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The characteristics of photon and phonon standing waves in a periodic medium

G Knuyt[1,3] **and M Nesládek**[1,2]

[1] Institute for Materials Research, Limburgs Universitair Centrum, Wetenschapspark 1, B-3590 Diepenbeek, Belgium
[2] IMEC vzw, division IMOMEC, Wetenschapspark 1, B-3590 Diepenbeek, Belgium

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Abstract
The main characteristics of the spatial variation of the photon and phonon wave fields at the band gap boundaries are analysed for a one-dimensional medium with periodic optical or acoustic parameters. The derivations are based on symmetry considerations and on analytical results derived from the basic differential equation for the wave field. A simple relation is derived between the band gap width and the derivative of the field intensity at the interface between the regions of high and low wave velocity. The general field characteristics are derived for some examples. Using the analysis a remarkable asymmetric behaviour of the wave absorption near the Brillouin zone boundaries can be explained in a straightforward way.

1. Introduction

In recent years a lot of research has been done on waves in media with periodic properties, both for scientific and technical reasons. This can concern acoustic waves in so-called phononic crystals (e.g. acoustic superlattices) or electromagnetic waves in photonic crystals. Just like for electrons in a periodic potential, frequency gaps will be present [1–4] and near the band edges interesting phenomena occur [5–9].

In this paper special attention will be paid to the explanation of the results of Kuzmiak *et al* [10] where a periodic system was studied, consisting of thin metallic regions in combination with non-dissipating regions. These authors found a remarkable behaviour of the absorption coefficients and electromagnetic wave lifetimes for wavevectors near the zone boundaries. These physical parameters showed asymmetric behaviour according to the frequency value (larger or smaller values depending on the position of the frequency with respect to the band gap). In order to explain results like that of Kuzmiak *et al* it is necessary not only to have a good knowledge of the photonic (phononic) band structure, but also to have a clear physical picture of the spatial variation of the (acoustic or electromagnetic) field for frequencies near the

[3] Author to whom any correspondence should be addressed.

gap. A number of studies on one-dimensional periodic media have been done already [11–21], some of them using the Kronig–Penney treatment [22, 23]. In the present paper we concentrate our attention on the properties of the field near the band edges (the standing wave field). The explanation of the results of Kuzmiak *et al* will be straightforward then.

2. The dispersion relation and spatial variation of the field

In our study of the propagation of electromagnetic or elastic waves, we start with the one-dimensional wave equation (the Helmholtz equation; see e.g. [1])

$$c^2(x)\,\frac{\mathrm{d}^2U(x)}{\mathrm{d}x^2} + \omega^2 U(x) = 0. \tag{1}$$

The field $U(x)$ represents the spatial dependence of e.g. an electric field component, or the deviation of an atomic coordinate from its equilibrium value. $c(x)$ is the local wave velocity which is chosen as a piecewise constant function, and ω is the frequency. We adopt the following notation. In regions I (layers of thickness d_1) the velocity equals c_1; for regions II (thickness d_2) the velocity is c_2 with $c_2 < c_1$. Near the origin ($x = 0$) region I extends from $x = 0$ to d_1 and region II from $x = -d_2$ to 0. The period for the function $c(x)$ equals $d = d_1 + d_2$.

Due to the periodicity of c^2 in equation (1) the field $U(x)$ is a Bloch-type function: $U(x + d) = \exp(\mathrm{i}\mathbf{k}d)U(x)$ where $\mathbf{k}$ is the quasi-wavenumber. By expressing $U(x)$ as a linear combination of two exponentials in each region, and by demanding continuity for $U(x)$ and $\mathrm{d}U/\mathrm{d}x$ at interface points, the field $U(x)$ and the dispersion relation $\omega = \omega(\mathbf{k})$ can be determined by solving an eigenvalue problem. In order to obtain transparent results we introduced dimensionless quantities $\alpha = c_1/c_2$, $\beta = d_1/d_2$, $\omega^* = \omega d/\langle c\rangle$, $x^* = x/d$ and $\mathbf{k}^* = \mathbf{k}d$. The quantity $\langle c\rangle$ is a weighted mean wave velocity [24] defined by $\langle c\rangle^{-1} = d_1/c_1d + d_2/c_2d$. Explicit calculations lead to the dispersion relation

$$\cos\mathbf{k}^* = \cos\omega^* - \frac{1}{2}\frac{(1-\alpha)^2}{\alpha}\left(\sin\frac{\beta\omega^*}{\alpha+\beta}\right)\left(\sin\frac{\alpha\omega^*}{\alpha+\beta}\right). \tag{2}$$

The explicit expressions for $U(x)$ can be obtained in a straightforward way, but are rather lengthy and will not be reproduced here. The main characteristics of U will become clear using the methods explained in the following sections.

3. The behaviour of ω^* and the band gaps

Because the rhs of equation (2) can run out of the interval $[-1, 1]$, band gaps for ω^* will open at the centre and boundary of the first Brillouin zone ($\mathbf{k}^* = 0, \pm\pi$). Each gap can be characterized by two boundary frequencies which we denote as ω^*_{n-} and ω^*_{n+}. n is the number of the gap, and ω^*_{n-} and ω^*_{n+} respectively the low and high ω^* values at the gap boundaries. The fields corresponding to these ω^* will be denoted further as U_{n-} and U_{n+}. The successive gaps ($n = 1, 2, \ldots$) are attained for $\mathbf{k}^* = n\pi$ (extended zone scheme) and the frequency gaps are situated near $\omega^* \approx n\pi$.

The band gap disappears when the second term in the rhs of equation (2) is zero. This can occur in the trivial case $\alpha = 1$, but also if one of the sine functions is zero. This condition leads to the following possible zero-gap values for the β/α ratio: $(\beta/\alpha)_{\mathrm{zg}} = n'/(n-n')$ where n' is an integer with $0 \leqslant n' \leqslant n$. In figure 1 the gap width for $n = 3$ is shown as a function of β/α for $\alpha = 1.5$. It disappears for $\beta/\alpha = 0$, 1/2, 2 and ∞. Some results on the behaviour of U_{n-} and U_{n+} will be discussed further in relation to figure 1.

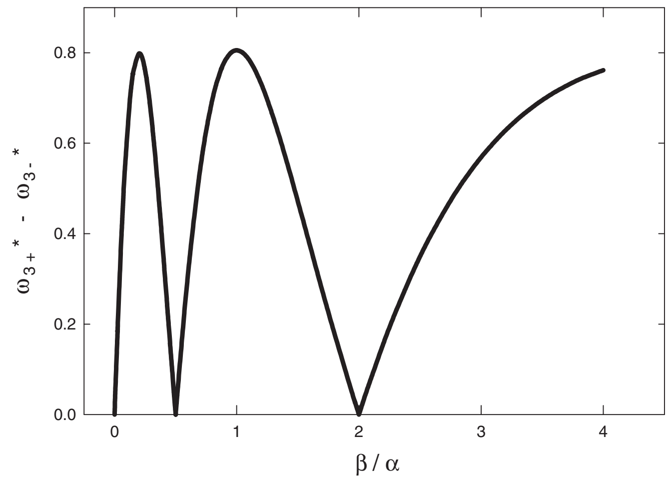

Figure 1. The dimensionless band gap width as a function of the parameter $\beta/\alpha = (d_1/d_2)(c_1/c_2)^{-1}$ for the third band gap. Zero gap width occurs at $\beta/\alpha = (\beta/\alpha)_{zg} = 0$, 1/2, 2 and ∞.

4. Analysis of the behaviour of the fields U_{n-} and U_{n+}

4.1. Periodicity, number of oscillations and parity

Because $\mathbf{k}^* = n\pi$ (modulo 2π) at the gap boundaries, the Bloch condition becomes $U_{n\pm}(x+d) = (-1)^n U_{n\pm}(x)$. Hence for even n, $U_{n\pm}$ has period d, while for odd n only a shift over $2d$ reproduces U (see e.g. the paper by de Sterke and Sipe on periodic media [25]). $U_{n\pm}^2(x)$ shows n oscillations over its period d. Because $c^2(x)$ in equation (1) is invariant under reflection with respect to the points $x = d_1/2$ and $-d_2/2$, $U(x)$ will be symmetric or antisymmetric. This implies that the derivatives $\mathrm{d}U^2/\mathrm{d}x$ at $x = -d_2$ and 0 have opposite signs but the same absolute value.

4.2. Particular behaviour of U_{n-} versus U_{n+}

Further properties of $U_{n\pm}(x)$ are derived by analytical considerations. Multiplication of equation (1) with $U(x) = U_{n\pm}(x)$ and integration over an interval d leads to

$$\omega_{n\pm}^2 = -\int_{x=0}^{d} c^2(x) U_{n\pm}(x)(\mathrm{d}^2 U_{n\pm}/\mathrm{d}x^2)\,\mathrm{d}x \tag{3}$$

where U was normalized according to $\int_{x=0}^{d} U^2(x)\,\mathrm{d}x = 1$. In the case where $c(x)$ is piecewise constant and shows two discontinuities, partial integration of equation (3) leads to $\omega_{n\pm}^2 = (c_1^2 - c_2^2)(\mathrm{d}U_{n\pm}^2/\mathrm{d}x)_{x=0} + \int_{x=0}^{d}(\mathrm{d}U_{n\pm}/\mathrm{d}x)^2 c^2(x)\,\mathrm{d}x$. The continuity of U and $\mathrm{d}U/\mathrm{d}x$ together with the properties of U cited in section 4.1 were used. After subtracting the two equations for the + and $-$ cases one obtains $\omega_{n+}^2 - \omega_{n-}^2 = \mathrm{MC} + \mathrm{SC}$. Here the main contribution (MC) and secondary contribution (SC) are given by $\mathrm{MC} = (c_1^2 - c_2^2)[(\mathrm{d}U_{n+}^2/\mathrm{d}x)_{x=0} - (\mathrm{d}U_{n-}^2/\mathrm{d}x)_{x=0}]$ and $\mathrm{SC} = \int_{x=0}^{d} c^2(x)[(\mathrm{d}U_{n+}/\mathrm{d}x)^2 - (\mathrm{d}U_{n-}/\mathrm{d}x)^2]\,\mathrm{d}x$. Because $\omega_{n+} > \omega_{n-}$ these expressions indicate that $(\mathrm{d}U_n^2/\mathrm{d}x)_{x=0}$ is positive for $U_n = U_{n+}$ and negative for $U_n = U_{n-}$, on condition that the MC term dominates over the SC one. Numerical results indeed show that MC ≈ -2SC. The analytical proof goes as follows. The MC term can be transformed into the same expression for the SC, but with the square bracket in the integral replaced by $(1/2)(\mathrm{d}^2U_{n-}^2/\mathrm{d}x^2 - \mathrm{d}^2U_{n+}^2/\mathrm{d}x^2)$.

Hence MC and SC can be compared by comparing their integrand. Now the functions $U_{n\pm}(x)$ are approximately proportional to oscillating functions $\cos(\bar{k}_n x + \theta_{n\pm})$ with $\bar{k}_n$ a mean wavenumber. From the orthogonality of U_{n+} and U_{n-} one derives that $\theta_{n-} - \theta_{n+} = \pi/2$. Using this equality and the cosine expressions for $U_{n\pm}$, the integrands for MC and SC can be made explicit, and the above relation between MC and SC is easily checked. Using the results for MC and SC in $\omega_{n+}^2 - \omega_{n-}^2$ leads then (for relatively small gap widths) to the following relation between the band gap width and the derivative of the field intensity at the interface:

$$\omega_{n+} - \omega_{n-} \approx \frac{d(c_1^2 - c_2^2)}{2\pi n\langle c\rangle}\left(\frac{\mathrm{d}U_{n+}^2}{\mathrm{d}x}\right)_{x=0}. \tag{4}$$

Because the lhs of equation (4) is positive and $c_1 > c_2$, this equation directly illustrates the well known tendency of the intensity U_{n+}^2 to concentrate in the high c region; the reverse will be true for U_{n-}^2. A case in which the band gap (the lhs in equation (4)) is approximately zero will be discussed further. All the above analytical results were checked numerically. The just mentioned tendency for U_{n+}^2 corresponds to the specific behaviour of an electron conduction band wavefunction in solids (see e.g. [26]).

4.3. *The amplitude of $U_{n\pm}$ in the two regions*

A still more complete picture for the behaviour of the field U can be obtained by considering its amplitudes A. In region I e.g. it is defined by the exact expression $U_{\mathrm{I}}(x) = A_{\mathrm{I}}\cos(\omega x/c_1 + \varphi_{\mathrm{I}})$. Because U and $\mathrm{d}U/\mathrm{d}x$ have to be continuous at the interfaces, various relations between the amplitudes can be derived. Combination of these relations easily leads to an exact equation for the ratio of the amplitudes in regions I and II:

$$(A_{\mathrm{I}}/A_{\mathrm{II}})^2 = \frac{1 + (c_1/\omega)^2(U_0'/U_0)^2}{1 + (c_2/\omega)^2(U_0'/U_0)^2} \tag{5}$$

where for simplicity U and $\mathrm{d}U/\mathrm{d}x$ at $x = 0$ are denoted respectively as U_0 and U_0'.

4.4. *Examples*

In the previous sections a number of properties of the fields $U_{n\pm}$ and its intensities $U_{n\pm}^2$ were derived. We will not give a systematic description of the field and intensity behaviour for various n, α and β values. On the contrary, some examples will illustrate how the above properties can be combined into a clear picture for the field behaviour. In figures 2(a), (b) the fields $U_{1\pm}(x)$ and their intensities are shown in the interval $-d_2 < x < d_1$ $(-0.4 < x^* < 0.6)$ for $\alpha = \beta = 1.5$. Because β/α is well distinct from the zero-gap values, the frequency gap is relatively large, and so are the slopes of U^2 at the boundary between the two regions $(x^* = 0)$. Like for arbitrary n, U_{1-}^2 decreases when entering regions of higher c (going from negative to positive x), and U_{1+}^2 increases there. Because $n = 1$ both functions show only one node and one oscillation per period d. Therefore the mean value of U_{1-}^2 in region II is larger than in region I, although (using equation (5)) it can be shown that the field amplitude A_{II} is smaller than A_{I}. This is specific to the $n = 1$ situation.

In figures 3(a), (b) the fields $U_{3\pm}(x)$ and their squares are shown for $\alpha = 1.5$ and $\beta = 3.1$. For these parameters the ratio $\beta/\alpha \approx 2.07$ is slightly larger than the zero-gap value 2.0 (see figure 1). Because of equation (4), $(\mathrm{d}U_{3+}^2/\mathrm{d}x)_0$ will be very small and positive, and both $U_{3\pm}^2$ will show extrema very near $x = 0$. Further, $d_1/d_2 = \beta$ is somewhat larger than for the

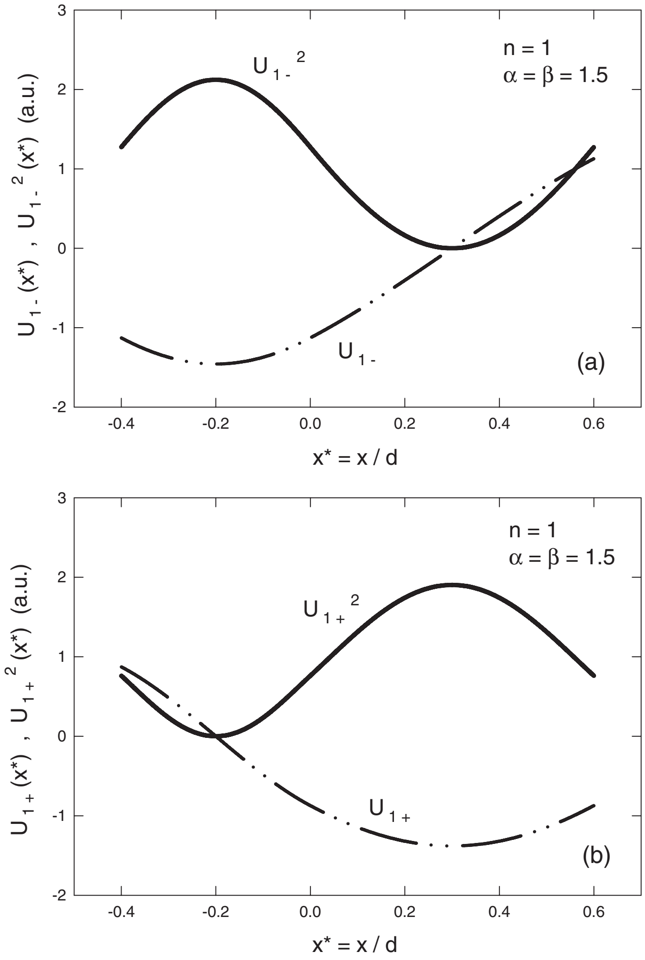

Figure 2. The dependence of U_{1-}^2 and U_{1+}^2 ((a) and (b) respectively) on $x^* = x/d$ for $\alpha = \beta = 1.5$. Only the interval $-d_2 < x < d_1$ ($-0.4 < x^* < 0.6$) is shown. The features of the curves are described in detail in section 4.4.

zero-gap situation, so the boundary ($x = 0$) lies at the left of the extrema. The only possibility is then that U_{3+}^2 has a maximum (antinode) and U_{3-}^2 a minimum (node) for a very small positive x value, in agreement with figures 3(a), (b). The U_0 and U_0' values for the + and − fields can easily be derived from the $U_\pm^2$ behaviour, and then equation (5) can be applied. The result is that for the − field the ratio $A_\mathrm{I}/A_\mathrm{II}$ equals a value c_1/c_2 larger than 1, while for the + field it is exactly 1. This is clearly illustrated in figures 3(a), (b).

In a study on nonlinear periodic media using the envelope function approach, de Sterke and Sipe [25] used a $\mathbf{k}\cdot\mathbf{p}$ method approximation in determining the eigenfunctions for the rapid field fluctuations. They find that the eigenfunctions for the lower edge of the lowest stop gap ($n = 1$) peak in the middle of the high refraction index (low c) material, while the eigenfunction for the higher edge does the same in the low index material. This was indeed found above, and also for higher n. The present treatment also gives information on the derivative of the intensity at the interface in various situations, on the presence of nodes and on the ratio of the field amplitudes in the two regions.

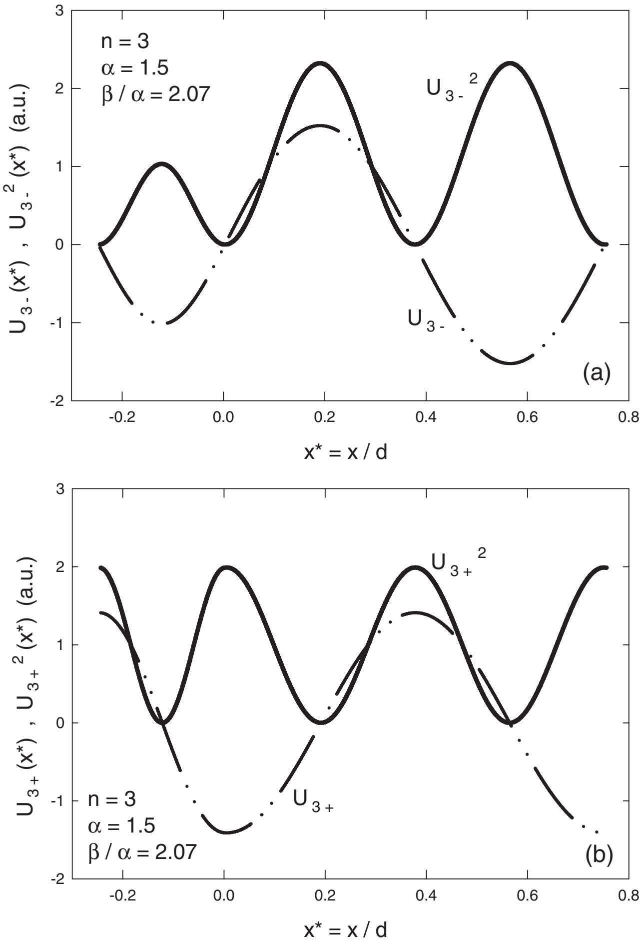

Figure 3. The dependence of U_{3-}^2 and U_{3+}^2 ((a) and (b) respectively) on $x^* = x/d$ for $\alpha = 1.5$, $\beta = 3.1$. The β/α value just exceeds the zero-gap value 2.0. The features of the curves are described in detail in section 4.4.

5. Concluding remarks

The behaviour of the standing waves $U_{n\pm}$ in a periodic medium was inferred from a number of analytical considerations. In particular, equation (4) relates the slope of the field intensity at the boundary to the gap width, and equation (5) yields the amplitude ratio for the different regions. In a few examples it was illustrated how the various results can be combined; it became clear that the character of the field intensity can change substantially with the parameters describing the medium. The intensities calculated above show pronounced extrema, the number of which increases with the gap number, which is in agreement with the behaviour of the local density of states (LDOS) as calculated by Moroz [19] using Green function techniques. Comparison of the various examples discussed above suggests that the LDOS can seriously change the character for varying n, or in cases of relatively small frequency gaps.

The analysis of the previous sections can be used in order to interpret remarkable results found by Kuzmiak *et al* [10]. These authors have studied the photonic band structure in periodic systems consisting of metallic components (thin regions showing dissipation) in combination with vacuum or a dielectric. They find a remarkable asymmetric behaviour of the absorption coefficients and electromagnetic wave lifetimes for wavevectors near the Brillouin zone boundaries. This asymmetry is represented by a decreasing absorption coefficient for waves with frequencies near the lower band edge at the Brillouin zone boundary, and a significant increase for waves with frequencies in the neighbourhood of the upper band edge at the zone boundary. This can be understood from the above results. Because of the large electronic density the relative dielectric constant for metals is smaller than 1 (plasma model), and the metallic regions thus have the highest c. For the low frequency standing wave the field amplitude will then decrease when entering the metallic regions. Because the latter are thin, the field will show a node in the metallic region, and little dissipation will occur, leading indeed to small absorption and a long wave lifetime. On the high frequency side, the field amplitude will increase when entering both sides of the thin metallic layers, and the field amplitude will show a local maximum. This indeed leads to a large absorption and a short wave lifetime. This asymmetric absorption behaviour is one illustration of the influence of the characteristics of the photon or phonon field on the physical properties of the periodic medium. The above results make it clear that even small variations (e.g. of the ratio β/α) can substantially change the field behaviour and hence the physical properties. Recently it was shown by a number of authors [27–30] that it is indeed possible to vary the periodic medium characteristics, even in a continuous way.

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