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2000 J. Phys. A: Math. Gen. 33 7137

(http://iopscience.iop.org/0305-4470/33/40/310)

J. Phys. A: Math. Gen. **33** (2000) 7137–7141. Printed in the UK PII: S0305-4470(00)12108-0

Poles and zeros of the scattering matrix associated with defect modes

D Felbacq
LASMEA UMR CNRS 6602, Complexe des Cézeaux, 63177 Aubière Cedex, France

Received 23 February 2000

Abstract. We analyse electromagnetic wave propagation in one-dimensional periodic media with single or periodic defects. The study is made from the point of view both of the modes and of the diffraction problem. We provide an explicit dispersion equation for the calculation of the modes, and we establish a connection between modes and poles and zeros of the scattering matrix.

Periodic media with defects have been intensively addressed in the field of quantum mechanics (see [1–3] and references therein) and also, since the development of photonic crystals, in electromagnetics [4–7]. On the general subject of photonic crystals, the interested reader can find an impressive bibliography on the Internet [8]. From the theoretical point of view, the quasi-totality of the studies is involved in the characterization of the spectrum of the infinite medium. Nevertheless, for working physicists, the main problem is that of the finite structure [9–11]. Indeed, one can only imagine experiments, such as the diffraction of a plane wave, by finite devices. The main question is then to relate the modes to the behaviour of the diffracted field. The simplest connection is that of the determination of the conduction bands: whenever the frequency belongs to the spectrum of the infinite structure, the finite one allows the guidance of waves while in the gap the electromagnetic field decreases exponentially. In this paper we study, as a model problem, the simple case of a one-dimensional periodic structure with defects, which may model for instance a quantum cavity. Such a device has also been intensively addressed [13–20]. Nevertheless, these studies involve the infinite structure for which a spectral analysis is given, whereas in the present communication we aim at establishing a link between the diffractive properties of a finite structure with a defect, and the known spectral properties of an infinite structure with a defect [12].

Throughout this paper, an orthonormal triaxial Cartesian coordinate system $(0, x, y, z)$ is used. We consider a periodic structure, described by a bounded real one-periodic function $\varepsilon(x)$ ($\varepsilon(x) = \varepsilon(x+1)$), representing the relative permittivity with respect to x, whereas the permeability is assumed to be μ_0, i.e. that of vacuum. The structure is assumed to be invariant in the y- and z-directions and the harmonic fields (time dependence of $\exp(-\mathrm{i}\omega t)$) are invariant along z. This way, the field is described by a function $u_n(x)\exp(\mathrm{i}\alpha y)$, where $\alpha \in (-\pi, +\pi]$ is the Bloch frequency (in the case of a scattering problem, the frequency α is equal to $k_0 \sin\theta$, where θ is the angle of incidence of an incident plane wave). When the electric field $\boldsymbol{E}$ is parallel to the z-axis ($E\|$ case) $u_N(x)\exp(\mathrm{i}\alpha y)$ represents the z-component of $\boldsymbol{E}$, and when the magnetic field $\boldsymbol{H}$ is parallel to the z-axis ($H\|$ case) it represents the z-component of $\boldsymbol{H}$.

Denoting $\beta^2(x) = k_0^2\varepsilon(x) - \alpha^2$, $\beta_0^2 = k_0^2 - \alpha^2$, and setting $U = (u, q^{-1}\partial_x u)$, the propagation equation takes the form

$$\partial_x U = \begin{pmatrix} 0 & q \\ -q^{-1}\beta^2 & 0 \end{pmatrix} U \tag{1}$$

with $q(x) \equiv 1$ for $E\|$ polarization, $q(x) \equiv \varepsilon(x)$ for $H\|$ polarization. The monodromy matrix of the equation, or Floquet operator, is the 2×2 matrix $\boldsymbol{T}_{k,\alpha}$ such that: $U(x+d) = \boldsymbol{T}_{k,\alpha}U(x)$. When considering only n periods of the medium embedded in vacuum and illuminated by a plane wave (the device extends over $[0, n]$), the following boundary conditions hold:

$$\begin{aligned} &\mathrm{i}\beta_0 u|_{x=0} + \partial_x u|_{x=0} = 2\mathrm{i}\beta_0 \\ &\mathrm{i}\beta_0 u|_{x=n} - \partial_x u|_{x=n} = 0 \end{aligned} \tag{2}$$

from which the reflection and transmission coefficients can be derived:

$$\begin{aligned} r_n &= u|_{x=0} - 1 \\ t_n &= u|_{x=n}. \end{aligned}$$

In the infinite medium, the conduction bands are characterized by the condition $|\operatorname{tr}(\boldsymbol{T})| \leqslant 2$; we thus define

$$\begin{aligned} \boldsymbol{G} &= \{(k,\alpha)/|\operatorname{tr}(\boldsymbol{T}_{k,\alpha})| > 2\} \\ \boldsymbol{B} &= \{(k,\alpha)/|\operatorname{tr}(\boldsymbol{T}_{k,\alpha})| < 2\}. \end{aligned}$$

For $(k, \alpha) \in \boldsymbol{G} \cup \boldsymbol{B}$, we denote by $(\boldsymbol{v}, \boldsymbol{w})$ a basis of eigenvectors of $\boldsymbol{T}_{k,\alpha}$, such that $\det(\boldsymbol{v}, \boldsymbol{w}) = 1$, associated with eigenvalues μ and $\frac{1}{\mu}$ (as a convention $|\mu| < 1$ for $(k, \alpha) \in \boldsymbol{G}$). We write in the canonical basis of $\mathbb{C}^2$: $\boldsymbol{v} = (v_1, v_2)$, $\boldsymbol{w} = (w_1, w_2)$.

Let us now introduce a defect in the crystal in the following way: we replace one period of the crystal by a layer of width h and permittivity $\varepsilon_d(x)$ (ε_d is simply assumed to be real and bounded). In view of the spectral problem, the structure is therefore made of two periodic half-spaces connected by an inhomogeneous layer extending over $[0, h]$. We denote by $\boldsymbol{T}_0$ the monodromy matrix of the defect, omitting here to explicitly write the dependence in (k, α). We have the following results.

Proposition 1. *[2, 3, 16]: The defect does not modify the conduction bands.*

Proposition 2. *The defect modes of the structure correspond to couples* (k, α) *such that* $\det(\boldsymbol{T}_0\boldsymbol{w}, \boldsymbol{v}) = 0$.

Proof. As we have introduced a defect, we may now accept an increasing solution in the left semi-crystal and a decreasing solution in the right semi-crystal. The problem is to match these two solutions. This is only possible if $\boldsymbol{T}_0$ switches increasing solutions to decreasing ones, that is if $\boldsymbol{T}_0\boldsymbol{w} \in V\mathrm{ect}(\boldsymbol{v})$. □

Suppose that the structure is finite and that the defect is switched between n periods. The monodromy matrix is $\boldsymbol{T}_{k,\alpha}^n\boldsymbol{T}_0\boldsymbol{T}_{k,\alpha}^n$. In basis $(\boldsymbol{v}, \boldsymbol{w})$, $\boldsymbol{T}_0$ is written

$$\boldsymbol{T}_0 = \begin{pmatrix} a_0 & c_0 \\ b_0 & d_0 \end{pmatrix}.$$

Denoting

$$\chi = (\chi_{ij}) = \begin{pmatrix} w_2 - \mathrm{i}\beta_0 w_1 & w_2 + \mathrm{i}\beta_0 w_1 \\ -v_2 + \mathrm{i}\beta_0 v_1 & -v_2 - \mathrm{i}\beta_0 v_1 \end{pmatrix} \tag{3}$$

an expression of the coefficients (r_n, t_n) can be easily obtained:

$$r_n(k,\alpha) = \frac{p(\mu^{2n})}{q(\mu^{2n})} \qquad t_n(k,\alpha) = \frac{-2\mathrm{i}\beta_0\mu^{2n}}{q(\mu^{2n})} \tag{4}$$

where

$$p(X) = \chi_{21}\chi_{11}a_0X^2 + (\chi_{21}^2c_0 - \chi_{11}^2b_0)X - \chi_{21}\chi_{11}d_0$$
$$q(X) = -\chi_{21}\chi_{12}a_0X^2 + (-\chi_{21}\chi_{22}c_0 + \chi_{11}\chi_{12}b_0)X + \chi_{11}\chi_{22}d_0.$$

Assume now that there exists some defect mode for a couple (k_0, α_0) such that $|\alpha_0| < k_0$, allowing us to define an angle of incidence θ_0 by $\alpha_0 = k_0\sin\theta_0$.

It is easily seen that the equation of proposition 2 is simply written $d_0(k_0, \alpha_0) = 0$, whence we obtain from (4)

$$r_n(k_0,\theta_0) = \frac{-\chi_{11}^2b_0 + \chi_{21}^2c_0 + \chi_{21}\chi_{11}\mu^{2n}a_0}{\chi_{11}\chi_{12}b_0 - \chi_{21}\chi_{22}c_0 - \chi_{21}\chi_{12}\mu^{2n}a_0}$$
$$t_n(k_0,\theta_0) = \frac{-2\mathrm{i}\beta_0}{-\chi_{21}\chi_{22}c_0 + \chi_{11}\chi_{12}b_0 - \chi_{21}\chi_{12}\mu^{2n}a_0}.$$

As n tends to infinity, we have the following limits:

$$\begin{aligned} r_n(k_0,\theta_0) &\longrightarrow \frac{\chi_{21}^2c_0 - \chi_{11}^2b_0}{\chi_{21}\chi_{11}b_0 - \chi_{22}\chi_{21}c_0} & t_n(k_0,\theta_0) &\longrightarrow \frac{-2\mathrm{i}\beta_0}{\chi_{21}\chi_{11}b_0 - \chi_{22}\chi_{21}c_0} \\ r_n(k,\theta_0) &\longrightarrow -\frac{\chi_{21}}{\chi_{22}} \quad \text{for} \quad k \neq k_0 & t_n(k,\theta_0) &\longrightarrow 0 \quad \text{for} \quad k \neq k_0. \end{aligned} \tag{5}$$

Remark 1. Obviously from (3) $|-\frac{\chi_{21}}{\chi_{22}}| = 1$, and so as a conclusion $|r_n(k_0,\theta_0)|$ tends pointwise towards a value that is strictly less than 1, whereas for any point different from k_0, in a small enough neighbourhood of k_0, $|r_n(k,\theta_0)|$ tends to 1 as $n \longrightarrow \infty$. This result means that the reflected energy admits a sharp minimum near k_0. It is important to note that the minimum of $|r_n(k,\theta_0)|$ is not *a priori* reached for value k_0 of the wavenumber, but the sharpness is all the more important as n is important. Clearly, for a given incidence θ_0, it is possible to transmit waves of wavenumber belonging to *a small interval near* k_0 and tending to $\{k_0\}$ as n tends to infinity.

It is known that for a fixed incidence θ, the scattering matrix admits a meromorphic extension to the complex half-space $\{\mathrm{Im}\,(k) < 0\}$ [21]. From (4), poles and zeros of r_n are solutions respectively of equations

$$\begin{aligned} &\mu^{4n}a_0 + \mu^{2n}\left(\frac{\chi_{21}}{\chi_{11}}c_0 - \frac{\chi_{11}}{\chi_{21}}b_0\right) = d_0 \\ &\mu^{4n}\frac{\chi_{21}\chi_{12}}{\chi_{11}\chi_{22}}a_0 + \mu^{2n}\left(\frac{\chi_{21}}{\chi_{11}}c_0 - \frac{\chi_{12}}{\chi_{22}}b_0\right) = d_0 \end{aligned} \tag{6}$$

and the limit of both equations as n tends to infinity is just $d_0(k, k\sin\theta) = 0$, which is the equation defining the defect modes. As both equations (6) are analytic perturbations of $d_0(k, k\sin\theta) = 0$ we can conclude the following.

Proposition 3. *One defect mode* $(k_0, k_0\sin\theta_0)$ *is associated with exactly one zero* k_z^n *of* r_n *and one pole* k_p^n *of* r_n *and* t_n*. Moreover* k_z^n *and* k_p^n *tend to* k_0 *as* n *tends to infinity.*

Remark 2. This suggests that, for sufficiently large n, there exist two positive numbers γ_n and δ_n such that

$$k_z^n = k_0 - \mathrm{i}\gamma_n\delta_n + \mathrm{O}(\delta_n)$$
$$k_p^n = k_0 - \mathrm{i}\delta_n + \mathrm{O}(\delta_n).$$

We know that, as n tends to infinity, δ_n tends to 0 and that $r_n(k_0, \theta_0)$ admits a limit given by (5). In the vicinity of k_0, we can write $r_n(k, \theta) \simeq -\frac{\chi_{21}}{\chi_{22}} \frac{k-k_z^n}{k-k_p^n}$ whence we obtain $r_n(k_0, \theta_0) \simeq -\frac{\chi_{21}}{\chi_{22}} \frac{\mathrm{Im}\,(k_z^n)}{\mathrm{Im}\,(k_p^n)}$, so that $\gamma_n = \frac{\chi_{11}^2 \chi_{21}^{-1} b_0 - \chi_{21} c_0}{\chi_{21} c_0 - \chi_{21} \chi_{11} \chi_{22}^{-1} b_0}$.

Remark 3. For real z, $z \mapsto -\frac{\chi_{21}}{\chi_{22}} \frac{z-k_z^n}{z-k_p^n}$ is the equation of a circle of diameter $\sqrt{1+\gamma_n^2}$, so that while in the gap the reflection coefficient belongs to the unit circle of the complex plane, it describes a circle for real k varying in the vicinity of k_0.

In order to be able to apply the Bloch-wave method to defect structures, an approximate method consists in periodizing the defect; this is the so-called supercell approximation. Let us apply this method to our simple example. We consider thus an infinite periodic structure whose period is made of one defect switched between n periods of the previous medium. We call it a superstructure. We know that the global monodromy matrix of the superstructure is $\tilde{\boldsymbol{T}}_{k,\alpha} = \boldsymbol{T}_{k,\alpha}^n \boldsymbol{T}_0 \boldsymbol{T}_{k,\alpha}^n$, and that the conduction bands are characterized by $|\operatorname{tr}(\tilde{\boldsymbol{T}})| < 2$. Now what happens at $k = k_0$? Obviously $\operatorname{tr}(\tilde{\boldsymbol{T}}_{k,\alpha}) = \mu^{2n} a_0 + \mu^{-2n} d_0$ so that for $(k, \alpha) = (k_0, \alpha_0)$ $\operatorname{tr}(\tilde{\boldsymbol{T}}_{k_0,\alpha_0}) = \mu^{2n} a_0$ and thus tends to 0 as n tends to infinity. This means that, at $\alpha = \alpha_0$, there exists an interval J_n of wavenumbers k over which $|\operatorname{tr}(\tilde{\boldsymbol{T}}_{k,\alpha_0})| < 2$ and therefore J_n is a conduction band in the superstructure. Of course the length of this interval depends upon n and tends to 0 as n tends to infinity because J_n tends to $\{k_0\}$. This is a crucial point as it justifies the use of Bloch-wave theory in the framework of the super-cell approximation, *at least in a small neighbourhood of* k_0. Finally, we can state the following.

Proposition 4. *In the superstructure, the existence of a defect* (k_0, α_0) *implies the opening of conduction bands inside gaps of the unperturbed structure that can support defect modes. The widths of these 'defect' conduction bands tend to zero exponentially with the number n of subperiods constituting one period of the superstructure.*

Remark 4. For a finite superstructure, and as the medium is periodic, we may apply a theory [15] allowing us to compute the superior envelope of the modulus of the reflection coefficient of a periodic structure. In the present problem, this is just the graph of

$$k \longmapsto \sqrt{1 - (4 - \operatorname{tr}(\tilde{\boldsymbol{T}})^2) \left(\tilde{\boldsymbol{t}}_{12}\beta_0 - \frac{\tilde{\boldsymbol{t}}_{21}}{\beta_0} \right)^{-2}}$$

where $\tilde{\boldsymbol{T}} = (\tilde{\boldsymbol{t}}_{ij})$.

We have analysed wave propagation in one-dimensional photonic crystals with one defect. We have shown a connection between the scattering properties and the modes: defect modes of the infinite structure give rise to a pole and a zero, explaining the behaviour of the refection coefficient. These results should help in the understanding of more complicated structures such as bi-dimensional photonic crystals, for which our paper could be used as an approximate theory [6, 7].

References

[1] Rarity J and Weisbuch C (ed) 1996 *Micro-Cavities and Photonic Band Gap: Physics and Applications* (Dordrecht: Kluwer)

[2] Carmona R and Lacroix B 1990 *Spectral Theory of Random Schrödinger Operator* (Basel: Birkhauser)

[3] Figotin A and Pastur L 1992 *Spectra of Random and Almost-Periodic Operators* (Berlin: Springer)

[4] Joannopoulos D, Meade R D and Winn J N 1995 *Photonic Crystals* (Princeton, NJ: Princeton University Press)

[5] Figotin A and Kuchment P 1996 *SIAM J. Appl. Math.* **56** 1561
[6] Centeno E and Felbacq D 1999 *J. Opt. Soc. Am.* A **16** 2705
[7] Maystre D 1994 *Pure Appl. Opt.* **3** 975
[8] Optoelectronics Group, Electrical Engineering Department, University of California, Los Angeles `http://www.ee.ucla.edu/labs/photon`
[9] Pendry J B and MacKinnon A 1992 *Phys. Rev. Lett.* **69** 2772
Bell P M, Pendry J B, Martin-Moreno L and Ward A J 1995 *Comput. Phys. Commun.* **85** 306
[10] Stefanou N, Karathanos V and Modinos A 1992 *J. Phys.: Condens. Matter* **4** 7389
Stefanou N, Yannopapas V and Modinos A 1998 *Comput. Phys. Commun.* **113** 49
[11] Ohtaka K and Tanabe Y 1992 *J. Phys. Soc. Japan* **65** 2265
[12] Karathanos V, Modinos A and Stefanou N 1994 *J. Phys.: Condens. Matter* **6** 6257
[13] Lekner J 1994 *J. Opt. Soc. Am.* A **11** 2892
[14] Felbacq D, Guizal B and Zolla F 1998 *Opt. Commun.* **152** 119
[15] Felbacq D, Guizal B and Zolla F 1998 *J. Math. Phys.* **39** 4604
[16] Figotin A and Gorenstein V 1998 *Phys. Rev.* B **58** 180
[17] Leung K M 1993 *J. Opt. Soc. Am.* B **10** 303
[18] Nian-hua Liu 1997 *Phys. Rev.* B **55** 4097
[19] Shanhui Winn Fan, Joshua N and Joannopoulos J D 1995 *J. Opt. Soc. Am.* B **12** 1267
[20] Bass F G, Slepyan G Ya and Gurevich A V 1994 *Phys. Rev.* B **50** 3631
[21] Reed R and Simon B 1979 *Methods of Modern Mathematical Physics* (New York: Academic)