Chapter 1

Force detection with nanowires

This chapter aims to provide a general background of theoretical notions and methods involved in the experiments presented later on in this thesis. In the main framework of force detection using a nanowire (NW) as mechanical resonator, we first provide an analytical model for vibrations of singly-clamped beams, deriving the normal equations of motion to model the NW's dynamics and introducing their bi-dimensional character. We discuss the main limitation to mechanical force sensing and their origin. Thereafter, the light-nanowire interaction, which allows the optical detection of NWs is presented. Finally, we briefly describe the fabrication method of the GaAs NWs used in our force sensing applications.

1.1 Mechanics of nanowires

In this thesis we will focus only on the flexural (transverse) vibrational modes, and specifically on the *fundamental transverse mode*, which is the mechanical mode with the lowest frequency and stiffness, ideal for force sensing applications. In fact, a NW is highly sensitive to the lateral components of a force, specially when on resonance. In beams with high aspect ratio, resonances of bending modes are much more accessible and force-'sensitive' than the other mechanical modes. Specifically, torsional modes and longitudinal (axial or 'breathing') modes related to axial forces causing a compression/extension of the NW.

1.1.1 Flexural vibration of a beam

The mechanics and governing equation of a NW in pure bending are accurately described by the Euler-Bernoulli beam theory, formulated in the mid-18th century. Also known as thin beam theory, it is applicable to beams for which the length L is much larger than the depth (at least by a factor 10) and for small deflections compared to the depth. Under these conditions, the following assumptions are valid and simplify the physical description:

1. the rotation of cross sections of the beam is neglected compared to the translation (i.e. the effects of the rotatory inertia are neglected compared with those of the linear inertia);

2. the angular distortion due to shear is considered negligible compared to the bending deformation. The rotation is such that the cross-sections do not deform and remain orthogonal to the center axis (pure bending). Hence, shear force is only produced by the bending moment.

Constitutive and kinematical relations By choosing a proper coordinate system, it is possible to reduce the problem of a three-dimensional body under bending to the a 1-D representation. The origin of the reference has to be placed at the center of mass of the cross-section[1] with the so-called *neutral axis* being orthogonal to it; in this way, a normal force N causes only strain [2] and no curvature (i.e. no moment). The stress applied to the side the structure causes a linear variation of the axial strain ϵ_{zz}, which is statically equivalent to only a moment and null at the neutral axis. The normal stress acting on a cross-section is in turn equivalent to a resultant normal force N along z and a moment M in the xy-plane [36]. Moreover, by arbitrarily orienting the xy reference axes on the cross-section, the *constitutive equation for bending* relates the moment M to the beam's curvature κ via the bending stiffness tensor as:

$$\begin{bmatrix} M_x \\ M_y \end{bmatrix} = - \begin{bmatrix} E_Y I_x & E_Y I_{xy} \\ E_Y I_{yx} & E_Y I_y \end{bmatrix} \begin{bmatrix} \kappa_x \\ \kappa_y \end{bmatrix} \tag{1.1}$$

where E_Y is Young's elastic modulus for the beam, I_x and I_y are the cross-sectional area moment of inertia[3] and $I_{xy} = I_{yx}$ is the product moment of area[4]. For any geometry, it is possible to diagonalize the system and obtain two directions for x and y which are *principal axes* of the second moment of area and in respect of which bending moments are fully uncoupled.

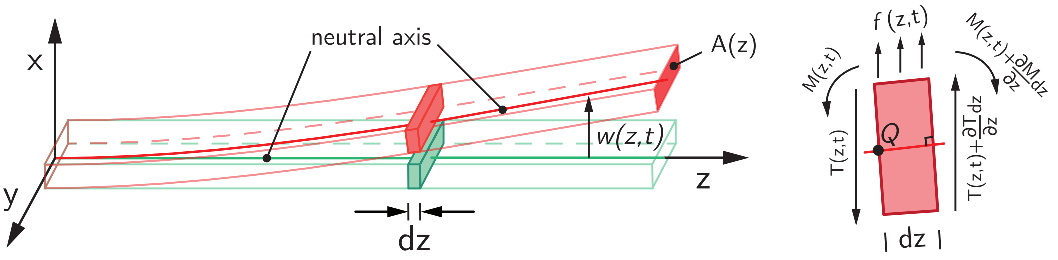

FIGURE 1.1 | **Singly-clampled beam in pure bending.**
On the left: a beam of length L and cross-sectional area $A(z) \ll L^2$. It is oriented along its principal axes x and y with the neutral axis coincident with the z-axis, at rest (in green). In red, bent beam under an homogeneous load along x, with displacement amplitude $w(z,t) \ll L$. On the right: a force and momentum balance for an infinitesimal section $dz \times A(z)$ at the point Q on the neutral axis.

With a beam in such coordinate system sketched in Fig. 1.1, we derive the beam equation for a bending moment M_y along the y-axis causing a transverse displacement $w(z,t)$ of the neutral axis in the x direction.
For pure bending we just have

$$M_y(z,t) = -E_Y I_y \kappa_y \simeq -E_Y I_y(z) \frac{\partial^2 w(z,t)}{\partial z^2} \tag{1.2}$$

where the curvature κ_y can be approximated by the second derivative of the displacement for small and smooth deflections.

It is intuitive to derive the equation of motion through expression of local equilibrium, considering the bending and shear resultants $M(z,t)$ and $T(z,t)$, respectively,

[1] $(x_0, y_0) = \frac{1}{\int_A dA} \left(\int_A x dA, \int_A y dA \right)$
[2] $N = E_Y A \epsilon_{zz}$
[3] $I_x = \int_A y^2 dA, I_y = \int_A x^2 dA$
[4] $I_{xy} = I_{yx} = \int_A xy dA$

on an infinitesimal beam's segment subjected to a distributed vertical load $f(z,t)$. In the limit of $dz \to 0$, the moment balance – neglecting rotatory inertia under Bernoulli's beam assumptions – gives

$$T(z,t) = -\frac{\partial M_y(z,t)}{\partial z} \; , \tag{1.3}$$

while the transverse force balance has to be equal to the element's inertial force gives $f(z,t) - \partial T(z,t)/\partial z = \rho A(z)\ddot{w}(z,t)$. The latter, by means of Eqs. (1.2) and (1.3), is expressed in terms of the displacement and applied load

$$\rho A(z)\frac{\partial^2 w(z,t)}{\partial t^2} + \frac{\partial^2}{\partial z^2}\left[E_Y I_y(z)\frac{\partial^2 w(z,t)}{\partial z^2}\right] = f(z,t) \tag{1.4}$$

where $\rho A(z)$ is mass per unit length. The beam's density ρ as well as the Young's modulus E_Y are assumed constant under the hypothesis of homogeneous beam.

Free vibration of the beam To calculate the characteristic modes of vibration of the beam, we need to study the free evolution of the system in absence of an applied external force, i.e. $f(z,t) = 0$. Assuming that the cross-section shape and area $A(z)$ remain constant over the beam length, also the bending stiffness $E_Y I_y$ will be constant and the equation of motion reduces to

$$\rho A\frac{\partial^2 w(z,t)}{\partial t^2} + E_Y I_y\frac{\partial^4 w(z,t)}{\partial z^4} = 0 \tag{1.5}$$

This equation can be solved by separation of variables using a Fourier decomposition of the displacement $w(z,t)$ into the sum of harmonic vibrations:

$$w(z,t) = \sum_{n=0}^{\infty} \mathbb{R}(w_n(z)e^{-i\omega_n t}) \tag{1.6}$$

where $\mathbb{R}(\cdots)$ refers to the real part of the quantity in parentheses, $w_n(z)$ describes the shape and amplitude of the bending and $e^{-i\omega_n t}$ accounts for the oscillatory temporal evolution. Being NWs highly under-damped resonators, the motion damping term $\Gamma_n \dot{w}$ is neglected for the moment. The separation ansatz leads to a spatial equation in the form of

$$\frac{d^4 w_n(z)}{dz^4} - \frac{\beta_n^4}{L^4}w_n(z) = 0 \quad \text{with} \quad \beta_n = L\left(\omega_n^2\frac{\rho A}{E_Y I_y}\right)^{\frac{1}{4}} \tag{1.7}$$

which admits an infinite number of solutions $w_n(z)$ (i.e. n^{th} flexural mode), each of them vibrating at a distinct eigenfrequency ω_n of the system. We expressed the parameter β_n as a dimensionless quantity to simplify and clarify the calculations. The dispersion relation for β_n in equation (1.7), relates the geometrical and structural properties of the cantilever to its eigenfrequencies, which can be calculated as:

$$f_n = \frac{\omega_n}{2\pi} = \frac{1}{2\pi}\frac{\beta_n^2}{L^2}\sqrt{\frac{E_Y I_y}{\rho A}} \tag{1.8}$$

Mode n	β_n	ω_n/ω_0
0	1.875	1
1	4.694	6.267
2	7.855	17.547
3	10.996	34.386
$n \geq 3$	$(n+1/2)\pi$	$[(n+1/2)\pi/\beta_0]^2$

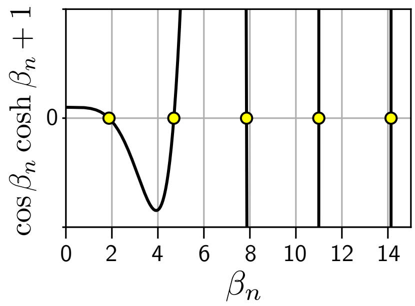

TABLE 1.1 | **Solutions of the dispersive equation**
Values of β_n and of the normalized eigenfrequencies to the fundamental ω_0. For $n \geq 3$, the asymptotic values can be expressed in closed form [37].

The lowest frequency f_0 is referred to as the *fundamental frequency*.
The differential equation (1.7) has a general solution expressed as:

$$w_n(z) = A_n \cos\left(\beta_n \frac{z}{L}\right) + B_n \cosh\left(\beta_n \frac{z}{L}\right) + C_n \sin\left(\beta_n \frac{z}{L}\right) + D_n \sinh\left(\beta_n \frac{z}{L}\right) \quad (1.9)$$

with β_n and 3 out of the 4 coefficients (A_n, B_n, C_n, D_n) defined through the boundary conditions of the physical problem, up to an arbitrary scaling factor of the eigenfunction's amplitude.

In our case, the NW is fixed at one end ($z = 0$) and free to vibrate at the other ($z = L$). This cantilever configuration implies that the deflection and slope must vanish at $z = 0$, while at the free end ($z = L$) the bending moment and shear force must be zero. That is, respectively:

$$w_n(0) = 0, \quad \left.\frac{dw_n}{dz}\right|_{z=0} = 0, \quad E_Y I_y \left.\frac{d^2 w_n}{dz^2}\right|_{z=L} = 0, \quad \frac{d}{dz}\left[E_Y I_y \left.\frac{d^2 w_n}{dz^2}\right|_{z=L}\right] = 0 \quad (1.10)$$

Applying these mathematical constraints to equation (1.9), allows to define the values of (A_n, B_n, C_n, D_n) up to one global parameter and to obtain the characteristic equation for the single-camped beam problem:

$$\cos\beta_n \cosh\beta_n + 1 = 0 \quad (1.11)$$

The infinite countable set of roots (i.e. eigenvalues) of the transcendental expression (1.11) are summarized in Table (1.1). Each root β_n is associated to the mode shape $w_n(z)$ of the n^{th} flexural mode, which is solution of the spatial equation (1.9) and is determined to be

$$w_n(z) = \frac{1}{K_n}\left\{(\cos\beta_n + \cosh\beta_n)\left[\sin\left(\beta_n \frac{z}{L}\right) - \sinh\left(\beta_n \frac{z}{L}\right)\right] - (\sin\beta_n + \sinh\beta_n)\left[\cos\left(\beta_n \frac{z}{L}\right) - \cosh\left(\beta_n \frac{z}{L}\right)\right]\right\} \quad (1.12)$$

Following a common choice of normalization [36, 37], we choose solutions $u_n(z)$ with $K_n = w_n(L) = 2(\sin\beta_n \cosh\beta_n - \cos\beta_n \sinh\beta_n)$ in order to ensure the condition $|w_n(z)|_{max} = 1$, which for a cantilever corresponds to $w_n(L) = 1$. Such normalized vibration profiles $u_n(z)$ are dimensionless and just describe the mode's shape, leaving the amplitude information (and physical unit of distance) to the time-dependent part of the general solution. In Fig. 1.2 are shown the mode shapes correspondent to the first five flexural modes.

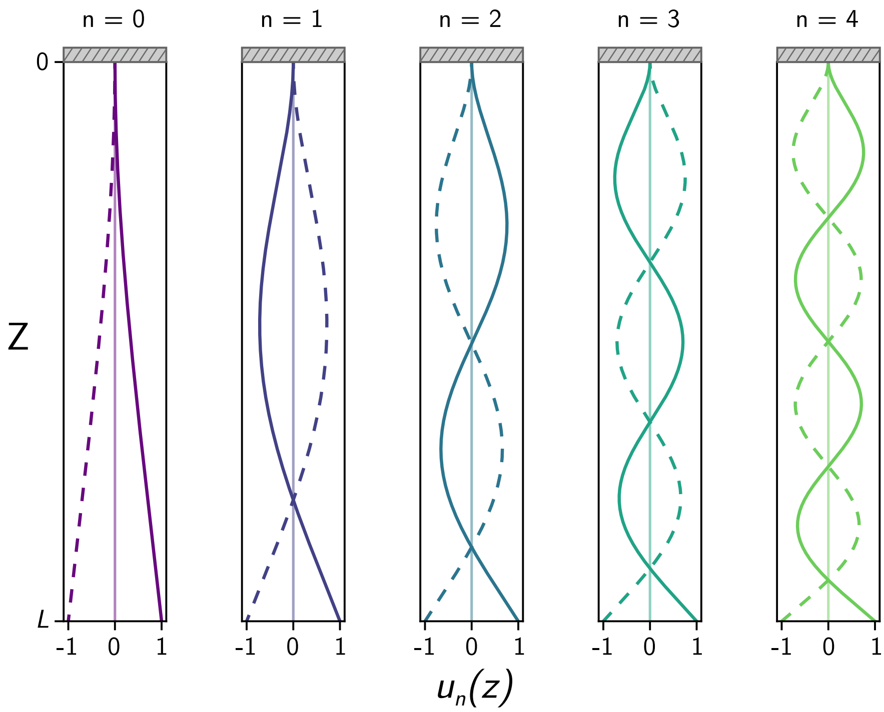

FIGURE 1.2 | **Flexural modes of vibration for a single-clampled beam.** Normalized vibrational profiles $u_n(z)$ for the first five flexural modes of a singly-clamped beam. The curves are describes by Eq.(1.12).

Orthogonality of modes and normal equations of motion

The eigenvalue problem for beams in bending can be written in compact form by introducing two linear differential operators; specifically: the inertial operator $\mathbb{m} = \rho A(z)$ and the stiffness operator $\mathbb{k} = \frac{\partial^2}{\partial z^2} E_Y I_y(z) \frac{\partial^2}{\partial z^2}$. In doing so, equation (1.5) resembles the expression describing lumped-mass systems, where each natural frequency ω_n and modal function u_n satisfies the relation

$$(\mathbb{k} - \omega_n^2 \mathbb{m}) u_n = 0 \tag{1.13}$$

By introducing the scalar product defined for continuous functions on $[0, L]$[5], it is possible to demonstrate that the natural modes $u_n(z)$ are mutually orthogonal[6] [38, 39]. In particular, the orthogonality relations are carried out in terms of the weighted inner product with respect to the inertial operator $\mathbb{m}$:

$$\langle u_n, u_p \rangle_{\mathbb{m}} = \int_0^L \rho A(z) u_n(z) u_p(z) dz = M_n \delta_{np} \tag{1.14}$$

[5] $\langle u_n, u_p \rangle = \int_0^L u_n(z) u_p(z) dz$

[6] but not ortho-normal since $\langle u_n, u_p \rangle = \frac{L}{4}$

where δ_{np} is the Kronecker delta[7] and $M_n = \int_0^L \rho A(z) u_n^2(z) dz$ is the generalized mass of the n^{th} mode. A dual expression for orthogonality can be derived respect to the stiffness operator $\mathbb{k}$:

$$\langle u_n, u_p \rangle_{\mathbb{k}} = \int_0^L \frac{d^2}{dz^2} \left[E_Y I_y(z) \frac{d^2 u_n(z,)}{dz^2} \right] u_p(z) dz = M_n \omega_n^2 \delta_{np} \tag{1.15}$$

Since the mutually orthogonal and complete set of modal functions $\{u_n\}$ is linearly independent, any transverse vibration of the beam $w(z,t)$, which satisfies the boundary conditions, can be represented as a linear combination of these functions. That is the convergent series

$$w(z,t) = \sum_{n=0}^{\infty} u_n(z) r_n(t) \tag{1.16}$$

where $r_n(t) = a_n \sin(\omega_n t + \phi_n)$ are time-dependent harmonic functions at the natural frequencies of the beam[8], with amplitude a_n and phase ϕ_n determined by the initial conditions on $w(z,0)$ and $\dot{w}(z,0)$. Note that, as a consequence of the expansion theorem, any deformation $w(z)$ of the cantilever is represented as a weighted combination of the normalized modes of the unforced cantilever $w(z) = \sum_n^{\infty} a_n u_n(z)$.

These are key concepts that allow to decompose the continuous vibrational problem into an infinite system of equations of motion with single degree of freedom, whose displacements correspond to the modal coordinates $r_n(t)$ [36]. Replacing the expression (1.16) into the generic governing equation (1.4), multiplying both sides by u_p and integrating over $[0, L]$, then results in the identity

$$\int_0^L \sum_{n=0}^{\infty} \left\{ \ddot{r}_n(t) \rho A u_n u_p + r_n(t) \frac{d^2}{dz^2} \left[E_Y I_y \frac{d^2 u_n}{dz^2} \right] u_p \right\} dz = \int_0^L u_p f(z,t) dz \tag{1.17}$$

Interchanging the order of integration and summation and applying the orthogonality relations (1.14) and (1.15) reduces equation (1.17) to a set of uncoupled differential equations in $r_n(t)$ called *normal equations of motion*:

$$\boxed{M_n \ddot{r}_n(t) + M_n \omega_n^2 r_n(t) = F_n(t)} \quad \text{for} \quad n = 0, \ldots, \infty \tag{1.18}$$

Each equation describes the amplitude of an individual mode and is equivalent to the one of a mass-spring lumped system. To each degree of freedom corresponds a *modal mass* $M_n = \langle u_n(z), u_n(z) \rangle_{\mathbb{m}}$ and a *modal stiffness* $k_n = M_n \omega_n^2 = \langle u_n(z), u_n(z) \rangle_{\mathbb{k}}$. The *modal forces* $F_n(t) = \langle u_n(z), f(z,t) \rangle$ (i.e. the forces acting on the modal masses M_n) account for the portion of the applied force distributed to each mode.

Effective mass The *modal mass* or *effective mass* M_n is a fundamental quantity in describing the dynamical behavior of a continuum system with position-dependent inertia. In fact, each volume element of the beam reacts to a transverse load with increasing inertia the closest it is to the free-end point.

By virtue of our normalization condition $|u_n(L)| = 1$, the equations of motion (1.18) describe the time evolution of the displacement $r_n(t)$ at the tip and the

[7] $\delta_{np} := \begin{cases} 1 & \text{for } n = p \\ 0 & \text{for } n \neq p \end{cases}$

[8] Can bee seen as a generalized Fourier Series

effective mass are measured at the position of maximum displacement $z = L$. From equation (1.14) it follows that:

$$\frac{M_n}{M_{tot}} = \frac{1}{L}\int_0^L |u_n(z)|^2 dz = \frac{1}{4} \qquad \forall n \tag{1.19}$$

Given the total potential energy of the mode $\mathcal{E}_P = \frac{1}{2}M_n\omega_n^2|r_n(t)|^2$, it is important to underline that, if the displacement is probed at another position $z = z_0 \neq L$, the correspondent effective mass value renormalized by a factor $|u_n(z_0)|^2$ as [37]:

$$M_n(z_0) = \frac{M_n}{|u_n(z_0)|^2} \geq \frac{1}{4} \quad \text{for} \quad 0 \leq z_0 \leq L \tag{1.20}$$

This follows from the fact that, for the same energy, the modal displacement scales as $r_n(z_0, t) = r_n(t)u_n(z_0)$.

> Since the modal mass is constant and equal to 1/4 of the total mass – independently of the mode n –, in the following will be indicated as M.

Mechanical dissipation The equations of motion in (1.18) describe the ideal case of a non-dissipative perfectly elastic cantilever. However, real resonators are non conservative systems and dissipate energy with consequent damping of their motion.

A common framework to introduce dissipation is to account for the internal damping of a viscoelastic material [40, 41]. Using Hooke's law for solids, the strain ϵ is linearly related to the applied stress σ via the Young modulus $E_Y = \frac{\sigma}{\epsilon}$. While for elastic material (i.e. conservative case) E_Y is constant and real, in the viscoelastic case the relation depends on the excitation's frequency and the strain is phase-lagged with respect to stress as

$$E_Y(\omega) = E_{Y,eff}(\omega)[1 + i\phi(\omega)] \tag{1.21}$$

The loss angle $\phi(\omega)$ represents a rate of energy loss meaning that a fraction $2\pi\phi$ of energy stored in the oscillatory motion $\mathcal{E}_{tot}$ is being dissipated during each cycle. $E_{Y,eff}$ and ϕ are assumed to be constant over the frequency range of interest $\omega \geq \omega_0$. We also introduce the quality factor Q as a figure of merit of the resonator according to its standard definition:

$$Q^{-1} = \phi = \frac{\Delta\mathcal{E}_{loss}}{2\pi\mathcal{E}_{tot}} = \frac{\mathbb{Im}(E_Y)}{\mathbb{Re}(E_Y)} \tag{1.22}$$

By replacing the complex Young modulus (1.21) in equation (1.7), the eigenfrequencies ω_n of the system are determined by a complex-valued dispersion relation for β_n. For good resonators such NW cantilevers, operating in the low dissipation regime (i.e. $\phi \ll 1$ and $Q \gg 1$), it is possible to approximate the complex expression (1.8) as $\omega_n^{diss} \propto \sqrt{E_{Y,eff}(1 + i\phi)} \approx \sqrt{E_{Y,eff}}(1 + i\frac{\phi}{2})$ and define the eigenfrequencies for an under-damped resonator

$$\omega_n^{diss} \approx \left(1 + i\frac{1}{2Q}\right)\omega_n \tag{1.23}$$

As a consequence, the full displacement solution for a free vibrating beam with very low damping maintains the mode shapes and the oscillating frequencies of the undamped case with the only addition of a characteristic exponential decay term

$$w(z,t) = \sum_{n=0}^{\infty} u_n(z) r_n(t) e^{-\frac{\omega_n}{2Q}t} \tag{1.24}$$

Finally, the expression of the normal equations of motion can be rederived by using the complex frequencies [9] in (1.23) and expressed as:

$$\boxed{M\ddot{r}_n(t) + \Gamma_n \dot{r}_n(t) + M\omega_n^2 r_n(t) = F_n(t)} \quad \text{for} \quad n = 0, \ldots, \infty \tag{1.25}$$

where $\Gamma_n = \frac{M\omega_n}{Q}$ is the resonator's *mechanical dissipation*. This equation, corresponding to a damped harmonic oscillator (mass-damper-spring system), will be used in the following to describe the linear response of a flexural mode of the NW.

Note that, since M is identical for all the modes and we assumed the quality factor $Q^{-1} = \phi$ constant, Γ_n appears to increase proportionally to the mode's frequency. This is not generally true because Q is function of ω_n and higher order modes tend to have higher quality factors. In reality, the sources of mechanical dissipation are multiple, difficult to model individually and they all add up as $Q^{-1} = \sum_i Q_i^{-1}$[41]. In our case, since the NWs are operated in vacuum at 10^{-6} mbar, the acoustic dissipation is negligible [10] and Q is limited by intrinsic dissipation mechanisms. Mainly, vibrational energy can be dissipated by internal friction and via coupling to the substrate (clamping losses), due to the time-varying strain radiating elastic energy into the substrate at the clamping (i.e. point of maximum strain). Internal friction is associated with the viscoelastic model we adopted previously, and accounts for defects in the crystalline NW bulk (e.g. stacking faults) [42] and surface losses [20, 43]. The latter are related to the high surface-to-volume ratio of nano-mechanical resonators which amplifies the role of surface defects and impurities over the bulk's properties.

1.1.2 Mechanical polarizations

Up to this point, we gave the description of the flexural normal modes $\{u_n\}$ of a NW and its natural frequencies $\{\omega_n\}$ along one of the two *centroidal principal axes* of the generic NW's cross-section (i.e. x-axis) – concept we introduced at the beginning of subsection 1.1.1. The same equations apply to the NW bending along the other principal axis (i.e. y-axis): its displacement is still described by the same set of mode shapes $\{u_n\}$, while the natural frequencies might differ. In fact, from the eigenfrequency expression (1.8) follows that $\omega_{n,x} \propto \sqrt{I_y}$ with the second moment of area being the only parameter responsible – in case of if $I_y \neq I_x$ – for a difference of the natural frequencies sets $\{\omega_{n,x}\} \neq \{\omega_{n,y}\}$. Note that the eigenfrequency spacing is conserved since it depends on β_n, which is set by the mode shape's solution.

In general, the natural response of a NW to a transverse displacement in the xy-plane is oriented along the centroidal principal axes for which the bending moments result uncoupled. These two directions correspond to the axis of minimum and maximum moment of inertia for the cross-section.

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[9] $\langle u_n, u_n \rangle_{\mathbb{k}} = M\omega_n^2(1 + i/2Q)^2 \approx M\omega_n^2(1 - i/Q) = M\omega_n^2 + \frac{M\omega_n}{Q}\frac{d}{dt}$

[10] Below 10^{-3} mbar Q is not pressure limited