;
density = 1000*El(:,1);
clear M;
for nm = 1:size(density,1)
    E{nm} = 10^11*blkdiag([El(nm,2) El(nm,10) El(nm,9); 
    El(nm,10) El(nm,3) El(nm,8); 
    El(nm,9) El(nm,8) El(nm,4)],[... 
    El(nm,5),El(nm,6),El(nm,7)];
end
clear El;

COlt(:, :) = COlt(:, :)/100;
% change size of object, meter or centimeter
Row = zeros(144*size(CNlt,1),1);
Col = zeros(144*size(CNlt,1),1);
% creat row index for the assembled matrix, for each element
% it is 12*12 matrix, 144 entities in the matrix in total,
MAD = zeros(144*size(CNlt,1),1);
MBD = zeros(144*size(CNlt,1),1);
% MAD: matrix A(stiffness) data; MBD: matrix B(mass) data.

NN = size(COlt,1);         % # of nodes
L = size(CNlt,2)-1;        % # of tetrahedron elements
for k = 1:size(CNlt,1)
% loop over tetra elements, build up stiffness and mass matrix data;
% do not confuse this j with the complex number j.
    [Klt,Mlt] = KMlinearTetra(COlt(CNlt(k,1:L),:),E{CNlt(k,L+1)},... 
    density(CNlt(k,L+1)));

    Row(144*(k-1)+1:144*k) = kron([3*(CNlt(k,1:L)-1)+1,... 
    3*(CNlt(k,1:L)-1)+2,3*(CNlt(k,1:L)-1)+3],ones(1,12));
    Col(144*(k-1)+1:144*k) = repmat([3*(CNlt(k,1:L)-1)+1,... 
    3*(CNlt(k,1:L)-1)+2,3*(CNlt(k,1:L)-1)+3],1,12);

    MAD(144*(k-1)+1:144*k) = reshape(Klt,1,144);
    MBD(144*(k-1)+1:144*k) = reshape(blkdiag(Mlt,Mlt,Mlt),1,144);
end
A = sparse(Row,Col,MAD,3*NN,3*NN);
BM = sparse(Row,Col,MBD,3*NN,3*NN);
[v,d] = eigs(A,BM,n0,(2*pi*k0*1000)^2);
[freq, IX] = sort(diag(d));
freq = sqrt(freq)/(2*pi);

inum = 0;
im = 1;
while abs(freq(im))<10
    im = im+1;
inum = inum+1;
end
v = v(:,IX);
v(:,1:inum) = [];
v = v./repmat(sqrt(diag(v'*BM*v')),3*NN,1);
% normalize eigenvector with respect to mass matrix BM;
disp(freq); % display freqs in matlab command window
dlmwrite([femdata ' freqL2QAround' num2str(k0) 'KHz.txt'],...
    freq(inum+1:n0),'delimiter',' ','precision', '%.6f');
% export freqs data to text file
if(smode == 1)
    dlmwrite([femdata ' modeL2QAround' num2str(k0) 'KHz.txt'],v,' ');
    % export mode data to text file
end
toc;
end
function [Klt,Mlt] = KMlinearTetra(X,El,rho)

% calculates element stiffness and mass matrix of linear tetrahedron
% element.
% X is coordinates of the 4 nodes of the linear tetrahedron,
% size is 4*3, in format [x1, y1, z1; ... ; x4, y4, z4];
% E is elastic tensor, size 6*6.
% exports element stiffness matrix Klt size 12*12,
% element mass matrix Mlt size 4*4;
T = [1 1 1 1;X'];
V = 1/6*abs(det(T));
Q = 6*V*eye(4)/T;

a1 = Q(1,2); b1 = Q(1,3); c1 = Q(1,4);
a2 = Q(2,2); b2 = Q(2,3); c2 = Q(2,4);
a3 = Q(3,2); b3 = Q(3,3); c3 = Q(3,4);
a4 = Q(4,2); b4 = Q(4,3); c4 = Q(4,4);

B = 1/(6*V)*[a1 a2 a3 a4 0 0 0 0 0 0 0 0;
0 0 0 0 b1 b2 b3 b4 0 0 0 0;
0 0 0 0 0 0 0 0 c1 c2 c3 c4;
0 0 0 0 b1 b2 b3 b4 a1 a2 a3 a4 0 0 0 0;
0 0 0 0 c1 c2 c3 c4 b1 b2 b3 b4;
c1 c2 c3 c4 0 0 0 0 a1 a2 a3 a4];
Klt = V*B'*El*B;
Mlt = rho*V/20*[ 2 1 1 1;
1 2 1 1;
1 1 2 1;
1 1 1 2];
end
6. QuadTetra2Mode.m

This one is used to calculate normal modes of an empty cell, with a filled cell meshing data.

```matlab
function [freq2,v2]=QuadTetra2Mode(femdata,n2,k2,smode)
% calculates resonance frequency and mode when some of the material
% property are set to zero. The material that is set to zero should be
% material 2, and the material in contact with material 2 is material 1 and
% only material 1. femdata is mesh file and corresponding material file.
% n2 is total number of modes to calculate, k2 is the frequency interested
% in, if smode=1, the eigenvector file will be written in a file.

tic;
if nargin == 1
    n2=30;
    k2=30;
    smode=0;
end
if nargin == 2
    k2=30;
    smode=0;
end
if nargin==3
    smode=1;
end
M=importdata([femdata '.txt'],',1); % import mesh data file
CO=M.data;
CO(:,1) = [];  % delete first column, node index
M=importdata([femdata '.txt'],',size(CO,1)+3);
CN=M.data;
CN(:,1) = [];  % delete first column, element index
M=importdata([femdata '_2material.txt'],',1);
% import material property file
El=M.data;
density=1000*El(:,1);
clear M;
for nm=1:size(density,1)
    c12 = El(nm,2)-2*El(nm,3);
    E{nm}=10^11*blkdiag([El(nm,2),   c12,        c12;
                         c12,        El(nm,2),   c12;
                         c12,        c12,        El(nm,2)],...
                       El(nm,3),El(nm,3),El(nm,3));
    %
    % E{nm}=10^11*blkdiag([El(nm,2) El(nm,10) El(nm,9);
    %                      El(nm,10) El(nm,3) El(nm,8);
    %                      El(nm,9) El(nm,8) El(nm,4)],...
    %                      El(nm,5),El(nm,6),El(nm,7));
    %
end
clear El;
load Gausspoints.txt;
CO(:, :) = CO(:, :)/100;
% change size of object, meter or centimeter
```
Row = zeros(900*size(CN,1),1);
Col = zeros(900*size(CN,1),1);

% creat row index for the assembled matrix, for each element it is 30*30
% matrix, 900 elements in total, use a column vector to speed up
% calculation following Matlab advice.
MAD = zeros(900*size(CN,1),1);
MBD = zeros(900*size(CN,1),1);

% MAD: matrix A(stiffness) data; MBD: matrix B(mass) data.
NN = size(CO,1);
% # of nodes
L = size(CN,2)-1;
% nodes of each tetrahedron element

for j = 1:size(CN,1)
    % loop over tetra elements; j is not complex number j.
    if density(CN(j,L+1))~=0 && sum(sum(E{CN(j,L+1)}))~=0
        [K,M] = KM(CO(CN(j,1:L),:),Gausspoints,E{CN(j,L+1)},
density(CN(j,L+1)));
        Row(900*(j-1)+1:900*j) = kron([3*(CN(j,1:L)-1)+1,
            3*(CN(j,1:L)-1)+2,3*(CN(j,1:L)-1)+3],ones(1,30));
        Col(900*(j-1)+1:900*j) = repmat([3*(CN(j,1:L)-1)+1,
            3*(CN(j,1:L)-1)+2,3*(CN(j,1:L)-1)+3],1,30);
        MAD(900*(j-1)+1:900*j) = reshape(K,1,900);
        MBD(900*(j-1)+1:900*j) = reshape(blkdiag(M,M,M),1,900);
    end
end;
c=(Row==0);
Row(c)=[];
Col(c)=[];
MAD(c)=[];
MBD(c)=[];

A = sparse(Row,Col,MAD,3*NN,3*NN);
BM = sparse(Row,Col,MBD,3*NN,3*NN);

for i=1:size(density,1)
    nodes{i}=[];
end
for i=1:size(CN,1)
    nodes(CN(i,L+1))= union(nodes(CN(i,L+1)),CN(i,1:L));
end

nodes0=1:3*size(CO,1);
c=intersect(nodes{1},nodes{2});
c2=setdiff(nodes{2},c);
p2=[3*(c2-1)+1 3*(c2-1)+2 3*(c2-1)+3];
pl=setdiff(nodes0,p2);

% find all the 'empty' node
At=A(pl,pl);
BMt=BM(pl,pl);

if smode == 1
    [vt,d2]=eigs(At,BMt,n2,(2*pi*k2*1000)^2);
    [~, IX]=sort(diag(d2));
    ffreq2=sqrt(sort(diag(d2)))/(2*pi);
inum = 0;
im = 1;
while abs(freq2(im))<10
    im=im+1;
    inum=inum+1;
end
v=vt(:,IX);
v(:,1:inum) = [];

v = v./repmat(sqrt(diag(v'*BMt*v')) , size(p1,2),1);
% normalize eigenvector with respect to mass matrix BM; does not work if
% there is zero eigenvalues;
v2=zeros(3*size(CO,1),n2-inum);
for i=1:(n2-inum)
    v2(p1,i)=v(:,i);
end;
% 'distribute' the cropped eigenvector into the original eigenvector,
% the exported eigenvector is of the full size, so it can can compared
% with real cell filled with Helium.

disp(freq2);
dlmwrite([femdata '_'freq2Around' num2str(k2)
'KHz.txt' ],freq2(inum+1:n2)/10^6,...
'delimiter',' ','precision', '.7f');
% export mode data to text file
dlmwrite([femdata '_'mode2Around' num2str(k2) 'KHz.txt' ],v2,' ');
% vector for mode image
dlmwrite([vdotR' femdata '_'mode2Around' num2str(k2) 'KHz.txt' ],...
BM*v2,' ');
% vector for comparing with full cell.
else
    d2=eigs(At,BMt,n2,(2*pi*k2*1000)^2);
    freq2=sqrt(sort(d2))/(2*pi);
    disp(freq2);

    inum = 0;
    im = 1;
while abs(freq2(im))<10
    im=im+1;
    inum=inum+1;
end
dlmwrite([femdata '_'freq2Around' num2str(k2)
'KHz.txt' ],freq2(inum+1:n2)/10^6,...
'delimiter',' ','precision', '.7f');
end
toc;
7. QuadTetraModeT1Parallel.m

This is based on QuadTetraModeT1.m, modified using parfor (parallel for loop) in loop calculating element stiffness matrix. In order to used parfor, Parallel Computing Toolbox needs to be installed. Otherwise, ordinary for loop is used. This function calls subfunction KM.m and KMelement.m (not listed here, need to include these two codes at the end of the file, or subfunction and primary function need to be in the same folder.

```matlab
function [freq,v] = QuadTetraModeT1Parallel(femdata,n0,k0,smode)
% ----------------------------------------------------------------------
% QuadTetraModeT1.m modified to use parfor (parallel for loop).
% tic;
if nargin == 1
    n0 = 20;
    k0 = 20;
    smode = 0;
end
if nargin == 2
    k0 = 20;
    smode = 0;
end
M = importdata([femdata '.txt'],' ',1);
CO = M.data;
CO(:,1) = [];
% delete first column, # of elements
M = importdata([femdata '.txt'],' ',size(CO,1)+3);
CN = M.data;
CN(:,1) = [];
% delete first column, # of the nodes
M = importdata([femdata '_isomaterial.txt'],' ',1);
El = M.data;
density = 1000*El(:,1);
clear M;
E = cell(size(density,1),1);
for nm = 1:size(density,1)
    c12 = El(nm,2)-2*El(nm,3);
    E{nm}=10^11*blkdiag([El(nm,2), c12, c12;
                         c12, El(nm,2), c12;
                         c12, c12, El(nm,2)],...
                             El(nm,3),El(nm,3),El(nm,3));
end
clear El;
Gausspoints=importdata('Gausspoints.txt','
Row=[];
Col=[];
MAD=[];
MBD=[];
NN = size(CO,1);
L = size(CN,2)-1;
```
CN1=CN(:,1:L);
CO1=cell(1,size(CN,1));
E1=cell(size(CN,1),1);
density1=zeros(size(CN,1),1);
for j = 1:size(CN,1)
    CO1{j} = CO(CN(j,1:L),:);
    E1{j} = E{CN(j,L+1)};
    density1(j) = density(CN(j,L+1));
end
parfor j = 1:size(CN,1)
    % loop over tetra elements; j is not complex number j.
    [K,M] = KM(CO1{j},Gausspoints,E1{j},
                density1(j));
    Row = [Row, kron([3*(CN1(j,:)-1)+1,
                     3*(CN1(j,:)-1)+2,3*(CN1(j,:)-1)+3],ones(1,30))];
    Col = [Col, repmat([3*(CN1(j,:)-1)+1,
                        3*(CN1(j,:)-1)+2,3*(CN1(j,:)-1)+3],1,30)];
    MAD = [MAD, reshape(K,1,900)];
    MBD = [MBD, reshape(blkdiag(M,M,M),1,900)];
end
A = sparse(Row,Col,MAD,3*NN,3*NN);
BM = sparse(Row,Col,MBD,3*NN,3*NN);
[v2 d] = eigs(A,BM,n0,(2*pi*k0*1000)^2);
freq = sqrt(sort(diag(d)))/(2*pi);
[~, IX] = sort(diag(d));
inum = 0;
im = 1;
while abs(freq(im))<10
    im = im+1;
    inum = inum+1;
end
v = v2(:,IX);
v(:,1:inum) = [];
v = v./repmat(sqrt(diag(v'*BM*v'))',3*NN,1);
% normalize eigenvector with respect to mass matrix BM;
disp(freq);
dlmwrite([femdata '_freqLAround' num2str(k0) 'KHz.txt'],
        freq(inum+1:n0)/10^3, 'delimiter', ' ', 'precision', '%.7f');
if(smode == 1)
    dlmwrite([femdata '_modeLAround' num2str(k0) 'KHz.txt'],v,' ');
    % export mode data to text file
    % dlmwrite(['vdotR' femdata '_modeSAround'
    %    num2str(k0) 'KHz.txt'],BM*v,' ');
    % this 'normalized' mode file is used in similarity calculation,
    % ModeFinder.m
end
toc;
8. postQTModeImageT3.m

This program is used to show resonant mode image. It can be linear or quadratic mesh.

```
function postQTModeImageT3(femdata,Afreq)
% show resonance modes image of femdata file.
% files needed: mesh data file and output file from program
% 'QuadTetraModeT1.m', with file name 'femdat_modeAroundk0KHz.txt'
% for example, the following command will show the modes around 20KHz
% frequency from output of 'QuadTetraModeT1(femdata,25,30,1)' 
% postQTModeImageT3('femdata', 'Around30');
V=importdata(fullfile(femdata,'_mode' Afreq 'KHz.txt'),' ');
% freq=importdata(fullfile(femdata,'_freq' Afreq 'KHz.txt'),' ');
M=importdata(fullfile(femdata,'.txt'),' ',1); % import mesh data file
CO=M.data;
CO(:,1) = [];               % delete first column, node index.
CO(:,::) = CO(:,::)/100;      % change size of object, meter or centimeter
M=importdata(fullfile(femdata,'.txt'),' ',size(CO,1)+3);
CN=M.data;
CN(:,1) = [];  % delete first column, element index.
CNF10nodes=[CN(:,1:3);CN(:,[1 2 4]);CN(:,[1 3 4]);CN(:,[3 2 4])];
% get all faces of all the element;
% method a:
% CNF=unique(sort(CNF,2),'rows');
% just delete duplicated copies of faces, but still keeps all the faces,
% including those inside the volume.
% method b:
% this code tries to find all the element faces that are on the surface of
% the object, by deleting "element faces" that appear more than once in
% the 'faces' CNF data,
[~,m,n]=unique(sort(CNF10nodes,2),'rows');
t=unique(n);
v=[];
for kk=1:length(t)
    if(length(find(n==t(kk))))>1
        v=[v;find(n==t(kk))];
    end
end
n(v)=[];
CNF10nodes=CNF10nodes(m(n),:);
x0 = 1.05*max(CO(:,1));
y0 = 1.05*max(CO(:,2));
z0 = 1.05*max(CO(:,3));
nm=input('enter mode number,0 to quit.
');
Ap=input('amplification factor.
');
while nm~0
    COV = 0.001*Ap*reshape(V(:,nm)',,3,size(CO,1))';
    clf; % to erase old drawing, otherwise edges will show up in the
    % following graph.
    patch('Vertices',CO+sin(2*pi*(6+5)/20)*COV,'Faces',CNF10nodes,...
    'FaceVertexCData',[0.2,0.3,0.9],...
    'FaceColor','flat');
    view(45,18)
```
axis equal;
% axis([-1.1*x0 1.1*x0 -1.1*y0 1.1*y0 -0.1*z0 1.02*z0]);
% depending on situation, may need to adjust the axis option.
nm=input('enter mode number, 0 to quit.
');
Ap=input('amplification factor.
');
end
9. ModeFinder.m

This one is used to calculate similarity matrix between one changing group of modes (the helium property parameter changes, each change introduces a new set of eigen mode) with a fixed group of modes. The fixed group eigen vector needs to be imported. It calls subfunction KM.m and KMElement.m.

function [freq] = ModeFinder(femdata,n0)

tic;
k0 = importdata([femdata 'freqSAround75KHz.txt'], ',0);
M = importdata([femdata '.txt'], ',1);
CO = M.data;
CO(:,1) = [];
% delete first column,
M = importdata([femdata '.txt'], ',size(CO,1)+3);
CN = M.data;
CN(:,1) = [];
% delete first column,
M = importdata([femdata '_Lmaterial.txt'], ',1);
El = M.data;
density = 1000*El(:,1);
clear M;
E = cell(size(density,1),1);
for nm = 1:size(density,1)
    E{nm} = 10^11*blkdiag([El(nm,2) El(nm,10) El(nm,9);
                           El(nm,10) El(nm,3) El(nm,8);
                           El(nm,9) El(nm,8) El(nm,4)],...
                           El(nm,5),El(nm,6),El(nm,7));
end
clear El;

Gausspoints=importdata('Gausspoints.txt', ' ');
CO(:,:) = CO(:, :)/100;
% change size of object, meter or centimeter
Row=[];
Col=[];
MAD=[];
MBD=[];
NN = size(CO,1);
L = size(CN,2)-1;

CN1=CN(:,1:L);
CO1=cell(1,size(CN,1));
El=cell(size(CN,1),1);

density1=zeros(size(CN,1),1);
for j = 1:size(CN,1)
    CO1{1} = CO(CN(j,1:L),:);
    El{j} = E(CN(j,L+1));
    density1(j) = density(CN(j,L+1));
end

parfor j = 1:size(CN,1)
% loop over tetra elements; j is not complex number j.
    [K,M] = KM(CO1{j},Gausspoints,El{j},...
density1(j));
Row = [Row, kron([3*(CN1(j,:)-1)+1,...
3*(CN1(j,:)-1)+2,3*(CN1(j,:)-1)+3],ones(1,30))];
Col = [Col, repmat([3*(CN1(j,:)-1)+1,...
3*(CN1(j,:)-1)+2,3*(CN1(j,:)-1)+3],1,30)];
MAD = [MAD, reshape(K,1,900)];
MBD = [MBD, reshape(blkdiag(M,M,M),1,900)];
end

A = sparse(Row,Col,MAD,3*NN,3*NN);
BM = sparse(Row,Col,MBD,3*NN,3*NN);
freq=[];
vR = importdata(['vdotR' femdata '_modeSAround75KHz.txt',', ',0]);
parfor ik0=1:size(k0,1)
    [v2,d] = eigs(A,BM,n0,(2*pi*k0(ik0)*10^6)^2);
    freq =[freq sqrt(sort(diag(d)))/(2*pi)];
    [~, IX] = sort(diag(d));
    vt = v2(:,IX);
    %v = vt./repmat(sqrt(diag(vt'*BM*vt'))',3*NN,1);
    % normalize eigenvector with respect to mass matrix BM;
    vdotp=(vt./repmat(sqrt(diag(vt'*BM*vt'))',3*NN,1))'*vR;
    dlmwrite(['vdot' num2str(ik0) 'SL.txt'],vdotp,'delimiter',' ',
            'precision', '%.5f');
end
clear vt;
clear vR;
dlmwrite([femdata 'AllfreqSL.txt'],freq/10^6,...
            'delimiter', ' ', 'precision', '%.7f');
toc;
This program is used to find the best elastic constant so the experiment result agrees well with calculated result. It is not effective in our calculation.

```matlab
function Elfit = Elfit (femdata)
% program to fit elastic constant using function minimization.
% input femdata:
% includes:
% initial material value (guessing) femdata_2material.txt;
% mesh file, femdata.txt;
% experiment frequency, femdata_ext.txt;
% Gausspoints.txt;
% output: fitting result.

tic;
M = importdata([femdata '2material.txt'],' ',1);
% initial parameter value
El0 = M.data;
fp = @(El) parameterf(El,femdata);
%options = optimset('LevenbergMarquardt','on');
%Elfit = lsqnonlin(fp,El0,[],[],options);
Elfit = lsqnonlin(fp,El0);
disp(Elfit);
toc;

function freqpara=parameterf(El,femdata)
M=importdata([femdata '.txt'],' ',1);
% import mesh data file
CO=M.data;
CO(:,1) = [];
% delete first column, # of elements
CO(:,:) = CO(:,:)/100;
% change size of object, meter or centimeter
M=importdata([femdata '.txt'],' ',size(CO,1)+3);
CN=M.data;
CN(:,1) = [];
% delete first column, # of the nodes
clear M;
Gausspoints=importdata('Gausspoints.txt',' ');
freq0 = importdata([femdata '_exp.txt'],' ');
density=1000*El(:,1);
for nm=1:size(density,1)
c12 = El(nm,2)-2*El(nm,3);
E{nm}=10^11*blkdiag([El(nm,2), c12, c12;
c12, El(nm,2), c12;
c12, c12, El(nm,2)],...
El(nm,3),El(nm,3),El(nm,3));
end

Row = zeros(900*size(CN,1),1);
Col = zeros(900*size(CN,1),1);
% create row index for the assembled matrix, for each element it is 30*30
% matrix, 900 elements in total.
MAD = zeros(900*size(CN,1),1);
MBD = zeros(900*size(CN,1),1);
% MAD: matrix A(stiffness) data; MBD: matrix B(mass) data.
```
NN = size(CO,1); % # of nodes
L = size(CN,2)-1; % nodes of each tetrahedron element
for j = 1:size(CN,1)
  % loop over tetra elements; j is not complex number j.
  [K,M] = KM(CO(CN(j,1:L),:),Gausspoints,E(CN(j,L+1)),...
    density(CN(j,L+1)));
  Row(900*(j-1)+1:900*j) = kron([3*(CN(j,1:L)-1)+1,...
    3*(CN(j,1:L)-1)+2,3*(CN(j,1:L)-1)+3],ones(1,30));
  Col(900*(j-1)+1:900*j) = repmat([3*(CN(j,1:L)-1)+1,...
    3*(CN(j,1:L)-1)+2,3*(CN(j,1:L)-1)+3],1,30);
  MAD(900*(j-1)+1:900*j) = reshape(K,1,900);
  MBD(900*(j-1)+1:900*j) = reshape(blkdiag(M,M,M),1,900);
end

n0=20;
% number of eigenvalues to calculate
k0=20;
% frequency around k0 KHz.
A = sparse(Row,Col,MAD,3*NN,3*NN);
BM = sparse(Row,Col,MBD,3*NN,3*NN);
d=eigs(A,BM,n0,(2*pi*k0*1000)^2);
freqpara = sqrt(sort(d))/(2*pi);

% following is used to delete the 6 rigid motion.
inum = 0;
im = 1;
while abs(freqpara(im))<10
  im = im+1;
  inum = inum+1;
end
freqpara(1:inum)=[];
freqpara=(freqpara-freq0);
This program is used to calculate dislocation theory result.

```matlab
function dislocation
% dislocation theory, shear modulus, attenuation, and decrement.
% the parameter is used to fit our own experiment.
% reference:
% [1]. J. Appl. Phys. 27, 583 (1956);
% Theory of Mechanical Damping Due to Dislocations
% A. Granato and K. Lücke
% % Phys.—JETP 60, 537 (1984)].
clc;
global L RL rho c44 b poisson RA  n t0 v0 vt
F=63*10^3;
L=6*10^-6;
RA=5*10^9;
RL=0.6*10^-8;
n=3;
poisson=0.28;
t0=40*10^-9;
VM=20.0*10^-6;
A=(VM/(6.022*10^23))^(1/3);
b=1.1*A;
c44=0.0124*10^9*((20.97*10^-6)/VM)^5.73;
rho=0.004003/VM;
vt=sqrt(c44/rho);
v0=vt;
fexp1=[1
0.996655379
0.994138565
0.992050264
0.990426648
0.988957463
0.987567581
0.986074745
0.984979813
0.983914097
0.983037595
0.982195875
0.981541976];
Texp=[2.1:-0.1:0.9];
%fplot(@(T) (1+idm2(T,F))/(1+idm2(0,F)),[0,2.1], 'b');
fplot(@(T) idm2(T,F)*100,[0.001,2.1], 'r');
hold on;
percent=100*(idm2(0.9,F)-idm2(2.1,F))
cof=idm2(2.1,F);
plot(Texp,-((1-fexp1.^2)-cof).*100,'or');
```

11. dislocation.m
function idm2=idm2(T,F)
% shear modulus change, DG/G,
% integration over dislocation length.
idm1=@(l) idm(l,T,F);
idm2=quadgk(idm1,0,inf,'MaxIntervalCount',30000);

function idm=idm(l,T,F)
% shear modulus, dG/G,
global L RL poisson RA c44 n rho b t0 v0

N=l./L^2.*exp(-1./L);
Tension=c44*b^2*(log(2*l./b)-1/(4*(1-poisson))-1-log(4))/(4*pi);
f1=sqrt(Tension.*(1-poisson)./(4*1.^2*rho*b^2));

Q=f1.*2*pi*rho*b^2/((1-poisson)*(RL*T^n));
O=F./f1;
dm=(1-O.^2)/((1-O.^2).^2+(O./Q).^2);
c1=2.*rho.*v0.^2*b.^2*1.^2./(pi^3.*Tension);

%idm=-RA.*c1.*dm*N;
relax=(1+(2*pi.*F*t0*T^(-2.75)).^2);
idm=-RA.*c1.*dm*N./relax;
Bibliography

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67. Rose-Innes, A.C., Low Temperature Laboratory Techniques: The Use of Liquid Helium in the Laboratory. 1973: Hodder General Publishing Division.
91. J. R. Beamish and J. P. Franck, Physical Review B 26, 6104 (1982). “Sound propagation at frequencies from 3 to 21 MHz in hcp and bcc He3 and its interaction with dislocations”.
Vita

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Guoxing Liu was born in Jiangsu, China. He graduated with a B.S. in Physics in 2006. The same year, he attended graduate school in Physics Department at Penn State. His Ph.D. research is about applying resonant ultrasound spectroscopy technique to solid helium 4 study.