Band Gap Formation and Multiple Scattering in Photonic Quasicrystals with a Penrose-Type Lattice

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This Letter presents a study of the local density of states (LDOS) in photonic quasicrystals. We show that the LDOS of a Penrose-type quasicrystal exhibits small additional band gaps. Among the band gaps, some exhibit a behavior similar to that typical of photonic crystals, while others do not. The development of certain band gaps requires large-size quasicrystals. It is explained by the long-range interactions involved in their formation. Moreover, the frequencies where the band gaps occur are not necessarily explained using single scattering and should therefore involve multiple scattering.

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One of the major recent revolutions in photonics, the photonic crystal, was pioneered by E. Yablonovitch [1]. The basic idea proposed was that if one is able to build a material that can forbid the propagation of electromagnetic waves, then one will be able to control spontaneous emission. Recalling from solid state physics the way periodic potentials create band gaps for the electrons in semiconductors, the idea proposed for obtaining such photonic band gaps was based on the use of periodic arrangements of dielectric materials. Rapidly, photonic crystals with a full band gap, i.e., a domain of wavelengths in which the propagation of electromagnetic waves is completely forbidden, have been identified, and infrared band gaps have been demonstrated experimentally [2,3].

Since these pioneering works, numerous different phenomena and applications have been identified. One of the most advanced in terms of industrial development is certainly the photonic crystal fiber (now available commercially) [4,5]. Novel exciting phenomena could be exploited in the near future in practical optical circuits. One can cite phenomena such as superprism [6], self-guiding [7], and others effects that are based on the richness of the dispersion relation of photonic crystals [8,9].

The existence of more complex ordered structures was found in nature with the discovering of icosahedral phase of metallic alloys [10]. These structures, named quasicrystals, were discovered by D. Shechtman *et al.*, and exhibit unique electronic properties. Since their discovery, these structures have intrigued scientists from various communities (principally from solid-state physics, but also mathematics, and now photonics). Aperiodically driven 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 [10].

Following up on the solid-state-physics analogy underlying Yablonovich's idea, some researchers considered aperiodically-ordered systems, i.e., photonic quasicrystals. Thus, the question about the properties of photonic quasicrystals arose naturally.

Recently, it has been shown theoretically that two-dimensional photonic quasicrystals could exhibit photonic band gaps [11,12]. Moreover, it has been noted that one advantage of these aperiodic structures is to present many inequivalent sites, and consequently many possible different defects [11,13]. A remarkable property of photonic quasicrystals is that total band gaps can be obtained in the presence of sufficiently high (e.g., twelvefold) statistical symmetry [14,15], even if the value of the minimal index contrast has been subject of controversy.

It is worth noticing that earlier studies in connection with Fibonacci-like one-dimensional quasicrystals have shown the existence of photonic band gaps, as well as the experimental evidence of light waves localization [16,17]. Band gaps at extremely large wavelengths with respect to the average thickness of the layers have been exhibited [18]. Moreover, band edge resonances have been studied in similar structures, and field enhancement and group velocity reduction have been observed experimentally [19].

Recently, M. Notomi *et al.* have studied the emission in aperiodically-ordered structures, considering a Penrose-type quasicrystal laser [20]. They found localized modes, at variance with typical extended modes in photonic crystal lasers.

In this Letter, we shall consider a two-dimensional Penrose tiling, obtained as a combination of two types of rhombuses whose edges have the same length denoted as a [21]. This geometry is characterized by a tenfold statistical rotational symmetry [21]. The quasicrystal of interest here is generated by placing identical 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 nondispersive, 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.

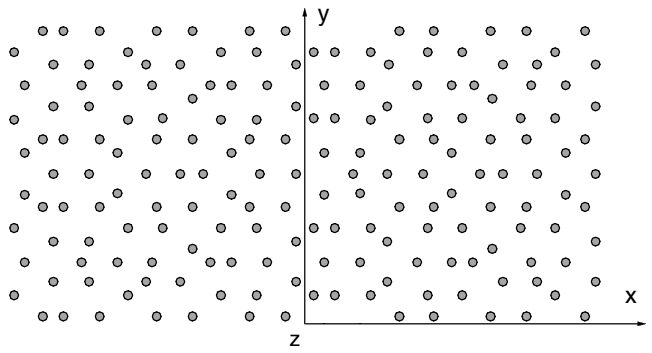

FIG. 1. Upper part ($y > 0$) of a photonic quasicrystal made of 530 dielectric rods (permittivity ε_a and radius r_a) lying in vacuum. The rods are located at the vertices of a Penrose tiling made with two types of rhombuses whose edges length are a.

As mentioned previously, one of the main differences between standard photonic crystals and the Penrose quasicrystal is the lack of spatial periodicity, and hence of a unit cell, which renders impossible the definition of a Brillouin zone, and numerically intractable the study of infinite structure. To overcome these problems, two approaches have been proposed: the first one relies on the introduction of an artificial periodicity (supercell approximation), whereas the second one directly considers a finite structure. From the modeling point of view, the second approach seems more satisfactory, as the actual structure will necessarily be finite. Then a natural question arises about the physically meaningful characterization of finite-size structure. In this connection, one of the most insight-providing quantities that can be studied by numerical modeling is the density of states. We note that in Ref. [11], calculations of density of states have been performed within a supercell approximation, though the authors have carefully checked that the artificially-introduced periodicity does not undermine their conclusions.

In our investigation, we decided to consider a finite number of rods in a homogeneous host medium. The method we utilize for numerical characterization of finite-size quasicrystals has been developed simultaneously by our group and others several years ago, and is based on a multipolar expansion of the fields around (and inside) each cylindrical rod [22,23]. This method is closely related to the Korringa-Kohn-Rostocker method used in solid states physics [24] that is itself derived from a pioneering work by Lord Rayleigh in electrostatics [25]. It has also been recently applied to the study of the local density of states (LDOS) in finite photonic crystals [26,27].

Before moving on to the actual investigation, for the sake of clarity, we define up front the normalized LDOS $\rho(\mathbf{r}_0, \omega)$, to which we shall refer frequently in what follows. As we consider a two-dimensional geometry, with all fields and quantities invariant along the z axis, the symbol $\mathbf{r}$ will be used here to denote a two-dimensional vector in the xOy plane. The normalized LDOS, $\rho(\mathbf{r}_0, \omega)$, can be expressed as the imaginary part of the Green's function $G(\mathbf{r}, \omega)$

$$\rho(\mathbf{r}_0, \omega) = \Im m[G(\mathbf{r} = \mathbf{r}_0, \omega)]. \quad (1)$$

The Green's function in (1) is given by the solution of the equation

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

where $\varepsilon(\mathbf{r})$ is the relative permittivity ($\varepsilon = \varepsilon_a$ inside the rods, and $\varepsilon = 1$ outside), c the vacuum wave speed, and ω the radian frequency. Note that $G(\mathbf{r}, \omega)$ must also fulfill an outgoing wave condition. To better understand the physical meaning of the normalized LDOS, it is worth mentioning that, for a lossless structure, $\rho(\mathbf{r}_0, \omega)$ is proportional to the total power that would be emitted by a line source located at position $\mathbf{r}_0$. Note that the normalization of $\rho(\mathbf{r}_0, \omega)$ has been chosen so as to have $\rho(\mathbf{r}_0, \omega) = 1$ in vacuum. For interested readers, Ref. [27] explains also the relationship with the total density of states.

We begin with investigating how the photonic quasicrystals properties vary with the structure size (i.e., the number of rods). Since for one-dimensional photonic quasicrystals it has been shown that some of the interesting effects appear only for very large number of layers [18], it appears reasonable to consider the same issues for the two-dimensional photonic quasicrystals of interest here. In this connection, it is worth pointing out that two-dimensional extension of conclusions drawn for one-dimensional structures is not necessarily straightforward. For instance, in one-dimensional photonic crystals band gaps appear even for arbitrarily small permittivity contrast, whereas for two-dimensional crystals one needs a suitably large contrast.

Figure 2 shows the normalized LDOS at a given point (the center of the quasicrystal) versus the normalized frequency for the Penrose-type photonic quasicrystal in Fig. 1 (530 rods). Note that the structure has no specific symme-

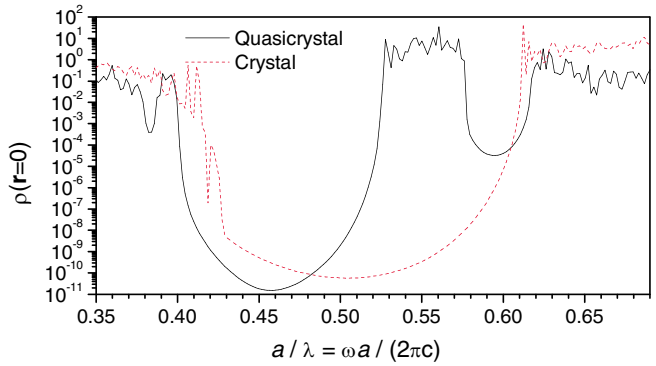

FIG. 2 (color online). Solid line: normalized local density of states at the center of the photonic quasicrystal of Fig. 1 (530 rods, with $\varepsilon_a = 12$ and radius $r_a = 0.116a$) vs the normalized frequency. Dashed line: idem for a photonic crystal made of 576 rods (square lattice, with period $d = 0.77a$, and same rod parameters, so as to guarantee the same filling factor as in the quasicrystal case).

try (the symmetries of the square shape of the whole quasicrystal and of the Penrose tiling are different). We have verified that the choice of the central point does not affect the results.

In the same figure, as a reference for comparison, it is shown the normalized LDOS at the central point of a photonic crystal with a square lattice of period d, made with rods with same relative permittivity $\varepsilon_a = 12$ and radius $r_a = 0.116a$. Quantitative comparisons between the two cases are not straightforward and necessarily meaningful, since there are several possible choices in the parameters (filling factor, distance between the rods, etc.) to be kept constant. In our simulations, we decided to keep the same filling factor and rod diameter (this resulted in $d = 0.77a$). Looking at the quasicrystal LDOS curve, one can observe smaller band gaps appearing on each side of the large central band gap. As it will be shown hereafter, this unique behavior can be attributed to the long-range interactions in the quasicrystal, i.e., interactions averaged over a long range. Such long range should extend over a distance accommodating all possible significant interactions between contiguous and almost contiguous cylinders.

To understand the nature of the interactions involved, we have studied the LDOS with respect to the size of the photonic quasicrystal. Figure 3 shows the minimum LDOS value (in logarithmic scale) versus the square root of the number of rods for the three different band gaps observed in Fig. 2, and for structure size up to 797 rods. Also shown is the LDOS for the photonic crystal with square lattice, for which the exponential decay is clearly visible, even for very small sizes. For the photonic quasicrystal, the behavior of the band gaps is quite different. Specifically, the central band gap exhibits a behavior that is similar to that observed for the photonic crystal, with only a slight deviation from the perfect exponential decay which is attributable to the inherent ambiguity in the definition of the quasicrystal size. This observation seems to indicate that the central band gap stems from relatively short-distance interactions. Further support to this speculation is provided by the fact that this band gap is present even for small-size structures. Conversely, the behavior of the smaller lateral band gaps is far from being exponential for small sizes; in fact, it gets rather difficult to unambiguously identify possible band gaps for a small number of rods. Accordingly, this is the evidence that these lateral band gaps stem from long-range interactions. The dashed lines in Fig. 3 show the asymptotic (large-size) exponential fits, from which we could give a rough estimate of the necessary size to establish the exponential decay, i.e., when the computed samples are reasonably close to the fits. We obtain minimum sizes of about 190 and 260 rods for the higher and lower band gaps, respectively (i.e., lengths of about $7.5a$ and $8.7a$, respectively).

In order to further explore the physical mechanisms involved in the band gap formation in photonic quasicrystals, we now consider the Fourier transform of the permittivity profile of the finite-size structure,

$$\tilde{\varepsilon}(\boldsymbol{\sigma}) = \iint \varepsilon(\mathbf{r}) \exp(-2i\pi\boldsymbol{\sigma}\cdot\mathbf{r}) d\mathbf{r}, \tag{3}$$

with $\boldsymbol{\sigma} \equiv (\sigma_x, \sigma_y)$ denoting a two-dimensional spectral vector. The spectrum (magnitude) is shown in Fig. 4, and its tenfold rotational symmetry, inherited by the statistical symmetry of the structure, is clearly visible. A simple first-order model, such as Born approximation [28], would yield the usual Bragg condition

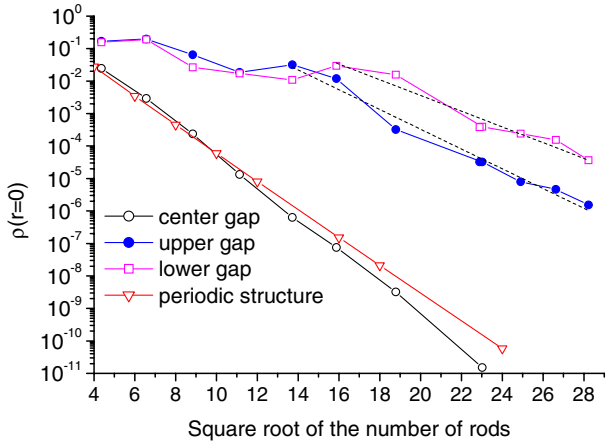

FIG. 3 (color online). Normalized local density of states at the origin vs the crystal size (square root of the number of rods) at the frequency corresponding to the minimum of the band gap. Photonic crystal (triangles), central gap of the quasicrystal (hollow circles), upper gap of the quasicrystal (filled circles), and lower gap of the quasicrystal (squares). The dashed lines represent exponential fits for the large-size region.

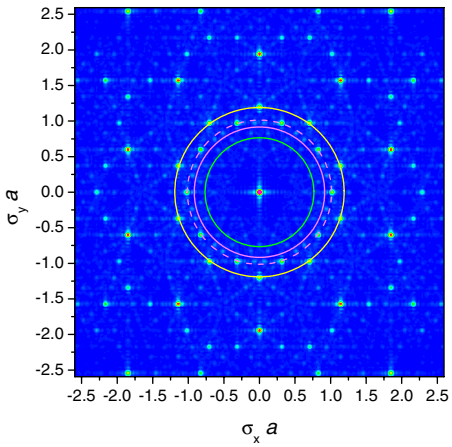

FIG. 4 (color online). Fourier spectrum (magnitude, in false-color scale) given by (3) of the permittivity profile for the quasicrystal in Fig. 1. The solid-line circles correspond to the Bragg condition in (4) for the highest-frequency band gap (largest radius), the central band gap (medium radius), and the lowest-frequency band gap (smallest radius) for $\varepsilon_a = 12$. The dashed-line circle corresponds to the Bragg condition for the central band gap and for $\varepsilon_a = 8$.

$$2\pi\|\boldsymbol{\sigma}\| = 2k_0 \quad (4)$$

(with $k_0 = \omega/c$ denoting the wave number in vacuum), which merely represents a constructive interference condition, and can also be written more conveniently as $\sigma = \|\boldsymbol{\sigma}\| = \omega/\pi c$. In essence, the Born approximation consists of replacing, in the relevant integral equation, the total field with the incident field (see Ref. [28] for more details). It is generally admitted that this approximation is valid when $k_0^2(\varepsilon - 1)V$ is small enough with respect to unity, where V is the volume of the scatterer, and ε its relative permittivity. Similar approximations have been successfully used to design periodic structures with nearly isotropic photonic band gaps [29].

Obviously, this model takes into account only single scattering, and its validity is restricted to low-permittivity-contrast scenarios. Considering the previous configuration parameters, the three band gaps in Fig. 2 are obtained for normalized frequency values $[\omega a/(2\pi c) = a/\lambda]$ of 0.38, 0.46, and 0.60, which [from (4)] correspond to $\sigma a =$ 0.76, 0.92, 1.19, respectively. We have also performed similar calculations for a lower permittivity value ($\varepsilon_a = 8$, instead of 12), which better fulfills the Born-approximation-related low-contrast conditions. In this case, only the central gap is observed for a normalized frequency of 0.51 (corresponding to $\sigma a \approx 1$). In Fig. 4, the solid-line circles correspond to $\varepsilon_a = 12$, while the dashed-line circle corresponds to $\varepsilon_a = 8$. Note that changes in the dielectric permittivity affect the spectral pattern only via a scaling of the spectral variables.

It emerges that the two higher-frequency band gaps are unambiguously explained using the Bragg condition in (4) and the location of the maxima in the Fourier spectrum of the permittivity in the (σ_x, σ_y) plane. However, in the case $\varepsilon_a = 12$ the locations of the gaps deviate from the Born-approximation prediction. The nature of the lowest-frequency band gap seems to be more complex, and should be attributable to multiple scattering phenomena that are not taken into account in this simple model. A further remark is in order: clearly, multiple interactions are always present and important in scattering phenomena, especially with photonic crystals and quasicrystals, and must be taken into account when, for example, the diffracted field is evaluated. However, usually, the frequency position of the lower band gaps can be predicted using a single scattering model (like the one used here) that basically gives a constructive interference condition for all of the scattered contributions by the rods (Bragg condition).

In conclusion, it has been shown that long-range interactions are involved in the formation of band gaps with two-dimensional finite-size Penrose-type photonic quasicrystals. The nature of the highest-frequency band gaps has been related, via a simple model, to the Fourier spatial spectrum of the permittivity profile. Unlike these band gaps, the small low-frequency band gap observed cannot be unambiguously explained through simple first-order approximations, indicating that this band gap stems from multiple scattering processes. To the best of our knowledge, this represents the first example where this phenomenon has been shown. The physical mechanisms involved in photonic quasicrystals are quite different from those encountered in connection with photonic crystals, as shown in this Letter, and opportunities of new applications could follow from their full understanding.

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