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Fundamentals of Nanomechanical Resonators

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ISBN 978-3-319-28689-1 ISBN 978-3-319-28691-4 (eBook)
DOI 10.1007/978-3-319-28691-4

Library of Congress Control Number: 2016942892

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Preface

Back in December 1959, future Nobel laureate Richard Feynman gave a visionary and now oft-quoted talk entitled “There’s Plenty of Room at the Bottom.” The occasion was an American Physical Society meeting at the California Institute of Technology. Although he did not intend it, Feynman’s 7000 words were a defining moment in nanotechnology, long before anything “nano” appeared on the horizon. The breadth of Feynman’s vision is staggering. In that lecture 42 years ago, he anticipated a spectrum of scientific and technical fields that are now well established, among them electron-beam and ion-beam fabrication, molecular beam epitaxy, nanoimprint lithography, atom-by-atom manipulation, quantum-effect electronics, spin electronics (also called spintronics), and microelectromechanical systems (MEMS) or, even smaller, nanoelectromechanical systems (NEMS).

It is the latter topic which has been the focus of our research careers: mechanical systems with at least one dimension below $1\ \mu\text{m}$ ($10^{-6}\ \text{m}$) where the number of atoms departs from what is usually considered *macroscale* and enters into the *mesoscale*.

NEMS have been developed for a bit more than two decades now. Fabrication technology has evolved and improved enormously for these devices which allows, for reproducibility and yield, two *sine qua non* conditions for an eventual commercialization and, with it, a direct impact on society. The two driving forces for NEMS research have been *metrology* and *fundamental science*.

Matter at this mesoscale is often awkward to explore. It contains too many atoms to be easily understood by straightforward application of quantum mechanics (although the fundamental laws still apply). Yet these systems are not so large as to be completely free of quantum effects; thus, they do not simply obey the classical physics governing the macroworld. It is precisely in this intermediate domain, the mesoworld, that unforeseen properties of collective systems might emerge. Indeed, many efforts have been invested into cooling mechanical resonators down to their *ground state*, which has been recently proven. In addition, interaction between NEMS and q-bits, operation within Coulomb blockade, etc., have been also studied over the years.

On the other hand, NEMS can also be used as extremely good sensors. After the first pioneering experiments on measuring the quanta of electrical conductance and the one of thermal conductance, NEMS have also been targeted to detect spins, radiation, temperature, mass, etc. The theoretical limits for the performance of NEMS-based sensors are outstanding. However, these devices have seldom made it to the market. Comparing to their *bigger brothers*, MEMS, which it took them around 35 years to start having a great impact in consumer market, we can learn several lessons to foster the applicability of NEMS:

- *Standardized fabrication*: Fabrication should be reproducible, with high yield and the fabrication process should be standard (or very similar) across many different foundries.
- *Education*: An educated and trained workforce is required to tackle the problems that arise within these systems. Unfortunately, almost no university in the world offers a course in these type of devices, covering both the electrical and mechanical aspects.

It is the latter point that this book aims to address: to be a textbook for a course for engineers, not going into the details of atomic-scale simulation and analysis but rather taking an approach such as “top-down,” i.e., using macroscopic formulas to model the devices.

At this point, it is important to note that this book focused on NEMS, that is, electrically transduced nanomechanical resonators, in contrast to cavity optomechanics, which fully transduces and controls nanomechanical resonators by optic techniques. However, in particular, the mechanical models introduced in this book are key to the understanding and optimization of nanomechanical resonators used in optomechanics. There are also natural overlaps between the fields in hybrid devices, as it is the case, e.g., in microwave-based cavity optomechanics, which is based on electrostatic transduction but uses optomechanical techniques.

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Chapter 1

Resonance Frequency

Abstract Nanomechanical resonators are continuum mechanical structures, such as beams, strings, plates, or membranes. In this chapter the eigenmodes of such ideal lossless continuum mechanical structures are estimated by simple analytical models. Specific resonance modes of a damped continuum mechanical structure are best described by an effective lumped-element model. In this chapter, the eigenmodes of the most common continuum mechanical structures used as nanomechanical resonators are derived. Then linear, coupled, and nonlinear damped and driven resonators are discussed by means of lumped-element models.

At the *eigenfrequency* of an ideal (lossless) mechanical structure, according to the equipartition theorem, the kinetic energy of a specific mechanical vibration is equal to the potential energy stored in the respective vibrational deformation of the structure. Continuum mechanical structures have many such vibrational modes, called *eigenmodes*, at which this situation occurs. At the eigenfrequency, the total energy in the mechanical system is passed back and forth endlessly between kinetic and potential energy. Thus, once energy is added, e.g. by a kick, such a system would endlessly oscillate precisely at its eigenfrequency with a constant vibrational amplitude.

In a real mechanical structure however, not the entire energy is commuting between kinetic and potential energy, but a little part of the energy is lost during every cycle of vibration. There are many different mechanisms by which energy can dissipate, as will be discussed in Chap. 2 on page 57. Hence, a real mechanical structure will oscillate only for a finite amount of time, until all the energy that was initially entered into the system, e.g. by the kick, has been lost. In real mechanical structures with inherent energy loss, the eigenmode mechanism is called *resonance*. And the predominant frequency at which the energy is commuting between kinetic and potential energy is called the *resonance frequency*. The resonance frequency is typically close (slightly lower) to the eigenfrequency of the same system assumed without losses.

The resonance frequency of a micro- or nanomechanical resonator is typically estimated from the respective eigenfrequency, which can be calculated by means of analytical continuum mechanical models, as discussed in Sect. 1.1, or finite element method (FEM) simulations. FEM tools are readily available and are the

most convenient way to obtain a precise estimate of the eigenmodes of specific micro- and nanomechanical resonators. On the one hand, compared to FEM, analytical models represent idealized mechanical structures and often do not reproduce specific features of the mechanical resonator to be modelled. But on the other hand, analytical models give valuable insight in the effect of geometry and material parameters on the resulting eigenmodes. Therefore, despite FEM, analytical continuum mechanical models are indispensable for the design process of micro- and nanomechanical resonators.

As analytical continuum mechanical models, for simplicity, typically do not consider energy losses, it is convenient to represent an individual eigenmode of a mechanical resonator by an equivalent lumped-element model, as discussed in Sect. 1.2 on page 29. It is straightforward to include energy losses in lumped-element models, which allows for a more accurate description of the dynamic response of an individual eigenmode of a real dissipative micro- and nanomechanical resonator.

1.1 Eigenmodes of Ideal Continuum Mechanical Structures

In this section, analytical models are introduced to describe the free and lossless (conservative) vibration of continuum mechanical structures typically used as micro- and nanomechanical resonators. Bending vibrations of “one-dimensional” resonators, such as *beams* and *strings*, are introduced in Sect. 1.1.1. A string is a special case of a doubly clamped beam that is under tensile stress, such that the effect of the tensile stress is dominating over the beam’s bending stiffness (flexural rigidity). In other words, the difference between beams and strings lies in the way potential energy is stored. While in beams the potential energy is stored in the elastic bending, in strings it is stored in the work done against the strong tensile stress during deflection. In Sect. 1.1.2 “one-dimensional” bulk modes are described. Bending vibrations of “two-dimensional” plates are introduced in Sect. 1.1.3. Here the distinction is made between pure stress-free *plates* and pre-stressed *membranes*, similar to the distinction between beams and strings in the one-dimensional case. Finally, in Sect. 1.1.4 torsional vibration in slender rods are discussed.

The classical way to find the eigenmodes of a continuum mechanical structures is by deriving the differential equation of motion, which can be obtained by equalizing all the forces (inertial and elastic) acting on an infinitesimally small piece of structure (Newton’s third law). In this way it is readily possible to derive exact solutions for many simple and idealized continuum mechanical structures, such as beams, strings, or membranes. But for some structures, such as plates, it can be very hard to find the solution of the resulting differential equations. In that case the eigenmodes can be approximated by methods based on energy assumptions.

Rayleigh’s method is a useful tool to obtain a good approximation for the fundamental eigenfrequency of a conservative system (a system without loss of energy). The method is based on the complete commute of the energy between its

kinetic and potential state (equipartition theorem), as explained previously. Hence, we can assume that the maximal kinetic energy ($W_{\text{kin,max}}$) must be equal to the maximal potential energy ($W_{\text{pot,max}}$)

$$W_{\text{kin,max}} = W_{\text{pot,max}}. \quad (1.1)$$

All the potential and kinetic energies of a few common ideal structures introduced in this chapter are listed in Table 1.1. It is obvious that in order to calculate the energies, the structure specific mode shape $u(x, y, t)$ is required. It is possible to separate the spatial modal shape from the temporal variations. Separating the variables, the mode shape function of a specific normal mode can be written in the form

$$u(x, y, t) = U(x, y) \cos(\omega t) \quad (1.2)$$

where the spatial mode shape function $U(x, y)$ gets modulated by the temporal sinusoidal function $\cos(\omega t)$ with the angular velocity ω .¹ The separation of variables is done likewise with polar coordinates.

Since the maximal value of the temporal function is unity ($\max\{\cos(\omega t)\} = 1$), the potential energy maximum is readily given by

$$W_{\text{pot,max}} = \max\{W_{\text{pot}}(u(x, y, t))\} = W_{\text{pot}}(U(x, y)). \quad (1.3)$$

Because for the kinetic energy it is essential that

$$W_{\text{kin}} \propto \left(\frac{\partial u(x, y, t)}{\partial t} \right)^2, \quad (1.4)$$

and with the Ansatz (1.2) the maximal kinetic energy readily can be written as

$$W_{\text{kin,max}} = \max\{W_{\text{kin}}(u(x, y, t))\} = \omega^2 W_{\text{kin}}(U(x, y)). \quad (1.5)$$

Substituting (1.3) and (1.5) in (1.1), it is now possible to calculate the eigenfrequency Ω of a specific eigenmode

$$\Omega^2 = \omega^2 = \frac{W_{\text{pot}}(U(x, y))}{W_{\text{kin}}(U(x, y))} \quad (1.6)$$

for a suitable displacement function $U(x, y)$. Rayleigh's method yields the exact eigenfrequency if the exact mode shape is known. But typically, the correct mode shape function is unknown and a suitable approximation has to be assumed that satisfies all the boundary conditions. A common approach is to use the displacement

¹For convenience, the term "frequency" is subsequently used in place for the actual correct term "angular velocity."

Table 1.1 Strain and kinetic energies of various continuum mechanical structures with E : Young's modulus, I_y : geometrical moment of inertia, h : structure thickness, w : beam width, $A = hw$: cross section, ρ : mass density, G shear modulus, I_p : polar moment of inertia, ν : Poisson's ratio, $D_P = Eh^3/(12(1 - \nu^2))$: flexural rigidity of plate, σ : tensile stress [1–4]

Member	Potential energy (W_{pot})	Kinetic energy (W_{kin})
Beam of length L in bending vibration	$\frac{1}{2}EI_y \int_0^L \left(\frac{\partial^2 u}{\partial x^2} \right)^2 dx$	$\frac{1}{2}A\rho \int_0^L \left(\frac{\partial u}{\partial t} \right)^2 dx$
String of length L in bending vibration	$\frac{1}{2}\sigma A \int_0^L \left(\frac{\partial u}{\partial x} \right)^2 dx$	
Beam or String of length L in bending vibration	Energy stored in longitudinal extension $\frac{1}{8}EA \int_0^L \left(\frac{\partial u}{\partial x} \right)^4 dx$	
Rod of length L in longitudinal vibration	$\frac{1}{2}EA \int_0^L \left(\frac{\partial u}{\partial x} \right)^2 dx$	
Rod of length L in torsional vibration	$\frac{1}{2}GI_p \int_0^L \left(\frac{\partial u}{\partial x} \right)^2 dx$	$\frac{1}{2}I_p\rho \int_0^L \left(\frac{\partial u}{\partial t} \right)^2 dx$
Rectangular plate of size S in bending vibration	$\frac{D_P}{2} \iint_S \left\{ \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)^2 + 2(1 - \nu) \left[\left(\frac{\partial^2 u}{\partial x \partial y} \right)^2 - \frac{\partial^2 u}{\partial x^2} \frac{\partial^2 u}{\partial y^2} \right] \right\} dx dy$	$\frac{1}{2}\rho h \iint_S \left(\frac{\partial u}{\partial t} \right)^2 dx dy$
Circular plate of radius R in center symmetrical bending vibration	$\pi D_P \int_0^R \left\{ \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} \right)^2 - 2(1 - \nu) \frac{\partial^2 u}{\partial r^2} \frac{1}{r} \frac{\partial u}{\partial r} \right\} r dr$	$\pi\rho h \int_0^R r \left(\frac{\partial u}{\partial t} \right)^2 dr$
Rectangular membrane of size S in bending vibration	$\frac{1}{2}\sigma h \iint_S \left\{ \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 \right\} dx dy$	$\frac{1}{2}\rho h \iint_S \left(\frac{\partial u}{\partial t} \right)^2 dx dy$
Circular membrane of radius R in bending vibration	$\sigma h \pi \int_0^R \left(\frac{\partial u}{\partial r} \right)^2 r dr$	$\pi\rho h \int_0^R r \left(\frac{\partial u}{\partial t} \right)^2 dr$

function of the respective static deflection of the structure of interest due to a uniform load. An assumed approximate mode shape is always stiffer than the correct function and the resulting eigenfrequency obtained by Rayleigh's method is always slightly higher than the exact eigenfrequency.

Rayleigh's method gives a decent approximation for the fundamental eigenfrequency. But in order to obtain more accurate solutions, also of higher modes, Rayleigh's method is often combined with *Ritz's method*. This method is a so-called *variational method* used to approximate various mechanical boundary value problems. The Ritz method is based on minimizing the total potential energy in a mechanical system. The minimum energy is found by varying free variables of a test solution that obeys all boundary conditions. The combined method to approximate the eigenfrequencies of specific mechanical boundary value problems is often called the *Rayleigh–Ritz method*. According to the Ritz method, n free variables c_i are introduced to the spatial mode shape function $U(x, y)$ [1]

$$U(x, y) = \sum_{i=1}^n c_i U_i(x, y). \quad (1.7)$$

The set of variables c_i that minimize the total energy in the structure resulting in a minimum eigenfrequency can be found by minimizing the so-called *Rayleigh quotient* (1.6)

$$\frac{\partial}{\partial c_i} \omega^2 = \frac{\partial}{\partial c_i} \left\{ \frac{W_{\text{pot}}(U(x, y))}{W_{\text{kin}}(U(x, y))} \right\} = 0 \quad (i = 1, 2, 3, \dots, n) \quad (1.8)$$

which by applying the quotient derivation rule and with (1.6) becomes

$$\frac{\partial}{\partial c_i} \{W_{\text{pot}}(U(x, y)) - \omega^2 W_{\text{kin}}(U(x, y))\} = 0 \quad (i = 1, 2, 3, \dots, n). \quad (1.9)$$

Substituting (1.7) into (1.9) yields a homogeneous linear system of equations of n variables, which can be written as

$$\mathbf{M}_n(\omega) \mathbf{c}_i = 0 \quad (1.10)$$

with the square matrix $\mathbf{M}_n(\omega)$ of order n multiplied by the c_i values of the vector \mathbf{c}_i . In order to get the non-trivial solution, the determinant of this system has to be equal to zero

$$\det(\mathbf{M}_n(\omega)) = 0. \quad (1.11)$$

This results in the *frequency* or *characteristic equation* yielding the corresponding n eigenfrequencies ω_i . It is clear from (1.9) that the Rayleigh–Ritz method for $n = 1$ reduces to the Rayleigh method (1.6).

In this chapter, the eigenfrequencies of a few exemplary structures, such as beams, strings, and rectangular membranes are derived exactly. For all other structures, the fundamental eigenfrequency is approximated by Rayleigh's method, yielding the basic terms of the particular eigenfrequencies. Approximations for the higher modes, which typically were derived by the Rayleigh–Ritz method, are taken from mechanics textbooks.

1.1.1 One-Dimensional Bending Vibrations

One-dimensional bending vibrations of beams and strings are among the most common nanomechanical structures. By some definitions, they are the only actual nanomechanical resonators with at least 2 dimension below the size of $1\ \mu\text{m}$. A few typical examples are shown in Fig. 1.1.

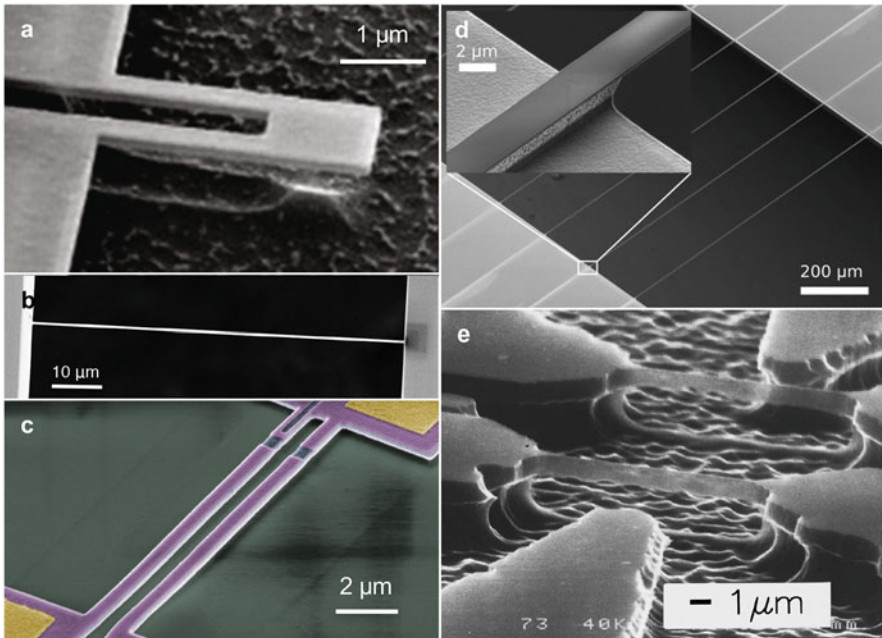


Fig. 1.1 Examples of flexural one-dimensional nanomechanical resonators. (a) Silicon nitride nanocantilever for gravimetric gas chromatography. (Reprinted with permission from [5]. Copyright 2010 American Chemical Society.) (b) Silicon nitride nanostring for airborne nanoparticle detection [6]. (c) Aluminium nitride beam resonators. (d) High-Q silicon nitride string resonators. (Reprinted with permission from [S. Schmid, K.D. Jensen, K.H. Nielsen, A. Boisen, Damping mechanisms in high-Q micro and nanomechanical string resonators. *Phys. Rev. B* 84(16), 165307 (2011)]. Copyright 2011 by the American Physical Society.) (e) Silicon nanobridges. (Reprinted from [10], with permission from AIP Publishing)

1.1.1.1 Free Bending Vibration of Beams

The eigenmode problem of bending beams is one of the prominent cases that can be solved exactly. The model is based on the beam bending theory finalized in the eighteenth century by the Swiss mathematicians Leonard Euler and Daniel Bernoulli, hence the name *Euler–Bernoulli beam theory*. The bending behavior of beams can be modelled under the of assumptions that the beam is slender ($L/h > 10$) (see Fig. 1.2), and that the rotational inertia and the shear deformation can be neglected. The equation of motion of a thin beam can be derived by means of the equilibrium of forces for an infinitesimal piece of beam. Assuming a linear elastic material and small deflections $u(x, t)$, the equation of motion of a thin beam (Euler–Bernoulli beam) is given by [12, 13]

$$\rho A \frac{\partial^2 u(x, t)}{\partial t^2} + EI_y \frac{\partial^4 u(x, t)}{\partial x^4} = 0, \quad (1.12)$$

where ρ is the mass density, A is the cross sectional area, E is the Young's modulus, and I_y is the geometric moment of inertia. The solution to this differential equation is a superposition of normal modes that can be separated into a position dependent and a time-dependent term via a separation of variables [14]

$$u(x, t) = \sum_{n=1}^{\infty} U_n(x) \cos(\omega t), \quad (1.13)$$

where ω is the frequency of motion and n denotes the modal number. A general solutions to the displacement function of the beam $U_n(x)$ can be written in the form

$$U_n(x) = a_n \cos \beta_n x + b_n \sin \beta_n x + c_n \cosh \beta_n x + d_n \sinh \beta_n x \quad (1.14)$$

with the *wavenumber* β_n . The first two terms with the trigonometric functions represent the standing waves in the beam center, while the last two hyperbolic terms represent the influence of the clamping. From this equation it is clear that a beam will vibrate in certain vibrational modes each with a distinct spatial shape.

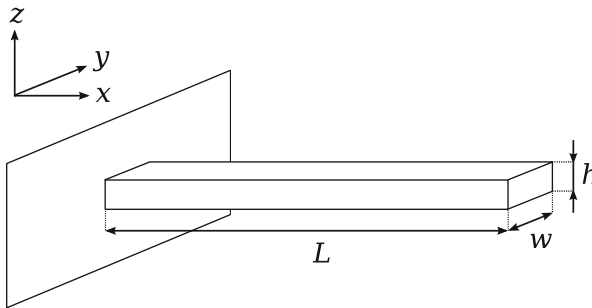


Fig. 1.2 Schematic drawing of a single-clamped beam

By insertion of Eq. (1.14) into (1.12), the differential equation can be rewritten as

$$-\rho A \omega^2 u(x, t) + EI_y \beta_n^4 u(x, t) = 0 \quad (1.15)$$

which results in the *dispersion relationship* which yields the eigenfrequency Ω as a function of the wavenumber

$$\Omega = \omega = \beta_n^2 \sqrt{\frac{EI_y}{\rho A}}. \quad (1.16)$$

The dispersion relationship can be written as

$$\Omega = \beta_n^2 c_E \sqrt{\frac{I_y}{A}}. \quad (1.17)$$

with the wavevelocity c_E in the elastic beam

$$c_E = \sqrt{\frac{E}{\rho}}. \quad (1.18)$$

Assuming a rectangular cross section with beam thickness h the geometric moment of inertia is given by $I_y = \frac{Ah^2}{12}$. By defining a flexural rigidity of a square beam

$$D_E = \frac{Eh^3}{12} \quad (1.19)$$

the eigenfrequency of a beam can be written as

$$\Omega = \beta_n^2 \sqrt{\frac{D_E}{\rho h}}. \quad (1.20)$$

The Euler–Bernoulli beam theory assumes a thin and long beam. If the beam width to height ratio becomes larger $w/h > 5$, the flexural rigidity of a Euler–Bernoulli beam has to be replaced by the flexural rigidity of a plate

$$D_P = \frac{Eh^3}{12(1-\nu^2)} \quad (1.21)$$

where ν is the Poisson's ratio to account for the suppression of the in-plane dilatation accompanying axial strain which makes a plate stiffer than a beam [1, 3].

In the next step, the wavenumber of specific eigenmodes of a beam is derived. This is done by finding the unknown coefficients a_n, b_n, c_n, d_n in (1.14) by means of the specific boundary conditions of the beam. We take into account two specific

cases: (1) singly clamped beams, also called cantilevers, and (2) doubly clamped beams, also called bridges.

Cantilevers

Cantilevers are fixed at one end, while the free end is curvature free and does not experience a momentum. The boundary conditions of a cantilever are hence described by

$$U_n(0) = \frac{\partial}{\partial x} U_n(0) = \frac{\partial^2}{\partial x^2} U_n(L) = \frac{\partial^3}{\partial x^3} U_n(L) = 0. \quad (1.22)$$

These fourth boundary conditions create a system of linear equations of fourth order, which can be written as

$$\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -\cos(\beta_n L) & -\sin(\beta_n L) & \cosh(\beta_n L) & \sinh(\beta_n L) \\ \sin(\beta_n L) & -\cos(\beta_n L) & \sinh(\beta_n L) & \cosh(\beta_n L) \end{bmatrix} \begin{Bmatrix} a \\ b \\ c \\ d \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix}. \quad (1.23)$$

A non-trivial solution exists for this homogeneous system if the determinant is zero, that is

$$\cos(\beta_n L) \cosh(\beta_n L) + 1 = 0 \quad (1.24)$$

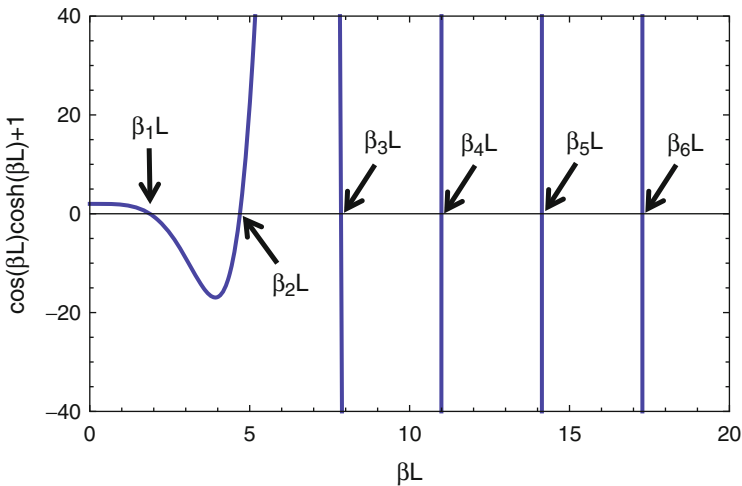


Fig. 1.3 Depiction of the roots of the frequency equation (1.24) for a cantilever

which is the frequency equation. The equation is plotted in Fig. 1.3. From this equation has discrete solutions for specific wavenumbers β_n , which correspond to the specific eigenfrequencies of the cantilever. This transcendental equation can be solved numerically for the lower order modes. The cosine is a periodic function while the hyperbolic cosine is exponentially increasing with increasing $\beta_n L$. The number of roots of (1.24) are hence corresponding to the number of periods of $\cos(\beta_n L)$. For higher eigenvalues (1.24) simplifies to

$$\cos(\beta_n L) \approx 0 \quad \forall n \geq 3 \quad (1.25)$$

and $\beta_n L \approx (2n - 1)\pi/2$. In conclusion, the roots of the frequency equation of a cantilever beam are

$$\lambda_n = \beta_n L = 1.8751, 4.6941, 7.8548, (2n - 1)\pi/2. \quad (1.26)$$

We can now write the eigenfrequency of a cantilever as

$$\Omega_n = \frac{\lambda_n^2}{L^2} \sqrt{\frac{EI_y}{\rho A}}. \quad (1.27)$$

The mode shape function $U_n(x)$ of a cantilever can be obtained from the boundary conditions (1.22). From the first two boundary conditions we obtain

$$U_n(0) = 0 : a_n + c_n = 0 \quad (1.28)$$

$$\frac{\partial U_n(0)}{\partial x} = 0 : b_n + d_n = 0 \quad (1.29)$$

and (1.14) reduces to

$$U_n(x) = a_n(\cos \beta_n x - \cosh \beta_n x) + b_n(\sin \beta_n x - \sinh \beta_n x). \quad (1.30)$$

With the third boundary condition we obtain the ratio of the coefficients a_n and b_n

$$\frac{\partial^2}{\partial x^2} U_n(L) = 0 : \frac{b_n}{a_n} = -\frac{\cos(\beta_n L) + \cosh(\beta_n L)}{\sin(\beta_n L) + \sinh(\beta_n L)} \quad (1.31)$$

and (1.14) becomes

$$U_n(x) = a_n \left[\cos \beta_n x - \cosh \beta_n x - \frac{\cos(\beta_n L) + \cosh(\beta_n L)}{\sin(\beta_n L) + \sinh(\beta_n L)} (\sin \beta_n x - \sinh \beta_n x) \right]. \quad (1.32)$$

The first four mode shapes of a cantilever are shown in Fig. 1.4. It can be seen from the figure that certain areas of the cantilever have a large vibrational amplitude whereas other areas (near the nodal points) are moving with low amplitude. The number of nodal points increases with increasing mode number.