Notes & Report

Vibrations of thick plates

A "concise" walk-through of the calculations and programs, with a selection of results

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Contents

PART I

Introduction & Important Results

I
FOREWORD

The following report will make use of the Einstein summation notation, that is to say, repeated indices imply a sum over all possible values of the index. Usually this will mean $i \in \{x, y, z\}$, but later when looking at the equations of motion for our membrane, the z direction will be summed over, but equal to 0.

Additionally, this development does not use tensor calculus and differential geometry to its fullest extend and should be iterated over in a completely covariant notation to be more rigorous and more versatile. This will be left for later however, as using plain Cartesian will be plenty enough for the theory and for our numerical solutions.

Before the lengthy development, a small formula cheat-sheet is given, with links to relevant parts later down the document. The document aims to be as self consistent as can be, within reason, and so a large number of calculations are explicitly done for the reader's help.

The two parts are in principle independent, but some context will be left out if one chooses to read one without some understanding of the other. It is however possible to accept some of the results and ignore the sometimes verbose calculations.

II
LIST OF IMPORTANT MATHEMATICAL RESULTS FROM PART II

I General continuous medium

I.1 Basics The strain is defined (4):

$$u_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_l}{\partial x_i}\frac{\partial u_l}{\partial x_j}\right]$$

From the strain (4), the stress σ_{ij} is defined as the divergence (9) of the forces on and in the body:

$$f^i = \nabla_j \sigma^{ij}$$

and it can be written as (10):

$$F_i = \oint_{\partial V} \sigma_{ij}\, dS_j = \oint_{\partial V} \sigma_{ij}\, n_j\, dS$$

I.2 Thermodynamics The variation of energy in a body under deformation can be written (13):

$$dU = TdS + \sigma_{ij} \cdot du_{ij}$$

We define the elasticity tensor (20) of a material as:

$$\lambda_{ijkl} = \left[\frac{\partial^2 F}{\partial u_{ij}\partial u_{kl}}\right]_{u_{ij}=0,\,T}$$

Using it, we can write the free energy as (21):

$$F = \frac{1}{2}\lambda_{ijkl}\, u_{ij}\, u_{kl}$$

This leads us to Hooke's law or the constitutive law of the media (23):

$$\sigma_{kl} = \lambda_{ijkl}\, u_{ij}$$

II Plate theory results

II.1 Unstressed homogeneous plate In this case, we use the Kirchhoff approximation (26) to write the strain (28):

$$\varepsilon_{ij} = -z\partial_{ij} w$$

Define a new tensor (29):

$$D_{ijkl} = \lambda_{ijkl} \int_{-\frac{h}{2}}^{+\frac{h}{2}} z^2 dz = \lambda_{ijkl}\, \frac{h^3}{12}$$

The equation of motion, with a source is (33):

$$-\partial_{ij}[D_{ijkl}\, \partial_{kl} w] + A(x,y)\cos(\omega t) = \rho h \partial_{tt} w$$

II.2 Stressed homogeneous plate Changing our assumptions we get the strain for Von Kármán plates (35):

$$\varepsilon_{ij} = \varepsilon^0_{ij} - z\, \partial_{ij} w + \frac{1}{2}\partial_i w\, \partial_j w$$

we again define a new tensor (36):

$$\lambda_{ijkl}\, T_{kl}\, h = h\, \sigma_{ij} = N_{ij}$$

For a stressed plate, without source, the equation of motion becomes (39):

$$+\frac{1}{2}\partial_j\left(N_{ij}\, \partial_i w\right) - \partial_{kl}\left(D_{ijkl}\, \partial_{ij} w\right) = \rho h \partial_{tt} w$$

II.3 Multilayered stressed plate For a laminated composite plate, we need to define new tensors (47):

$$A_{ijkl} = \sum_{a=0}^{N} \overline{\lambda^a_{ijlk}}\,(z_{a-1} - z_a)$$
$$B_{ijkl} = \sum_{a=0}^{N} \frac{\overline{\lambda^a_{ijlk}}}{2}\,(z^2_{a-1} - z^2_a)$$
$$C_{ijkl} = \sum_{a=0}^{N} \frac{\overline{\lambda^a_{ijlk}}}{3}\,(z^3_{a-1} - z^3_a)$$

Which we plug in the previous expression using (48):

$$\begin{bmatrix} N_{ij} \\ M_{ij} \end{bmatrix} = \begin{bmatrix} A_{ijkl} & B_{ijkl} \\ B_{ijkl} & C_{ijkl} \end{bmatrix} \begin{bmatrix} T_{kl} \\ -\partial_{kl} w \end{bmatrix}$$

To finally give, for a composite plate (49):

$$\frac{1}{2}\partial_j[(A_{ijkl}\, T_{kl} - B_{ijkl}\, \partial_{kl} w)\, \partial_i w] - \partial_{ij}[B_{ijkl} T_{kl} - C_{ijkl}\, \partial_{kl} w] = \rho h \partial_{tt} w$$

III Material symmetries

III.1 Voigt notation When doing calculation using the strain, stress or elastic tensors, it is often useful to change representation and to use the Voigt notation (50), making vectors out of matrices (1):

$$(u) = \begin{bmatrix} u_{xx} & u_{xy} & u_{xz} \\ u_{xy} & u_{yy} & u_{yz} \\ u_{xz} & u_{yz} & u_{zz} \end{bmatrix} \longrightarrow \mathbf{u} = \begin{bmatrix} u_{xx} \\ u_{yy} \\ u_{zz} \\ u_{yz} \\ u_{xz} \\ u_{xy} \end{bmatrix}$$

III.2 FePS3 result After applying symmetries, it can be shown that the elastic tensor for $FePS_3$ (66) can be reduced to 13 independent components, this depends on the type of crystal we consider (2):

$$(\lambda^{FePS_3}) = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} & 0 & 0 \\ \lambda_{12} & \lambda_{22} & \lambda_{23} & \lambda_{24} & 0 & 0 \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & \lambda_{34} & 0 & 0 \\ \lambda_{14} & \lambda_{24} & \lambda_{34} & \lambda_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \lambda_{55} & \lambda_{56} \\ 0 & 0 & 0 & 0 & \lambda_{56} & \lambda_{66} \end{bmatrix}$$

PART II

Continuous Media

III
CRASH COURSE IN ELASTICITY

I Strain and Stress

I.1 The Strain tensor Let us consider a continuous and deformable body in $\mathbb{R}^3$. The position vector of any point in or on the body is given by:

$$\vec{r} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix}$$

and, after subjecting the body to a very small deformation, this same vector becomes :

$$\vec{r}' = \begin{bmatrix} r_1' \\ r_2' \\ r_3' \end{bmatrix} = \begin{bmatrix} r_1 + \Delta r_1 \\ r_2 + \Delta r_2 \\ r_3 + \Delta r_3 \end{bmatrix}.$$

Thence, we can define the displacement of a point in a continuous media:

$$\vec{u} = \vec{r}' - \vec{r} = \begin{bmatrix} r_1' - r_1 \\ r_2' - r_2 \\ r_3' - r_3 \end{bmatrix} \tag{1}$$

which will we can simply write as: $u_i = r_i' - r_i$, which is a much lighter notation, and we can express the post- or pre- deformation coordinate $r_i' = r_i + u_i$ or $r_i = r_i' - u_i$. Taking its differential, we get the following:

$$du_i = \frac{\partial u_i}{\partial x_j} dx_j, \tag{2}$$

as the displacement on every axis can depend on all 3 coordinates.

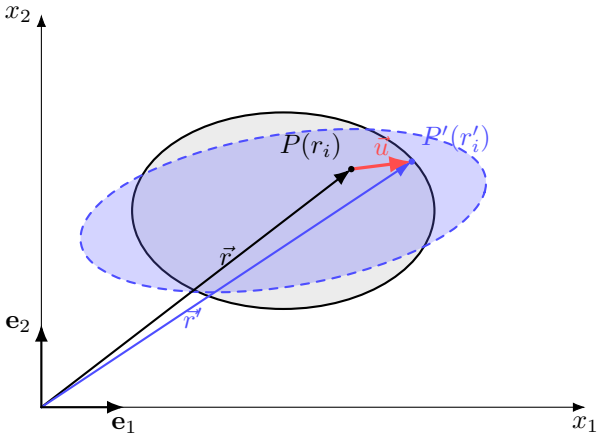

FIG. i Deformation of a body creates

Consider now 2 points inside the medium, situated at $\vec{r_1}$ and $\vec{r_2}$, separated by $d\vec{x}$. Before deformation, the distance between the two points is given by : $dl^2 = d\vec{x} \cdot d\vec{x} = dx_i dx_i = dx_1^2 + dx_2^2 +$

dx_3^2. After deformation of the solid, the distance changes, and the two points are now separated by: $dl'^2 = dx'_i dx'_i$. From before, we can write $dx'_i = dx_i + du_i$, and insert it into dl'^2:

$$\begin{aligned}
dl'^2 &= (dx_i + du_i)(dx_i + du_i) \\
dl'^2 &= dx_i^2 + 2du_i dx_i + du_i \\
dl'^2 &= dx_i^2 + 2\left[\frac{\partial u_i}{\partial x_j}dx_j\right]dx_i + \left[\frac{\partial u_i}{\partial x_k}dx_k\right]\left[\frac{\partial u_i}{\partial x_l}dx_l\right] \\
dl'^2 &= dx_i^2 + 2\frac{\partial u_i}{\partial x_j}dx_i dx_j + \frac{\partial u_i}{\partial x_k}\frac{\partial u_i}{\partial x_l}dx_k dx_l \\
dl'^2 &= dx_i^2 + \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)dx_i dx_j + \frac{\partial u_{i\to l}}{\partial x_{l\to i}}\frac{\partial u_{i\to l}}{\partial x_{k\to j}}dx_{k\to j}dx_{l\to i}
\end{aligned}$$

Finally giving us the following equation, where we see the factor $dx_i dx_j$ in the last 2 terms, and the first one is just the expression of $dl^2 = dx_i^2$.

$$dl'^2 = dl^2 + \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)dx_i dx_j + \frac{\partial u_l}{\partial x_i}\frac{\partial u_l}{\partial x_j}dx_j dx_i$$

With one last step of refactoring and shuffling terms around the previous expression, we get:

$$dl'^2 - dl^2 = \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_l}{\partial x_i}\frac{\partial u_l}{\partial x_j}\right]dx_i dx_j = 2u_{ij}\,dx_i dx_j \tag{3}$$

The Strain Tensor is thus defined as:

$$u_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_l}{\partial x_i}\frac{\partial u_l}{\partial x_j}\right] \tag{4}$$

In a first part, we will neglect the crossed term, as being of a higher order, it plays a smaller part in the small displacement cases. In such a case, we have:

$$u_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] \tag{5}$$

I.2 A few results In general, this tensor can be made diagonal at a certain point on a body, but not multiple. When it is diagonal, only the the u_{ii} terms remain, as eigenvalues of the new basis vectors. These 3 terms are then called "principal values", and usually labelled : $u^{(1)}$, $u^{(2)}$ and $u^{(3)}$.

Where the tensor is diagonal, we can simplify the previous expression for dl'^2:

$$\begin{aligned}
dl'^2 &= dx_i^2 + 2u_{ii}dx_i dx_i = (\delta_{ii} + 2u^{(i)}\delta_{ij})dx_i dx_j \\
dl'^2 &= (1 + 2u^{(1)})dx_1^2 + (1 + 2u^{(2)})dx_2^2 + (1 + 2u^{(3)})dx_3^2
\end{aligned}$$

If we define $\eta = \frac{dx'_i - dx_i}{dx_i}$, we can write the relative extension of the deformation for the i-th coordinate at a certain point if the displacement is small enough, in the diagonal basis as:

$$\eta = \frac{\sqrt{1 + u^{(i)}}dx_i - dx_i}{dx_i} \approx (1 + u^{(i)}) \tag{6}$$

And similarly defining $\tau = \frac{dV' - dV}{dV}$, the relative expansion of the elementary volume element of the solid at a particular point:

$$dV = dx_1\,dx_2\,dx_3 \quad ; \quad dV' = dx_1'\,dx_2'\,dx_3'$$
$$dV' = \sqrt{1+u^{(1)}}\,\sqrt{1+u^{(2)}}\,\sqrt{1+u^{(3)}}dV$$
$$dV' \approx (1+u^{(1)})(1+u^{(2)})(1+u^{(3)})dV$$
$$dV' \approx (1+u^{(1)}+u^{(2)}+u^{(3)})dV$$

We recognize the sum of the principal values to be the trace of the tensor, which **is** an invariant, so that this result (with the caveat that the value of u_{ij} is a function of (x,y,z,t)) is true whether or not we are near the point where we diagonalised. If we keep to small deformations.

$$\tau = \frac{dV'-dV}{dV} = \frac{[1+\mathrm{tr}(u_{ij})]dV - dV}{dV} = \mathrm{tr}(u_{ij}) = u_{ii} \tag{7}$$

I.3 The Stress tensor Next up, we consider the total force $\vec{F}$ acting in and on the body, that is, the integral of the density of forces $\vec{f}$ over the whole volume V:

$$\vec{F} = \int_V \vec{f}(x_i)dV \tag{8}$$

Making a crucial assumption here, we can write the force f_i as stemming from the divergence of a quantity, which, here would need to be an object with 2 indices, that is to say, a tensor of rank 2. In a later part, if I'm not too lazy, doing this properly would lead us to write:

$$f^i = \nabla_j \sigma^{ij} \tag{9}$$

because the force is a vector, and not a covector, its components need to be contravariant, and so, the covariant derivative would need to act on a (2,0)-form. This is needlessly complicated, though more mathematically correct. I would need a lot more differential geometry and tensor calculus to make stuff work though. So no full covariance, no Christoffel symbols. Yet.

In the rest of this report, we will lighten the visual load by writing $\frac{\partial}{\partial x_i}$ as ∂_i. Again, this should be the covariant derivative, but we'll make do with a partial.

$$F_i = \int_V f_i\,dV = \int_V \partial_j\,\sigma_{ij}\,dV$$

This assumption is great, because we can apply Green-Ostrogradsky to integrate over the contour instead of the volume:

$$F_i = \oint_{\partial V} \sigma_{ij}\,dS_j = \oint_{\partial V} \sigma_{ij}\,n_j\,dS \tag{10}$$

This is formally the definition of the Stress Tensor, σ_{ij}. The stress tensor is mathematically defined as the source of the sum total of the forces acting on the body. No stress means no forces, no sum total of forces means no stress.

II Thermodynamics of a membrane

II.1 Work of the internal forces Consider a body that is deformed in such a manner that: $u_i \to u_i + \delta u_i$, the elementary work done by the internal forces per unit volume is then, from simple thermodynamics, and using our Stress Tensor (10) expression:

$$\delta W = F_i \cdot dl_i = \nabla_j \sigma_{ij} \cdot \delta u_i \tag{11}$$

which can be integrated over the whole volume of the body to find the elementary work in the body. We can again use the divergence trick here, yielding:

$$\int_V \delta W dV = \int_V \left[\nabla_j(\sigma_{ij}) \cdot \delta u_i\right] dV$$
$$\int_V \delta W dV = \int_V \nabla_j(\sigma_{ij} \cdot \delta u_i) dV - \int_V \sigma_{ij} \cdot \nabla_j(\delta u_i) dV$$
$$\int_V \delta W dV = \cancelto{0}{\oint_{\partial V} \left[\sigma_{ij} \cdot \delta u_i\right] dV} - \int_V \sigma_{ij} \cdot \nabla_j(\delta u_i) dV.$$

If we let the stress be $\sigma_{ij} \approx 0$ when $\vec{r} \in \partial V$ we can kill off the first term. This is a well justified assumption for a vibrating plate, where the stress is mostly internal to the plate and the lateral boundaries are under Dirichlet or Von Neumann conditions. We can continue by splitting the volume term as before to find back the Strain Tensor (5).

$$\int_V \delta W dV = -\int_V \sigma_{ij} \cdot \nabla_j(\delta u_i) dV$$
$$\int_V \delta W dV = -\frac{1}{2} \int_V \sigma_{ij} \left[\nabla_j \delta u_i + \nabla_i \delta u_j\right] dV$$
$$\int_V \delta W dV = -\int_V \sigma_{ij} \cdot \delta \left[\frac{1}{2}(\nabla_j u_i + \nabla_i u_j)\right] dV$$
$$\int_V \delta W dV = -\int (\sigma_{ij} \cdot \delta u_{ij}) dV$$

And of course, we can readily identify δW in the right hand side, giving us finally:

$$\delta W = -\sigma_{ij} \cdot \delta u_{ij} \tag{12}$$

the work is thus proportional to the Stress times the variation in Strain, with a minus sign. Physically, this means that deforming a body by a certain amount forces the internal stresses to oppose this deformation by an amount linearly dependant on the size of the deformation.

II.2 Thermodynamics Applying the first law of thermodynamics, we can write:

$$\Delta U = \Delta Q - \Delta W$$
$$dU = \delta Q - \delta W$$
$$dU = TdS - (-\sigma_{ij} \cdot du_{ij})$$
$$dU = TdS + \sigma_{ij} \cdot du_{ij} \tag{13}$$

Stopping for a quick sanity check here, imagining a purely hydrostatic pressure, no shear and only stressing the normals on every side gives us a $\sigma_{ij} = -p\delta_{ij}$, and plugging it back in we get:

$$dU = TdS + \sigma_{ij} \cdot du_{ij}$$
$$dU = TdS + (-p\,\delta_{ij}) \cdot du_{ij}$$
$$dU = TdS - p \cdot \mathrm{tr}(u_{ij}) = TdS - p \cdot u_{ii}$$

Where we recognize a previous result, the relative expansion (7), which is simply dV in this case. In the case of simple hydrostatic pressure, we find a familiar expression:

$$dU = TdS - pdV \tag{14}$$

We can also write out the other thermodynamical potentials, the free energy F, the enthalpy H and the free enthalpy G using their well known expressions:

$$F = U - TS \qquad \Longrightarrow dF = -SdT + \sigma_{ij} \cdot du_{ij} \tag{15}$$
$$H = U + PV \qquad \Longrightarrow dH = TdS - u_{ij} \cdot d\sigma_{ij} \tag{16}$$
$$G = U - TS + PV \qquad \Longrightarrow dG = -SdT - u_{ij} \cdot d\sigma_{ij} \tag{17}$$

We can then extract for these relations the following relations for the two Stress and Strain tensors :

$$\sigma_{ij} = \left[\frac{\partial E}{\partial u_{ij}}\right]_S = \left[\frac{\partial F}{\partial u_{ij}}\right]_T \tag{18}$$
$$u_{ij} = \left[\frac{\partial H}{\partial \sigma_{ij}}\right]_S = \left[\frac{\partial G}{\partial \sigma_{ij}}\right]_T \tag{19}$$

II.3 Hooke's law To proceed forward, we choose the free energy F as our potential. We assume an isothermal system, so that we can remove our first term:

$$dF = \cancelto{0}{-SdT} + \sigma_{ij} \cdot du_{ij} = \sigma_{ij} \cdot du_{ij}$$

When the strain is equal to 0, that is, when the body is not deformed at all, we assume that the stress is also 0. With this assumption, from (18) we can write:

$$\sigma_{ij}(u_{ij} = 0) = \left[\frac{\partial F}{\partial u_{ij}}\right]_{u_{ij}=0,T} = 0$$

With this, we can Taylor expand the free energy around $u_{ij} = 0$ to second order, that is to say, we limit ourselves to small deformations. Given that experimentally we see amplitudes of displacement $\approx$ 90nm in the on a drum $\approx$ 5000nm in diameter, we fall well within this limit.

$$F = F_0 + \cancelto{0}{\left[\frac{\partial F}{\partial u_{ij}}\right]_{u_{ij}=0,T}} u_{ij} + \frac{1}{2}\left[\frac{\partial^2 F}{\partial u_{ij}\,\partial u_{kl}}\right]_{u_{ij}=0,T} u_{ij}\,u_{kl}$$
$$F = F_0 + \frac{1}{2}\left[\frac{\partial^2 F}{\partial u_{ij}\,\partial u_{kl}}\right]_{u_{ij}=0,T} u_{ij}\,u_{kl}$$

By defining the second derivative of F as a new tensor of rank 4, λ_{ijkl}, we get this expression:

$$\lambda_{ijkl} = \left[\frac{\partial^2 F}{\partial u_{ij}\partial u_{kl}}\right]_{u_{ij}=0,\,T} \tag{20}$$

and using the gauge symmetry, removing the constant, of the free energy we can write the free energy F as:

$$F = \frac{1}{2}\lambda_{ijkl}\,u_{ij}\,u_{kl} \tag{21}$$

This is going to be our starting point later for the equation of motion of the membrane. Before that, we'll first show Hooke's law, or the constitutive law of the medium. Later still, we'll show a few results about the λ_{ijkl} tensor and its symmetries.

For now we can take the derivative of our (21) with respect to deformation. Because we have both u_{ij} and u_{kl}, we can do the derivation the old fashioned way:

$$\delta F = \lim_{\varepsilon \to 0} \frac{F(u_{ij} + \epsilon \delta u_{ij}) - F(u_{ij})}{\varepsilon}$$
$$\delta F = \lim_{\varepsilon \to 0} \frac{\frac{1}{2}\lambda_{ijkl}(u_{ij} + \varepsilon \delta u_{ij})(u_{kl} + \varepsilon \delta u_{kl}) - \frac{1}{2}\lambda_{ijkl}\, u_{ij}\, u_{kl}}{\varepsilon}$$
$$\delta F = \lim_{\varepsilon \to 0} \frac{\frac{1}{2}\lambda_{ijkl}(u_{ij}u_{kl} + \varepsilon \delta u_{ij}u_{kl} + \varepsilon \delta u_{ij}u_{kl} + \varepsilon^2 \delta u_{ij}\delta u_{kl}) - \frac{1}{2}\lambda_{ijkl}\, u_{ij}\, u_{kl}}{\varepsilon}$$

Since we have to enforce the $(ij) \longleftrightarrow (kl)$ symmetry, we can combine the two ε factors:

$$\delta F = \lim_{\varepsilon \to 0} \frac{\frac{1}{2}\lambda_{ijkl}(u_{ij}u_{kl} + 2\varepsilon u_{ij}\delta u_{kl} + \varepsilon^2 \delta u_{ij}\delta u_{kl}) - \frac{1}{2}\lambda_{ijkl}\, u_{ij}\, u_{kl}}{\varepsilon}$$

Now we can very easily subtract the two equal parts and divide the remaining factors by ε:

$$\delta F = \lim_{\varepsilon \to 0} \frac{1}{2}\lambda_{ijkl}(2u_{ij}\delta u_{kl} + \varepsilon \delta u_{ij}\delta u_{kl})$$

Applying the limit to our expression we get rid of the 2nd order term, and we are left with and taking the limit $\delta u_{ij} \to du_{ij}$:

$$\frac{\partial F}{\partial u_{ij}} = \lambda_{ijkl} u_{ij} \tag{22}$$

But we can recall from before (18) that this is also equal to the Stress Tensor, σ_{ij}, and thence, we get Hooke's law, or the constitutive law of the material:

$$\sigma_{kl} = \lambda_{ijkl}\, u_{ij} \tag{23}$$

The tensor λ_{ijkl} is called the Elasticity Tensor or the Stiffness Tensor. It is inherent to a particular material, and refers broadly to the amount of energy it takes to deform a material along a particular axis. It is given in units of pressure, usually in the MPa for our crystalline structures.

IV
EQUATIONS OF MOTION

For what follows, the partial derivative with respect to the i-th coordinate, $\frac{\partial}{\partial i}$, will be written ∂_i wherever possible to ease the notation.

I Kirchhoff-Love Plate Theory, Unstressed Plate

In the case of plates, it is common to make what is known as the KIRCHHOFF approximation. The approximation assumes a small enough deformation, with no shearing of the membrane, that we can write the following:

$$u_x = u_x^0 - z\,\partial_x w \tag{24}$$
$$u_y = u_y^0 - z\,\partial_y w \tag{25}$$
$$u_z = w(x,\,y,\,t) \tag{26}$$

Let us first compute the components of the STRAIN TENSOR (5), we will need to assume that we can apply SCHWARZ's theorem to w, and we remember that $\partial_i i = \delta_{ii}$ as well as that $\partial_z w = 0$ (no shearing):

$$\varepsilon_{xx} = \frac{1}{2}[\partial_x(u_x^0 - z\,\partial_x w) + \partial_x(u_x^0 - z\,\partial_x w)] = -z\,\partial_x^2 w = -z\,\partial_{xx} w$$
$$\varepsilon_{yy} = \frac{1}{2}[\partial_y(u_y^0 - z\,\partial_y w) + \partial_y(u_y^0 - z\,\partial_y w)] = -z\,\partial_{yy} w$$
$$\varepsilon_{zz} = \frac{1}{2}[\partial_z w + \partial_z w] = \partial_z w = 0$$
$$\varepsilon_{xy} = \frac{1}{2}[\partial_x(u_y^0 - z\,\partial_y w) + \partial_y(u_x^0 - z\,\partial_x w)] = -z\partial_{xy} w$$
$$\varepsilon_{xz} = \frac{1}{2}[\partial_x w + \partial_z(u_x^0 - z\,\partial_x w)] = \frac{1}{2}[\partial_x w - \cancelto{1}{\partial_z z}\cdot\partial_x w - z\partial_{xz} w] = -\frac{1}{2}z\partial_{xz} w = 0$$
$$\varepsilon_{yz} = \frac{1}{2}[\partial_y w + \partial_z(u_y^0 - z\,\partial_y w)] = -\frac{1}{2}z\partial_{yz} w = 0$$

In the KIRCHHOFF picture, the STRAIN TENSOR can be written as the matrix:

$$(\varepsilon) = \begin{bmatrix} -z\,\partial_{xx} w & -z\,\partial_{xy} w & 0 \\ -z\,\partial_{yx} w & -z\,\partial_{yy} w & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{27}$$

or in the tensorial notation,

$$\varepsilon_{ij} = -z\partial_{ij} w \tag{28}$$

We recall the free energy of an elementary volume given by (21), we will consider the free energy per unit surface, by integrating over the thickness, h, of the plate. We can write:

$$U = \int_{-\frac{h}{2}}^{+\frac{h}{2}} F dz = \int_{-\frac{h}{2}}^{+\frac{h}{2}} \left[\frac{1}{2}\lambda_{ijkl}\,u_{ij}\,u_{kl}\right] dz$$

Then, we can simply insert the previously found expression for the STRAIN TENSOR, (28), such that we have:

$$U = \int_{-\frac{h}{2}}^{+\frac{h}{2}} \left[\frac{1}{2}\lambda_{ijkl}\,(-z\partial_{ij} w)\,(-z\partial_{kl} w)\right] dz = \frac{1}{2}\left[\int_{-\frac{h}{2}}^{+\frac{h}{2}} z^2\lambda_{ijkl} dz\right]\partial_{ij} w\,\partial_{kl} w = \frac{1}{2}D_{ijkl}\,\partial_{ij} w\,\partial_{kl} w$$

Computing D_{ijkl} is straight forward, as the Stiffness Tensor is constant with respect to position in a material and can be pulled out of the integral, it would only change if we traversed an interface, which we do not in this model.

$$D_{ijkl} = \lambda_{ijkl} \int_{-\frac{h}{2}}^{+\frac{h}{2}} z^2 dz = \lambda_{ijkl} \frac{h^3}{12} \tag{29}$$

With this, U becomes:

$$U[w] = \frac{1}{2}\left[\frac{h^3}{12}\,\lambda_{ijkl}\,\partial_{ij}w\,\partial_{kl}w\right] = \frac{1}{2}D_{ijkl}\,\partial_{ij}w\,\partial_{kl}w \tag{30}$$

This expression inherits the symmetries of the free energy, that is to say, it is left invariant by the swaps $(ij) \to (kl)$ as well as $i \to j$ (and of course $k \to l$). And to get to the equations of motions, we will need to take the functional derivative of the energy with respect to w. We'll use the previously mentioned symmetries to group together cross terms in the product.

$$\begin{aligned}
\delta U &= \lim_{\varepsilon \to 0} \frac{U(w+\varepsilon\delta w) - U(w)}{\varepsilon} \\
\delta U &= \lim_{\varepsilon \to 0} \frac{\frac{1}{2}\left[D_{ijkl}\,\partial_{ij}(w+\varepsilon\delta w)\,\partial_{kl}(w+\varepsilon\delta w)\right] - \frac{1}{2}\left[D_{ijkl}\,\partial_{ij}w\,\partial_{kl}w\right]}{\varepsilon} \\
\delta U &= \lim_{\varepsilon \to 0} \left[\frac{1}{2}D_{ijkl}\right] \frac{(\partial_{ij}w + \varepsilon\partial_{ij}\delta w)(\partial_{kl}w + \varepsilon\partial_{kl}\delta w) - \partial_{ij}w\,\partial_{kl}w}{\varepsilon} \\
\delta U &= \lim_{\varepsilon \to 0} \left[\frac{1}{2}D_{ijkl}\right] \frac{\cancel{\partial_{ij}w\,\partial_{kl}w} + \varepsilon\partial_{ij}\delta w\,\partial_{kl}w + \varepsilon\partial_{kl}\delta w\,\partial_{ij}w + \varepsilon^2\partial_{kl}\delta w\,\partial_{ij}\delta w - \cancel{\partial_{ij}w\,\partial_{kl}w}}{\varepsilon} \\
\delta U &= \lim_{\varepsilon \to 0} \left[\frac{1}{2}D_{ijkl}\right] \frac{2\cancel{\varepsilon}\partial_{ij}\delta w\,\partial_{kl}w + \cancel{\varepsilon^2}\partial_{kl}\delta w\,\partial_{ij}\delta w}{\cancel{\varepsilon}} \\
\delta U &= D_{ijkl}\,\partial_{ij}\delta w\,\partial_{kl}w
\end{aligned}$$

From here, we integrate by parts twice and toss the integrated boundary terms into a constant that we will set equal to 0 to get the natural resonant modes of the plate.

Which we can write, letting $\delta w,\ \delta U \to 0$:

$$\frac{\partial U}{\partial w} = \partial_{ij}\left[D_{ijkl}\,\partial_{kl}w\right] \tag{31}$$

And we can easily get the expression of our force per unit surface with (31), using the trusty $\vec{F} = -\vec{\nabla}U$:

$$\vec{F}_{\text{bending}} = -\partial_{ij}\left[D_{ijkl}\,\partial_{kl}w\right]\ \hat{e}_z \tag{32}$$

The tensor D_{ijkl} is a constant of the material, or at least, a constant in the plane, we can pull it out of the derivative and simply apply 4 derivatives to w. It is NOT customary to do so, however, because $M_{ij} = D_{ijkl}\,\partial_{kl}w$ has units of force. It is usually referred to as the "bending moment" of the plate. It can be useful to write the previous equation using this moment, as this notation will be relevant later in the laminate version of the theory.

$$\vec{F}_{\text{bending}} = -\partial_{ij}\left[M_{ij}\right]\ \hat{e}_z$$

The summation is over all 3 indices, but the derivative with respect to z is simply equal to 0, as our initial assumptions had $w(x, y, \cancel{z}, t)$ as NOT a function of z. This condition is the **no shear** hypothesis and collapses our sum over $i \in \{x, y, z\}$ to a sum over $i \in \{x, y, z\}$.

For the Kirchhoff-Love plate theory, we get the following differential equation using Newton's principle, with an actuation force thrown in for good measure:

$$-\partial_{ij}[D_{ijkl}\,\partial_{kl}w] + A(x,y)\cos(\omega t) = \rho h \partial_{tt} w \tag{33}$$

where, of course, ρh is simply the surface density of the material, $\partial_{tt}w$ is the acceleration and $A(x,y)\cos(\omega t)$ is any laser type force, with a pulsation ω and a power by unit surface given by $A(x,y)$. The equation has non vanishing components only on the z axis, and so we directly write it as a scalar equation.

We will not attempt to solve this analytically and will rely on the finite difference method to find the eigenvalues. Doing this makes us remove the actuation term, but this isn't a problem, indeed, the only thing the laser force would do is excite a specific eigenmode and eigenfrequency.

To recap what we have done :

- Chosen the Kirchhoff approximation (26) for plates
- Calculated the strain generated (28) by the displacement
- Used the strain to get the free energy by unit volume, using (21), and integrated it over the thickness
- Took the functional derivative (31) with respect to w to get the force by unit surface (32)
- Collapsed the sum over $i \in \{x,y,z\}$ into just $i \in \{x,y\}$ to get the final differential equation (33) for the motion

II Föppl–von Kármán Plate Theory, Stressed Plate

Most of the following development is very similar to the previous section. The starting point is the same, as we, once again assume our displacement to follow the same Kirchhoff approximation (26), taking a more general form, with a displacement u_x^0 and u_y^0 that are position dependant, as is the case when the membrane is strained. The main difference, however, comes in the form of the strain tensor, as we will, this time consider the neglected term in (4).

Let us directly compute our tensor term by term as before:

$$\varepsilon_{xx} = \frac{1}{2}\left[\partial_x(u_x) + \partial_x(u_x) + \partial_x(u_x)\partial_x(u_x) + \partial_x(u_y)\partial_x(u_y) + \partial_x(u_z)\partial_x(u_z)\right]$$

$$\varepsilon_{xx} = \partial_x(u_x^0 - z\,\partial_x w) + \frac{1}{2}[\partial_x(u_x^0 - z\,\partial_x w)]^2 + \frac{1}{2}[\partial_x(u_y^0 - z\,\partial_y w)]^2 + \frac{1}{2}[\partial_x w]^2$$

$$\varepsilon_{xx} = \partial_x u_x^0 - z\,\partial_{xx} w + \cancelto{\approx 0}{\text{lots of small terms}} + \frac{1}{2}[\partial_x w]^2$$

$$\varepsilon_{xx} = \partial_x u_x^0 - z\,\partial_{xx} w + \frac{1}{2}[\partial_x w]^2$$

$$\varepsilon_{yy} = \partial_y u_y^0 - z\,\partial_{yy} w + \frac{1}{2}[\partial_y w]^2$$

$$\varepsilon_{zz} = 0 \text{ } w \text{ is not function of } z$$

$$\varepsilon_{xz} = \frac{1}{2}\left[\partial_z(u_x) + \partial_x(u_z) + \partial_x(u_x)\partial_z(u_x) + \partial_x(u_y)\partial_z(u_y) + \partial_x(u_z)\partial_z(u_z)\right]$$

$$\varepsilon_{zz} = \frac{1}{2}[\partial_z(\cancel{u_x^0} - z\,\partial_x w) + \partial_x w + \cdots + \partial_x w\,\cancel{\partial_z w}] = \frac{1}{2}[-\partial_x w - z\cancel{\partial_{xz} w} + \partial_x w + \cancelto{\approx 0}{\text{lots of small terms}}]$$

$$\varepsilon_{xz} \approx 0 \qquad \& \qquad \varepsilon_{yz} \approx 0$$

$$\varepsilon_{xy} = \frac{1}{2}[\partial_y(u_x^0 - z\,\partial_x w) + \partial_x(u_y^0 - z\,\partial_y w) + \cdots + \partial_x w\,\partial_y w]$$

$$\varepsilon_{xy} = \frac{1}{2}(\partial_y w + \partial_x w) - z\,\partial_{xy} w + \frac{1}{2}\partial_x w\,\partial_y w$$

As before we can write the obtained strain tensor in a matrix form, as follows :

$$(\varepsilon) = \begin{bmatrix} \partial_x u_x^0 - z\,\partial_{xx} w + \frac{1}{2}[\partial_x w]^2 & \frac{1}{2}(\partial_y w + \partial_x w) - z\,\partial_{xy} w + \frac{1}{2}\partial_x w\,\partial_y w & 0 \\ \frac{1}{2}(\partial_y w + \partial_x w) - z\,\partial_{xy} w + \frac{1}{2}\partial_x w\,\partial_y w & \partial_y u_y^0 - z\,\partial_{yy} w + \frac{1}{2}[\partial_y w]^2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{34}$$

But it is usually more useful and less of an eyesore to write it out in tensor notation, which gives us :

$$\varepsilon_{ij} = \frac{1}{2}(\partial_i u_j^0 + \partial_j u_i^0) - z\,\partial_{ij} w + \frac{1}{2}\partial_i w\,\partial_j w$$

And of course, the first term looks an awful lot like (5), and so, we can write it out as just that, a pre-strain, written ε_{ij}^0 :

$$\varepsilon_{ij} = \varepsilon_{ij}^0 - z\,\partial_{ij} w + \frac{1}{2}\partial_i w\,\partial_j w \tag{35}$$

It is interesting to note that by adding what we have added we see a first derivative in w appear, that gives the product of the slope on both axis for the component considered. We can even refactor a step further, writing:

$$\varepsilon_{ij} = T_{ij} - z\,\partial_{ij} w$$

This is more of a calculation trick than a physically relevant regrouping of terms, though this term written like this will give rise to a tension-like force in our differential equation. Nevertheless, we again recall (21) and insert our strain in the equation:

$$\begin{aligned} F &= \frac{1}{2}\lambda_{ijkl}\,\varepsilon_{ij}\,\varepsilon_{kl} \\ F &= \frac{1}{2}\lambda_{ijkl}\,\left[T_{ij} - z\,\partial_{ij} w\right]\left[T_{kl} - z\,\partial_{ij} w\right] \\ F &= \frac{1}{2}\lambda_{ijkl}\,\left[T_{ij}T_{kl} - 2z\,\partial_{ij} w T_{kl} + z^2\,\partial_{ij} w\,\partial_{kl} w\right] \end{aligned}$$

Here again, we have combined the two crossed terms into the middle term to complete the identity because our system is left invariant by the swap of the pair $(ij) \to (kl)$ (and vice-versa). We can now continue by integrating our free energy by unit volume over the thickness of the plate to have our energy by unit surface, as before.

$$\begin{aligned} U &= \int_{-h/2}^{+h/2} F\,dz = \int_{-h/2}^{+h/2} \frac{1}{2}\lambda_{ijkl}\,\left[T_{ij}T_{kl} - \cancelto{0\,\text{odd}}{2z\,\partial_{ij} w T_{kl}} + z^2\,\partial_{ij} w\,\partial_{kl} w\right]\,dz \\ U &= \frac{1}{2}\lambda_{ijkl} T_{ij} T_{kl}\,h + \frac{1}{2}\lambda_{ijkl}\,\frac{h^3}{12}\,\partial_{ij}\,\partial_{kl} \end{aligned}$$

And by using the constitutive law of the material (23), we can contract, in the first term, the λ_{ijkl} and the first T_{kl} tensors into:

$$\lambda_{ijkl}\,T_{kl}\,h = h\,\sigma_{ij} = N_{ij} \tag{36}$$

Which we can directly insert and expanding back the remaining $T_{ij} = \left[\varepsilon_{ij}^0 + \frac{1}{2}\partial_i w\,\partial_j w\right]$ and contracting the second term using our now familiar D_{ijkl}:

$$U[w] = \frac{1}{2}N_{ij}\,\left[\varepsilon_{ij} + \frac{1}{2}\partial_i w\,\partial_j w\right] + \frac{1}{2}D_{ijkl}\,\partial_{ij} w\,\partial_{kl} w \tag{37}$$

And, similarly as before [or by using simpler means of calculation] we can take the derivative with respect to w, to get the restoring force of the membrane:

$$F = -\frac{dU}{dw} = +\frac{1}{2}\partial_j \left(N_{ij}\,\partial_i w\right) - \partial_{kl}\left(D_{ijkl}\,\partial_{ij} w\right) \tag{38}$$

And finally, we can write out the full differential equation, again, adding a pulsed laser force for flavour, using Newton's laws :

$$+\frac{1}{2}\partial_j \left(N_{ij}\,\partial_i w\right) - \partial_{kl}\left(D_{ijkl}\,\partial_{ij} w\right) + A(x,\,y)\cos\left(\omega t\right) = \rho h \partial_{tt} w \tag{39}$$

Compared to the previous expression of (33), the only change is the apparition of the first term. Let us come back to a previous remark, that the first term was a "tension-like" term. Indeed, if we do a little sanity check, by letting our membrane be isotropic and with infinitesimal thickness $h \to 0$, we find the classic d'Alembert equation: if the membrane is isotropic, σ_{ij} reduces to basically just a constant c if we consider no in-plane shear, and if the membrane's thickness becomes vanishingly small then during the integration over h step (and also dividing by h because we don't really have an energy by unit volume anymore), the bending moment term will die because of the h^3 factor in the result.

$$\begin{aligned}
\lim_{h\to 0}\frac{F}{h} &= \lim_{h\to 0}\frac{+\frac{1}{2}\partial_j\left(\sigma_{ij}\,\cancel{h}\,\partial_i w\right) - \partial_{kl}\left(\lambda_{ijkl}\,\frac{\cancel{h}^3}{12}\,\partial_{ij} w\right)}{\cancel{h}} \\
\lim_{h\to 0}\frac{F}{h} = f &= +\frac{1}{2}\partial_j\left(\sigma_{ij}\,\partial_i w\right) - \lim_{h\to 0}\partial_{kl}\left(\lambda_{ijkl}\,\frac{h^2}{12}\,\partial_{ij} w\right) \\
f &= \frac{1}{2} c\,\partial_{ii} w
\end{aligned}$$

Which you can plug into the differential equation, shutting off the laser term I add for flair, to give:

$$\frac{1}{2} c\,\partial_{ii} w = \rho\,\partial_{tt}$$

The expected result for a vibrating thin membrane, or thin rope.

III Laminate von Kármán plates

To build on the previously obtained result, we first need to back-track a little bit. In the case of a laminate plate, where the individual layers are of different material, as is our own situation with 2D heterostructures, we need to specify as many λ_{ijkl} as there are materials. Additionally, the trick we used to use the central symmetry of the plate to rid ourselves of the linear terms in the differential equation does not hold in general for a laminate.

To start, we need to orient properly each layer with respect to the other, if possible. As we are dealing with crystals, it is possible that there exists an anisotropy for the tensor on its λ_{xxxx} and λ_{yyyy}, which deal with the forces on the Cartesian axis. To do this, we simply need to rotate our system such that we are considering the proper stack. To rotate a 4 indices (a (0,4)-form if we want to be exact), we need to multiply it 4 times by the rotation matrix of the transformation:

$$\mathcal{R}_x(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix};\ \mathcal{R}_y(\theta) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix};\ \mathcal{R}_z(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{40}$$

But of course, in our case only the z rotation is relevant for this operation, as we are turning the (xy)-plane to align the crystalline axis. To transform λ_{ijkl} we write:

$$\overline{\lambda_{ijkl}} = [\mathcal{R}_z(\theta)]_{im}[\mathcal{R}_z(\theta)]_{jn}[\mathcal{R}_z(\theta)]_{ko}[\mathcal{R}_z(\theta)]_{lp}\,\lambda_{mnop} \tag{41}$$

This is of course best done with computers, and we assume any sensible person will agree. Let us now consider the a-th layer in the stack which will have, after being rotated to its correct axis, the ELASTICITY TENSOR (20) denoted $\overline{\lambda^{(a)}_{ijkl}}$.

Let us then recall the von Kármán differential equation from before (39), and write it in terms of the bending moment M_{ij}, which we saw previously (32):

$$+\frac{1}{2}\partial_j\left(N_{ij}\,\partial_i w\right) - \partial_{ij}\,M_{ij} + A(x,\,y)\cos\left(\omega t\right) = \rho h \partial_{tt} w$$

To your (I hope), and everyone else's surprise, we are done ! This **is** the differential equation for a laminate plate ! It is however with a heavy heart that I must admit that it isn't the full picture of the horror, as indeed the definitions of both N_{ij} and M_{ij} have stayed the same, but their expression have changed an awful lot. We define, for a N layer laminate:

$$\overline{\sigma^a_{ij}} = \overline{\lambda^a_{ijlk}}\,[\varepsilon^0_{kl} - z\,\partial_{kl} w] \tag{42}$$

$$\overline{N_{ij}} = \int_{-h/2}^{h/2} \sum_{a=0}^{N} \overline{\sigma^a_{ij}}\,dz \tag{43}$$

$$\overline{M_{ij}} = \int_{-h/2}^{h/2} \sum_{a=0}^{N} \overline{\sigma^a_{ij}}\,z\,dz \tag{44}$$

We can swap the sum and the integral easily by changing the boundaries of the integral. Let z_{a-1} and z_a be the z-coordinates of the boundaries of the a-th layer, we can write:

$$\overline{N_{ij}} = \sum_{a=0}^{N} \int_{z_{a-1}}^{z_a} \overline{\sigma^a_{ij}}\,dz$$

$$\overline{M_{ij}} = \sum_{a=0}^{N} \int_{z_{a-1}}^{z_a} \overline{\sigma^a_{ij}}\,z\,dz$$

We can now continue and compute the explicit values of both these tensors for a general case, starting with N_{ij}, the tension like term:

$$\overline{N_{ij}} = \sum_{a=0}^{N} \int_{z_{a-1}}^{z_a} \overline{\sigma^a_{ij}}\,dz$$

$$\overline{N_{ij}} = \sum_{a=0}^{N} \int_{z_{a-1}}^{z_a} \overline{\lambda^a_{ijlk}}\,[\varepsilon^0_{kl} - z\,\partial_{kl} w]\,dz$$

$$\overline{N_{ij}} = \sum_{a=0}^{N} \overline{\lambda^a_{ijlk}} \left[\int_{z_{a-1}}^{z_a} \varepsilon^0_{kl}\,dz - \int_{z_{a-1}}^{z_a} z\,\partial_{kl} w\,dz\right]$$

$$\overline{N_{ij}} = \sum_{a=0}^{N} \overline{\lambda^a_{ijlk}} \left[\varepsilon^0_{kl}(z_{a-1} - z_a) - \partial_{kl} w\left(\frac{z^2_{a-1}}{2} - \frac{z^2_a}{2}\right)\right]$$

And for M_{ij}, the bending moment, we can proceed similarly:

$$\overline{M_{ij}} = \sum_{a=0}^{N} \int_{z_{a-1}}^{z_a} \overline{\sigma_{ij}^a}\, z\, dz$$
$$\overline{M_{ij}} = \sum_{a=0}^{N} \int_{z_{a-1}}^{z_a} \overline{\lambda_{ijlk}^a}\, [\varepsilon_{kl}^0 - z\, \partial_{kl} w] z\, dz$$
$$\overline{M_{ij}} = \sum_{a=0}^{N} \overline{\lambda_{ijlk}^a} \left[\int_{z_{a-1}}^{z_a} \varepsilon_{kl}^0\, z\, dz - \int_{z_{a-1}}^{z_a} \partial_{kl} w\, z^2\, dz \right]$$
$$\overline{M_{ij}} = \sum_{a=0}^{N} \overline{\lambda_{ijlk}^a} \left[\varepsilon_{kl}^0 \left(\frac{z_{a-1}^2}{2} - \frac{z_a^2}{2} \right) - \partial_{kl} w \left(\frac{z_{a-1}^3}{3} - \frac{z_a^3}{3} \right) \right]$$

Here, it is useful to define new terms, to write this in a nicer and cleaner fashion. Doing this also lets us pre-compute these quantities and declutters the differential equation, they are not intrinsic constants of the material but are still specific and unique to each and every plate and should be a function of neither x, y nor t.

$$A_{ijkl} = \sum_{a=0}^{N} \overline{\lambda_{ijlk}^a}\, (z_{a-1} - z_a) \tag{45}$$
$$B_{ijkl} = \sum_{a=0}^{N} \frac{\overline{\lambda_{ijlk}^a}}{2}\, (z_{a-1}^2 - z_a^2) \tag{46}$$
$$C_{ijkl} = \sum_{a=0}^{N} \frac{\overline{\lambda_{ijlk}^a}}{3}\, (z_{a-1}^3 - z_a^3) \tag{47}$$

With this, we can write out our N_{ij} and M_{ij} tensors in a sleek matrix equation:

$$\begin{bmatrix} N_{ij} \\ M_{ij} \end{bmatrix} = \begin{bmatrix} A_{ijkl} & B_{ijkl} \\ B_{ijkl} & C_{ijkl} \end{bmatrix} \begin{bmatrix} T_{kl} \\ -\partial_{kl} w \end{bmatrix} \tag{48}$$

Beyond being a pretty way of writing it, the matrix here illustrates directly one thing and that is that if $B_{ijkl} = 0$ our matrix is diagonal, and by plugging in the numbers of a homogeneous plate, we find ourselves back in a familiar territory (as expected, of course):

$$\begin{bmatrix} N_{ij} \\ M_{ij} \end{bmatrix} = \begin{bmatrix} \overline{\lambda_{ijkl}}\, [h/2 - (-h/2)] & 0 \\ 0 & \frac{\overline{\lambda_{ijkl}}}{3}\, [(h/2)^3 - (-h/2)^3] \end{bmatrix} \begin{bmatrix} T_{kl} \\ -\partial_{kl} w \end{bmatrix} = \begin{bmatrix} \overline{\lambda_{ijkl}}\, h\, T_{kl} \\ -\overline{\lambda_{ijkl}}\, \frac{h^3}{12}\, \partial_{kl} w \end{bmatrix}$$

Which we can easily compare to (37). Why is $B_{ijkl} = 0$ in the case of a homogeneous plate ? Well, it is because a homogeneous plate is symmetric with respect to the middle plane. In such a case, it is easy to see that the definition of B_{ijkl}, which takes the square of the z-coordinates and subtracts them would give 0. In any case, we can write the differential equation for the motion of the plate as:

$$\frac{1}{2} \partial_j [(A_{ijkl}\, T_{kl} - B_{ijkl}\, \partial_{kl} w)\, \partial_i w] - \partial_{ij} [B_{ijkl} T_{kl} - C_{ijkl}\, \partial_{kl} w] = \rho h \partial_{tt} w \tag{49}$$

This differential equation is much meaner and much harder to solve. If we assume no mirror symmetry with respect to the middle plane, the terms in B_{ijkl} remain and this is no longer just an eigenvalue problem. In this case, the plate would no longer have eigenmodes, as the operator applied on w is itself a function of w, in addition, it is also non-linear with a product of the first and the second derivatives of w. To proceed in the numerical resolution, we will need to limit ourselves to symmetric plates. They can be heterogeneous just fine, so long as they are symmetrical.

V
ELASTICITY TENSOR AND ITS SYMMETRIES

I Head-count for our tensor

In (20) we defined a λ_{ijkl} tensor that we then extensively used in the previous section to find equations of motion. We will take a closer look at it now, and see what its components mean and how many of them remain after applying the many symmetries of our crystals. It is our goal to give an applicable blueprint to find steps of calculation for the well known results of other types of crystals should it be needed. First let's recall the definition of the free energy (21):

$$F = \frac{1}{2}\lambda_{ijkl}\, u_{ij}\, u_{kl}$$

We also know that Hooke's law, or the constitutive law, (23) gives:

$$\sigma_{kl} = \lambda_{ijkl}\, u_{ij}$$

From these two equations, and the definition of u_{ij} that is a symmetric tensor, we know that the tensor **has to be left invariant by the following swaps:** $i \longleftrightarrow j$ and $k \longleftrightarrow l$. From these two equations we can also see that the tensor is left invariant by the swap of the **pairs**: $(ij) \longleftrightarrow (kl)$.

In a 3-dimensional space, a tensor of rank 0 (a scalar of course) has 3^0 components, a tensor of rank 1 (a vector) has 3^1 components, a tensor of rank 2 like u_{ij} or σ_{ij} has 3^2 components before symmetry, but of course these two have the added symmetry with respect to the diagonal, and so a quick count lets us see that they have only 6 independent components (4, 10). In matrix formulation it's very obvious:

$$(u) = \begin{bmatrix} u_{xx} & u_{xy} & u_{xz} \\ u_{xy} & u_{yy} & u_{yz} \\ u_{xz} & u_{yz} & u_{zz} \end{bmatrix} \quad ; \quad (\sigma) = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix}$$

And of course, a rank-4 tensor has $3^4 = 81$ components before applying the symmetries. All of what we will do is in reality quite similar to the simple counting we did above. However, the human brain is not very well suited to the visualisation of 4-dimensional objects, and paper even less so, so we will be relying on a few tricks to simplify our calculations. Most of said tricks will be to change the vector space we are looking at whenever convenient, as for instance, we can see the tensor as having at once $9{\cdot}9$ components or $27{\cdot}3$ or any such combination, instead of 3^4.

II First symmetry: $i \longleftrightarrow j$

Let us first fix the pair (kl) to be constant; we are brought down to a sub-space of the full tensor. This is simply a $3{\times}3$ matrix with nine components. We can write it, applying directly the symmetry with respect to the diagonal, and we see only six independent terms:

$$(\lambda_{kl}) = \begin{bmatrix} (\lambda_{kl})_{xx} & (\lambda_{kl})_{xy} & (\lambda_{kl})_{xz} \\ (\lambda_{kl})_{xy} & (\lambda_{kl})_{yy} & (\lambda_{kl})_{yz} \\ (\lambda_{kl})_{xz} & (\lambda_{kl})_{yz} & (\lambda_{kl})_{zz} \end{bmatrix}$$

Of course this is an expected result; it follows simply from the previous u_{ij} and σ_{ij} matrices. By applying this first symmetry, our tensor was reduced to $6 \times 9 = 54$ independent components! Obviously this works similarly by fixing (ij) and looking at the other sub-space. We have reduced our tensor from $3 \times 3 \times 3 \times 3 = 81 \to 6 \times 6 = 36$ independent components.

III Second symmetry: $(ij) \longleftrightarrow (kl)$, Voigt notation

The Voigt notation expresses our u_{ij} tensor as a six-component vector in the following fashion:

$$(u) = \begin{bmatrix} u_{xx} & u_{xy} & u_{xz} \\ u_{xy} & u_{yy} & u_{yz} \\ u_{xz} & u_{yz} & u_{zz} \end{bmatrix} \longrightarrow \mathbf{u} = \begin{bmatrix} u_{xx} \\ u_{yy} \\ u_{zz} \\ u_{yz} \\ u_{xz} \\ u_{xy} \end{bmatrix} \tag{50}$$

By ridding ourselves of the redundant terms and arranging this matrix into a vector, we have both saved ourselves a few calculations in the matrix multiplication and also made the problem easier to visualise. Using the Voigt notation changes the vector space that we are working in from a tensor product of four three-dimensional spaces to a tensor product of two copies of the 6-dimensional space of symmetric second-order tensors. This means simply that we can rewrite (without loss of information!) Hooke's law (23), for instance, as:

$$\sigma_{ij} = \lambda_{ijkl}\, u_{kl} \longrightarrow \sigma_P = \lambda_{PQ}\, u_Q \tag{51}$$

If we carefully assign each pair of indices (ij) a number we can write the full λ_{PQ} tensor as a matrix, and by applying the symmetry with respect to the diagonal we can again count the independent components.

Pairs	$\longleftrightarrow$	Voigt index
(xx)	$\longleftrightarrow$	1
(yy)	$\longleftrightarrow$	2
(zz)	$\longleftrightarrow$	3
(yz)	$\longleftrightarrow$	4
(xz)	$\longleftrightarrow$	5
(xy)	$\longleftrightarrow$	6

Table 1 Assignment of axis pairs to Voigt indices

With this we can write the λ tensor in a more readable, reduced (but still complete) form:

$$(\lambda) = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} & \lambda_{15} & \lambda_{16} \\ \lambda_{12} & \lambda_{22} & \lambda_{23} & \lambda_{24} & \lambda_{25} & \lambda_{26} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & \lambda_{34} & \lambda_{35} & \lambda_{36} \\ \lambda_{14} & \lambda_{24} & \lambda_{34} & \lambda_{44} & \lambda_{45} & \lambda_{46} \\ \lambda_{15} & \lambda_{25} & \lambda_{35} & \lambda_{45} & \lambda_{55} & \lambda_{56} \\ \lambda_{16} & \lambda_{26} & \lambda_{36} & \lambda_{46} & \lambda_{56} & \lambda_{66} \end{bmatrix} \tag{52}$$

Now, it's rather easy to just count the number of independent components, but being lazy physicists, we can instead notice that this is just the trick used by Gauss to count the sum of the numbers from 1 to n, with n being the size of the space or subspace. Let us illustrate:

$$(\lambda) = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} & \lambda_{15} & \lambda_{16} \\ \lambda_{12} & \lambda_{22} & \lambda_{23} & \lambda_{24} & \lambda_{25} & \lambda_{26} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & \lambda_{34} & \lambda_{35} & \lambda_{36} \\ \lambda_{14} & \lambda_{24} & \lambda_{34} & \lambda_{44} & \lambda_{45} & \lambda_{46} \\ \lambda_{15} & \lambda_{25} & \lambda_{35} & \lambda_{45} & \lambda_{55} & \lambda_{56} \\ \lambda_{16} & \lambda_{26} & \lambda_{36} & \lambda_{46} & \lambda_{56} & \lambda_{66} \end{bmatrix}$$

Of course, the first line of n is all independent components, the second line has $n-1$ independent components because of the terms is already repeated, and so on, so we are indeed calculating:

$$\text{Number of terms} = n + (n-1) + \cdots + 2 + 1$$

The trick, for those who have not used it in a long while, to find the general formula here is to double the sum on each side and to pair terms together:

$$\begin{aligned}
\text{Number of terms} &= n + (n-1) + \cdots + 2 + 1 \\
2 \cdot \text{Number of terms} &= n + (n-1) + \cdots + 2 + 1 \quad + \quad n + (n-1) + \cdots + 2 + 1 \\
2 \cdot \text{Number of terms} &= \underbrace{n+1}_{n+1} + \underbrace{(n-1)+2}_{n+1} + \cdots + \underbrace{2+(n-1)}_{n+1} + \underbrace{1+n}_{n+1} \\
2 \cdot \text{Number of terms} &= \underbrace{(n+1) + (n+1) + \cdots + (n+1) + (n+1)}_{n} \\
2 \cdot \text{Number of terms} &= n \cdot (n+1) \\
\text{Number of terms} &= \frac{n \cdot (n+1)}{2}
\end{aligned}$$

If we apply it here to our (λ) matrix, we get $\frac{6(6+1)}{2} = 21$ independent components. We can also use the formula for the 3×3 subspaces, where we have $\frac{3(3+1)}{2} = 6$, which is what we counted.

So, applying the symmetries on the swap of the indices, we can reduce the number of independent components in the tensor from 81 to 21, which is then the **maximum** number possible. But these symmetries are not all the symmetries present in materials, indeed, any textbook or general Wikipedia page will inform that the point groups associated with the Bravais cells in crystal reduce further the number of independent components. Here is the table, taken and expanded from Landau[1].

Crystal family	Point groups	Independent components
Triclinic	C_1, C_i	21
Monoclinic	C_2, C_s, C_{2h}	13
Orthorhombic	D_2, C_{2v}, D_{2h}	9
Tetragonal	C_4, S_4, C_{4h}	7
Tetragonal	C_{4v}, D_{2d}, D_4, D_{4h}	6
Rhombohedral	C_3, S_6	7
Rhombohedral	C_{3v}, D_3, D_{3d}	6
Hexagonal	C_6, C_{6h}, D_6, C_{6v}, D_{6h}	5
Cubic	T, T_h, O, T_d, O_h	3

Table 2 Number of independent components by crystal type.

IV Third symmetry: Monoclinic crystal

Let us take an example that is relevant to our systems, the case of $FePS_3$. The crystal is monoclinic and so belongs to the $2/m$ point group. In practice it means that: a rotation of 180° around one axis leaves the crystal invariant, a reflection about the plane orthogonal to the previous rotation axis leaves the crystal invariant, and an inversion of all the coordinates also leaves the crystal unchanged (in bulk at least). Making the **choice** to have the x-axis align with the a-axis in the crystal, and the y-axis with the b-axis, we can associate a matrix with each of the different symmetries, representing the group in 3D space. The matrices for the group $C_{2h} : \{\mathcal{G} \,|\, E,\, i,\, \sigma_h,\, C_2\}$ can be written:

[1] Landau & Lifshitz, Volume 7, 1970

$$(E) = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1 \end{bmatrix} \quad ; \quad (i) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$
$$(\sigma_h) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1 \end{bmatrix} \quad ; \quad (C_2) = \begin{bmatrix} +1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{53}$$

Now however, we are not working with a 3D but with our Voigt notation to make the visualisation possible, so let's see how we can transform our transformations into the appropriate space. Let's recall (41), a rank n tensor transforms with n matrix multiplication of the proper application, such that, with $\mathcal{R}$ being any application:

$$\varepsilon'_{ij} = \mathcal{R}_{ik}\mathcal{R}_{jl}\,\varepsilon_{kl} \tag{54}$$

$$\lambda'_{ijkl} = \mathcal{R}_{im}\mathcal{R}_{jn}\mathcal{R}_{ko}\mathcal{R}_{lp}\,\lambda_{mnop} \tag{55}$$

And, using Voigt notation, we write the same transformation using an $\mathcal{L}$ application that such that:

$$\varepsilon'_{P} = \mathcal{L}_{PQ}\,\varepsilon_{Q} \tag{56}$$

$$\lambda'_{PQ} = \mathcal{L}_{PR}\mathcal{L}_{QS}\,\lambda_{RS} \tag{57}$$

While there **are** far cleverer methods to obtain $\mathcal{L}$ as a function of $\mathcal{R}$, the more visual way of writing it is perhaps to simply brute force the calculation in (54) and shoe-horn it into (56), giving us:

$$\begin{aligned}
\varepsilon'_{xx} &= \mathcal{R}^2_{xx}\,\varepsilon_{xx} + \mathcal{R}^2_{xy}\,\varepsilon_{yy} + \mathcal{R}^2_{xz}\,\varepsilon_{zz} + 2\,\mathcal{R}_{xx}\mathcal{R}_{xy}\,\varepsilon_{xy} + 2\,\mathcal{R}_{xx}\mathcal{R}_{xz}\,\varepsilon_{xz} + 2\,\mathcal{R}_{xy}\mathcal{R}_{xz}\,\varepsilon_{yz} \\
\varepsilon'_{yy} &= \mathcal{R}^2_{yx}\,\varepsilon_{xx} + \mathcal{R}^2_{yy}\,\varepsilon_{yy} + \mathcal{R}^2_{yz}\,\varepsilon_{zz} + 2\,\mathcal{R}_{yx}\mathcal{R}_{yy}\,\varepsilon_{xy} + 2\,\mathcal{R}_{yx}\mathcal{R}_{yz}\,\varepsilon_{xz} + 2\,\mathcal{R}_{yy}\mathcal{R}_{yz}\,\varepsilon_{yz} \\
\varepsilon'_{zz} &= \mathcal{R}^2_{zx}\,\varepsilon_{xx} + \mathcal{R}^2_{zy}\,\varepsilon_{yy} + \mathcal{R}^2_{zz}\,\varepsilon_{zz} + 2\,\mathcal{R}_{zx}\mathcal{R}_{zy}\,\varepsilon_{xy} + 2\,\mathcal{R}_{zx}\mathcal{R}_{zz}\,\varepsilon_{xz} + 2\,\mathcal{R}_{zy}\mathcal{R}_{zz}\,\varepsilon_{yz} \\
\varepsilon'_{yz} &= \mathcal{R}_{yx}\mathcal{R}_{zx}\,\varepsilon_{xx} + \mathcal{R}_{yy}\mathcal{R}_{zy}\,\varepsilon_{yy} + \mathcal{R}_{yz}\mathcal{R}_{zz}\,\varepsilon_{zz} + \big(\mathcal{R}_{yx}\mathcal{R}_{zy} + \mathcal{R}_{yy}\mathcal{R}_{zx}\big)\varepsilon_{xy} \\
&\quad + \big(\mathcal{R}_{yx}\mathcal{R}_{zz} + \mathcal{R}_{yz}\mathcal{R}_{zx}\big)\varepsilon_{xz} + \big(\mathcal{R}_{yy}\mathcal{R}_{zz} + \mathcal{R}_{yz}\mathcal{R}_{zy}\big)\varepsilon_{yz} \\
\varepsilon'_{xz} &= \mathcal{R}_{xx}\mathcal{R}_{zx}\,\varepsilon_{xx} + \mathcal{R}_{xy}\mathcal{R}_{zy}\,\varepsilon_{yy} + \mathcal{R}_{xz}\mathcal{R}_{zz}\,\varepsilon_{zz} + \big(\mathcal{R}_{xx}\mathcal{R}_{zy} + \mathcal{R}_{xy}\mathcal{R}_{zx}\big)\varepsilon_{xy} \\
&\quad + \big(\mathcal{R}_{xx}\mathcal{R}_{zz} + \mathcal{R}_{xz}\mathcal{R}_{zx}\big)\varepsilon_{xz} + \big(\mathcal{R}_{xy}\mathcal{R}_{zz} + \mathcal{R}_{xz}\mathcal{R}_{zy}\big)\varepsilon_{yz} \\
\varepsilon'_{xy} &= \mathcal{R}_{xx}\mathcal{R}_{yx}\,\varepsilon_{xx} + \mathcal{R}_{xy}\mathcal{R}_{yy}\,\varepsilon_{yy} + \mathcal{R}_{xz}\mathcal{R}_{yz}\,\varepsilon_{zz} + \big(\mathcal{R}_{xx}\mathcal{R}_{yy} + \mathcal{R}_{xy}\mathcal{R}_{yx}\big)\varepsilon_{xy} \\
&\quad + \big(\mathcal{R}_{xx}\mathcal{R}_{yz} + \mathcal{R}_{xz}\mathcal{R}_{yx}\big)\varepsilon_{xz} + \big(\mathcal{R}_{xy}\mathcal{R}_{yz} + \mathcal{R}_{xz}\mathcal{R}_{yy}\big)\varepsilon_{yz}
\end{aligned}$$

We immediately see that this is again just a linear system, and so we can use the colour highlights to build the 6×6 matrix in Voigt notation that corresponds to the transformation:

$$(\mathcal{L}) = \begin{bmatrix}
\mathcal{R}^2_{xx} & \mathcal{R}^2_{xy} & \mathcal{R}^2_{xz} & 2\mathcal{R}_{xy}\mathcal{R}_{xz} & 2\mathcal{R}_{xx}\mathcal{R}_{xz} & 2\mathcal{R}_{xx}\mathcal{R}_{xy} \\
\mathcal{R}^2_{yx} & \mathcal{R}^2_{yy} & \mathcal{R}^2_{yz} & 2\mathcal{R}_{yy}\mathcal{R}_{yz} & 2\mathcal{R}_{yx}\mathcal{R}_{yz} & 2\mathcal{R}_{yx}\mathcal{R}_{yy} \\
\mathcal{R}^2_{zx} & \mathcal{R}^2_{zy} & \mathcal{R}^2_{zz} & 2\mathcal{R}_{zy}\mathcal{R}_{zz} & 2\mathcal{R}_{zx}\mathcal{R}_{zz} & 2\mathcal{R}_{zx}\mathcal{R}_{zy} \\
\mathcal{R}_{yx}\mathcal{R}_{zx} & \mathcal{R}_{yy}\mathcal{R}_{zy} & \mathcal{R}_{yz}\mathcal{R}_{zz} & \mathcal{R}_{yy}\mathcal{R}_{zz}+\mathcal{R}_{yz}\mathcal{R}_{zy} & \mathcal{R}_{yx}\mathcal{R}_{zz}+\mathcal{R}_{yz}\mathcal{R}_{zx} & \mathcal{R}_{yx}\mathcal{R}_{zy}+\mathcal{R}_{yy}\mathcal{R}_{zx} \\
\mathcal{R}_{xx}\mathcal{R}_{zx} & \mathcal{R}_{xy}\mathcal{R}_{zy} & \mathcal{R}_{xz}\mathcal{R}_{zz} & \mathcal{R}_{xy}\mathcal{R}_{zz}+\mathcal{R}_{xz}\mathcal{R}_{zy} & \mathcal{R}_{xx}\mathcal{R}_{zz}+\mathcal{R}_{xz}\mathcal{R}_{zx} & \mathcal{R}_{xx}\mathcal{R}_{zy}+\mathcal{R}_{xy}\mathcal{R}_{zx} \\
\mathcal{R}_{xx}\mathcal{R}_{yx} & \mathcal{R}_{xy}\mathcal{R}_{yy} & \mathcal{R}_{xz}\mathcal{R}_{yz} & \mathcal{R}_{xy}\mathcal{R}_{yz}+\mathcal{R}_{xz}\mathcal{R}_{yy} & \mathcal{R}_{xx}\mathcal{R}_{yz}+\mathcal{R}_{xz}\mathcal{R}_{yx} & \mathcal{R}_{xx}\mathcal{R}_{yy}+\mathcal{R}_{xy}\mathcal{R}_{yx}
\end{bmatrix} \tag{58}$$

Since our symmetry matrices are all diagonal, we have coloured all such terms. In the general case, more terms survive, but in our special case of a monoclinic crystal we see only diagonal terms remain here again.

Plugging in the expressions of $\mathcal{R}$ we have, we get the following results:

$$\mathcal{L}^{(E)} = \text{diag}(+1,+1,+1,+1,+1,+1) \tag{59}$$
$$\mathcal{L}^{(i)} = \text{diag}(+1,+1,+1,+1,+1,+1) \tag{60}$$
$$\mathcal{L}^{(\sigma_h)} = \text{diag}(+1,+1,+1,+1,-1,-1) \tag{61}$$
$$\mathcal{L}^{(C_2)} = \text{diag}(+1,+1,+1,+1,-1,-1) \tag{62}$$

And so, finally we can carry out the last matrix multiplication to get the fully reduced form of our tensor λ_{ijkl} in the Voigt notation, we need to apply each symmetry and see what terms are removed or made dependent on other terms. We set the transformed tensor equal to the untransformed tensor:

$$\lambda'_{PQ} = \mathcal{L}_{PR}\mathcal{L}_{QS}\,\lambda_{RS} = \lambda_{PQ} \tag{63}$$

Since the matrices are diagonal, we don't need to worry about taking their transpose or any such, and we can simply do the matrix multiplication, which is an easy thing to do, and with it done we get the following:

$$(\lambda') = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} & -\lambda_{15} & -\lambda_{16} \\ \lambda_{12} & \lambda_{22} & \lambda_{23} & \lambda_{24} & -\lambda_{25} & -\lambda_{26} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & \lambda_{34} & -\lambda_{35} & -\lambda_{36} \\ \lambda_{14} & \lambda_{24} & \lambda_{34} & \lambda_{44} & -\lambda_{45} & -\lambda_{46} \\ -\lambda_{15} & -\lambda_{25} & -\lambda_{35} & -\lambda_{45} & \lambda_{55} & \lambda_{56} \\ -\lambda_{16} & -\lambda_{26} & -\lambda_{36} & -\lambda_{46} & \lambda_{56} & \lambda_{66} \end{bmatrix} \tag{64}$$

Which we set equal to the original λ_{PQ} matrix from before (52)

$$\begin{bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} & -\lambda_{15} & -\lambda_{16} \\ \lambda_{12} & \lambda_{22} & \lambda_{23} & \lambda_{24} & -\lambda_{25} & -\lambda_{26} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & \lambda_{34} & -\lambda_{35} & -\lambda_{36} \\ \lambda_{14} & \lambda_{24} & \lambda_{34} & \lambda_{44} & -\lambda_{45} & -\lambda_{46} \\ -\lambda_{15} & -\lambda_{25} & -\lambda_{35} & -\lambda_{45} & \lambda_{55} & \lambda_{56} \\ -\lambda_{16} & -\lambda_{26} & -\lambda_{36} & -\lambda_{46} & \lambda_{56} & \lambda_{66} = \end{bmatrix} = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} & +\lambda_{15} & +\lambda_{16} \\ \lambda_{12} & \lambda_{22} & \lambda_{23} & \lambda_{24} & +\lambda_{25} & +\lambda_{26} \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & \lambda_{34} & +\lambda_{35} & +\lambda_{36} \\ \lambda_{14} & \lambda_{24} & \lambda_{34} & \lambda_{44} & +\lambda_{45} & +\lambda_{46} \\ +\lambda_{15} & +\lambda_{25} & +\lambda_{35} & +\lambda_{45} & \lambda_{55} & \lambda_{56} \\ +\lambda_{16} & +\lambda_{26} & +\lambda_{36} & +\lambda_{46} & \lambda_{56} & \lambda_{66} \end{bmatrix}$$

And obviously, all the terms in colour have to be equal to 0 for the symmetries to hold true. So this gives us, finally, the full λ_{PQ} tensor for a monoclinic tensor. A quick count of the number of remaining, independent coefficients give us, as tabulated in (Table 2), 13 coefficients. To compute or find them, we can rely either on experimental data, usually in the bulk crystals, or using DFT for the monolayer limit. For DFT, one would use the equation (20), inducing a deformation in the lattice and seeing the change in energy.

$$(\lambda^{FePS_3}) = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} & \lambda_{14} & 0 & 0 \\ \lambda_{12} & \lambda_{22} & \lambda_{23} & \lambda_{24} & 0 & 0 \\ \lambda_{13} & \lambda_{23} & \lambda_{33} & \lambda_{34} & 0 & 0 \\ \lambda_{14} & \lambda_{24} & \lambda_{34} & \lambda_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \lambda_{55} & \lambda_{56} \\ 0 & 0 & 0 & 0 & \lambda_{56} & \lambda_{66} \end{bmatrix} \tag{65}$$

PART III

Numerical Resolution

VI
RESOLUTION METHODS

Our goal should now be to apply our theory to real situations. Along the previous developments, we came out with a couple of models, each of them adding a layer of depth onto the previous one.

The first equation we saw is the von Kármán differential equation (39) which takes into account the pre-stress N_{ij} and elasticity D_{ijkl}, both deriving from the stiffness λ_{ijkl} as (29) & $N_{ij} = h\lambda_{ijkl}T_{kl} = h\lambda_{ijkl}\left[\varepsilon^0_{ij} + \frac{1}{2}\partial_i w\,\partial_j w\right]$... We will assume we know λ_{ijkl} at the temperature of study, and we now want to solve the vibration of our sample according to its material characteristics. For example, the $FePS_3$ at room temperature and in GPa table is :

$$(\lambda^{FePS_3}) = \begin{bmatrix} 120.5 & 34.1 & 5.7 & 0.85 & 0 & 0 \\ 34.1 & 119.8 & 5.3 & -1.55 & 0 & 0 \\ 5.7 & 5.3 & 28.4 & -0.05 & 0 & 0 \\ 0.85 & -1.55 & -0.05 & 1.18 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9.88 & -1.05 \\ 0 & 0 & 0 & 0 & -1.05 & 1.68 \end{bmatrix} \tag{66}$$

I Assuming homogeneous strain

The first goal is not to solve the von Kármán differential equation in time, but to find the eigenmodes of w following this equation, derived from (39) :

$$\frac{1}{2}N_{ij}\partial_{ij}w - D_{ijkl}\partial_{ijkl}w = \rho h\partial_{tt}w \tag{67}$$

as N_{ij} and D_{ijkl} are supposed to be constant. What allows us to say that w will oscillate along specific eigenmodes is that we can rearrange the previous equation as an eigenvalue equation :

$$Kw = \omega^2 w \tag{68}$$

with :

$$K = \frac{1}{\rho h}(\frac{1}{2}N_{ij}\partial_{ij} - D_{ijkl}\partial_{ijkl}) \tag{69}$$

So now we just have to *build* K and solve the eigen-w and their eigenfrequencies.

To do that we will use finite elements techniques by dividing w as a pixelated map. By the way, this will enable us to apply different masks to w to emulate the *real* shapes of the holes. So now w is like a $(N \times N)$ matrix. But we cannot solve (68) with a square matrix w, so we *flatten* it to a $(1 \times N^2)$ vector (by slicing it horizontally !).

Now, time to build K! Let us imagine w is (originally) only one $(N \times 1)$ vertical *slice*. With that in mind, one can easily figure out that the ∂_x matrix takes the following shape :

$$(\partial) = \frac{1}{2dx}\begin{bmatrix} -2 & 2 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & -2 & 2 \end{bmatrix} \tag{70}$$

with a $(-1, 0, 1)$ diagonal. And the same for (∂^2) with a $(1, -2, 1)$ diagonal, (∂^3) with a $(-1, 2, -2, 1)$ diagonal, and (∂^4) with a $(1, -4, 6, -4, 1)$ diagonal. Now to forge the hyper-derivation matrix applying on the $(1 \times N^2)$ w vector, you can convince yourself that it comes down to using a

Kronecker product ! So for example : $(\partial_{xxxy}) = (\partial^3) \otimes (\partial\,)$. In general, with $x \equiv 0$ and $y \equiv 1$, we can write $(\partial_{ijkl}) = (\partial^{i+j+k+l}) \otimes (\partial^{4-i-j-k-l})$.

So now, to build simply need to do the (69) Einstein summation ! And then we use a simple solver to get the eigen-everything. Note that it is at this step that we can apply our mask. This mask is just a boolean $(N \times N)$, so now $(1 \times N^2)$, array, and what we do is to simply remove the n False-value cells out of K, which will yield $(1 \times N^2 - n)$ eigen-vectors which you can patch to a fresh $(N \times N)$ zero-matrix to find the final result.

II With non-homogeneous strain

Now let's assume that there is an uneven strain over the membrane. This is described by the equation (49) based on the definition of (41). We will assume that $B_{ijkl} = 0$ to overcome non linearity issues – which would make the search of some kind of eigenmodes meaningless. This case actually happens when our sample is symmetric along z (eg. A-B-C-B-A) which we will assume. With that, those equations can be reformulated as :

$$K = \frac{1}{\rho h}\Big(\frac{1}{2}A_{ijkl}\underbrace{\partial_j e_{kl}(x,y)\partial_i}_{\big(\partial_j e_{kl}(x,y)\big)\partial_i + e_{kl}(x,y)\partial_{ij}} + C_{ijkl}\partial_{ijkl}\Big) \tag{71}$$

with :

$$A_{ijkl} = \sum_{a=0}^{N} \lambda^a_{ijlk}\,(z_{a-1} - z_a) \tag{72}$$

$$C_{ijkl} = \sum_{a=0}^{N} \frac{\lambda^a_{ijlk}}{3}\,(z^3_{a-1} - z^3_a) \tag{73}$$

$$\rho h = \sum_{a=0}^{N} \rho_a h_a \tag{74}$$

and :

$$(e)(x,y) = \begin{bmatrix} \cos^2\theta & \sin\theta\cos\theta \\ \sin\theta\cos\theta & \sin^2\theta \end{bmatrix} \frac{r^2}{L^2} 4\epsilon_{\max} \tag{75}$$

which is simply constructed on our *pixelated* $(N \times N)$ grid. Then we compute its gradient along x and y to obtain the $(\partial_j e)(x,y)$ matrix, and finally we flatten everything as $(1 \times N^2)$ and use the matrix product with the same derivative matrices we used in the first part. The resolution of K also follows the same process as in the first part.

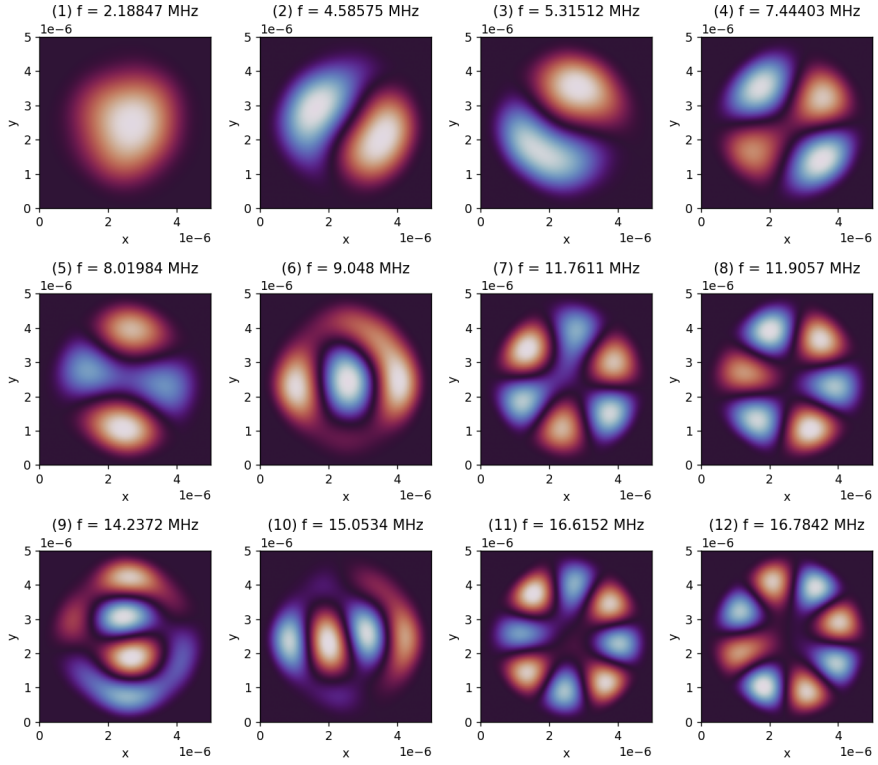

FIG. ii 9 $FePS_3$ layers – real hole shape – $N = 100$ – $\epsilon_{\max} = 0.01\%$

VII
HOW TO USE THE CODE?

Everything can be found on **this repository**. There is all the code and the hole masks in a separate folder.

Basically, all the functions can be found in the `integrator.py` which works as a *module* file. Then the files `integrator1-1b-2-3.py` import it to use these functions differently, with `integrator3.py` as the most advanced one using non-homogenous strain (so the one you should use). `integrator3b.py` serves to create a fancy 3D matplotlib animation of the membrane after executing `integrator3.py`.

Inside `integrator.py` you may find some λ_{ijkl} values found online in the `Lambda_val` dictionary, as well as density ρ, thickness h and gap size with the `rho_val`, `h_val` and `gap_val` dictionaries. Then there is a bunch of functions, first to compute the K matrix we want to solve, for different cases and assumptions, the ones which create the masks, the animation, and finally the proper function which solves K.

Assuming you use `integrator3.py` you can tweak the length `L` of the membrane, the size `N` of the finite-element grid we use, the types of layers of the membrane `layer_materials` (succession of the names of those layers, found in `Lambda_val`) and `eps_max`. Then you choose your mask, `meb_good100.png` is our most spherical hole using `N=100` but you can use other masks, or even shapes by choosing something different than `"image"`. And that's it.