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Localized modes in photonic quasicrystals with Penrose-type lattice

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Abstract: We investigate the properties of the resonant modes that occur in the transparency bands of two-dimensional finite-size Penrose-type photonic quasicrystals made of dielectric cylindrical rods. These modes stem from the natural local arrangements of the quasicrystal structure rather than, as originally thought, from fabrication-related imperfections. Examples of local density of states and field maps are shown for different wavelengths. Calculations of local density of states show that these modes mainly originate from the interactions between a limited numbers of rods.

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1. Introduction

Periodic structures have properties that have been subject of important theoretical developments in both solid-state physics [1] and photonics [2]. In solid-state physics, it has been long believed that periodic crystals were the only ordered structures. The existence of more complex type of order was found in nature with the discovery of the icosahedral phase of metallic alloys [3]. D. Shechtman et al. discovered these structures, which were named quasicrystals. Since then, *aperiodic order* has been subject of attention from solid-state physicists, but also mathematicians, and now photonic physicists. Aperiodically-ordered structures may exhibit a variety of weak (e.g., local and/or statistical) forms of rotational symmetries, which are not necessarily bounded by the crystallographic restriction typical of periodic structures [3]. While electronic properties of quasicrystals have been studied thoroughly, their *photonic* counterparts have been subject of less attention and deserve further investigations.

The earliest studies of Fibonacci-like one-dimensional quasicrystals have shown the existence of photonic bandgaps, and localization of the light [4,5]. Bandgaps at large wavelengths (with respect to the average layer thickness) have been shown to exist [6]. Field enhancement and group velocity reduction at the band-edge have been observed experimentally [7]. Numerical studies have shown that two-dimensional photonic quasicrystals can also exhibit photonic bandgaps [8,9]. Complete bandgaps can be obtained for relatively low index contrast [10,11] thanks to higher (e.g. 12-fold) statistical symmetries. One advantage of these aperiodic structures is their capability of exhibiting many inequivalent sites, and consequently many possible different defects [8,12]. It has also been shown that long-range interactions play an important role in the formation of bandgaps in such structures [13]. Recently, M. Notomi et al. have studied the stimulated emission in aperiodically-ordered structures, considering a Penrose-type quasicrystal laser [14]. Contrary to the typical extended modes of the band-edge photonic crystal lasers, Penrose laser modes were found to be localized. Note that a very interesting theoretical study of localized modes in defect-free quasiperiodic photonic crystal has shown that transmission within the bandgap could be attributed to a competition between the nonperiodicity and self-similarity [15].

Our aim is to provide some physical insight in the nature of these resonant modes via an analysis based on the calculation of the *local density of states* (LDOS) for finite-size photonic quasicrystals. We first recall the basic elements of the numerical method we use, and of the computation of the LDOS. Then, we show that the LDOS maps present evidence of modes attributable only to the constructive interference of the field diffracted by a very limited number of rods. This shows the *localized* nature of the modes, opposite to the *extended* nature of the resonant modes that can be observed in the transparency bands of finite-size periodic photonic crystals. Indeed, these latter can easily be interpreted as Fabry-Perot modes (*i.e.* a standing wave mode) for a given Bloch mode, whereas the aperiodic-order-induced modes here are found to stem essentially from the *local* arrangement of rods.

2. Modelling and LDOS

We consider a two-dimensional Penrose tiling built as a combination of two types of rhombus tiles, whose edges have the same length denoted as a [16]. This geometry is characterized by a fivefold symmetry [16]. The quasicrystal of interest here is generated by placing identical

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dielectric rods at the vertices of the rhombuses of the Penrose tiling, as shown in Fig. 1. The rods are assumed to lay in vacuum and to be made of nondispersive dielectric material, with relative permittivity $\varepsilon_a = 12$, and with radius $r_a = 0.116a$. The electric field is assumed to be parallel to the axis of the rods (E parallel polarization).

A computationally-effective and physically-insightful modeling of such a finite-size structure is addressed here, without any supercell approximation, via the LDOS analysis.

The numerical method we utilize is based, first, on a multipolar expansion of the fields around (and inside) each rod, giving rise to Fourier-Bessel series that can be separated into two parts: the local incident field and the outgoing scattered fields. Note that the local incident field on a rod includes the field scattered by the other rods. Obviously, the scattered field is related to the local incident field through the diffraction process, i.e. the coefficients of the series representing the incoming and outgoing waves are related to each other by a scattering matrix. Enforcing the suitable matching conditions at the rods interfaces, one is eventually led to a linear system whose solution gives the coefficients of the multipolar expansions. A detailed presentation of the method can be found in Refs. 17 and 18. This method is known as the Korringa-Kohn-Rostocker method in solid states physics [19] and is often called "multipole expansion method" or "scattering matrix method" in the optics community. The method has recently been extended to handle the calculation of the local density of states (LDOS) in finite-size photonic crystals [20,21].

In the following computations, the normalized LDOS $\rho(\mathbf{r}_0, \omega)$ at any arbitrary location \mathbf{r}_0 is easily evaluated using the method described above. It is worth noticing that we consider a two-dimensional geometry invariant along the *z*-axis, and consequently all the electromagnetic field components are also *z*-invariant. The symbol \mathbf{r} will be used throughout the paper to denote a two-dimensional vector in the *xOy* plane. It is well known that in the case of interest, i.e. a set of two dimensional lossless rods, the normalized LDOS, $\rho(\mathbf{r}_0, \omega)$, is

given by the imaginary part of the Green's function $G(\mathbf{r}, \omega)$ evaluated at the source location:

$$\rho(\mathbf{r}_0, \boldsymbol{\omega}) = \Im m \big(G(\mathbf{r} = \mathbf{r}_0, \boldsymbol{\omega}) \big) \,. \tag{1}$$

The Green's function in Eq. (1) is defined via the following equation:

$$\Delta G(\mathbf{r}, \boldsymbol{\omega}) + \varepsilon \left(\mathbf{r}\right) \left(\frac{\boldsymbol{\omega}}{c}\right)^2 G(\mathbf{r}, \boldsymbol{\omega}) = 4\delta(\mathbf{r} - \mathbf{r}_0), \qquad (2)$$

where $\varepsilon(\mathbf{r})$ is the relative permittivity ($\varepsilon = \varepsilon_a$ inside the rods, and $\varepsilon = 1$ outside), c the vacuum light celerity, ω the angular frequency, and the standard radiation condition (outgoing field) is implied. The normalization of $\rho(\mathbf{r}_0, \omega)$ has been chosen so as to have $\rho(\mathbf{r}_0, \omega) = 1$ in vacuum. The LDOS has the key feature of being intrinsically related to the response of the structure to any type of excitation. In solid-state physics, the LDOS is informative about the dynamics that an atom would undergo if located at a given point. In our electromagnetic analogy, the LDOS maps practically provide information about the total power emitted versus the excitation point.

3. Results and discussion

Figure 1 shows a Penrose quasicrystal structure made of 530 rods (left), and the LDOS at the center point $\mathbf{r}_0 = (0,0)$ versus the normalized frequency (right). Several bandgaps can be observed in the frequency range displayed: A large central one, and two less pronounced (at higher and lower frequencies). A previous study by the same authors has shown that bandgap

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formation in photonic quasicrystals may involve long-range interactions and multiple scattering [13].



Fig. 1. Left: A Penrose photonic quasicrystal made of 530 dielectric rods placed at the vertices of the rhombus tiles. Right: LDOS computed at x = 0, y = 0. Distances are normalized with respect to *a* in all figs.

Here, we will concentrate on the behavior of the modes when a frequency in a transparency band is considered. Figure 2 shows a typical map of LDOS for the quasicrystal in Fig. 1 at a normalized frequency $a/\lambda = 0.415$ between the two lower-frequency bandgaps. The map shows that, in a large quasicrystal, several localized resonances can be observed at the same frequency. A typical nearly-fivefold-symmetric localized mode is magnified by the zoom in Fig. 2. The deviance from perfect fivefold symmetry is likely attributable to the finite size of the structure. Figure 3 shows other typical LDOS maps at a higher normalized frequency) at a chosen location x/a = 1.05 and y/a = 4.6. This location has been chosen to be in the region of the localized mode on which we will focus, and we will show later that its choice is not critical (see movie). We have chosen these two examples as being representative of the observed field maps of the modes, but we have found many others analogous situations corresponding to different wavelengths within the transparency bands.

It should be noticed that, in periodic crystals, a local deviance from periodicity (defect) could induce a transition from the extended modes to localized modes. Indeed, for example, removing a rod in a perfectly periodic structure is a well-known device to create a localized mode. Our numerical computations have confirmed the existence of such localized modes in the transparency bands of quasicrystals (without resizing or displacing any rod). As the authors of Ref. [14] implicitly assumed, we confirm that the behavior observed in their experiments is not a consequence of unavoidable fabrication-related deviance from the quasicrystalline ideal structure, but it rather represents one of its inherent properties.

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Fig. 2. Left: LDOS map in linear false-color scale (red=high; blue=low) pertaining to the upper region of the photonic quasicrystal in Fig. 1, at a normalized frequency $a/\lambda = 0.415$. Right: Zoom of a region (dashed square) where a fivefold symmetry of the field distribution is clearly visible. Distances are normalized with respect to *a* in all figs.



Fig. 3. As in Fig. 2, but for a normalized frequency $a / \lambda = 0.726$.

Figure 4 shows the maps of the modulus and phase of the field at the normalized frequency $a/\lambda = 0.726$ when the structure is excited by a single electric line source located at x/a = 1.05 and y/a = 4.6 (see the previous discussion, pertaining to Fig. 3: For that source location, the LDOS is maximum at $a/\lambda = 0.726$). As can be expected, the distribution of the modulus of the field is very similar to that of the LDOS map shown in Fig. 3, and the phase map also reveals the fivefold symmetry of the mode. Note that we have checked that the field vanishes outside the part shown in Fig. 4, thus the source excites no other localized mode in the structure at this frequency

The quasicrystal laser experiment reported in Ref. [14] has demonstrated that the mode described above could be used for lasing, and that lasers could take advantage of the richness of the possible symmetries of quasicrystals. Performance optimisation of such lasers would need a fine understanding of the quasiverystals properties and physical origins of the modes. The following observations may hopefully contribute to a deeper understanding.

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Fig. 4. Electric line source excitation at x/a = 1.05 and y/a = 4.6, with normalized frequency $a/\lambda = 0.726$. Modulus (left) and phase (right) of the electric field.

In order to investigate the process of formation of the localized modes, such that in Fig. 4, we modified the structure by removing parts of the quasicrystal outside the resonant region. In a previous paper [13] we have shown that certain bandgaps of a quasicrystal involve longrange interactions. Thus the question of the role of such long-range interactions in the appearance of the observed modes arises naturally even if the two effects are not physically related (the studied modes are outside the bandgap). Figure 5 shows some examples of LDOS maps (computed in the same region as in Fig. 4) pertaining to increasingly smaller quasicrystals obtained by progressively eliminating certain rods outside the region displayed. The amplitude of the LDOS associated with the mode slightly changes (about 20 percent) but the distribution does not. This behavior suggests that the modes have indeed a highly localized nature. This is clearly visible from the last case (rightmost plot), where, in spite of a very drastic reduction of the number of rods (the quasicrystal has been reduced along both x and y dimensions to keep only 47 rods located inside a square centered at x/a = -0.25 and y/a =4.25, with edge length equal to 5.9a), a behavior similar to that of the larger structures is observed. The reduction in the LDOS amplitude can be mainly attributed to a resonance frequency shift rather than a real decrease in the resonance strength. The movie in Fig. 6 shows the LDOS for the smallest quasicrystal made of 47 rods when the frequency a/λ varies from 0.712 to 0.739. It can be observed that the LDOS maximum arises now at a normalized frequency of 0.729 (instead of the 0.726 value observed for the larger structure). The frequency shift is accompanied by only a small weakening of the resonance strength, as shown by the maximum of the LDOS map. Thus we have shown that long-range order does not play a major role in the lasing effect observed, contrarily to the hypothesis of the authors of Ref. [14]. This result is fully consistent with the analysis made in Ref. [15]: Localized modes may appear due to the non-periodicity of the structure, but in our case they appear outside the bandgap region, which is unexpected.



Fig. 5. LDOS maps for photonic quasicrystals of different sizes (same color scale). From left to right: 488, 384, and 47 rods, respectively.

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Fig. 6. LDOS map for a photonic quasicrystal of 47 rods, at a normalized frequency of 0.729. See also the movie that shows the variations for normalized frequencies varying from 0.712 to 0.739. Color scales are identical to that in Fig. 5

4. Conclusions

We have presented a numerical study of localized resonant modes in two-dimensional finitesize Penrose-type photonic quasicrystals. The existence of the localized modes observed by other authors in the quasicrystal lasers has been numerically confirmed. It has been shown that these modes probably originate from interactions among a small number of rods, rather than from undesired fabrication-related defects, and should accordingly be considered as an inherent property of quasicrystalline geometries. Indeed, the observed localized modes are only slightly modified by the elimination of several rods around (and even relatively close to) the localization region. These conclusions are nontrivial and somehow *counterintuitive*, since it is well known that band-edge modes in periodic crystals are not localized. The fact that localization is not much affected by long-range interactions strengthens the difference with the bandgap effect.

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