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Photonic band gaps and localization in the Thue–Morse structures

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Both theoretically and experimentally, we demonstrate that the photonic band gaps in Thue–Morse aperiodic systems can be separated into two flavors, the fractal gaps and the traditional gaps, distinguished by the presence or absence of fractal structure, respectively. The origin of two kind gaps is explained by the different interface correlations. This explanation is confirmed by the gap width behaviors. In addition, the eigenstates near the fractal gaps have a cluster-periodic form, while those near the traditional gaps have the Bloch wavelike form. Our detailed study of these differences is essential for understanding the spectra and light localization in aperiodic systems. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1928317]

Similar to atomic crystals, the spectra of photonic crystals have photonic bandgaps (PBGs)[1] that are products of the translational periodicity. The Fourier spectrum (FS) of an infinite periodic crystal has δ-function peaks at wave vectors corresponding to the reciprocal lattice vectors (this is the origin of Bragg scattering). On the other hand, the FS of an infinite random system is nearly homogeneous.[2] A quasicrystal (QC) does not possess periodicity but is still deterministically generated, and has a FS lying somewhere between the two extremes of periodic and random systems.[3] One fascinating property of QCs is the presence of band gaps in their spectra.[3–11,13,14] Several theoretical methods have been used to understand the band gaps in one-dimensional (1D) electronic QCs, such as the trace map approach,[7,9,11,12] the weak perturbation approach,[10] and the renormalization-group approach.[13–15] The most common examples of 1D QCs are the Fibonacci and the Thue-Morse (TM) structures. These two types are distinguished by the presence of delta-functionlike peaks in the FS of Fibonacci structures, and singularities in the FS of TM structures.[7,8] TM lattices, also known as *aperiodic* structures, were thought to be more random than Fibonacci lattices (quasi-periodic structures), and hence the TM eigenstates were expected to be more localized. However, the reality of photonic TM eigenstates is more complex.[16] In the diagonal tight-binding model for TM QCs, the origin of the electronic band gaps is the FS singularities, which are the fixed points of the FS recursion relation.[7] Although the tight-binding electronic TM lattices have been extensively studied, very few theoretical and even fewer experimental work[17,18] has been done on the PBGs of TM dielectric structures, which form an important class of photonic quasi-crystals (PQCs). Furthermore, the PBGs of TM PQCs can be quite different in character from the band gaps in electronic TM QCs, even when both have similar FS singularities. Such differences between optical/photonic and electronic waves have been emphasized in Anderson localization studies of random systems,[2] but thus far not in the study of aperiodic systems. Analysis of TM PQCs reveals that PBGs can result not only from periodicity but also from other complex spatial correlations. A more complete understanding of TM PQCs is essential for future applications, such as the design of optical/photonic cavities.

TM lattices can be generated by an inflation rule where the $(n+1)$st TM lattice is obtained from the nth lattice by replacing A by AB and replacing B by BA. The lowest-order TM lattice are represented by the strings $S_0=A$, $S_1=AB$, $S_2=ABBA$, $S_3=ABBABAAB$, etc. In this letter, we report our theoretical and experimental investigations of the PBGs and the localization properties of the eigenstates of TM PQCs. Our systems are composed of layers A and B with widths a and b, indices of refraction n_a and n_b, and phase modulations $\theta_a=k_a a=n_a\omega a/c$ and $\theta_b=k_b b=n_b\omega b/c$, respectively. The electric field in the ith layer can be written as $E_i(z)=A_i^+ e^{ik_i(z-z_i)}+A_i^- e^{-ik_i(z-z_i)}$. Matching boundary conditions, we obtain $(A_{i-1}^+,A_{i-1}^-)^T=M_i(A_i^+,A_i^-)^T$ where M_i is the transfer matrix between layers.[19] From the product of the 2^n transfer matrices, we can obtain the transmission and reflection of an S_n TM lattice.

The numerical results reveal that two kinds of PBGs exist in TM PQCs. The fractal gaps (FGs) and the traditional gaps (TGs) are distinguished by their behavior as the system length increases, as shown in Fig. 1. As the system length increases, there are fractal structures generated in the FGs, in contrast to the TGs which maintain a resemblance to a common PBG in a periodic PC. The conditions satisfied by the central frequency of the basic FG (BFG) and the basic TG (BTG) are $\theta_a+\theta_b=2/3\pi$ and $\theta_a+\theta_b=\pi$, respectively. In the previous studies[7,8] of electronic TM systems, using a tight-binding model, it was found analytically that the $2/3\pi$ and π singularities (both with the largest scaling exponents) have different singular properties, but there was no study of gap different behaviors. However, due to the more complex form of the optical transfer matrix, a strict criterion for the PBG kind is not available now. Nevertheless, we can infer from our numerical results that a gap is of the TG kind when $(\theta_a+\theta_b)/\pi$ takes on a integer value, and of the FG kind for other value.

To understand the physical origin of the BTG and BFG, we present a simple explanation based on the two kinds of correlations between the interfaces, which are the

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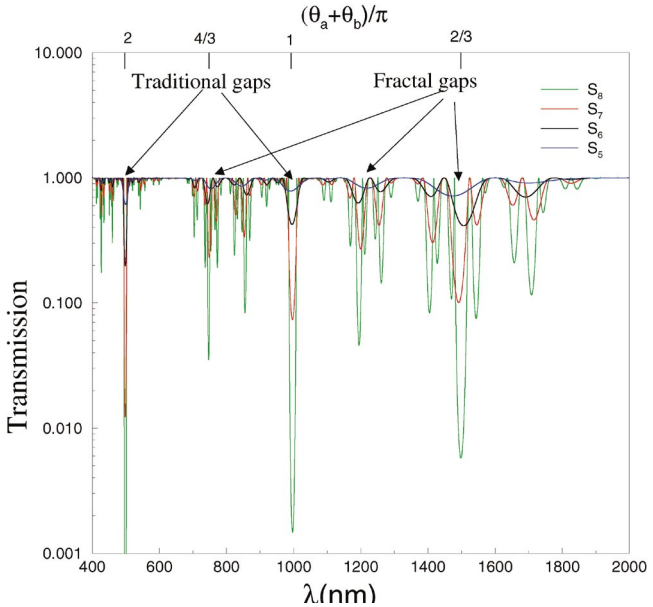

FIG. 1. (Color) Numerical simulations of the transmission spectra of S_5, S_6, S_7, and S_8 TM lattices with $n_a=3.3$, $n_b=3.014$, $a=93.5$ nm, and $b=63$ nm. Certain gaps, labeled FGs, have fractal structure that is not present in the other gaps, labeled TGs.

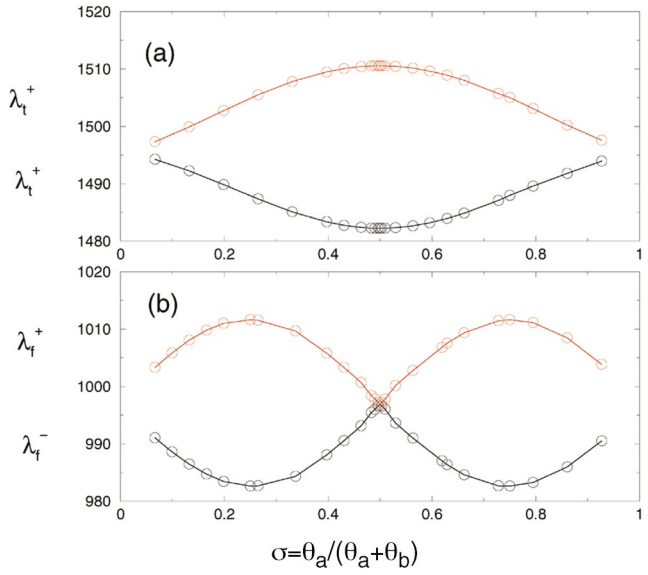

FIG. 2. (Color) The upper (red) and lower (black) edges of (a) the BFG and (b) the BTG as the phase modulations are changed. The structural parameters are the same as in Fig. 1.

scattering points in 1D systems. Taking the S_5 structure *ABBABAABBAABABBABAABABBAABBABAAB* as an example, the first kind of interface correlation is found by dividing between every other layer as follows: *A*|*BB*|*AB*|*AA*|*BB*|*AA*|*BA*|*BB*|*AB*|*AA*|*BA*|*BB*|*AA*|*BB*|*AB*|*AA*|*B*. Here, every interface (with the sign |) is between an *A* layer and a *B* layer. The BTG (and other TGs) are generated by backscattering from these interfaces. This correlation is homogeneously distributed, so the TGs do not change when the system length increases. The next correlation is found by dividing between every third layer in three different ways as follows:

(*i*) *A*|*BBA*|*BAA*|*BBA*/*ABA*|*BBA*|*BAA*|*BAB*/*BAA*|*BBA*|*BAA*|*B*,
(*ii*) *AB*/*BAB*|*AAB*/*BAA*|*BAB*/*BAB*|*AAB*|*ABB*|*AAB*/*BAB*|*AAB*,
and (*iii*) *ABB*|*ABA*/*ABB*|*AAB*|*ABB*|*ABA*/*ABA*|*BBA*/*ABB*|*ABA*/*AB*,

where the symbols / and | distinguish whether the interface separates like or unlike layers, respectively. These correlations correspond to the BFG. This correlation is clearly much more complex than the first kind of interface correlation and depends on the system length. A detailed study of the nature of these correlations will be performed elsewhere.[20]

The gap width should reach its maximum when the backscattering waves from the most relevant interfaces constructively interfere with each other. This condition is satisfied for the BTG when $\sigma=0.25$ or 0.75 (all backscattered waves are in phase), and for the BFG when $\sigma=0.5$, where $\sigma=\theta_a/(\theta_a+\theta_b)$. In Fig. 2, we tune σ by changing the layer thicknesses and study the effect on the gap width. We show the upper and lower edges of the BFG [λ_f^+ and λ_f^- in Fig. 2(a)] and the BTG [λ_t^+ and λ_t^- in Fig. 2(b)]. In good agreement with our prediction, the gap width is indeed maximal at these conditions. One interesting feature is the disappearance of the BTG when $\sigma=0.5$. This is also easily explained by our simple picture, because the backscattering waves from two kind interfaces $f_a=A|B$ and $f_b=B|A$ are out-of-phase and cancel each other. We would like to point out that the BTG is not "a trivial gap from the periodic background" as remarked in Ref. 7. The gap width behavior in Fig. 2 confirms that the BTG is quite different from the fundamental gap in a periodic system, even though they look similar and their central frequencies are the same. Physically, it is because the first interface correlation is not trivial in many aspects, such as the two kind relevant interfaces in a S_5 lattice compose a sequence as $f_af_bf_bf_af_bf_af_af_bf_bf_af_af_bf_af_bf_bf_a$ which is a S_4 TM *interface lattice*. In our numerical simulations, both the BFG and BTG are quite robust, e.g., to 10% deviation of the thickness and the dielectric constants.

The difference between the FGs and TGs is also obvious when we investigate the properties of the eigenstates around these two kinds of gaps. The states near the FGs behave in a quite complex manner when the system length increases. In Fig. 3(a), we plot the profile of the gap-edge state near the BFG in an S_{10} TM lattice. The state appears localized, but when the system size increases from the S_{10} lattice to the S_{12}

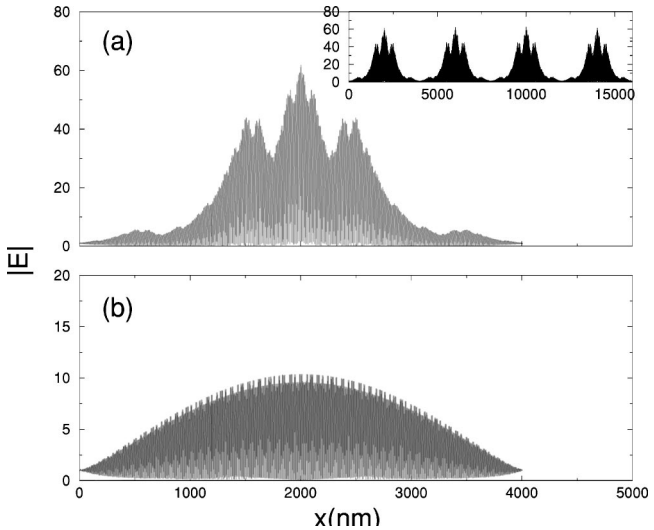

FIG. 3. The field magnitude $|E|$ vs position x. (a) The gap-edge state near the BFG in an S_{10} TM lattice. The inset shows the state at the same frequency in an S_{12} TM lattice. (b) The gap-edge state near the BTG in an S_{10} TM lattice. All structural parameters are the same as in Fig. 1.

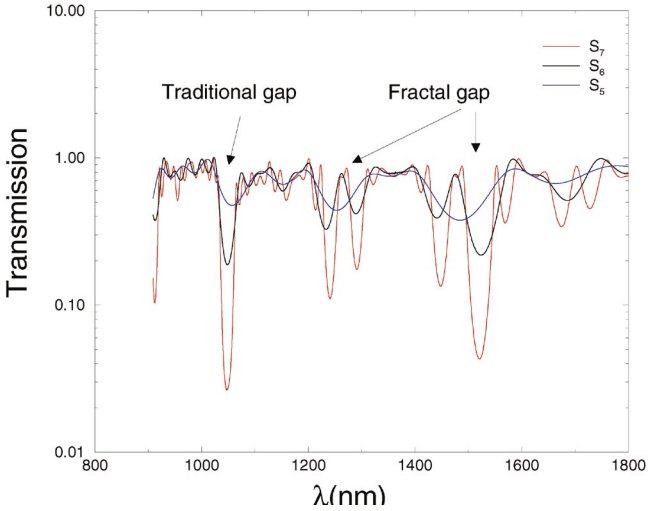

FIG. 4. (Color) The experimental spectra of S_5, S_6, and S_7 TM lattices with identical structural parameters to Fig. 1. The agreement with the FG and TG behaviors in Fig. 1 is evident.

lattice, at same frequency we find that the state [shown in the inset to Fig. 3(a)] now resembles a cluster-periodic state with large magnitude fluctuations. Strictly, such states are extended in an infinite long lattice. However, given their field distribution, we can think of them as quasi-localized states, with characteristics lying somewhere between the localized states and Bloch states. Due to the large magnitude fluctuations, these quasi-localized states can have a very high quality factor, indicating their potential usefulness in the design of optical cavities. Using the cluster-expansion technique, which is developed in the study of electronic TM lattices,[9] the optical quasi-localized states can also be explained similarly.[20] However, the eigenstates near the TGs are Bloch-wavelike states [see in Fig. 3(b)] whose magnitude displays little fluctuation. Their profile shows a sine functional behavior in a finite TM PQC, just like a band-edge Bloch state in a finite periodic system. This similarity results from the homogeneity of the first interface correlation.

To confirm our theoretical predictions, we fabricated several TM structures. Previous experiments have employed dielectric or elemental semiconductor media, such as porous Si, TiO_2, and SiO_2.[4,18] With potential active optoelectronic applications in mind, we chose the III-V compound semiconductors GaAs and $Al_xGa_{1-x}As(x=0.6)$. The samples were grown by gas source molecular-beam epitaxy and all parameters are the same as Fig. 1 (with less than 5% deviation). The spectra of three TM lattices S_5 (32 layers), S_6 (64 layers), and S_7 (128 layers) are shown in Fig. 4. The experimental results clearly agree very well with the numerical results in Fig. 1.

In conclusion, we have identified and studied both theoretically and experimentally the detailed differences between the two kinds of PBGs and the eigenstate localization properties in TM PQCs. The two kinds of gaps are distinguished by the presence (or lack of) of fractal structure within the gap. Based on the spatial correlation of the interfaces, we have provided a simple explanation for the physical origin of the two kinds of gaps. The behavior of the gap widths of the BFG and the BTG are in agreement with our proposed explanation. We have also found that the eigenstates near the FGs have a cluster-periodic form, while those near the TGs resemble Bloch waves. Our experimental results for several TM structures confirm our theoretical predictions about the optical spectra. The results further our understanding of light transport in aperiodic systems, and could lead to future applications of PQCs, such as the design of multifrequency PQC lasers, PQC filters and optical cavities.

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