Expressions for reflection and transmission coefficients for one-dimensional photonic quasicrystals

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Abstract. We give general expressions for the light reflection and transmission coefficients for one-dimensional (1D) photonic quasicrystals in the framework of the so-called two-wave approximation. A special attention is paid to quasicrystals composed of dielectric layers, where the reflection and transmission coefficients as a function of the length of the structure take a simple form. The expression for the diffraction vectors of a 1D quasicrystal with an arbitrary number of different constituent segments is discussed as well.

Introduction

Quasicrystals (QCs) belong to a wide class of aperiodic systems possessing long-range order and allowing coherent Bragg diffraction of electron or electromagnetic waves [1,2]. In the case of light waves such structures are called resonant or active photonic quasicrystals if the constituting materials produce dipole-like excitations; such systems are, for instance, multiple-quantum-well structures (MQWs). The theory of the propagation of electromagnetic waves in MQWs in the framework of the two-wave approximation was developed in work [3] and then generalized on the case of dielectric contrast [4]. It should be noted that in distinction from 1D periodic systems for which one can obtain analytically exact solutions, for 1D non-periodic systems it generally appears to be impossible and one has to resort to some approximations, in particular to that stated here.

In this work we theoretically study the propagation of electromagnetic waves in 1D quasi-periodic media and deterministic aperiodic structures (DAS) [3,4], in particular, in quasicrystals. Firstly, we deduce a general expression for diffraction vectors of an arbitrary 1D quasicrystal. Secondly, we consider the two-wave approximation in a general form to calculate the light reflection and transmission coefficients for a one-dimensional DAS with non-zero value of the structure factor. Thirdly, we present the expressions for the reflection and transmission coefficients in the case of an all-dielectric photonic quasicrystal; the expression for the Fourier components ε_G of the dielectric function of a DAS expressed by the structure factor is also given.

1. The structure factor and diffraction vectors of 1D quasicrystals

We use the standard definition of the structure factor [2,3]:

$$f(q) = \lim_{N\to\infty} \frac{1}{N} \sum_{m=1}^{N} e^{2iqz_m} = \sum_G f_G \delta_{2q,G} \, . \tag{1}$$

Here q is the light wave vector, the coordinates z_m give the positions of the scattering elements, which in our case are interfaces between the dielectric layers, and symbol $\delta_{2q,G}$ is the Kronecker symbol for arbitrary, not necessarily integer-valued quantities $2q$ and G. It is assumed that the structure factor of the semi-infinite system can be different from 0, i.e. $f_G \neq 0$ for any G. The vectors G are diffraction vectors of a quasicrystal (or any other DAS), which can be found from a given sequence z_m determined by DAS under consideration. For example, for 1D quasicrystals constructed from two segments (A and B) the vectors G and the corresponding structure factors f_G are given by two integer indices, h and h', i.e. $G = G(h, h')$. The analogous definition of the structure factor (equation (1)) is applied to a sublattice. It is worth mentioning that vectors G of the sublattices of a quasicrystal are equal, i.e. $G_a(h, h') = G_b(h, h') = G(h, h')$. A calculation of the structure factor f_G of a quasicrystal is a separate problem and is made in [2,5].

Let us consider a one-dimensional disordered quasicrystal, with the interfaces between the segments placed along z-axis in points $z'_m = z_m + \delta z_m$, where δz_m are independent and randomly distributed variables so that $\overline{\delta z_m} = 0$, $\overline{\delta z_m^2} = \sigma^2$. The structure factor averaged over the disorder realization has a form

$$f(q) = \sum_{h,h',h''\dots} \delta_{2q,G(h,h',h''\dots)} f_{hh'h''\dots} \exp(-(q\sigma)^2/2) \, .$$

The long-range correlations in the positions of the layers are still present in such a structure, and consequently the Bragg diffraction is determined by the same diffraction vectors as in the non-disordered quasicrystalline lattice. Evidently, the theory presented in the work is suitable for such correlated disordered structures as well.

We shall give a simple but not rigorous derivation of the expression for the diffraction vectors of an unlimited 1D quasicrystal composed of n types of different segments (i.e. of various constituting layers). Let us denote by a_i the length of i-type segment and by N_i the number of such segments in the structure. Thus, the full length of the quasicrystal is $L = \sum_{i=1}^{n} N_i a_i$. Using a more general definition of the structure factor $f_N(q) = N^{-1} \sum_{j=1}^{N} e^{iqx_j}$, where $N = \sum_{i=1}^{n} N_i$ is the full number of segments of the quasicrystal, and by dividing the whole quasicrystal into self-similar parts, in the limit $N \to \infty$ one can obtain that $GL = 2\pi m$, $m \in Z$. Then, by taking into account the linear independence of the solutions, one can present $m = \sum_{i=1}^{n} M_i h_i$, where $h_j \in Z$ are integers determining the diffraction vectors $G \equiv G(h_1, h_2, h_3, \dots)$ and M_i are also integers, but not arbitrary. From the equality $G \sum_{i=1}^{n} N_i a_i = 2\pi \sum_{i=1}^{n} M_i h_i$ and independence of the sought solution for G on values N_i ($N_i \to \infty$), one can get $M_i = N_i$ ($i = 1, 2, \dots n$). Using the notion of the average period of a quasicrystal, which is $\bar{d} = L/N$ (when $L \to \infty$, $N \to \infty$), and changing indices so that $h = h_1$, $h' = h_2 - h_1$, $h'' = h_2 - h_1$ and so on, we eventually come to the following expression for the diffraction vectors

$$G(h, h', h'', h'''\dots) = \frac{2\pi}{\bar{d}} \left(h + \frac{h'}{t_1} + \frac{h''}{t_2} + \frac{h'''}{t_3} + \dots \right) ,$$

where the numbers $h, h', h'', h''', \dots \in Z$, and values of t_k are defined by the relations $t_k = 1 + \lim_{N_i\to\infty} \sum_{i=1, i\neq k}^{i=n} N_i/N_k$. In particular, the diffraction vectors of a two-segment quasicrystal are defined by expression $G(h, h') = (2\pi/\bar{d})(h + h'/t)$ [2], where $t = 1 + \lim_{N\to\infty} N_1/N_2$. The simplest and well-known example is the so-called Fibonacci quasicrystal, which can be constructed by the help of the substitution rule $A \to B$, $B \to AB$, thus, starting with a sequence $ABAABABA\dots$. For this quasicrystal the value of t is the golden ratio, i.e. $t = (\sqrt{5} + 1)/2$.

2. Pseudo-band gaps in aperiodic systems

We consider a propagation (along z-axis) of electromagnetic waves in a 1D structure for which the modulation function $F(z)$, describing variation of the medium parameters (e.g. the dielectric permittivity) along z-direction, can be decomposed into the Fourier series $F(\omega, z) = \sum_G F_G e^{iGz}$. Besides periodic structures, which obviously satisfy this property, there are a number of deterministic aperiodic structures generating coherent Bragg diffraction, in particular, quasicrystals and incommensurate modulated crystals [1]. The frequency functions F_G depend on the system under consideration and require a separate calculation. As long as the function $F(z)$ is almost-periodic [6] (or periodic when considering a periodic structure) the electromagnetic field $E_K(z)$ with the wave vector K can be sought as a linear superposition $\sum_G E_{K-G} e^{i(K-G)z}$, and the wave equation is written as

$$-d^2 E_K(z)/dz^2 = F(\omega, z) E_K(z) \tag{2}$$

Hereafter we consider the situations where in RHS of equation (2) only the components with vectors $G = 0$ and $\pm G$ (where $G \equiv |G|$) are kept and one can take into account only two wave vectors, K and $K - G$, at the condition $|K - G/2| \ll G/2$. The last is valid if $|F_G| \ll |F_0|$, which allows neglecting the rest of diffraction vectors G. Thus, $E_K(z) \approx E_K e^{iKz} + E_{K-G} e^{i(K-G)z}$, where the wave vector magnitude K can be presented as $K = G/2 \pm Q$. Substituting the last expression for $E_K(z)$ in equation (2) and neglecting the other components except E_K and E_{K-G} we obtain that $E_{K-G} = E_K(K^2 - F_0)/F_G$ and $Q = \sqrt{(G/2)^2 + F_0 \pm \sqrt{G^2 F_0 + F_G F_{-G}}}$, where the positive sign must be ignored since $Q \ll G/2$ and the real part of F_0 is positive, consequently

$$Q = \sqrt{(G/2)^2 + F_0 - \sqrt{G^2 F_0 + F_G F_{-G}}}\,. \tag{3}$$

By neglecting the absorption in the system one can get $F_0 = F_0^*$ and $F_G = F_{-G}^*$, and if the radicand (under the big root sign) is negative we find ourselves in the region of a pseudo-band gap. The latter strongly resembles the typical band gaps in periodic structures: a high reflectivity in the pseudo-band gap region is due to the constructive interference of the light waves competing with the effect of nonperiodicity of the structure. The edges of the pseudo-band gap satisfy the condition $Q = 0$ and can easily be found from equation (3): $(G/2)^2 - F_0 \pm |F_G| = 0$. Similar to 1D quasi-periodic media, two-dimensional quasicrystals made from materials with a small dielectric contrast can also demonstrate wide pseudo-band gaps [7]; however, in this case the derivation of the explicit analytical expressions is complicated.

The above two-wave approximation can be justified by the help of the perturbation theory which allows one to evaluate the convergence of an infinite sum over all diffraction vectors except G and to determine pseudo-band gap edges placed around a Bragg frequency. Primarily, this approach was applied to the so-called 1D resonant photonic crystals for which the Bragg frequency coincides with the resonant one [3].

In the simplest cases, the Bragg condition for a DAS is defined in such a way that it would lead to the only pseudo-band gap in the energy spectrum or to two pseudo-band gaps of almost the same width. The first case is realized in 1D photonic quasicrystals with non-frequency-dependent dielectric constants of the constituent materials. Since while decreasing the dielectric contrast the value F_G converts to 0 (see section 3), the polariton wave vector becomes $Q = |G/2 - \sqrt{F_0}|$ and at a frequency $\bar{\omega}$ the Bragg condition $G/2 = \sqrt{F_0(\bar{\omega})}$ is fulfilled. The second case corresponds to a situation where the segments of a photonic quasicrystal are characterized by some frequency function symmetric about a special frequency, e.g., the exciton resonance frequency for MQWs [3]. One can show that for MQWs the calculation of the corresponding Fourier-components leads to the following expressions:

$$F_0 = \left(\frac{\omega}{c}\right)^2 \bar{\varepsilon} - \frac{2ir}{1+r}\frac{\omega\sqrt{\varepsilon_a}}{c\,\bar{d}}\;, \qquad F_G = \left[\left(\frac{\omega}{c}\right)^2 (\varepsilon_a - \varepsilon_b) - \frac{2ir}{1+r}\frac{\omega\sqrt{\varepsilon_a}}{c\,a}\right]\frac{f_{-G}}{\pi G}\sin\frac{Ga}{2}\,. \tag{4}$$

Here we have used the following notations: ε_a and ε_b are the background dielectric constants of the quantum well and the barrier, respectively, a is the well width, $\bar{d}$ is the mean period defined as the average distance between quantum wells, and r is the amplitude reflection coefficient of light for a single quantum well (reduced to the plane in the centre of the well), calculated for the case $\varepsilon_a = \varepsilon_b$. In addition, equation (4) contains the structure factor f_G which for quasi-crystalline sequences is equal to $2\pi f_{hh'}/\bar{d}$, and $f_{-G} = f_G^*$. The optical spectra and pseudo-band gaps for light propagation in MQWs were studied in [3,4,5]. In this case the resonant Bragg condition is $\omega_0 n/c = G/2$ (where $n \approx \sqrt{\varepsilon_b}$) and in the energy spectrum there are two pseudo-band gaps which in the reflection spectra manifest themselves as two "shelves" of almost the same width being located at about equal distances from the frequency ω_0.

Now we will find the general expressions for the amplitude reflection and transmission coefficients (at normal light incidence) for a structure of the length L with an arbitrary quasi-crystalline sequence of the constituent layers of different types. For this purpose we define the field $E(z)$ as

$$E_0 e^{iqz} + E_r e^{-iqz} \quad (z < 0)\,; \qquad E_t e^{iq(z-L)} \quad (z > L)$$

$$E_{K_1} e^{iK_1 z} + E_{K_1-G} e^{i(K_1-G)z} + E_{K_2} e^{iK_2 z} + E_{K_2-G} e^{i(K_2-G)z} \quad (0 < z < L)$$

where $K_1 = G/2 - Q$, $K_2 = G/2 + Q$, and $q = (\omega/c)\sqrt{\varepsilon_{out}}$ is the wave vector magnitude of the plane light wave incident from a uniform medium surrounding the quasicrystal. By using the boundary conditions for the field $E(z)$ and its derivative $dE(z)/dz$ at the interfaces $z = 0$ and $z = L$ and introducing the notations $\xi_{1,2} = (K_{1,2}^2 - F_0)/F_G$,

$$A(K_{1,2}) = q - K_{1,2} + (q + K_{2,1})\xi_{1,2}$$

$$B(K_{1,2}) = q + K_{1,2} + (q - K_{2,1})\xi_{1,2}$$

$$C(K_{1,2}) = K_{1,2} - q - (q + K_{2,1})\xi_{1,2} e^{-iGL}$$

the reflection coefficient $r_L = E_r/E_0$ can be reduced to the form

$$r_L = \frac{A(K_2)C(K_1) - A(K_1)C(K_2)e^{2iQL}}{B(K_2)C(K_1) - B(K_1)C(K_2)e^{2iQL}} \tag{5}$$

and the transmission coefficient $t_L = E_t/E_0$ to

$$t_L = 2qe^{iK_2 L} \frac{C(K_1)(1 + \xi_2 e^{-iGL}) - C(K_2)(1 + \xi_1 e^{-iGL})}{B(K_2)C(K_1) - B(K_1)C(K_2)e^{2iQL}}\,. \tag{6}$$

The analysis of expressions (5) and (6) under condition $|F_G| \to 0$ shows that if $q^2 = F_0$, then $r_L = 0$ and $t_L = e^{iqL}$, therefore the dielectric constant of the surrounding medium must be equal to $\varepsilon_{out} = F_0(c/\omega)^2$. This equality can be strictly satisfied for any frequency only for purely dielectric photonic quasicrystals because in this case $F_0 = (\omega/c)^2\bar{\varepsilon}$ (see section 3), nevertheless it can be approximately used in other cases also. In fact, the dielectric constant ε_{out} of the surrounding medium should be set to $\bar{\varepsilon} = L^{-} \int_0^L \varepsilon(\tilde{\omega}, z)dz$, where $\tilde{\omega}$ must satisfy the condition $|F_G(\tilde{\omega})| \ll 1$. We pay attention that the above expressions for r_L and t_L can be exploited only in the frequency ranges for which the criterion for the validity of the two-wave approximation is satisfied, and for each individual system these expressions should be checked numerically. In the case where the value of the dielectric constant of the medium surrounding a quasicrystal is arbitrary the reflection and transmission coefficients, instead of expressions (5) and (6), can be found by using the transfer-matrix technique, see [4].

In the pseudo-band gap region, in the limit as $L \to \infty$, $|r_\infty| = 1$ and from equation (5) one can obtain the dispersion relation between the frequency ω and imaginary part Q'' of the polariton wave vector Q, which is just equation (3). Let us introduce the following notations: $\eta = \sqrt{G^2F_0 + |F_G|^2}$, $X = 2GQ''F''_G + 2|F_G|^2 + G^2F'_G - 2\eta F'_G$, where F'_G and F''_G denote the real and imaginary parts of F_G, respectively, and $Q'' = \sqrt{\eta - (G/2)^2 - F_0}$. Then the reflection coefficient of light from a semi-infinite structure can be written as $r_\infty = e^{i\phi} = Re(r_\infty) + iIm(r_\infty)$ (where ϕ is the reflection coefficient phase), and its real and imaginary parts after some transformations may be reduced to the following forms:

$$Re(r_\infty) = \frac{(q^2 + F_0)X + 2|F_G|^2(F'_G - \eta)}{(q^2 - F_0)X + 2|F_G|^2(\eta - F'_G)}\ ,\ \ Im(r_\infty) = \frac{2q[2Q''(F'_G\eta - |F_G|^2) + GF''_G(2F_0 - \eta)]}{(q^2 - F_0)X + 2|F_G|^2(\eta - F'_G)} \tag{7}$$

These expressions can be used to calculate the phase change ϕ on reflection from the interface between the structure and the surrounding medium and also to state the conditions under which the phase of the light wave changes by a given value ϕ. The latter has a direct relation to different types of 1D topological insulators, e.g., 1D dielectric topological insulator [8]. Since for such systems $F_0 = q^2$, the frequency ω at which $\phi = \pi$, as is seen from the first equation (7), can be found from the condition $X = 0$, which can be simplified to the form $2GQ''\sin\psi + 2|\varepsilon_G|(\omega/c)^2 + (G^2 - 2\eta)\cos\psi = 0$, where ψ is the phase of $\varepsilon_G = |\varepsilon_G|e^{i\psi}$.

3. The dielectric photonic quasicrystals

If a 1D photonic quasicrystal consists of layers characterized with non-frequency dependent dielectric susceptibilities (and magnetic permeability $\mu = 1$), one can find the Fourier-components $F_0 = (\omega/c)^2\varepsilon_0$ and $F_G = (\omega/c)^2\varepsilon_G$, where ε_0 and ε_G are Fourier-components of the dielectric profile function $\varepsilon(z) = \sum_G \varepsilon_G e^{iGz}$. The function $\varepsilon(z)$ can be represented in terms of the unit step functions, from where one can obtain the expression for ε_G which for a two-segment quasicrystal is

$$\varepsilon_G = \varepsilon_a f^{(a)}_{-h,-h'}\frac{(1 - e^{-iGa})}{iG\bar{d}_a} + \varepsilon_b f^{(b)}_{-h,-h'}\frac{(1 - e^{-iGb})}{iG\bar{d}_b}\ , \tag{8}$$

where $\bar{d}_a = \lim_{N\to\infty}(N_a a + N_b b)/N_a$ and $\bar{d}_b = \lim_{N\to\infty}(N_a a + N_b b)/N_b$ are the mean periods of sublattices of the initial quasi-crystalline lattice, and $f^{(a)}_{hh'}$ and $f^{(b)}_{hh'}$ are the structure factors related to the corresponding sublattices. The generalization of equation (8) on an arbitrary number of segments is trivial.

It is useful to mention the second simplest case of a dielectric photonic QC, when a deterministic aperiodic structure consists of dielectric layers A with the width a incorporated into a dielectric medium with the dielectric constant ε_b in such a way that their centres, lying along z-axis, form a sequence given by the expression $z_m = z_0 + m\bar{d} + \Delta\{m/t + \varphi\}$. Here z_0 is an arbitrary constant, Δ, t, φ are the parameters of the structure, $\bar{d}$ its average period, and $\{x\}$ denotes the fractional part of a number. In this case the Fourier components F_0 and F_G can be found from equation (4) by setting $r \to 0$.

The edges of a pseudo-band gap calculated on the basis of the two-wave approximation are found from equation (3) under condition $Q = 0$: $\omega_\pm = (Gc/2)/\sqrt{\varepsilon_0 \pm |\varepsilon_G|}$. The value of the wave vector of the light propagating in the surrounding medium, q, must be chosen equal to $\omega\sqrt{\bar{\varepsilon}}/c$ because it leads to zero reflection coefficient when $F_G \to 0$; $\varepsilon_0 = \bar{\varepsilon}$ is the average dielectric constant and L is the length of a quasicrystal. After some transformations and by dividing the numerators and denominators of the expressions for r_L (equation (5)) and t_L (equation (6)) by $Z(\omega) = F_G e^{iGL/2} + (Q^2 - (q + G/2)^2)e^{-iGL/2}$ the amplitude reflection coefficient of light can be reduced to the following form

$$r_L = \frac{(F_G + Q^2 - (q + G/2)^2)(Q^2 - (q - G/2)^2)}{(F_G + Q^2 - (q - G/2)^2)((G/2)^2 - q^2 - Q^2 - 2iqQ\cot QL)} \tag{9}$$

and the amplitude transmission coefficient to

$$t_L = \frac{-2iqQ[F_G e^{iGL/2} + (Q^2 - (q - G/2)^2)e^{-iGL/2}]}{(F_G + Q^2 - (q - G/2)^2)((G/2)^2 - q^2 - Q^2 - 2iqQ\cot QL)\sin QL}\,. \tag{10}$$

A further simplification of the above expressions for r_L and t_L leads to the following answers:

$$r_L = \frac{F_G(qG - \sqrt{q^2G^2 + |F_G|^2}) + |F_G|^2}{(F_G + qG - \sqrt{q^2G^2 + |F_G|^2})(\sqrt{q^2G^2 + |F_G|^2} - 2q^2 - 2iqQ\cot QL)}\,, \tag{11}$$

$$t_L = \frac{-2iqQ[F_G e^{iGL/2} + (qG - \sqrt{q^2G^2 + |F_G|^2})e^{-iGL/2}]}{(F_G + qG - \sqrt{q^2G^2 + |F_G|^2})(\sqrt{q^2G^2 + |F_G|^2} - 2q^2 - 2iqQ\cot QL)\sin QL}\,. \tag{12}$$

The equations (11) and (12) can be used when $|\varepsilon_G| \ll \bar{\varepsilon}$, in particular, for low-contrast photonic quasicrystals. Since these expressions contain explicitly the length L of a structure, it allows one to determine the length at which the formation of pseudo-band gaps occurs in different 1D deterministic aperiodic structures.

A typical reflection spectrum $|r_L(\omega)|^2$ for a quasicrystal calculated by equation (11) in the vicinity of frequency $\bar{\omega} = Gc/2\sqrt{\bar{\varepsilon}}$ is almost symmetrical about $\bar{\omega}$ and resembles in much the reflection spectrum for an analogous periodic structure. Since the equation $Z(\omega) = 0$ determines some of the eigenfrequencies of the system and the function $Z(\omega)$ is reduced in expressions for r_L and t_L (equation (5) and (6)), one can conclude that the set of eigenfrequencies and the reflection and transmission spectra for 1D purely dielectric photonic quasicrystals are much poorer than those for photonic quasicrystals composed of constituent layers with a frequency-dependent dielectric function.

We note that in the pseudo-band gap region in the limit as $L \to +\infty$ the product $Q\cot QL$ gives Q'', where $Q'' = \sqrt{\eta - (G/2)^2 - q^2}$, and $|\sin QL| \to +\infty$ leading to zero transmission coefficient ($t_\infty = 0$). Another possible approximation is $qG - \sqrt{q^2G^2 + |F_G|^2} \approx -|F_G|^2/(2qG)$, which is valid for very low-contrast structures. With these simplifications, equations (11) and (12) for the optical coefficients r_L and t_L can be considerably simplified, especially in the cases of the pseudo-band gap edges (at frequencies $\omega_\pm$) and the gap "centre" (at frequency $\bar{\omega}$).

In conclusion, we have given the general expression for the diffraction vectors of 1D quasicrystals and generalized the theory of light propagation in quasicrystals (and in other deterministic aperiodic structures) developed in works [3,4]. An analysis of the obtained expressions allows one to optimize the parameters of different 1D photonic quasicrystals to get pseudo-band gaps in the frequency range of interest. Also the developed theory can be generalized to the case of inclined light incidence or the propagation of acoustic waves in phononic quasicrystals, and as a particular case it can give answers for the corresponding periodic systems.

Acknowledgments
The author is grateful to M.M. Glazov and E.L. Ivchenko for useful discussions.

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