Geometric approach based on optimal toric packings for photonic crystals and metamaterials design.

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Abstract

We introduce new classes of nanostructures—optimal toric packings of particles and their Voronoi tessellations—that exhibit remarkable properties for photonic and potentially for plasmonic/phononic crystals design. These structures connect the classical problem of optimal packings on tori with the development of optimized photonic architectures.

1. Introduction

Design of photonic crystals [1, 2, 3] with large bandgaps above a specified band is a well-known problem with diverse applications. Usually, such a design is achieved numerically using optimization methods or machine learning (ML) techniques. Optimality of the final designs is not easy to determine: combinatorial complexity of the design space is too large. Therefore, despite advances in numerical and ML techniques [4, 5], theoretical understanding of design principles of photonic bandgap structures remains being an important topic, and may be useful for many adjacent areas of scientific knowledge (e.g. plasmonics, phononics, and magnonics). In fact, in the field of photonic crystals, approximate design principles do exist thanks to insightful classic work of O.Sigmund and K. Hougaard [6]. Their conjecture linked optimal structures for bandgaps between bands n and n+1 to centroidal Voronoi tessellations (CVT): rods being placed at locations of CVT generators (in the case of transverse magnetic (TM) polarization), and walls of the CVT (in the case of transverse electric (TE) polarization). We found another mathematical approach [7]: optimal disc packings in square and triangular tori. While geometric idea behind CVT is some kind of uniformity in distribution of optical elements (coincidence of Voronoi tesselation generators with corresponding cell center of mass), optimal disk packings realise a simpler geometric objective: maximisation of minimal distance between the elements. Arrays of particles placed at the centers of optimally packed discs on tori and nets formed by walls of their Voronoi tessellations produce qualitatively different structures that sometimes significantly enlarge bandgaps. The new classes of periodic structures might have many applications in photonics and beyound. Optimal packing problems have arisen throughout the history of humankind, one of the most famous example is probably the Kepler problem concerning densiest arrangement of (many) identical spheres, where a close-packed structure was conjectured to be a solution [8]. It took more than 300 years to prove 2D version of the Kepler conjecture, and then much more difficult 3D case [8]. These results were about infinite space. We use somehow related and much more recent results for finite spaces [9]: optimal packings in ”containers” with periodic boundary conditions. Indeed, even though a photonic crystal occupies an infinite space, it is obtained by periodic arrangement of a finite elementary unit cell. Considering a square or rhombic unit cell with periodic boundary, one obtains a square torus or triangular torus geometry, correspondingly [7]. Several mathematical and numerical methods had been used to find point configurations maximising minimal distance between points [9, 10, 11, 12]. In [7], we compared symmetry constrained CVT recipes of [6] with toric optimal configurations (OP). Here, we additionally study toric CVT configurations (tCVT, with generators of centroidal Voronoi tesselations being distributed on tori *without* symmetry restrictions). Part of the achieved advantage of OP over CVT comes from absence of symmetry restrictions. It is therefore logical to study also tCVT without those symmetry restrictions. We find that they are able to outperform toric OP in certain (rare) cases.

2. CVT, toric CVT, and toric OP configurations for photonic bandgap structures

Toric optimal packing configurations studied in [7] are illustrated on Fig. 1. CVT configurations of [6] with symmetry restrictions are shown on Fig. 2 and toric CVT configurations (without symmetry restrictions) are shown in Fig. 4. Here we illustrate only the square lattice geometry, for the triangular lattice case see [6, 7]. Bandgaps of optimised structures are shown in Fig. 3. Permittivity of the inclusions is the same as in Ref.[6]: $\varepsilon = 11.56$, while host media is air with $\varepsilon = 1$. 1-parameter optimisation (with only radius of rods or width of wires being the optimisation parameter) was applied to OP structures and obtained in this way OP_1 structures were compared with topology optimised (TO) structures of [6] (CVT_{top}), and with 1-parameter optimised CVT and tCVT structures (CVT_1 and $tCVT_1$, correspondingly). If 1-parameter optimisation is comparable with or better than TO (which involves hundreds of parameters), it is a clear sign of success. Indeed the OP_1 structures clearly have certain advantages compared to classic CVT

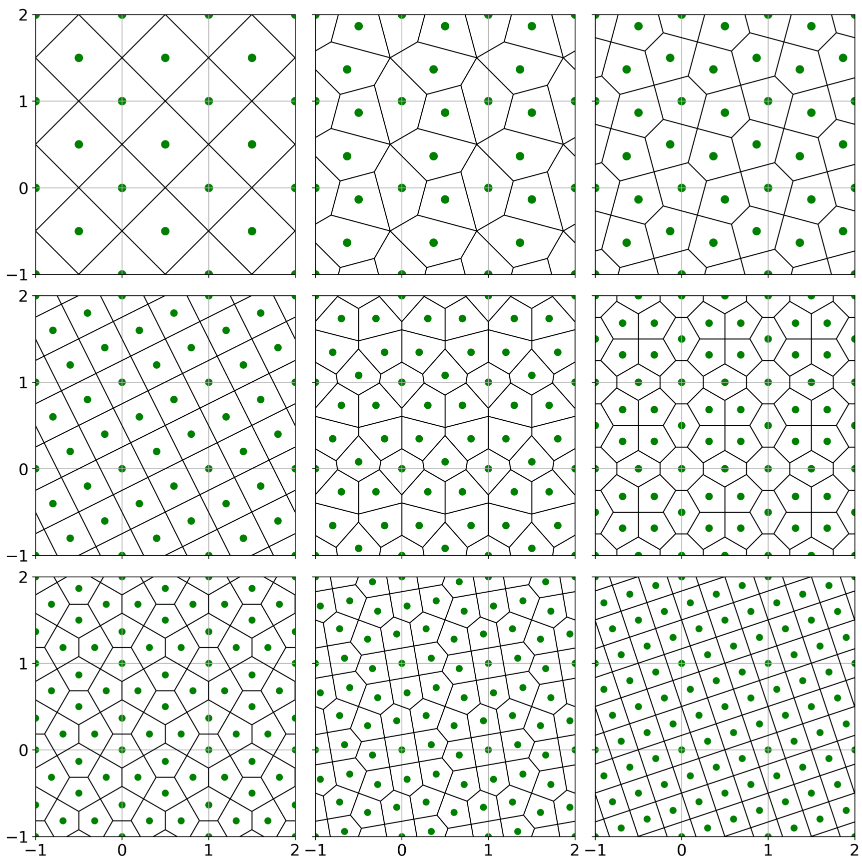

Figure 1: Optimal packing configurations (green dots) and their Voronoi tesselations (black lines) from N=2 (top left) to N=10 (bottom right). Each panel shows 3x3 supercell (numbers just mark the unit cells)

structures of [6]. In square lattice geometry, bandgaps of CVT structures for TE modes cannot reach levels that are achieved in triangular lattice geometry (approx. 52 %). However, for OP_1 structures, surprisingly, it is possible. In some cases OP_1 structures for TM modes also outperform CVT_{top}. One of the most peculiar structures arises at N=4 and N=8: for TM modes, arrays of points form one of the Archimedean square-triangular patterns, and for TE modes its corresponding Voronoi tesselations form Cairo pentagonal tiling [14, 15]. For triangular lattice geometry, the optimal packing recipe allows to predict "magic" band numbers where maximal bandgaps can be achieved [7]. Toric CVT structures (without symmetry restrictions) are shown in Fig. 4. We use results of [13] where toric CVT configurations were achieved using L-BFGS method. These structures, unlike OP, are not unique: there could be many different realisations, in particular it is possible to find fully hexagonal patterns in most cases. In some cases (e.g. N=5), toric CVT configurations coincide with toric OP structures. We chose fully hexagonal toric CVT patterns where it was possible, and found that for N=4 and N=8 they outperform toric OP structures (Cairo pentagonal tilings). At the same time, neither CVT nor toric CVT property, even being supplied with fully hexagonal patterning, is not enough to ensure optimal photonic bandgap: hexagons should also be somehow "round", e.g. for N=7 tCVT performs considerably worse than either OP or CVT (Fig 3c).

3. Further connections to art, math, and physics

Cairo tesselation [14, 15] is encountered in architecture, decorative design, and crystallography, but was not used in photonic crystals yet, to the best of our knowledge. In architecture, it can be found in Cairo (obviously), but also in Hamburg ([14, 15], see also Fig.6) and some other cities.

Mathematically, it is connected to one of the 11 Archimedean tilings via duality (see Fig.5). Archimedean tilings were already studied from the point of view of photonic structure design, but not from the point of view of optimal packings.

When discussing low-contrast limit of photonic bandgap structures, some kind of optimal packings in reciprocal space appear [17, 18].

Some of the structures of [7] may hopefully find applications in topological photonics and plasmonics: e.g. Ref.[16] studied lasing in arrays of quadrumers, while our N=4 configurations provides another route for packing of quadrumers on lattice.

There are certain connections with phononic structures studied in [19].

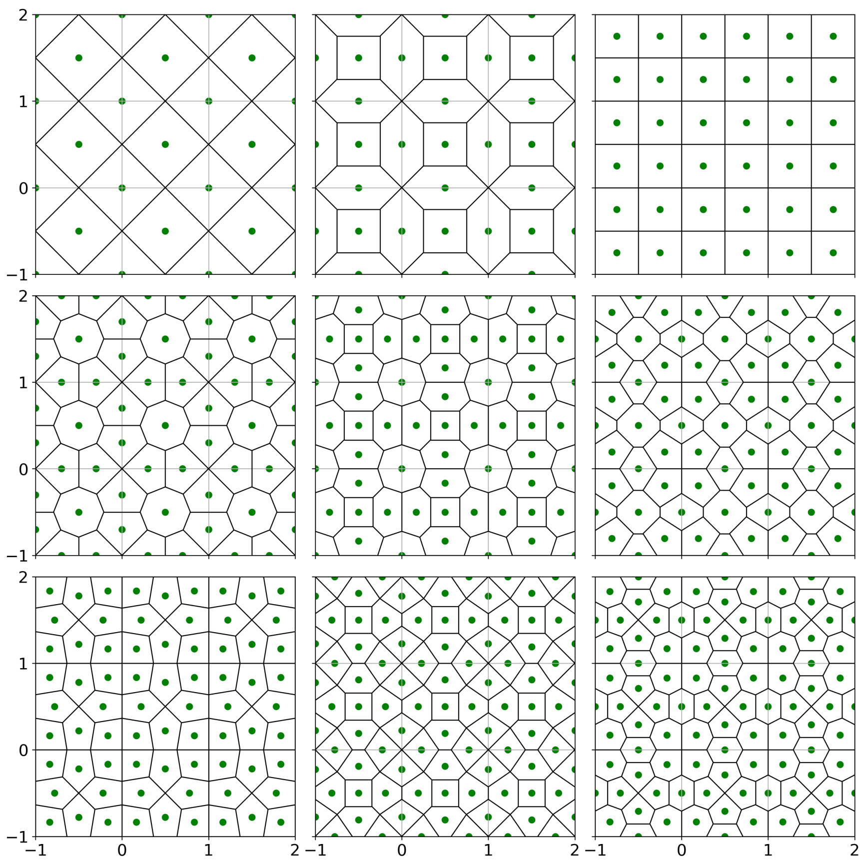

Figure 2: Centroidal Voronoi tesselations with symmetry constraints (black lines) and their generators (green dots) from N=2 (top left) to N=10 (bottom right). Each panel shows 3x3 supercell (numbers just mark the unit cells)

4. Conclusions

Splitting the process of topology optimisation on two steps, as suggested in [6], with the first step being purely geometric one, is very attractive and inspirational idea. So far systematic applications of this approach have been done in photonics, but it should be possible to extend to other realms of physics: plasmonics, phononics, etc. A peculiar historical fact is worth noting: in the very same year the first bandgap structure was ever discussed [3] (1887), a study appeared on an optimal geometric structure realising tiling of space [20]. These two scientific fields remain being intrinsically connected, providing interesting new findings. In [7] and here we considered toric optimal packing configurations and toric CVT configurations which sometime demonstrate certain advantages compared to classic CVT configurations of [6].

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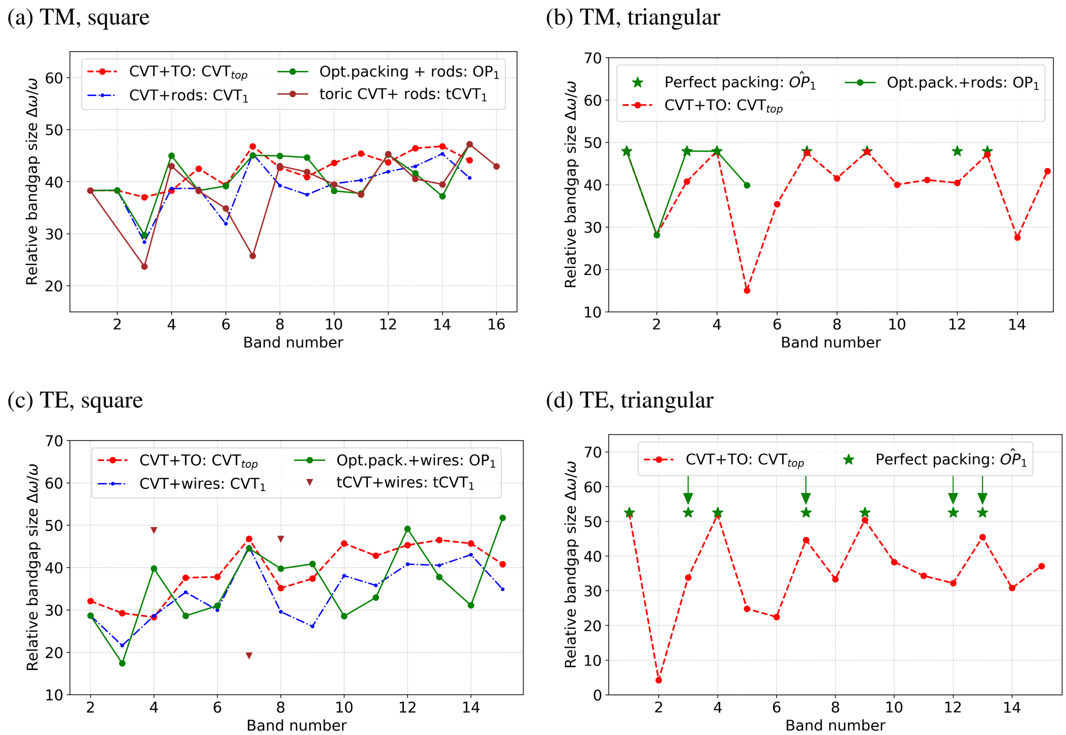

Figure 3: Relative bandgap vs. band number for square lattice geometry (left panels) and triangular lattice (right panels). Upper(bottom) panels: TM(TE) modes. Dot-dashed line ("CVT+rods(wires): CVT$_1$"): configurations realising centroidal VT (CVT) are taken from Ref. [6], and circular rods of equal radius are placed at each point of the configuration for TM modes, or wires of equal width are placed along walls of VT for TE modes. The rod radius (wire width) is optimised to achieve the highest bandgap (1-parameter optimisation). Dashed line ("CVT+TO: CVT$_{top}$"): results of Ref.[6], where topology optimisation was done on top of CVT. Solid line ("Opt.packing+ rods(wires): OP$_1$" for TM(TE) modes): our results, where configurations are obtained from optimal packing solutions and circular rods of equal and optimised radius are placed there for TM modes, or wires of optimised width are placed along walls of VT for TE modes. Triangles denote $tCVT$ configurations (CVT without symmetry constraints). Stars denote perfect packing solutions (close-packed structures), those VT in TE case produce honeycomb-like structures with maximal bandgaps. They are realised for "magic" band numbers $N = 1, 4, 9$ found both in [6] and in our approach [7], and at additional "magic" band numbers $N = 3, 7, 12, 13$ obtained via our approach only [7] (highlighted by vertical arrows).

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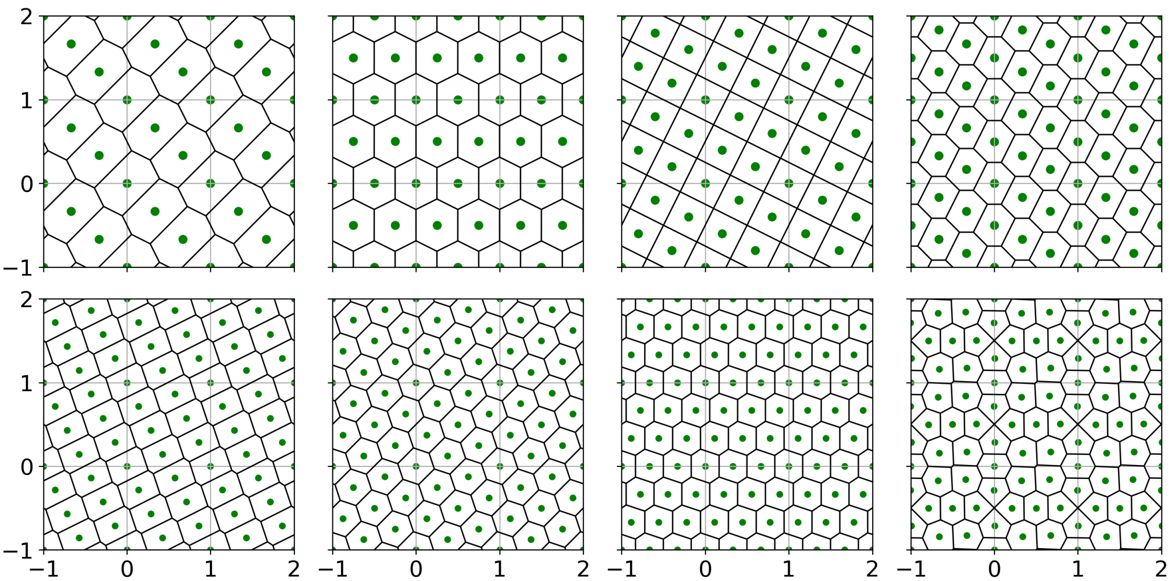

Figure 4: Toric centroidal Voronoi tesselations (black lines) and their generators (green dots) from N=3 (top left) to N=10 (bottom right). Each panel shows 3x3 supercell

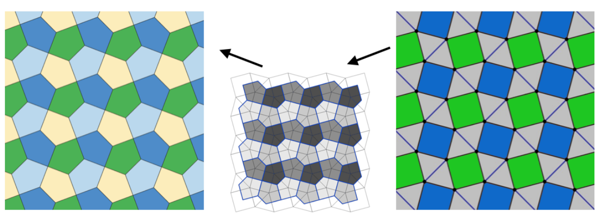

Figure 5: The Cairo pentagonal tiling (left), an Archimedean square-triangular tiling (right), and duality procedure transforming them between each other is in the center

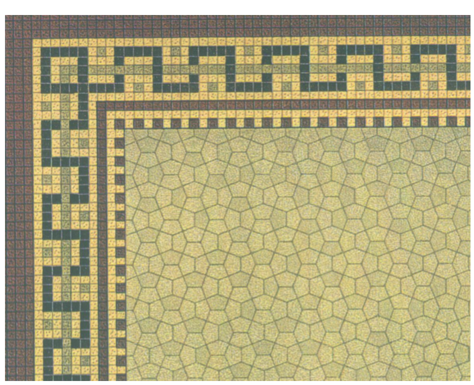

Figure 6: Photo of floor tiling from catalog of Villeroy & Boch, between 1900 and 1920. In Laeiszhalle music pavilion in Hamburg, constructed in 1908, the floor in the foyer is covered with such tiles. [15]

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