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Acoustic Metamaterials and Phononic Crystals

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Chapter 2
Discrete One-Dimensional Phononic and Resonant Crystals

Pierre A. Deymier and L. Dobrzynski

Abstract The objective of this chapter is to introduce the broad range of concepts necessary to appreciate and understand the various aspects and properties of phononic crystals and acoustic metamaterials described in subsequent chapters. These concepts range from the most elementary concepts of vibrational waves, propagating waves, and evanescent waves, wave vector, phase and group velocity, Bloch waves, Brillouin zone, band structure and band gaps, and bands with negative group velocities in periodic or locally resonant structures. Simple models based on the one-dimensional harmonic crystal serve as vehicles for illustrating these concepts. We also illustrate the application of some of the tools used to study and analyze these simple models. These analytical tools include eigenvalue problems (ω(k) or k(ω)) and Green's function methods. The purpose of this chapter is primarily pedagogical. However, the simple models discussed herein will also serve as common threads in each of the other chapters of this book.

2.1 One-Dimensional Monoatomic Harmonic Crystal

The one-dimensional (1-D) monoatomic harmonic crystal consists of an infinite chain of masses, m, with nearest neighbor interaction modeled by harmonic springs with spring constant, β. The separation distance between the masses at rest is defined as a. This model system is illustrated in Fig. 2.1.

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Fig. 2.1 Schematic illustration of one 1-D mono-atomic harmonic crystal

In the absence of external forces, the equation describing the motion of atom "*n*" is given by

$$m\frac{d^2u_n}{dt^2} = \beta(u_{n+1} - u_n) - \beta(u_n - u_{n-1}). \tag{2.1}$$

In this equation, u_n represents the displacement of the mass "*n*" with respect to its position at rest. The first term on the right-hand side of the equal sign is the harmonic force on mass "*n*" resulting from the spring on its right. The second term is the force due to the spring on the left of "*n*." The dynamics of the 1-D monoatomic harmonic crystal can, therefore, be studied by solving (2.2):

$$m\frac{d^2u_n}{dt^2} = \beta(u_{n+1} - 2u_n + u_{n-1}). \tag{2.2}$$

The next subsections aim at seeking solutions of (2.2).

2.1.1 Propagating Waves

We seek solutions to (2.2) in the form of propagating waves:

$$u_n = A\mathrm{e}^{\mathrm{i}kna}\mathrm{e}^{\mathrm{i}\omega t}, \tag{2.3}$$

where k is a wave number and ω is an angular frequency. Inserting solutions of the form given by (2.3) into (2.2) and simplifying by $A\mathrm{e}^{\mathrm{i}kna}\mathrm{e}^{\mathrm{i}\omega t}$, one obtains the relation between angular frequency and wave number:

$$\omega^2 = -\frac{\beta}{m}\left(\mathrm{e}^{\frac{\mathrm{i}ka}{2}} - \mathrm{e}^{-\frac{\mathrm{i}ka}{2}}\right)^2. \tag{2.4}$$

We use the relation $2i\sin\theta = \mathrm{e}^{\mathrm{i}\theta} - \mathrm{e}^{-\mathrm{i}\theta}$ and the fact that ω is a positive quantity to obtain the so-called dispersion relation for propagating waves in the 1-D harmonic crystal:

$$\omega(k) = \omega_0\left|\sin k\frac{a}{2}\right|, \tag{2.5}$$

with $\omega_0 = 2\sqrt{\frac{\beta}{m}}$ representing the upper limit for angular frequency. Since the monoatomic crystal is discrete and waves with wave-length $\lambda = \frac{2\pi}{k}$ larger than $2a$

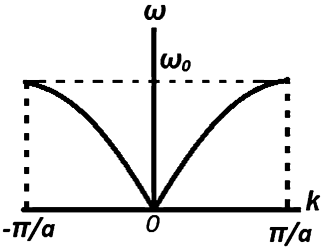

Fig. 2.2 Illustration of the dispersion relation for propagating waves in 1-D mono-atomic harmonic crystal

are physically equivalent to those with wave-length smaller than $2a$, the dispersion relation of (2.5) needs only be represented in the symmetrical interval $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ (see Fig. 2.2). This interval is the first Brillouin zone of the 1-D monoatomic periodic crystal.

2.1.2 *Phase and Group Velocity*

The velocity at which the phase of the wave with wave vector, k, and angular frequency, ω, propagates is defined as

$$v_{\varphi} = \frac{\omega}{k}. \tag{2.6}$$

The group velocity is defined as the velocity at which a wave packet (a superposition of propagating waves with different values of wave number ranging over some interval) propagates. It is easier to understand this concept by considering the superposition of only two waves with angular velocities, ω_1 and ω_2, and wave vectors, k_1 and k_2. Choosing, $\omega_1 = \omega - \frac{\Delta\omega}{2}$ and $\omega_2 = \omega + \frac{\Delta\omega}{2}$, and, $k_1 = k - \frac{\Delta k}{2}$ and $k_2 = k + \frac{\Delta k}{2}$. The superposition of the two waves, assuming that they have the same amplitude, A, leads to the displacement field at mass "n":

$$u_n^s = 2A\mathrm{e}^{\mathrm{i}kna}\mathrm{e}^{\mathrm{i}\omega t}\cos\left(\frac{\Delta k}{2}na + \frac{\Delta\omega}{2}t\right). \tag{2.7}$$

The first part of the right-hand side of (2.7) is a traveling wave that is modulated by the cosine term. This later term represents a beat pulse. The velocity at which this modulation travels is the group velocity and is given by

$$v_{\mathrm{g}} = \frac{\Delta\omega}{\Delta k}. \tag{2.8}$$

In the limit of infinitesimally small differences in wave number and frequency, the group velocity is expressed as a derivative of the dispersion relation:

$$v_{\mathrm{g}} = \frac{\mathrm{d}\omega(k)}{\mathrm{d}k}. \tag{2.9}$$

In the case of the 1-D harmonic crystal, the group velocity is given by $v_{\mathrm{g}} = \omega_0 \frac{a}{2} \cos k \frac{a}{2}$.

We now open a parenthesis concerning the group velocity and show that it is also equal to the velocity of the energy transported by a propagating wave. To that effect, we calculate the average energy density as the sum of the potential energy and the kinetic energy averaged over one cycle of time. The average energy is given by

$$\langle E \rangle = \frac{1}{2}\beta(u_n - u_{n-1})(u_n - u_{n-1})^* + \frac{1}{2} m \dot{u}_n \dot{u}_n^*. \tag{2.10}$$

In (2.10), the * denotes the complex conjugate and $\dot{u}$ the time derivative of the displacement (i.e., the velocity of the mass "n"). Inserting into (2.10) the displacements given by (2.3) and the dispersion relation given by (2.5) yields the average energy density:

$$\langle e \rangle = \frac{\langle E \rangle}{a} = 4A^2 \frac{\beta}{a} \sin^2 k \frac{a}{2}. \tag{2.11}$$

We now calculate the energy flow through one unit cell of the 1-D crystal in the form of the real part of the power, Φ, defined as the product of the force on mass "n" due to one spring and the velocity of the mass:

$$\Phi = \mathrm{Re}\left\{\beta(u_{n+1} - u_n)\dot{u}_n^*\right\} = \beta A^2 \omega_0 \left|\sin k \frac{a}{2}\right| \sin ka. \tag{2.12}$$

The velocity of the energy, v_{e}, is therefore the ratio of the energy flow to the average energy density, which after using trigonometric relations yields: $v_{\mathrm{e}} = \omega_0 \frac{a}{2} \cos k \frac{a}{2}$. This expression is the same as that of the group velocity. In summary, the group velocity represents also the velocity of the energy transported by the propagating waves in the crystal.

2.1.3 Evanescent Waves

In Sect. 2.1.1, we sought solutions to the equation of motion (2.2) in the form of propagating waves (Eq. (2.3)). We may also seek solutions in the form of nonpropagating waves with exponentially decaying amplitude:

$$u_n = A\mathrm{e}^{-k''na}\mathrm{e}^{\mathrm{i}k'na}\mathrm{e}^{\mathrm{i}\omega t}. \tag{2.13}$$

Equation (2.13) can be obtained by inserting a complex wave number $k = k' + ik''$ into (2.3). Combining solutions of the form given by (2.13) and the equation of motion (2.2), one gets

$$-m\omega^2 = \beta\left(e^{ik'\frac{a}{2}}e^{-k''\frac{a}{2}} - e^{-ik'\frac{a}{2}}e^{k''\frac{a}{2}}\right)^2. \tag{2.14}$$

Since the mass and the angular frequency are positive numbers, (2.14) possesses solutions only when the difference inside the parenthesis is imaginary. This condition is met at the edge of the Brillouin zone, when, $k' = \frac{\pi}{a}$. In this case, (2.14) yields the dispersion relation:

$$\omega = \omega_0 \cosh k'' \frac{a}{2}. \tag{2.15}$$

This condition is only met for angular frequencies greater than ω_0, that is, for frequencies above the dispersion curves of propagating waves illustrated in Fig. 2.2.

The solutions of (2.2) in the form of propagating and evanescent waves did not need to be postulated as was done above and in Sect. 2.1.1. We illustrate below a different path to solving (2.2). Instead of solving for the frequency as a function of wave number, this approach solves for the wave number as a function of frequency. This approach is particularly interesting as it will enable us to determine isofrequency maps in wave vector space when dealing with 2-D or 3-D phononic structures.

We start with (2.4) and rewrite it in the form

$$-m\omega^2 = \beta(e^{ika} - 2 + e^{-ika}). \tag{2.16}$$

We now define the new variable: $X = e^{ika}$. Consequently, equation (2.16) becomes a quadratic equation in terms of X:

$$X^2 + \left(\frac{m}{\beta}\omega^2 - 2\right)X + 1 = 0. \tag{2.17}$$

This equation has two solutions, which in terms of ω_0 are

$$X = \frac{1}{\omega_0^2}\left(\omega_0^2 - 2\omega^2\right) \pm \frac{2}{\omega_0^2}\sqrt{\omega^2\left(\omega^2 - \omega_0^2\right)}. \tag{2.18a}$$

The solutions given by (2.18a) are real or complex depending on the value of the angular frequency. Let us consider first the case, $\omega \leq \omega_{0,}$ for which

$$X = \frac{1}{\omega_0^2}\left(\omega_0^2 - 2\omega^2\right) \pm \frac{2i}{\omega_0^2}\sqrt{\omega^2\left(\omega_0^2 - \omega^2\right)}. \tag{2.18b}$$

We now generalize the problem to complex wave numbers $k = k' + ik''$. In this case, X should take the form

$$X = \mathrm{e}^{-k''a}\cos k'a + i\mathrm{e}^{-k''a}\sin k'a. \tag{2.19}$$

We identify the real and imaginary parts of equations (2.18b) and (2.19) and solve for k'' and k'. We find using standard trigonometric relations that $k'' = 0$ and $\sin^2 k' \frac{a}{2} = \frac{\omega^2}{\omega_0^2}$. This solution corresponds to propagating waves with a dispersion relation equivalent to that previously found in Sect. 2.1.1 (Eq. (2.5)).

In contrast, when we consider $\omega > \omega_0$, (2.18a) remains purely real. The real part of (2.19) should then be equal to the right-hand side term of (2.18a). We will denote this term $h^{\pm}(\omega)$. The imaginary part of (2.19) is zero. A trivial solution exists for $k' = 0$. However, in this case, the function $h^{\pm}(\omega)$ is always negative and one cannot find a corresponding value for k''. There exists another solution, namely, $k' = \frac{\pi}{a}$ (there is also a similar solution $k' = -\frac{\pi}{a}$), for which, we obtain

$$k''^{\pm}(\omega) = -\frac{1}{a}\ln(-h^{\pm}(\omega)). \tag{2.20}$$

One of the solutions given by (2.20) is positive and the other negative. In the former case, the displacement is representative of an exponentially decaying evanescent wave. In the latter case, the displacement grows exponentially. This second solution is unphysical. This unphysical solution is a mathematical artifact of the approach used here as it leads to a quadratic equation in X (i.e., k) for a 1-D monoatomic crystal. Since this crystal has only one mass per unit cell "a" it should exhibit only one solution for $\omega(k)$ in the complex plane. We illustrate in Fig. 2.3 the dispersion relations for the propagating and evanescent waves in the complex plane $k = k' + ik''$.

2.1.4 Green's Function Approach

In anticipation of subsequent sections where Green's function approaches will be used to shed light on the vibrational behavior of more complex harmonic structures, we present here the Green's function formalism applied to the 1-D monoatomic crystal. Considering harmonic solution with angular frequency ω, the equation of motion (2.2) can be recast in the form

$$\frac{1}{m}[\beta u_{n+1} + (m\omega^2 - 2\beta)u_n + \beta u_{n-1}] = 0. \tag{2.21}$$

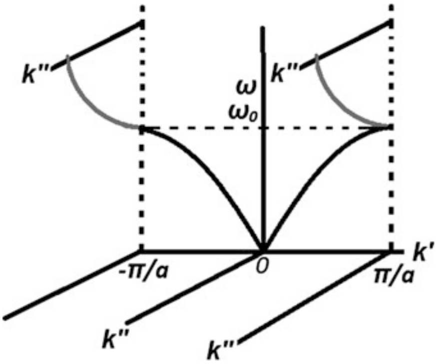

Fig. 2.3 Dispersion curves for the 1-D mono-atomic harmonic crystal extended to the wave-number complex plane. The *black solid curves* are for propagating waves, and the *grey solid curve* is for the evanescent waves

We now rewrite (2.21) in matrix form when applying it to all masses in the 1-D monoatomic crystal:

$$\overleftrightarrow{H_0}\,\vec{u} = \frac{1}{m}\begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \ldots & 0 & \beta & -\gamma & \beta & 0 & 0 & 0 & \ldots \\ \ldots & 0 & 0 & \beta & -\gamma & \beta & 0 & 0 & \ldots \\ \ldots & 0 & 0 & 0 & \beta & -\gamma & \beta & 0 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}\begin{bmatrix} \vdots \\ u_{n-1} \\ u_n \\ u_{n+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \quad (2.22)$$

where $\gamma = 2\beta - m\omega^2$. The operator, $\overleftrightarrow{H_0}$, is a more compact representation of the dynamic matrix in (2.22), and $\vec{u}$ is the vector whose components are the displacements of the masses in the crystal. With this notation, the Green's function, $\overleftrightarrow{G_0}$, associated with $\overleftrightarrow{H_0}$ is defined by the relation

$$\overleftrightarrow{H_0}\overleftrightarrow{G_0} = \overleftrightarrow{I}. \quad (2.23)$$

In this equation, $\overleftrightarrow{I}$ is the identity matrix. Equation (2.23) is written in component form as

$$\sum\nolimits_{n''} H_0(n, n'')G_0(n'', n') = \delta_{nn'}. \quad (2.24)$$

Here, we have used the Kroenecker symbol δ'_{nn} to represent the components of the identity matrix, that is 1 when $n = n'$ and 0 when $n \neq n'$. Since $\overleftrightarrow{H_0}$ is tridiagonal (harmonic interactions are limited to first nearest neighbors), (2.23) becomes

$$\frac{1}{m}[\beta G_0(n+1, n') - \gamma G_0(n, n') + \beta G_0(n-1, n')] = \delta_{nn'}. \quad (2.25)$$

From a physical point of view, the Green's function $G_0(n, n')$ is the displacement of mass "n" when a unit external force is applied at the site of mass "n'". The solution of (2.25) is known [1] and has the general form

$$G_0(n, n') = \frac{m}{\beta} \frac{t^{|n-n'|+1}}{t^2 - 1}. \tag{2.26}$$

The quantity, t, is determined by inserting this general solution into (2.25) and choosing $n = n'$. In this case, we obtain the simple quadratic equation:

$$t^2 - 2\xi t + 1 = 0, \tag{2.27}$$

with $\xi = \frac{\gamma}{2\beta} = 1 - \frac{m\omega^2}{2\beta} = 1 - \frac{2\omega^2}{\omega_0^2}$. The resolution of the quadratic equation yields

$$t = \begin{cases} \xi - (\xi^2 - 1)^{1/2} & \text{if} \quad \xi > 1 \\ \xi + (\xi^2 - 1)^{1/2} & \text{if} \quad \xi < -1 \\ \xi + i(1 - \xi^2)^{1/2} & \text{if} \quad -1 \le \xi \le 1 \end{cases}. \tag{2.28}$$

We note that for $\omega \epsilon\, [0,\ \omega_0]$ and $\xi \epsilon\, [-1, 1]$ t is a complex quantity. We introduce some wave number, k, and write this complex quantity, $t = e^{ika}$. We equate the real part and the imaginary part of this quantity with those of the third form of the solution in (2.28) and using standard trigonometric relations, we obtain the dispersion relation given by (2.5). We therefore recover the propagating wave solution in the crystal. For, $\omega > \omega_0$ and $\xi < -1$, $t \epsilon\, [-1, 0]$. Introducing a wave number, k, we can therefore rewrite $\xi = -\cosh ka$ and $t = -e^{-ka}$represents an evanescent wave.

As a final note, we recast the operator, $\overleftrightarrow{H_0}$, as the difference, $\overleftrightarrow{H'_0} - \omega^2 \overleftrightarrow{I}$, where the operator, H'_0, depends on the spring constant β only. Equation (2.23) then states that

$$\overleftrightarrow{G_0} = \overleftrightarrow{I}\left(\overleftrightarrow{H'_0} - \omega^2\right)^{-1}, \tag{2.29}$$

meaning that the poles (zeros of the denominator) of the Green's function are the eigenvalues of the operator, $\overleftrightarrow{H'_0}$. According to (2.26), the poles of the Green's function of the 1-D monoatomic harmonic crystal are, therefore, given by the equation

$$t^2 - 1 = 0. \tag{2.30}$$

This condition is met when $t = e^{ika} = \cos ka + i \sin ka$. In the case, $\omega \epsilon [0, \omega_0]$, $t = \xi + i(1 - \xi^2)^{1/2}$ if $-1 \le \xi \le 1$. We can subsequently write $\cos ka = \xi = 1 - \frac{2\omega^2}{\omega_0^2}$, which, using trigonometric relation, reduces to the dispersion relation of propagating waves in the crystal (Eq. (2.5)).

2.2 Periodic One-Dimensional Harmonic Crystals

2.2.1 *One-Dimensional Monoatomic Crystal and Super-Cell Approach*

We consider again the 1-D monoatomic harmonic crystal but treat it as a periodic system with a super-period, $R = Na$ i.e., a super-cell representation of the crystal. This system is represented in Fig. 2.4.

We will solve the equation of motion of the mass, "l" in the first super-cell, that is, $l \epsilon [0, N-1]$. Equation (2.21) applied to "l" is

$$-m\omega^2 u_l = \beta(u_{l+1} - 2u_l + u_{l-1}). \tag{2.31}$$

In contrast to Sect. 2.1, we now assume that the displacement obeys Block's theorem [2]. The solutions of (2.31) are the product of plane waves and a periodic function of the super-cell structure:

$$u_1(k) = \mathrm{e}^{\mathrm{i}kla}\tilde{u}_l(k). \tag{2.32}$$

The periodic function, $\tilde{u}_l(k)$, satisfies the condition: $\tilde{u}_l(k) = \tilde{u}_{l+N}(k)$. The wave number, k, is now limited to the interval: $\left[-\frac{\pi}{R}, \frac{\pi}{R}\right]$. The periodic function $\tilde{u}_l(k)$ is subsequently written in the form of a Fourier series:

$$\tilde{u}_l(k) = \sum\nolimits_g u_g\,(k)\,\mathrm{e}^{\mathrm{i}gla}, \tag{2.33}$$

where the reciprocal lattice vector of the periodic structure of super-cells $g = \frac{2\pi}{Na}m$ with m being an integer. Inserting (2.33) and (2.32) into (2.31) gives after some algebra

$$\sum\nolimits_g u_g(k)\mathrm{e}^{\mathrm{i}(k+g)la}\left[-m\omega^2 - \beta\left(\mathrm{e}^{\mathrm{i}(k+g)a} - 2 + \mathrm{e}^{-\mathrm{i}(k+g)a}\right)\right] = 0. \tag{2.34}$$

In addition to the trivial solution, $u_g(k) = 0$, (2.34) admits nontrivial dispersion relations:

$$\omega(k) = \omega_0\left|\sin\,(k+g)\frac{a}{2}\right|. \tag{2.35}$$

We illustrate this dispersion relation for a super-cell 2a long and containing two masses. For $N = 2$, the reciprocal space vectors, $g = \frac{\pi}{a}n$. Equation (2.35) becomes

$$\omega(k) = \omega_0\left|\frac{\sin\left(k + \frac{\pi}{a}n\right)a}{2}\right|.$$

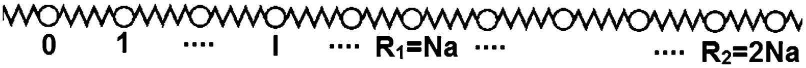

Fig. 2.4 Schematic representation of the 1-D mono-atomic crystal as a periodic structure with super-period Na

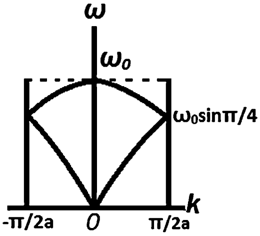

Fig. 2.5 Schematic illustration of the dispersion relation of the 1-D monoatomic harmonic crystal in the super-cell representation, $N = 2$

When $n = 0$, this dispersion relation is identical to that given by (2.5) that was illustrated in Fig. 2.2. The dispersion relation when $n = 1$is equivalent to that of (2.5) translated along the wave number axis by $\frac{\pi}{a}$. For $n = 2a$ and other even values, one obtains again the same result than for $n = 0$. The case $n = 3$ and other odd values are identical to the case $n = 1$. There are therefore only two possible nonequivalent representations of the dispersion relation (2.35). These dispersion relations are only valid in the interval of wave number: $\left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right]$. They are illustrated in Fig. 2.5.

In the super-cell representation, the dispersion relation consists of two branches that can be obtained graphically by folding the dispersion curve of Fig. 2.2 about two vertical lines at wave numbers $-\frac{\pi}{2a}$ and $\frac{\pi}{2a}$. The super-cell representation of the band structure of the monoatomic crystal is a purely mathematical representation. In general, one can construct the band structure of a super-cell with period $R = Na$ by folding the single dispersion curve of Fig. 2.2 N times inside a reduced Brillouin zone: $\left[0, \frac{\pi}{Na}\right]$. We will show in the next section that this representation may be useful in interpreting the band structure of the 1-D diatomic harmonic crystal.

2.2.2 *One-Dimensional Diatomic Harmonic Crystal*

The 1-D diatomic harmonic crystal is illustrated in Fig. 2.6.

The equations of motion of two adjacent odd and even atoms are

$$\begin{cases} m_1\,\ddot{u}_{2n} = \beta(u_{2n+1} - u_{2n} + u_{2n-1}) \\ m_2\ddot{u}_{2n+1} = \beta(u_{2n+2} - u_{2n+1} - u_{2n}) \end{cases}. \tag{2.36}$$

Fig. 2.6 Schematic illustration of the 1-D diatomic harmonic crystal. The atoms with an even label have a mass m_1, and the odd atoms have a mass m_2. The force constant of the springs is β. The periodicity of the crystal is $2a$

We seek solutions in the form of propagating waves with different amplitudes for odd or even atoms as their masses are different:

$$\begin{cases} u_{2n} = A\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}k2na} \\ u_{2n+1} = B\mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}k(2n+1)a} \end{cases}. \tag{2.37}$$

Inserting these solutions into (2.36) leads, after some algebraic manipulations and using the definition of the cosine in terms of complex exponentials, to the set of two linear equations in A and B:

$$\begin{cases} (2\beta - m_1\omega^2)A - 2\beta\cos ka\,B = 0 \\ -2\beta\cos ka\,A + (2\beta - m_1\omega^2)B = 0 \end{cases}. \tag{2.38}$$

This is an eigenvalue problem in ω^2. This set of equations admits nontrivial solutions (i.e., $A \neq 0, B \neq 0$) when the determinant of the matrix composed of the linear coefficients in equation (2.38) is equal to zero, that is,

$$\begin{vmatrix} 2\beta - m_1\,\omega^2 & -2\beta\ \cos\ ka \\ -2\beta\ \cos\ ka & 2\beta - m_2\omega^2 \end{vmatrix} = 0. \tag{2.39}$$

Setting $\alpha = \omega^2$, (2.39) takes the form of the quadratic equation:

$$\alpha^2 - 2\beta\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\alpha + \frac{4\beta^2}{m_1\,m_2}\sin^2 ka = 0, \tag{2.40}$$

which admits two solutions:

$$\omega^2 = \alpha = \beta\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \pm \sqrt{\beta^2\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\beta^2}{m_1\,m_2}\sin^2 ka}. \tag{2.41}$$

These two solutions are periodic in wave number, k, with a period of $\frac{\pi}{a}$. These solutions are represented graphically in the band structure of Fig. 2.7 over the interval, $k\,\epsilon\,\left[0, \frac{\pi}{2a}\right]$. This interval is the smallest interval, the so-called irreducible Brillouin zone, for representing the band structure. The complete band structure is reconstructed by mirror symmetry with respect to a vertical line passing though the origin.

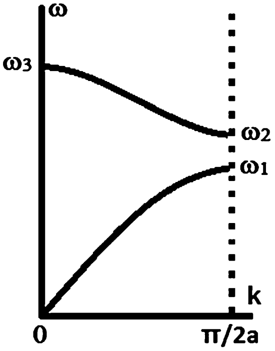

Fig. 2.7 Schematic representation of the band structure of the 1-D diatomic harmonic crystal in the irreducible Brillouin zone

The frequencies ω_1, ω_2 and ω_3 are given by $\omega_1 = \sqrt{\frac{2\beta}{m_1}}$, $\omega_2 = \sqrt{\frac{2\beta}{m_2}}$, and $\omega_3 = \sqrt{2\beta\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}$ if one chooses $m_1 > m_2$. The band structure of Fig. 2.7 exhibits two branches since the unit cell of the 1-D diatomic crystal contains two atoms. These branches are separated by a gap in the interval of frequency $[\omega_1, \omega_2]$. The low-frequency branch is called the acoustic branch. The high-frequency branch is called the optical branch. In the limit $m_1 = m_2 = m$, the diatomic crystal reduces to a monoatomic crystal. The band structure of Fig. 2.7 becomes that of the 1-D monoatomic harmonic crystal in the super-cell representation with $N = 2$ (see Fig. 2.5). The construction of the band structure of the diatomic crystal may then be understood conceptually by first considering the folded band structure of the monoatomic crystal with a super-period $R = 2a$. The waves with wave number $k = \frac{\pi}{2a}$ have a wavelength $\lambda = \frac{2\pi}{k} = 4a$. The wavelength is twice the period of the diatomic crystal. Then, we label alternating atoms with odd and even numbers in the monoatomic crystal. If at some instant an even atom undergoes a zero displacement, then the displacement of all other even atoms will also be zero. At the same time, all odd number atoms will be subjected to a maximum displacement. The even atom and odd atom sublattices support the $\lambda = 4a$ wave with the same frequency as long as their masses are the same. However, if now one perturbs the monoatomic crystal by making the mass of atoms on one sub-lattice different from the atoms on the other (leading to the formation of a diatomic crystal), the frequency of the $\lambda = 4a$ wave will be lower for the heavier atoms than for the lighter ones. Approaching the diatomic crystal by perturbing the masses of the monoatomic crystals separates the folded branches of the monoatomic crystal at $k = \frac{\pi}{2a}$ leading to the formation of a gap.

It is interesting to note that in contrast to the acoustic branch, the optical branch has a negative slope, i.e., a negative group velocity. The group velocity and energy velocity point in a direction opposite to the direction of the wave vector and of the phase velocity. This observation is particularly important when dealing with the concept of negative refraction. However, since the diatomic crystal is one dimensional, we cannot address the phenomenon of refraction yet. However, we rewrite the real part of the displacement of a superposition of waves given by (2.7) in the form

$$u_n^s = 2A\,\cos(k(na + v_\varphi t))\cos\left(\frac{\Delta k}{2}(na + v_{\mathrm{g}}t)\right). \tag{2.42}$$

Equation (2.42) shows that the envelope of the wave packet appears to propagate in the opposite direction of the superposition of waves when the phase velocity and the group velocity have opposite signs.

2.2.3 *Evanescent Waves in the Diatomic Crystal*

In this section, we use the method introduced in Sect. 2.1.3 to shed some light on the nature of waves with frequencies corresponding to the gap of Fig. 2.7. For this, we start with (2.38) and recast it in the form

$$\begin{cases} -m_1\omega^2 A = \beta B \mathrm{e}^{\mathrm{i}ka} - 2\beta A + \beta B \mathrm{e}^{-\mathrm{i}ka} \\ -m_2\omega^2 B = \beta A \mathrm{e}^{\mathrm{i}ka} - 2\beta B + \beta A \mathrm{e}^{-\mathrm{i}ka} \end{cases}. \tag{2.43}$$

We set $X = \mathrm{e}^{\mathrm{i}ka}$ and insert it into the equations of motion (2.43) to obtain after some algebraic manipulations the set of two quadratic equations:

$$\begin{cases} X^2 A = -A + X\left(2 - \dfrac{m_2\omega^2}{\beta}\right)B \\ X^2 B = -B + X\left(2 - \dfrac{m_1\omega^2}{\beta}\right)A \end{cases}. \tag{2.44}$$

Equation (2.44) is recast further in the form of an eigenvalue problem taking the matrix form

$$X\begin{pmatrix} A \\ B \\ XA \\ XB \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 2 - \dfrac{m_2\omega^2}{\beta} \\ 0 & -1 & 2 - \dfrac{m_1\omega^2}{\beta} & 0 \end{pmatrix}\begin{pmatrix} A \\ B \\ XA \\ XB \end{pmatrix}. \tag{2.45}$$

There exists a nontrivial solution when

$$\begin{vmatrix} -\alpha & 0 & 1 & 0 \\ 0 & -\alpha & 0 & 1 \\ -1 & 0 & -\alpha & 2 - \dfrac{m_2\omega^2}{\beta} \\ 0 & -1 & 2 - \dfrac{m_1\omega^2}{\beta} & -\alpha \end{vmatrix} = 0 \tag{2.46}$$

In (2.46), the eigenvalues are $\alpha = \mathrm{e}^{\mathrm{i}ka}$. This equation yields a fourth-order equation:

$$\alpha^4 + \alpha^2\left[2 - \left(2 - \frac{m_2\omega^2}{\beta}\right)\left(2 - \frac{m_1\omega^2}{\beta}\right)\right] + 1 = 0. \tag{2.47}$$

By setting $\zeta = \alpha^2 = \mathrm{e}^{\mathrm{i}2ka}$, we transform (2.47) in a quadratic equation whose solutions are

$$\zeta = \frac{1}{\omega_1^2\omega_2^2}\left(\omega_1^2\omega_2^2 + 2\omega^4 - 2\omega^2\omega_3^2\right) \pm \frac{2}{\omega_1^2\omega_2^2}\sqrt{\omega^2\left(\omega^2-\omega_1^2\right)\left(\omega^2-\omega_2^2\right)\left(\omega^2-\omega_3^2\right)}. \tag{2.48}$$

To obtain (2.48), we have used the relations $\omega_1 = \sqrt{\frac{2\beta}{m_1}}$, $\omega_2 = \sqrt{\frac{2\beta}{m_2}}$ and $\omega_3 = \sqrt{2\beta\left(\frac{1}{m_1}+\frac{1}{m_2}\right)} = \sqrt{\omega_1^2+\omega_2^2}$. If $0<\omega<\omega_1$ or $\omega_2<\omega<\omega_3$, then the argument of the square root in equation (2.48) is negative and ζ is a complex function of frequency corresponding to propagating waves (i.e., real wave number k). These cases represent the acoustic and optical branches of the band structure of the diatomic crystal. Inside the gap ($\omega_1<\omega<\omega_2$), ζ is a real function. Introducing a complex wave number $k = k' + ik''$, we redefine ζ as the quantity:

$$\zeta = \mathrm{e}^{-2k''a}\cos 2k'a + i\mathrm{e}^{-2k''a}\sin 2k'a. \tag{2.49}$$

ζ is therefore real only when $\sin 2k'a = 0$, that is when $k' = \frac{\pi}{2a}$. Equating the real part of (2.49) to (2.48) leads to two solutions for k''. The positive solution is unphysical as it represents an exponentially increasing wave. Again, the emergence of this unphysical solution results from the fact that in the current eigenvalue problem we used a 4×4 matrix (Eq. (2.45)) that is two times larger than the actual 2×2 dynamical matrix of the diatomic harmonic crystal. The negative solution for k'' corresponds to an evanescent wave with exponentially decaying amplitude. Similarly, the vibrational modes for frequencies beyond ω_3 also correspond to evanescent waves. The complete band structure of the 1-D diatomic harmonic crystal is illustrated schematically in Fig. 2.8.

2.2.4 Monoatomic Crystal with a Mass Defect

To shed additional light on the origin of the band gap in the band structure of the diatomic harmonic crystal, we investigate the propagation of waves in a 1-D monoatomic harmonic crystal with a single mass defect. This is accomplished by substituting one atom with mass m by another atom with mass m'. The diatomic crystal may subsequently be created as a periodic substitution of atoms with different masses. We address the following question: does the gap originate from

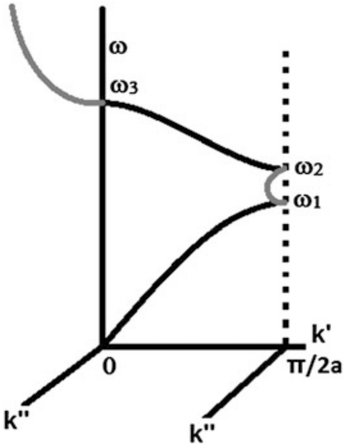

Fig. 2.8 Complete band structure of the 1-D diatomic harmonic crystal. The *black solid lines* correspond to propagating waves. The *gray lines* correspond to evanescent waves

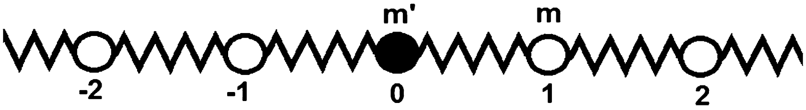

Fig. 2.9 Schematic illustration of the 1-D mono-atomic harmonic crystal with a single mass defect at site 0. The springs are all identical with the same spring constant

the scattering of propagating waves by mass defects independently of their periodicity or does the gap originate from the periodic arrangement of the mass defects?

The defected monoatomic crystal is illustrated in Fig. 2.9.

The equations of motion of the atoms in the defected crystal are

$$\begin{cases} -m\omega^2 u_n = \beta(u_{n+1} - 2u_n + u_{n-1}) & \text{for} \quad n \neq 0 \\ -m'\omega^2 u_o = \beta(u_1 - 2u_0 + u_{-1}) \end{cases}. \tag{2.50}$$

Let us consider an incident wave (i) propagating from the left of the crystal:

$$u_n^{(\mathrm{i})} = A_i \mathrm{e}^{\mathrm{i}kna} \quad \text{for} \quad n \leq -1. \tag{2.51}$$

Part of this wave will be reflected by the mass defect. Another part of the incident wave will be transmitted through the defect. We write the displacements associated with these reflected and transmitted waves in the form

$$\begin{aligned} u_n^{(\mathrm{r})} &= A_\mathrm{r} \mathrm{e}^{-\mathrm{i}kna} \quad \text{for} \quad n \leq -1 \\ u_n^{(\mathrm{t})} &= A_\mathrm{t} \mathrm{e}^{\mathrm{i}kna} \quad \text{for} \quad n \geq 1. \end{aligned} \tag{2.52}$$

In (2.52), the upper-scripts (r) and (t) stand for reflected and transmitted waves, respectively. The total displacement on the left of the defect is the sum of the incident and reflected displacement. The displacement on the right of the defect consists only of the transmitted wave. The total displacement is therefore given by

$$\begin{aligned} u_n &= u_n^{(\mathrm{i})} + u_n^{(\mathrm{r})} \quad \text{for} \quad n \le -1 \\ u_n &= u_n^{(\mathrm{t})} \quad \text{for} \quad n \ge 1. \end{aligned} \tag{2.53}$$

The continuity of the displacement at the defected site "0" imposes the condition

$$u_0 = u_0^{(\mathrm{i})} + u_0^{(\mathrm{r})} = u_0^{(\mathrm{t})}. \tag{2.54}$$

Substituting (2.51) and (2.52) into the condition (2.54) yields a relation between the amplitudes of the incident, the reflected, and the transmitted waves:

$$A_\mathrm{i} + A_\mathrm{r} = A_\mathrm{t}. \tag{2.55}$$

We now substitute equations (2.51), (2.52), and (2.54) into (2.50) for the motion of the mass m'. After some algebraic steps, this equation becomes

$$\left(-m'\,\omega^2 + 2\beta - \beta e^{ika}\right)A_T = A_i \beta e^{-ika} + A_R \beta e^{ika}. \tag{2.56}$$

Equations (2.55) and (2.56) constitute a set of linear equations in the amplitudes of the incident, reflected, and transmitted waves. We can express the amplitude of the reflected and transmitted waves in terms of the amplitude of the incident wave to define a transmission coefficient and a reflection coefficient:

$$\begin{aligned} T &= \frac{A_\mathrm{t}}{A_\mathrm{i}} = \frac{\beta 2i \sin ka}{(m'-m)\omega^2 + \beta 2i \sin ka} \\ R &= \frac{A_\mathrm{r}}{A_\mathrm{i}} = \frac{-(m'-m)\omega^2}{(m'-m)\omega^2 + \beta 2i \sin ka}. \end{aligned} \tag{2.57}$$

To obtain (2.57), we have used the fact that for the 1-D monoatomic harmonic crystal, the dispersion relation of (2.5) can be recast in the form $m\omega^2 = 2\beta(1-\cos ka)$. To analyze the behavior of the defected crystal further, we calculate the square of the modulus of the transmission coefficient:

$$T^2 = TT^* = \frac{4\beta^2 \sin^2 ka}{(m'-m)^2\omega^4 + 4\beta^2 \sin^2 ka}. \tag{2.58}$$

We note that when $m' = m$, the incident wave propagates without reflection, i.e., the transmission coefficient ((2.58)) is equal to 1. We also note that for $k = \frac{\pi}{2a}$, i.e., the edge of the Brillouin zone for the diatomic crystal, the transmission coefficient simplifies to $T^2 = \frac{4\beta^2}{(m'-m)^2\omega^4+4\beta^2}$. The transmission coefficient decreases monotonically as a function of frequency showing no sign of resonance or any other localized vibration phenomenon. In the absence of such a resonant phenomenon, the band structure of the diatomic harmonic crystal can, therefore, be ascribed to the periodicity of the structure, only. The presence of an acoustic branch and of an optical branch separated by a gap results from scattering of waves by the periodic crystal, namely, Bragg's scattering.

2.2.5 Monoatomic Harmonic Crystal with a General Perturbation

The approach of Sect. 2.2.4 is generalized by introducing a frequency dependent perturbation, $V(\omega)$, of the 1-D monoatomic crystal at site 0. The equations of motion of the atoms in this defected crystal are

$$\begin{cases} -m\omega^2 u_n = \beta(u_{n+1} - 2u_n + u_{n+1}) & \text{for} \quad n \neq 0 \\ -m\omega^2 u_0 = \beta(u_1 - 2u_0 + u_{-1}) + V(\omega)u_0 \end{cases}. \tag{2.59}$$

Following the derivation of the transmission and reflection coefficients in the previous section, we obtain

$$\begin{aligned} T &= \frac{\beta 2i \sin ka}{V(\omega) + \beta 2i \sin ka} \\ R &= \frac{V(\omega)}{V(\omega) + \beta 2i \sin ka}. \end{aligned} \tag{2.60}$$

We note that if $V(\omega) = \infty$, then an incident wave is totally reflected. Such a condition may arise from a local resonance. This case is discussed in the next section.

2.2.6 Locally Resonant Structure

In this section, we are interested in the behavior of a monoatomic crystal with a structural perturbation taking the form of a side branch. The side branch is composed of *L'* atoms of mass *m'* interacting via harmonic springs with force constant β'. The side branch is attached to the monoatomic crystal at site "0" via a spring with stiffness β_I. We assume that the lattice parameter is the same in the

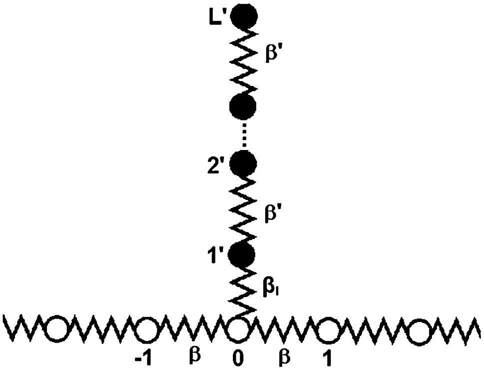

Fig. 2.10 Illustration of the 1-D mono-atomic crystal perturbed by a side branch

side branch and the infinite monoatomic crystal. This structure is illustrated in Fig. 2.10.

The derivation of an expression for the perturbation potential V begins with the equations of motion of atoms in the side branch:

$$\begin{cases} -m'\omega^2 u_{n'} = \beta'(u_{n'+1} - 2u_{n'} + u_{n'-1}) \quad \text{for} \quad n' \neq 1', L' & (a) \\ -m'\omega^2 u_{L'} = -\beta'(u_{L'} - u_{L'-1}) & (b). \\ -m'\omega^2 u_{1'} = -\beta_I(u_{1'} - u_0) + \beta'(u_{2'} - u_{1'}) & (c) \end{cases} \tag{2.61}$$

This set of equations is complemented by the equation of motion of site "0":

$$-m\omega^2 u_o = \beta(u_1 - 2u_0 + u_{-1}) + \beta_I(u_{1'} - u_0). \tag{2.62}$$

To find the perturbation potential, we are interested in coupling (2.61) and (2.62) to obtain an effective equation taking the form of equation (2.69) for site "0." Rewriting (2.62) as $\left(-m\omega^2 + \beta_I\left(1 - \frac{u_{1'}}{u_0}\right)\right)u_0 = \beta(u_1 - 2u_0 + u_{-1})$ yields

$$V = -\beta_I\left(1 - \frac{u_{1'}}{u_0}\right). \tag{2.63}$$

The ratio of displacements in equation (2.63) is found by considering the general solution to (2.61)(a):

$$u_{n'} = A'e^{\mathrm{i}k'n'a} + B'e^{-\mathrm{i}k'n'a}. \tag{2.64}$$

Inserting this solution in (2.61)(a) gives

$$m'\omega^2 = 2\beta'(1 - \cos k'a). \tag{2.65}$$

Should site *N'* have been in an infinite monoatomic crystal, its equation of motion would have been

$$-m'\omega^2 u_{L'} = \beta'(u_{L'+1} - 2u_{L'} + u_{L'-1}). \tag{2.66}$$

Subtracting (2.66) and (2.61)(b) gives

$$\beta'(u_{L'+1} - u_{L'}) = 0. \tag{2.67}$$

This equation serves as a boundary condition on site *N'* in the side branch. We define the displacement $u_{L'+1}$ at a fictive site "L' + 1" as support for the boundary condition (2.67). Similarly subtracting the equation of motion (2.61)(c) and that of site "1'" if it were embedded in an infinite monoatomic crystal leads to the boundary condition

$$-\beta_I(u_{1'} - u_0) + \beta'(u_{1'} - u_{0'}) = 0. \tag{2.68}$$

Fictive site "0'" is only used to impose the boundary condition. The two boundary conditions at sites "*1'*" and "*L'*" form the set of equations:

$$\begin{cases} u_{L'} - u_{L'+1} = 0 \\ (\beta_I - \beta')u_{1'} + \beta' u_{0'} = 0. \end{cases} \tag{2.69}$$

We insert the general solution (2.64) into (2.69) and obtain the set of linear equations

$$\begin{cases} A'\mathrm{e}^{\mathrm{i}k'L'a}\left(1 - \mathrm{e}^{\mathrm{i}k'a}\right) + B'\mathrm{e}^{-\mathrm{i}k'L'a}\left(1 - \mathrm{e}^{-\mathrm{i}k'a}\right) = 0 \\ A'\left[(\beta_I - \beta')\mathrm{e}^{\mathrm{i}k'a} + \beta'\right] + B'\left[(\beta_I - \beta')\mathrm{e}^{-\mathrm{i}k'a} + \beta'\right] = \beta_I u_0 \end{cases}. \tag{2.70}$$

Solving (2.70) gives

$$\begin{aligned} A' &= -\beta_I u_0 \mathrm{e}^{-\mathrm{i}k'L'a}\left(1 - \mathrm{e}^{-\mathrm{i}k'a}\right)/\Delta \\ B &= \beta_I u_0 \mathrm{e}^{\mathrm{i}k'L'a}\left(1 - \mathrm{e}^{\mathrm{i}k'a}\right)/\Delta, \end{aligned} \tag{2.71}$$

where

$$\Delta = -4i\sin\frac{k'a}{2}\left[(\beta_I - \beta')\cos k'\left(L' - \frac{1}{2}\right)a + \beta'\cos k'\left(L' + \frac{1}{2}\right)a\right]. \tag{2.72}$$

To obtain (2.72), we have used a variety of trigonometric relations.

It is worth noting that in the limit of $\beta_I = 0$, the set of (2.70) can be used to find the displacement of an isolated finite segment of monoatomic crystal. The existence of nontrivial solutions for the amplitudes A' and B' is ensured by the condition $\Delta = 0$. This condition is rewritten as $\cos k'\left(L' - \frac{1}{2}\right)a + \cos k'\left(L' + \frac{1}{2}\right)a = -2\sin k'L'a \sin \frac{k'a}{2} = 0$ or $\sin k'L'a = 0$. These solutions correspond to vibrational modes of the finite crystal of length L', i.e., standing waves with wave vectors: $k' = \frac{p\pi}{L'a}$, where p is an integer.

Finally, to find the perturbation V, we use (2.70) and (2.64) to obtain the displacement of atom "1'," which we subsequently insert into (2.63). After several algebraic and trigonometric manipulations, the perturbation becomes

$$V(\omega) = \frac{2\beta'\beta_I \sin \frac{k'a}{2} \sin L'k'a}{(\beta_I - \beta')\cos k'\left(L' - \frac{1}{2}\right)a + \beta' \cos k'\left(L' + \frac{1}{2}\right)a}. \tag{2.73}$$

The effect of the side branch on the propagation of waves along the infinite crystal is most easily understood by considering the limiting case: $\beta = \beta_I = \beta'$ and $m = m'$ such that $k = k'$. In this case, the side branch is constituted of the same material as the infinite crystal and equation (2.73) becomes

$$V(\omega) = \frac{2\beta \sin \frac{ka}{2} \sin L'ka}{\cos k\left(L' + \frac{1}{2}\right)a} \tag{2.74}$$

with the dispersion relation $\omega(k) = \omega_0 \left|\sin k\frac{a}{2}\right|$ (i.e., (2.5)). At the frequency (wave number) corresponding to the standing wave modes of the side branch, the perturbation $V = 0$. The transmission and reflection coefficients given by (2.60) are equal to 1 and 0, respectively. Zeros of transmission and complete reflection occur when $V = \infty$, that is, when $\cos k\left(L' + \frac{1}{2}\right)a = 0$ or $k = (2p + 1)\frac{\pi}{(2L'+1)a}$. These conditions correspond to resonances with the side branch. For instance for a single atom side branch, i.e., $L' = 1$, there is one zero of transmission in the irreducible Brillouin zone of the monoatomic crystal at $k = \frac{\pi}{3a}$. For a two-atom side branch, $L' = 2$, there are two zeros of transmission in the irreducible Brillouin zone of the monoatomic crystal at $k = \frac{\pi}{5a}$ and $k = \frac{3\pi}{5a}$. The number of zeros of transmission scales with the number of atoms in the side branch. Therefore, in contrast to the result of Sect. 2.2.4 where the mass defect did not introduce any zeros of transmission, the side branch leads to perturbations of the band structure of the supporting infinite 1-D monoatomic crystal. These perturbations arise from resonances $(V = \infty)$ of the side branch. The alterations to the band structure of the monoatomic crystal due to the side branch may be visualized as infinitesimally narrow band gaps. The crystal with a single side branch is not periodic, and the perturbed band structure results only from local resonances. In the next sections, we develop the formalism necessary to shed light on the interplay between Bragg's scattering and local resonances on the band structure of a 1-D monoatomic crystal with periodic arrangements of side branches. This formalism is based on the Green's function approach called the Interface Response Theory.

2.3 Interface Response Theory

2.3.1 Fundamental Equations of the Interface response Theory

In this section, we review the fundamental equations of the Interface Response Theory (IRT) for discrete systems [3]. This formalism allows the calculation of the Green's function of a perturbed system in terms of Green's functions of unperturbed systems. We recall (2.23) and (2.22) defining the Green's function, $\overleftrightarrow{G_0}$, by

$$\overleftrightarrow{H_0}\overleftrightarrow{G_0} = I.$$

The operator H_0 is the infinite tridiagonal dynamic matrix:

$$\overleftrightarrow{H_0} = \frac{1}{m}\begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & 0 & \beta & -\gamma & \beta & 0 & 0 & \cdots & \cdots \\ \cdots & \cdots & 0 & \beta & -\gamma & \beta & 0 & \cdots & \cdots \\ \cdots & \cdots & \cdots & 0 & \beta & -\gamma & \beta & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \tag{2.75}$$

where $\gamma = 2\beta - m\omega^2$. We initially consider a type of perturbation that cleaves the 1-D monoatomic harmonic crystal by severing a bond between two neighboring atoms (Fig. 2.11).

The equations of motion of the atoms 0 and 1 are

$$\begin{cases} \frac{1}{m}(-\alpha u_0 + \beta u_{-1}) = 0 \\ \frac{1}{m}(-\alpha u_1 + \beta u_2) = 0 \end{cases}, \tag{2.76}$$

with $\alpha = m\omega^2 - \beta$.

The dynamical operator for the cleaved crystal is written as

$$\overleftrightarrow{h_0} = \begin{bmatrix} \overleftrightarrow{h}_{S1} & \overleftrightarrow{0} \\ \overleftrightarrow{0} & \overleftrightarrow{h}_{S2} \end{bmatrix}$$

$$= \frac{1}{m}\left[\begin{array}{ccccccccc} \cdots & -3 & -2 & -1 & 0 & 1 & 2 & 3 & \cdots \\ \beta & -\gamma & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \beta & -\gamma & \beta & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \beta & -\gamma & \beta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta & -\alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\alpha & \beta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \beta & -\gamma & \beta & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta & -\gamma & \beta \end{array}\right]\begin{array}{c} \vdots \\ -3 \\ -2 \\ -1 \\ 0 \\ 1 \\ 2 \\ \vdots \end{array}. \tag{2.77}$$

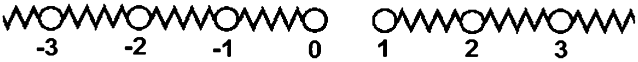

Fig. 2.11 Schematic illustration of the 1-D mono-atomic harmonic crystal cleaved between atoms 0 and 1

In (2.77), $\overleftrightarrow{h_0}$ is a block matrix composed of two independent matrices $\overleftrightarrow{h}_{S1}$ and $\overleftrightarrow{h}_{S2}$, corresponding to the two semi-infinite crystals on the left and right of the cleaved bond, respectively. The Green's function of the perturbed system, $\overleftrightarrow{g}_0$, is therefore defined through the relation

$$\overleftrightarrow{h}_0\overleftrightarrow{g}_0 = \overleftrightarrow{I}. \tag{2.78}$$

Since the dynamical matrix of the cleaved system is a block matrix, its associated Green's function is also a Block matrix:

$$\overleftrightarrow{g_0} = \begin{bmatrix} \overleftrightarrow{g}_{S1} & \overleftrightarrow{0} \\ \overleftrightarrow{0} & \overleftrightarrow{g}_{S2} \end{bmatrix}. \tag{2.79}$$

We define the perturbation operator or cleavage operator as the difference between the dynamical matrices of the cleaved and unperturbed crystals:

$$\overleftrightarrow{V}_0 = \overleftrightarrow{h}_0 - \overleftrightarrow{H}_0. \tag{2.80}$$

Using the matrix representation, the cleavage operator is a 2 × 2 matrix limited to the sites 0 and 1 of the crystal:

$$\overleftrightarrow{V}_0 = \begin{pmatrix} V_0(0,0) & V_0(1,0) \\ V_0(0,1) & V_0(1,1) \end{pmatrix} = \frac{1}{m}\begin{pmatrix} \beta & -\beta \\ -\beta & \beta \end{pmatrix}. \tag{2.81}$$

We rewrite (2.78) in the form $\overleftrightarrow{g}_0\overleftrightarrow{h}_0 = \overleftrightarrow{I}$ by using the commutative property of the product of a matrix with its inverse. Introduction (2.80) into this later relation, multiplying both sides of the equal sign by $\overleftrightarrow{G}_0$, applying the distributive property of the product of matrices, and finally using (2.23) yields

$$\overleftrightarrow{g}_0\left(\overleftrightarrow{I} + \overleftrightarrow{V}_0\overleftrightarrow{G}_0\right) = \overleftrightarrow{g}_0\left(\overleftrightarrow{I} + \overleftrightarrow{A}_0\right) = \overleftrightarrow{G}_0. \tag{2.82}$$

Equation (2.82) is called Dyson's equation. It enables the determination of the Green's function of a perturbed system in terms of the perturbation operator and the Green's function of the unperturbed system. In (2.82), we have defined the surface operator:

$$\overleftrightarrow{A}_0 = \overleftrightarrow{V}_0\overleftrightarrow{G}_0. \tag{2.83}$$

The Green's function of the perturbed system is then given by

$$\overleftrightarrow{g}_0 = \overleftrightarrow{G}_0 \left(\overleftrightarrow{I} + \overleftrightarrow{A}_0 \right)^{-1}. \tag{2.84}$$

The poles of $\overleftrightarrow{g}_0$ (i.e., the eigenvalues of the operator $\overleftrightarrow{h}_0$) are the zeros of $\overleftrightarrow{I} + \overleftrightarrow{A}_0$.

2.3.2 Green's Function of the Cleaved 1-D Monoatomic Crystal

We apply (2.84) to the calculation of the Green's function of the semi-infinite crystal on the right of the cleaved bond in Fig. 2.11 (i.e., $n \geq 1$). The components of the surface operator defined by (2.83) are written as

$$A_{S2}(n,n') = \sum\nolimits_{n''} V_0(n,n'')G_0(n'',n') \quad \text{with} \quad n,n' \geq 1. \tag{2.85}$$

The only nonzero components of the cleavage operator are for $n, n' \epsilon [0, 1]$, so (2.85) reduces to

$$A_{S2}(1,n') = V_0(1,0)G_0(0,n') + V_0(1,1)G_0(1,n'), \quad n' \geq 1. \tag{2.86}$$

Inserting the terms in (2.81) and (2.26) into (2.86) results in

$$A_{S2}(1,n') = \frac{t^{n'} - t^{n'+1}}{t^2 - 1}. \tag{2.87}$$

We now write equation (2.82) in component form:

$$g_{S2}(n,n') + g_{S2}(n,1)A_{S2}(1,n') = G_0(n,n'), \quad n,n' \geq 1. \tag{2.88}$$

Expressing (2.88) at site $n' = 1$and using the relation (2.87) gives

$$g_{S2}(n,1) = \frac{m}{\beta} \frac{t^n}{t-1}.$$

We can now combine that relation with (2.87), (2.26), and (2.88) to obtain the function sought

$$g_{S2}(n,n') = \frac{m}{\beta} \frac{t^{|n-n'|+1} + t^{n+n'}}{t^2 - 1}, \quad n,n' \geq 1. \tag{2.89}$$

The procedure used in this section to find the Green's function of the perturbed system can be generalized to obtain the universal equation of the IRT. All matrices in equation (2.82) are defined for, $n'\epsilon[-\infty,\infty]$. We now consider the space D for $n,n' \geq 1$ and rewrite equation (2.82) as

$$\overleftrightarrow{g}_{S2}(D,D)+\overleftrightarrow{g}_{S2}(D,M)\overleftrightarrow{A}_{S2}(M,D)=\overleftrightarrow{G}_{S2}(D,D). \tag{2.90}$$

The index S specifies that all functions are limited to the space of a semi-infinite truncated chain. Equation (2.88) is a particular case of the general equation (2.90) where we have specified the space corresponding to the location of the perturbation by M. In the case of the cleavage of the monoatomic crystal, $M = 1$. A particular form of (2.90) is

$$\overleftrightarrow{g}_{S2}(D,M)+\overleftrightarrow{g}_{S2}(D,M)\overleftrightarrow{A}_{S2}(M,M)=\overleftrightarrow{G}_{S2}(D,M). \tag{2.91}$$

We combine (2.91) and (2.90) to obtain the universal equation of the IRT:

$$\overleftrightarrow{g}_{S2}(D,D)=\overleftrightarrow{G}_{S2}(D,D)+\overleftrightarrow{G}_{S2}(D,M)\overleftrightarrow{\Delta}^{-1}(M,M)\overleftrightarrow{A}_{S2}(M,D), \tag{2.92}$$

where

$$\overleftrightarrow{\Delta}(M,M)=\overleftrightarrow{I}(M,M)+\overleftrightarrow{A_{S2}}(M,M). \tag{2.93}$$

Equation (2.93) introduces the diffusion matrix $\overleftrightarrow{\Delta}$.

The displacement vector $\vec{u}(D)$ is related to the Green's function $\overleftrightarrow{g}_S$ via the relation

$$\vec{u}(D)=\vec{f}(D)\overleftrightarrow{g}_{S2}(D,D), \tag{2.94}$$

where $\vec{f}$ is some force distribution applied in the space D. Inserting (2.92) into (2.94), we obtain the displacement vector of the perturbed system in terms of the displacement vector of the unperturbed system, U, as

$$\vec{u}(D)=\vec{U}(D)-\vec{U}(M)\overleftrightarrow{\Delta}^{-1}(M,M)\overleftrightarrow{A}_{S2}(M,D). \tag{2.95}$$

Applying (2.95) to the right side of the cleaved mono-atomic crystal yields

$$u(n')=U(n')-U(1)\Delta^{-1}(1,1)A_{S2}(1,n')\ \mathit{for}\ n'\geq 1,$$

with $\Delta^{-1}(1,1)=\frac{1}{1+A_{S2}(1,1)}=\frac{t^2-1}{t-1}$ and $A_{S2}(1,n')=\frac{t^{n'}-t^{n'+1}}{t^2-1}$. The displacement is therefore

$$u(n')=U(n')+U(1)t^{n'}\quad n'\geq 1.$$

If we choose $U(n') = t^{-n'}$, corresponding to an incident wave coming from $n' = +\infty$, the displacement field in the semi-infinite chain takes the form

$$u(n') = t^{-n'} + t^{n'-1} = \mathrm{e}^{-\mathrm{i}kn'a} + \mathrm{e}^{\mathrm{i}k(n'-1)a}.$$

This is a standing wave resulting from the superposition of an incident wave and a reflected wave. We can also obtain this result by writing the equation of motion at site 1 of the cleaved crystal:

$$-m\omega^2 u_1 = \beta(u_2 - u_1).$$

This equation implies that $u_1 - u_0 = 0$, where u_0 is the displacement of the site 0 taken as a fictive site imposing a zero force boundary condition on site 1. We assume that the displacement in the semi-infinite crystal is the sum of a reflected wave and a transmitted wave:

$$u_n = A_\mathrm{i}\mathrm{e}^{-\mathrm{i}kna} + A_\mathrm{r}\mathrm{e}^{\mathrm{i}kna}.$$

Inserting this general solution into the boundary condition leads to the relation between the incident and reflected amplitudes: $A_\mathrm{r} = A_\mathrm{i}\mathrm{e}^{-\mathrm{i}ka}$ leading to the displacement $u(n) = A_\mathrm{i}(\mathrm{e}^{-\mathrm{i}kna} + \mathrm{e}^{\mathrm{i}k(n-1)a})$.

2.3.3 Finite Monoatomic Crystal

The finite 1-D monoatomic crystal is formed by cleaving an infinite crystal at two separate locations. This doubly cleaved system is illustrated in Fig. 2.12.

The cleavage operator is a 4x4 matrix expressed in the space of the perturbed sites (0,1) and (*L*,*L* + 1):

$$\overset{\leftrightarrow}{V}_0 = \frac{1}{m}\begin{array}{c} \begin{array}{cccc} 0 & 1 & L & L+1 \end{array} \\ \left[\begin{array}{cccc} \beta & -\beta & 0 & 0 \\ -\beta & \beta & 0 & 0 \\ 0 & 0 & \beta & -\beta \\ 0 & 0 & -\beta & \beta \end{array}\right] \end{array} \begin{array}{c} \\ 0 \\ 1 \\ L \\ L+1 \end{array}. \tag{2.96}$$

The dynamical matrix is composed of three separate blocks corresponding to the three uncoupled regions of the cleaved system of Fig. 2.12, namely regions “1,” “2,” and “3.” Similarly, the Green’s function and the surface operators are also block diagonal matrices. Using (2.83), the nonzero components of the surface operator matrix corresponding to the block of the finite segment of crystal “2” are

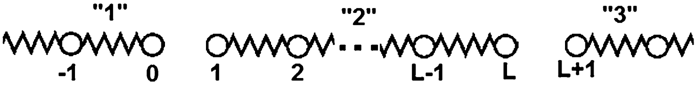

Fig. 2.12 Mono-atomic crystal cleaved between sites (0,1) and (L,L + 1) to obtain a finite crystal composed of atoms [1,L]

$$\begin{aligned} A_{S2}(1,n') &= V_0(1,0)G_0(0,n') + V_0(1,1)G_0(1,n') \\ A_{S2}(L,n') &= V_0(L,L)G_0(L,n') + V_0(L,L+1)G_0(L+1,n') \end{aligned} \quad n' \in [1,L]. \tag{2.97}$$

The Green's function of the infinite crystal given by (2.26) is inserted into (2.97) to obtain

$$\begin{aligned} A_{S2}(1,n') &= \frac{-t^{n'}}{t+1} \\ A_{S2}(L,n') &= \frac{-t^{L-n'+1}}{t+1} \end{aligned} \quad n' \in [1,L]. \tag{2.98}$$

To apply the universal equation of the IRT, we need the block "2" of the surface operator matrix in the space of the corresponding perturbed sites $M \epsilon\ [1,L]$, that is

$$\overleftrightarrow{A}_{S2}(M,M) = \begin{bmatrix} A_{S2}(1,1) & A_{S2}(1,L) \\ A_{S2}(L,1) & A_{S2}(L,L) \end{bmatrix} = \frac{-1}{t+1}\begin{bmatrix} t & t^L \\ t^L & t \end{bmatrix}. \tag{2.99}$$

The green's function of the finite segment of crystal takes the form

$$\begin{aligned} g_{S2}(n,n') = G_0(n,n') &- G_0(n,1)\Delta^{-1}(1,1)A_{S2}(1,n') - G_0(n,1)\Delta^{-1}(1,L)A_{S2}(L,n') \\ &- G_0(n,L)\Delta^{-1}(L,1)A_{S2}(1,n') - G_0(n,L)\Delta^{-1}(L,L)A_{S2}(L,n'), \quad n,n' \epsilon [1,L]. \end{aligned} \tag{2.100}$$

In (2.100),

$$\overleftrightarrow{\Delta}^{-1}(M,M) = \frac{1}{W}\frac{1}{t+1}\begin{bmatrix} 1 & t^L \\ t^L & 1 \end{bmatrix}, \tag{2.101}$$

with $W = \det\overleftrightarrow{\Delta} = \frac{1-t^{2L}}{(t+1)^2}$ and according to (2.93) $\overleftrightarrow{\Delta}(M,M) = \overleftrightarrow{I}(M,M) + \overleftrightarrow{A_{S2}}(M,M)$.

Inserting the expressions given by (2.26), (2.98), and (2.101) into (2.100) yields the Green's function of the finite crystal (for $n, n' \epsilon\, [1,L]$):

$$g_{S2}(n,n') = \frac{m}{\beta}\left[\frac{t^{|n-n'|+1} + t^{n+n'}}{t^2-1} + \frac{t^{2L+1}}{(t^2-1)(1-t^{2L})}\left(t^{n'-n} + t^{n-n'} + t^{1-n-n'} + t^{n+n'-1}\right)\right]. \tag{2.102}$$

According to (2.84), the poles of the Green's function are also those of $\overset{\leftrightarrow}{\Delta}^{-1}$. Here, these poles are the zeros of . The Eigen values of the finite crystals are, therefore, given by the condition $1 - t^{2L} = 0$. This condition may be rewritten as $t^{L} - t^{-L} = 0$. For angular frequencies, $\omega \epsilon [0, \omega_0], t = \mathrm{e}^{ika}$ and the modes of the finite crystal are given by $\mathrm{e}^{ikLa} - \mathrm{e}^{-ikLa} = \sin kLa = 0$. These modes correspond to standing waves with wave number conditioned by $k = \frac{p\pi}{La}$ with p being an integer. The displacement field of these standing waves is obtained from (2.95). In components form, (2.95) becomes

$$\begin{aligned} u(n') = {} & U(n') - U(1)\Delta^{-1}(1,1)A_{S2}(1,n') - U(1)\Delta^{-1}(1,L)A_{S2}(L,n') \\ & - U(L)\Delta^{-1}(L,1)A_{S2}(1,n') - U(L)\Delta^{-1}(L,L)A_{S2}(L,n'), \quad n, n' \epsilon [1, L]. \end{aligned} \tag{2.103}$$

Employing a reference displacement $U(n') = t^{n'}$, (2.103) gives

$$u(n') = t^{n'} + t^{n'}\frac{t}{1 - t^{2L}} + t^{-n'}\frac{t^{2L+2}}{1 - t^{2L}} + t^{n'}\frac{t^{2L}}{1 - t^{2L}} + t^{-n'}\frac{t^{2L+1}}{1 - t^{2L}}.$$

This expression diverges when $1 - t^{2L} = 0$. It is therefore necessary to obtain a finite displacement by renormalizing the previous expression by W. The renormalized displacement then reduces to $u(n') = t^{n'} + t^{-n'+1}$. This expression is that of the displacement of standing waves in the finite crystal.

2.3.4 One-Dimensional Monoatomic Crystal with One Side Branch

The calculation of the displacement in a system composed of a 1-D monoatomic crystal with a finite crystal branch coupled to its side via a spring with constant, β_I, as illustrated in Fig. 2.10, begins with the block matrix describing the Green's function of the uncoupled system $(\beta_I = 0)$

$$\overset{\leftrightarrow}{G}_S = \begin{pmatrix} \overset{\leftrightarrow}{G}_0 & \overset{\leftrightarrow}{0} \\ \overset{\leftrightarrow}{0} & \overset{\leftrightarrow}{g'}_{S2} \end{pmatrix}, \tag{2.104}$$

where $\overset{\leftrightarrow}{G}_0$ is the Green's function of the infinite crystal (whose components are given by (2.26)) and where $\overset{\leftrightarrow}{g}'_{S2}$ is the Green's function of the finite side crystal given by (2.102). This later Green's function is labeled with a "prime" sign to indicate that the spring constants and masses m' and $\beta'$of the finite crystal may be different from those of the infinite crystal m and β. The difference between the dynamic matrix of the coupled systems and of the dynamic matrix of the uncoupled system defines a coupling operator:

$$\overleftrightarrow{V}_I = \begin{pmatrix} V_I(0,0) & V_I(0,1') \\ V_I(1',0) & V_I(1',1') \end{pmatrix} = \begin{pmatrix} \dfrac{-\beta_I}{m} & \dfrac{\beta_I}{m} \\ \dfrac{\beta_I}{m'} & \dfrac{-\beta_I}{m'} \end{pmatrix}. \tag{2.105}$$

We note that if the masses in the finite and infinite crystals were the same, the coupling operator would simply be the opposite of the cleavage operator of (2.81). We now use the fundamental equation of the IRT to derive an expression for the displacement field in the coupled system in terms of the Green's function of the constituent crystals making up the uncoupled system and the perturbation operator of (2.105).

To that effect, we first write expressions for the surface operator:

$$\overleftrightarrow{A}_0(MD) = \begin{pmatrix} A(0,n) \\ A(0,n') \\ A(1',n) \\ A(1',n') \end{pmatrix} = \begin{pmatrix} V_I(0,0)G_0(0,n) \\ V_I(0,1')g'_{S2}(1',n') \\ V_I(1',0)G_0(0,n) \\ V_I(1',1')g'_{S2}(1',n') \end{pmatrix}. \tag{2.106}$$

In (2.106), n and n' refer to sites in the infinite crystals and the finite side branch, respectively. The diffusion matrix then takes the form of a 2x2 matrix in the space of the interface sites M:

$$\begin{aligned} \overleftrightarrow{\Delta}(MM) &= \begin{pmatrix} 1 + A(0,0) & A(0,1') \\ A(1',0) & 1 + A(1,1') \end{pmatrix} \\ &= \begin{pmatrix} 1 + V_I(0,0)G_0(0,0) & V_I(0,1')g'_{S2}(1',1') \\ V_I(1',0)G_0(0,0) & 1 + V_I(1',1')g'_{S2}(1',1') \end{pmatrix}. \end{aligned} \tag{2.107}$$

The inverse of the diffusion matrix is then

$$\overleftrightarrow{\Delta}^{-1}(MM) = \frac{1}{\det\overleftrightarrow{\Delta}} \begin{pmatrix} 1 + V_I(1',1')g'_{S2}(1',1') & -V_I(0,1')g'_{S2}(1',1') \\ -V_I(1',0)G_0(0,0) & 1 + V_I(0,0)G_0(0,0) \end{pmatrix}. \tag{2.108}$$

We use (2.95) to obtain the displacement field. For this we also need to assume a form for the reference displacement $U(D) = t^n$. This displacement corresponds to a wave propagating in the infinite crystal and launched from $n = -\infty$. The displacement inside the side crystal is also assumed to be equal to zero. The displacement in the space of the perturbed sites [0,1′] take the form

$$U(M) = (U(0), U(1')) = (1,0). \tag{2.109}$$

The displacement field at a site $n \geq 1$ along the infinite crystal (i.e., on the right side of the grafted branch) is therefore determined from the equation:

$$u_n = t^n - (1,0)\begin{pmatrix} \Delta^{-1}(0,0) & \Delta^{-1}(0,1') \\ \Delta^{-1}(1',0) & \Delta^{-1}(1',1') \end{pmatrix}\begin{pmatrix} A(0,n) \\ A(1',n) \end{pmatrix}. \tag{2.110}$$

Inserting (2.108) and (2.106) into (2.110) yields

$$u_n = t^n - \frac{1}{\det\overleftrightarrow{\Delta}} \overleftrightarrow{V}_I(0,0) G_0(0,n). \tag{2.111}$$

One then combines (2.26), (2.102), (2.105), and (2.111) to obtain

$$u_n = t^n \left(1 + \frac{\beta_I}{\beta} \frac{1}{\det\overleftrightarrow{\Delta}} \frac{t}{t^2 - 1} \right) = t^n T, \tag{2.112}$$

with

$$\det\overleftrightarrow{\Delta} = 1 - \frac{\beta_I}{\beta'} \frac{t' + t'^{2L'}}{(t' - 1)\left(1 - t'^{2L'}\right)} - \frac{\beta_I}{\beta} \frac{t}{t^2 - 1}. \tag{2.113}$$

In (2.112), T is the transmission coefficient. We can rewrite (2.113) in the form

$$\det\overleftrightarrow{\Delta} = -\frac{1}{V} - \frac{\beta_I}{\beta} \frac{1}{2i\sin ka}, \tag{2.114}$$

where $-\frac{1}{V} = 1 - \frac{\beta_I}{\beta'} \frac{t' + t'^{2L'}}{(t'-1)\left(1 - t'^{2L'}\right)}$. To obtain equation (2.114), we also defined $t = \mathrm{e}^{ika}$. With $t' = \mathrm{e}^{ik'a}$, one can show that the quantity V is that given by equation (2.73).

2.3.5 One-Dimensional Monoatomic Crystal with Multiple Side Branches

We now consider N_c side branches of various lengths grafted along an infinite 1-D monoatomic crystal. The spaces D and M for this system are defined as

$$\begin{aligned} D = {} & \{-\infty, \ldots, -1, 0, 1, \ldots \infty\} \\ & \cup \left\{ \{1', 2', \ldots L'\}, \{1'', 2'', \ldots, L''\}, \{1^{(3)}, 2^{(3)}, \ldots, L^{(3)}\} \ldots, \left\{1^{(N_c)}, 2^{(N_c)}, \ldots, L^{(N_c)}\right\} \right\} \end{aligned}$$

and

$$M = \left\{ p_1 = 0, 1', p_2, 1'', p_3, 1^{(3)}, \ldots, p_{N_c}, 1^{(N_c)} \right\}.$$

We have located the first finite crystal at site $p_1 = 0$ of the infinite crystal. The second finite crystal is located at site $p_2 > p_1$ of the infinite crystal. The third finite crystal is located at $p_3 > p_2$, etc. In this case, the coupling operator is a $2N_c \times 2N_c$ matrix, whose form is given by

$$\overleftrightarrow{V}_I = \frac{\beta_I}{m}\begin{pmatrix} -1 & 1 & 0 & 0 & \dots & 0 & 0 \\ 1 & -1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & -1 & 1 & \dots & 0 & 0 \\ 0 & 0 & 1 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix}. \tag{2.115}$$

To calculate $\overleftrightarrow{\Delta}(MM) = \overleftrightarrow{I}(MM) + \overleftrightarrow{V}_I(MM)\overleftrightarrow{G_S}(MM)$, one needs the Green's function of the uncoupled system, $\overleftrightarrow{G_S}(MM)$, which takes the form

$$\overleftrightarrow{G_S}(MM) = \begin{pmatrix} G_0(p_1p_1) & 0 & G_0(p_1p_2) & 0 & G_0(p_1p_3) & 0 & \dots & G_0(p_1p_{N_c}) & 0 \\ 0 & g_s(1'1') & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ G_0(p_2p_1) & 0 & G_0(p_2p_2) & 0 & G_0(p_2p_3) & 0 & \dots & G_0(p_2p_{N_c}) & 0 \\ 0 & 0 & 0 & g_s(1''1'') & 0 & 0 & \dots & 0 & 0 \\ G_0(p_3p_1) & 0 & G_0(p_3p_2) & 0 & G_0(p_3p_3) & 0 & \dots & G_0(p_3p_{N_c}) & 0 \\ 0 & 0 & 0 & 0 & 0 & g_s(1^{(3)}1^{(3)}) & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ G_0(p_{Nc}p_1) & 0 & G_0(p_{Nc}p_2) & 0 & G_0(p_{Nc}p_3) & 0 & \dots & G_0(p_{Nc}p_{Nc}) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & g_s\left(1^{(N_c)}1^{(N_c)}\right) \end{pmatrix}. \tag{2.116}$$

In this matrix, the odd entries (rows or columns) correspond to locations along the infinite crystal in M and the even entries correspond to the position of the first atom of the finite crystals (also in the space M). From (2.26) and (2.102), the elements of this matrix are therefore

$$G_0(p_ip_j) = \frac{\beta}{m}\frac{t^{\left|p_i - p_j\right|+1}}{t^2 - 1} \tag{2.117}$$

and

$$g_s(1^{(i)}1^{(i)}) = \frac{\beta'}{m'}\frac{t' + t'^{L'i}}{(t'-1)\left(1 - t'^{2L'i}\right)}. \tag{2.118}$$

We use (2.95) to obtain the displacement field. For this we also need to assume a form for the reference displacement $U(D) = t^n$. This displacement corresponds to a wave propagating in the infinite crystal and launched from $n = -\infty$. The displacement inside the side crystal is also assumed to be equal to zero. The displacement in the space M takes the form

$$\begin{aligned} U(M) &= (U(0), U(1'), U(p_2), U(1''), \dots, U(p_{N_c}), U(1^{N_c}) \\ &= (1, 0, t^{p_2}, 0, \dots, t^{p_{N_c}}, 0). \end{aligned} \tag{2.119}$$

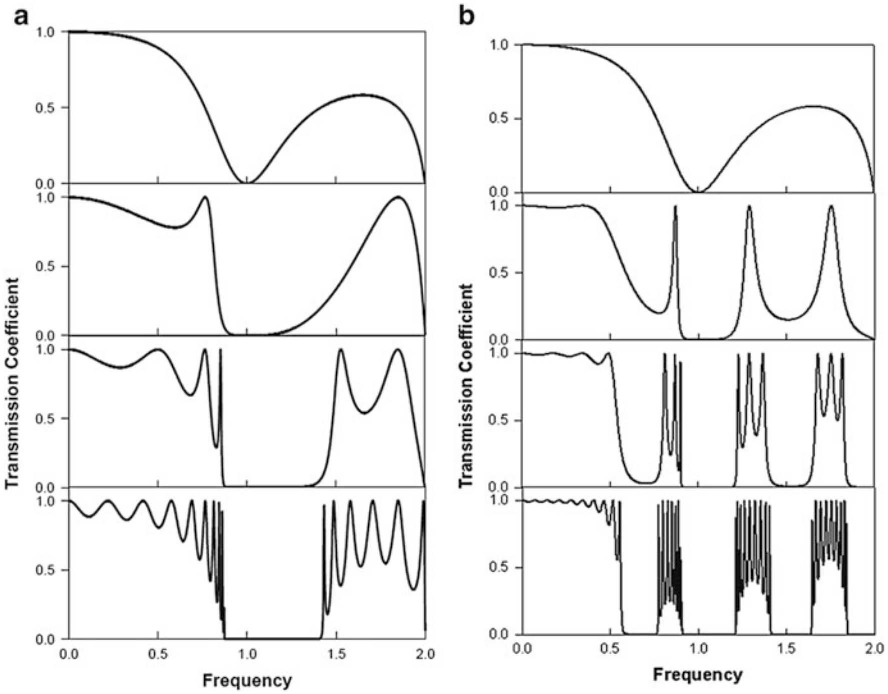

Fig. 2.13 Infinite mono-atomic crystal with (**a**) from top to bottom, a one-atom $(L' = 1)$ side branch located at $p_1 = 0$; two single-atom side branches located at $p_1 = 0$ and at $p_1 = 0$; four single-atom side branches at $p_1 = 0$, $p_2 = 1$, $p_3 = 2$, $p_4 = 3$; and ten one-atom side branches at $p_1 = 0, \ldots, p_{10} = 9$ and (**b**) from top to bottom, a one-atom $(L' = 1)$ side branch located at $p_1 = 0$; two single-atom side branches located at and at $p_1 = 0, p_2 = 4$; four single-atom side branches at $p_1 = 0, p_2 = 4, p_3 = 8, p_4 = 12$; and ten one-atom side branches at $p_1 = 0, \ldots, p_{10} = 36$, $\beta = \beta_I = 1, m = m\prime = 1$

The displacement field at a site $n \geq p_{N_c}$ along the infinite crystal (i.e., on the right side of the last grafted finite crystal) is therefore determined from (2.95), where we use

$$\overleftrightarrow{A}(M,n) = \begin{pmatrix} V_I(0,0)G_0(0,n) \\ V_I(1',0)G_0(0,n) \\ V_I(p_2,p_2)G_0(p_2,n) \\ V_I(1'',p_2)G_0(p_2,n) \\ \vdots \\ V_I(p_{N_c},p_{N_c})G_0(p_{N_c},n) \\ V_I(1^{p_{N_c}},p_{N_c})G_0(p_{N_c},n) \end{pmatrix} = \frac{\beta_I}{m}\frac{\beta}{m}\frac{t^n}{t^2-1}\begin{pmatrix} -t \\ t \\ -t^{1-p_2} \\ t^{1-p_2} \\ \vdots \\ -t^{1-pN_c} \\ t^{1-pN_c} \end{pmatrix}. \tag{2.120}$$

A transmission coefficient is subsequently defined as the ratio $T = u_n/t^n$. For a large number of grafted finite crystals, one has to resort to numerical calculation of the transmission coefficient by inserting (2.115)–(2.120) into (2.95). For the sake of illustration, we have performed such calculations using the limiting case: $\beta = \beta_I = \beta'$ and $m = m'$ (i.e., $t = t'$). The numerical calculation involves the following steps for a series of values of the angular frequency $\omega \leq \omega_0$:

(a) calculating $\xi = 1 - \frac{m\omega^2}{2\beta}$,
(b) calculating $t = \xi + i(1 - \xi^2)^{1/2}$ since $-1 \leq \xi \leq 1$
(c) inserting t into (2.115)–(2.120)
(d) Calculating the transmission coefficient $T(\omega)$

Figure 2.13 illustrates the formation of a band gap by (a) local resonances and (b) band folding effects (Bragg scattering) in the transmission coefficient as a function of frequency for $L' = 1,\ \beta = \beta_I = 1,\ m = m' = 1$. With these conditions, $\omega_0 = 2$. A single one-atom side branch produces one resonant zero of transmission at $\omega = 1$. As one increases the number of side branches, spaced regularly by one interatomic spacing, the periodicity of the infinite chain is conserved and the resonant zero of transmission broadens into a stop band. Two additional dips in transmission on both sides of the resonant stop band form if the side branches are spaced by four atomic spacings. For a large number of side branches spaced by four lattice parameters, these dips broaden and deepen approaching the band gaps that would result from the multiple scattering of waves by a periodic array of side branches.

This example clearly illustrates the contribution of local resonance to wave propagation as well as the contribution of scattering by a periodic array of scatterers. The former mechanism is the foundation of locally resonant structures that determines the properties of acoustic metamaterials. The latter is associated with Bragg's scattering, which is the fundamental mechanism underlying the properties of phononic crystals.

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