Lattice Vibrations in Aperiodic Self-Similar Low Dimension Phonon Lattice

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Phononic crystals are to sound what photonic crystals are to light and crystals are to electrons. A huge amount of application-driven research has been performed on photonic crystals, much less on phononic crystals, and almost nothing on phononic quasicrystals. In this paper we will exploring a phonic 1D quasicrystal and its 2D tiling. We consider 1D lattice vibrations (phonons) for quasicrystal. Using a Fibonacci sequence, we construct an aperiodic self-similar lattice and from that sequence, we construct a 2D tilting.

I. INTRODUCTION

Light and sound are the important carriers of information for live organisms. Historically the nature and characteristics of sound have been understood earlier than that of light because the progress in classical mechanics usually advanced the progress in electrodynamics. This is not the case for the in the areas of photonic and phononic crystals. In the last decade of the twentieth century there was a burst in study of photonic crystalsperiodic dielectric structures which may provide much higher efficiency than the traditional optical devices in generation, waveguiding, focusing, splitting, slowing down [6]. The works of Yablonovitch and John (see [18] and [6], respectively) proposed a photonic crystal which since then have been studied thoroughly (see [14]). The structure of photonic crystals is characterized but the periodic variation of their refractive index. This allows us to find the photonic band gaps (see [1]) and thus the photonic crystals have the property of control light propagation. If the wavelength is of the same order of magnitude as the typical distances between the objects in their ordered arrangement, then the interaction is dominated by diffraction besides refraction. Depending on the spectral properties of the material, band gaps appear for certain frequencies. In special cases, these gaps are omni-directional (see [17]).

The atomic structure of solids have been divided in two cases: glassy structure and crystal structure. The crystal structure are highly ordered, have translation order due to its periodic spacing, and symmetry. In 1982, Shechtman *et al.* (see [16]) discovered a quasicrystal and in 2011 was awarded the Nobel Prize in Chemistry. However, the concept of periodicity has long been studied, at least mathematically, by Bohr with periodic functions and later the works of Penrose and Ammann showed that we can partition a non-Euclidean spce in a nonperiodic way ([15]). Furthermore, Penrose has proposed a tiling on the plane, which is known as Pensore tiliting (see [10], [4], [5], [1]). These have been the foundation of the filed of quasi-periodic structures.

Quasicrystals are characterize by its non-periodic structure and thus it lacks translational symmetry. Additionally, they have found to exist universally in many metallic alloys and some polymers. Quasicrystals are found most often in aluminium alloys (Al-Li-Cu, Al-Mn-Si, Al-Ni-Co, Al-Pd-Mn, Al-Cu-Fe, Al-Cu-V, etc.), but numerous other compositions are also known (Cd-Yb, Ti-Zr-Ni, Zn-Mg-Ho, Zn-Mg-Sc, In-Ag-Yb, Pd-U-Si) [11].

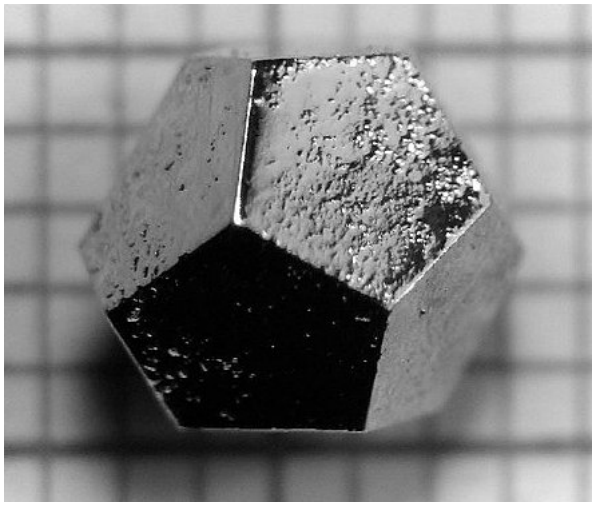

FIG. 1. Ho-Mg-Zn icosahedral quasicrystal formed as a pentagonal dodecahedron

II. PERIODIC PHONON LATTICE IN 1D

We assume that the elastic response of the crystal is a linear function of the forces. Furthermore, we assume that the force on the plane n caused by the displacement of difference of the plane $n+p$ is proportional to the difference $u[s+n]-u[n]$ of its displacements. For simplicity we ignore the effect of the beggining of the lattice and the end of the lattice. Lastly, will consider only the nearest neighbor interactions (i.e. $p=\pm 1$). So the force on the n is

$$F_n = K(u[a(n+1)] - u[an]) + K(u[a(n-1)] - u[an])$$

where K is the force constant between nearest particle.

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Linear Phonon Chain in 1D with Mono-atomic Lattice

We consider a 1D mono-atomic lattice (refer to FIG. 2) with separation **a** and mass M. Let k_1 be the force constant between nearest-neighbor. The general lattice vector is given by,

$$\mathbf{R}_n = na\hat{\mathbf{e}}_x$$

and so the nearest-neighbors vectors are given by

$$\mathbf{n}_1 = a\hat{\mathbf{e}}_x \text{ and } \mathbf{n}_2 = -a\hat{\mathbf{e}}_x.$$

So the harmonic potential is given by,

$$V = \frac{1}{2}k_1 \sum_n (u[na] - u[(n+1)a])^2.$$

FIG. 2. Monoatomic Lattice

The equation of motion is given by (Newton's Second Law of Motion)

$$\begin{aligned} M\frac{d^2u[an]}{dt^2} &= -\frac{-\partial V}{\partial(na)} \\ &= k_1(u[(n+1)a] - 2u[an] + u[a(n-1)]) \end{aligned}$$

We expect our solution to have the form (with wavevector k)

$$\begin{aligned} u[na] &= Ae^{\mathbf{i}(kna-\omega t)} = Ae^{\mathbf{i}(kna)}e^{-\mathbf{i}\omega t} \\ \Rightarrow u[(n\pm 1)a] &= Ae^{\mathbf{i}(k(n\pm 1)a)}e^{-\mathbf{i}\omega t} = u[na]e^{\pm \mathbf{i}ka} \end{aligned}$$

and inseting our solution to the equation of motion yields,

$$\begin{aligned} -\omega^2 M u[na] &= k_1(u[na]e^{\mathbf{i}ka} - 2u[na] + u[na]e^{-\mathbf{i}ka}) \\ &\Leftrightarrow \omega^2 M = -k_1(e^{\mathbf{i}ka} - 2 + e^{-\mathbf{i}ka}) \\ &\Leftrightarrow \omega^2 = \frac{2k_1}{M}(1 - \cos ka) \end{aligned}$$

III. LINEAR PHONON CHAIN IN 2D WITH DI-ATOMIC LATTICE

We consider a 2D di-atomic lattice (refer to FIG. 3) with blue circles of mass m_1 and purple rectangles of mass m_2. The general lattice vector is given by (using a basis around the blue circles),

$$\mathbf{R}_{nm} = na\hat{\mathbf{e}}_x + ma\hat{\mathbf{e}}_y = n\mathbf{a}_1 + m\mathbf{a}_2$$

We consider the following nearest neighbors:

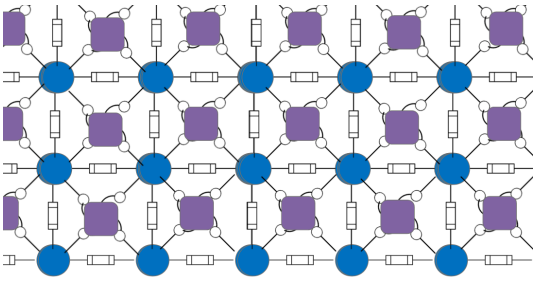

FIG. 3. di-atomic Lattice

- Blue circle to purple squares with distance $\mathbf{h}_i$ force constant k_1,
- Blue circle to blue circle (closest) horizontal and vertical distance $\mathbf{n}_i$ with force constant k_2
- Purple square to purple square (closest) horizontal and vertical distance $\mathbf{n}_i$ with force constant w_2
- Blue circle to blue circle (this is the diagonal) with distance $\mathbf{p}_i$ and force constant k_3
- Purple square to purple square (this is the diagonal) with distance $\mathbf{p}_i$ and force constant w_3

With this formalism, we have that the nearest neighbors are given by

$$(\mathbf{h}_i) = \begin{pmatrix} \frac{a\hat{\mathbf{e}}_x + a\hat{\mathbf{e}}_y}{2} \\ \frac{-a\hat{\mathbf{e}}_x + a\hat{\mathbf{e}}_y}{2} \\ \frac{-a\hat{\mathbf{e}}_x - a\hat{\mathbf{e}}_y}{2} \\ \frac{a\hat{\mathbf{e}}_x - a\hat{\mathbf{e}}_y}{2} \end{pmatrix}, \quad (\mathbf{n}_i) = \begin{pmatrix} a\hat{\mathbf{e}}_x \\ a\hat{\mathbf{e}}_y \\ -a\hat{\mathbf{e}}_x \\ -a\hat{\mathbf{e}}_y \end{pmatrix}, \quad (\mathbf{p}_i) = \begin{pmatrix} a\hat{\mathbf{e}}_x + a\hat{\mathbf{e}}_y \\ -a\hat{\mathbf{e}}_x + a\hat{\mathbf{e}}_y \\ -a\hat{\mathbf{e}}_x - a\hat{\mathbf{e}}_y \\ a\hat{\mathbf{e}}_x - a\hat{\mathbf{e}}_y \end{pmatrix}.$$

This means that the blue particle is being pulled by twelve forces and the purple also by twelve forces. Let u describe the motion of the blue particle and v will describe the motion of the purple particle. The equation of motion of the system (ignoring the cells in the boundary) is given by the following coupled equations ($\mathbf{d} = \frac{a\hat{\mathbf{e}}_x + a\hat{\mathbf{e}}_y}{2}$)

$$\begin{aligned} m_1\frac{\partial^2 \mathbf{u}[\mathbf{R}_{nm}]}{\partial t^2} = \sum_{i=1}^{4} \Bigg(& k_1\Big(v[\mathbf{R}_{nm} + \mathbf{h}_i] - u[\mathbf{R}_{nm}]\Big)\mathbf{h}_i \\ & + k_2\Big(u[\mathbf{R}_{nm} + \mathbf{n}_i] - u[\mathbf{R}_{nm}]\Big)\mathbf{n}_i \\ & + k_3\Big(u[\mathbf{R}_{nm} + \mathbf{p}_i] - u[\mathbf{R}_{nm}]\Big)\mathbf{p}_i \Bigg) \end{aligned}$$

and similarly

$$\begin{aligned} m_2\frac{\partial^2 \mathbf{v}[\mathbf{R}_{nm} + \mathbf{d}]}{\partial t^2} = \sum_{i=1}^{4} \Bigg(& k_1\Big(u[\mathbf{R}_{nm} + \mathbf{d} + \mathbf{h}_i] - v[\mathbf{R}_{nm} + \mathbf{d}]\Big)\mathbf{h}_i \\ & + w_2\Big(v[\mathbf{R}_{nm} + \mathbf{d} + \mathbf{n}_i] - v[\mathbf{R}_{nm} + \mathbf{d}]\Big)\mathbf{n}_i \\ & + w_3\Big(v[\mathbf{R}_{nm} + \mathbf{d} + \mathbf{p}_i] - v[\mathbf{R}_{nm} + \mathbf{d}]\Big)\mathbf{p}_i \Bigg). \end{aligned}$$

Let $\mathbf{K} = \alpha_1\mathbf{b}_1 + \alpha_2\mathbf{b}_2$, the reciprocal lattice basis are given by $\mathbf{b}_1$ and $\mathbf{b}_2$ (i.e $\langle \mathbf{b}_i|\mathbf{a}_j = 2\pi\delta_{ij}$). As before, we assume that our solutions are given by,

$$\begin{aligned}\begin{pmatrix}\mathbf{u}[\mathbf{R}_{nm}]\\ \mathbf{v}[\mathbf{R}_{nm}+\mathbf{d}]\end{pmatrix} &= \begin{pmatrix}\mathbf{u}[\mathbf{K}]\\ \mathbf{v}[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{d}\rangle}\end{pmatrix} e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}\\ &= \begin{pmatrix}\gamma_1\\ \gamma_2\end{pmatrix} e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}\\ &= \mathbf{\Gamma}(\mathbf{0})e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}.\end{aligned}$$

then for some displacement $\mathbf{Q}$ $(= \{\mathbf{h}_i,\ \mathbf{n}_i,\ \mathbf{p}_i\})$, our solution becomes,

$$\begin{aligned}\begin{pmatrix}\mathbf{u}[\mathbf{R}_{nm}+\mathbf{Q}]\\ \mathbf{v}[\mathbf{R}_{nm}+\mathbf{d}+\mathbf{Q}]\end{pmatrix} &= \begin{pmatrix}\mathbf{u}[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{Q}\rangle}\\ \mathbf{v}[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{d}+\mathbf{Q}\rangle}\end{pmatrix} e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}\\ &= \mathbf{\Gamma}(\mathbf{Q})e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}.\end{aligned}$$

With this notation, we have

$$\omega^2\begin{pmatrix}m_1 & 0\\ 0 & m_2\end{pmatrix}\mathbf{\Gamma}(\mathbf{0})e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)} = \begin{pmatrix}D_1\\ D_2\end{pmatrix}$$

where

$$\begin{aligned}D_1 =& \sum_{i=1}^{4}\Bigg(k_1\Big(v[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{h}_i\rangle}-u[\mathbf{K}]\Big)e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}\mathbf{h}_i\\ &+k_2\Big(u[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{n}_i\rangle}-u[\mathbf{K}]\Big)e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}\mathbf{n}_i\\ &+k_3\Big(u[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{p}_i\rangle}-u[\mathbf{K}]\Big)e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}\mathbf{p}_i\Bigg)\\ =& \sum_{i=1}^{4}\Bigg(k_1\Big(v[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{h}_i\rangle}-u[\mathbf{K}]\Big)\mathbf{h}_i\\ &+k_2\Big(u[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{n}_i\rangle}-u[\mathbf{K}]\Big)\mathbf{n}_i\\ &+k_3\Big(u[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{p}_i\rangle}-u[\mathbf{K}]\Big)\mathbf{p}_i\Bigg)e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}\end{aligned}$$

and

$$\begin{aligned}D2 =& \sum_{i=1}^{4}\Bigg(k_1\Big(u[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{d}+\mathbf{h}_i\rangle}-v[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{d}\rangle}\Big)\mathbf{h}_i\\ &+w_2\Big(v[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{d}+\mathbf{n}_i\rangle}-v[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{d}\rangle}\Big)\mathbf{n}_i\\ &+w_3\Big(v[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{d}+\mathbf{p}_i\rangle}-v[\mathbf{K}]e^{i\langle \mathbf{K}|\mathbf{d}\rangle}\Big)\mathbf{p}_i\Bigg)e^{i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}\end{aligned}$$

Thus, our equation of motion reduces to,

$$\omega^2\begin{pmatrix}m_1 & 0\\ 0 & m_2\end{pmatrix}\mathbf{\Gamma}(\mathbf{0}) = \begin{pmatrix}E_1\\ E_2\end{pmatrix}$$

with $E_{\{1,2\}} = D_{\{1,2\}}e^{-i(\langle \mathbf{K}|\mathbf{R}_{nm}\rangle-\omega t)}$ and so,

$$\omega^2 = \mathbf{\Gamma}(\mathbf{0})^{-1}\begin{pmatrix}m_1 & 0\\ 0 & m_2\end{pmatrix}^{-1}\begin{pmatrix}E_1\\ E_2\end{pmatrix}$$

IV. APERIODIC PHONON LATTICE IN LOW DIMENSION

In the literature, aperiodic quasicrystal are constructed from a Fibonacci sequence, namely if we define $F_1 = A$ and $F_2 = B$ then for $n > 2$

$$F_n = F_{n-1}\bigoplus F_{n-2}.$$

For instance, $F_3 = F_2\bigoplus F_2 = BA$, $F_4 = BAB$, $F_5 = BABBA$. Some interesting observations: every sequence will start with B and if n is odd the strand will end with B and A otherwise. Using Mathematica we can develop a code to generate such a sequence (refer to Appendix A for the source code). The following list contains the first ten sequences

$$\begin{gathered}A\\ B\\ BA\\ BAB\\ BABBA\\ BABBABAB\\ BABBABABBABBA\\ BABBABABBABBABABBABAB\\ BABBABABBABBABABBABABBABBABABBABBA\end{gathered}$$

Moreover, if we stack the sequence on the vertical axis (we pivot around the first atom) we can construct a tile set (such as in [10], [4], [1], [3]). This is similar how we had the 1D chain with diatomic basis and then we considered a 2D lattice with diatomic basis. While the sequences we constructed are aperiodic, in the tiling of such sequence we are getting ordered lattices (see FIG. 5-10 in Appendix C)

A. Vibrations due to Nearest atoms in 1D Aperiodic Lattice

Consider the Fibonacci sequence generated by $F_1 = A$ and $F_2 = BB$ (for lattices constructed from AB_2). The 10th Fibonacci sequence generated (see FIG. 4) is given by,

$$\begin{gathered}BBABBBBABBABBBBABBBBABBA\\ BBBBABBABBBBABBBBABBABBB\\ BABBBBABBABBBBABBABBBBBAB\\ BBBABBABBBBABBABB\end{gathered}$$

Consider a chain that follows the aperiodic arrange-

FIG. 4. 1D Tile constructed with first 70 atoms in the sequence of F_{10} with $F_1 = A$, $F_2 = BB$ and B being twice the size of A.

ment of Fibonacci sequence generated by $F_1 = A$ and $F_2 = BB$ (it does not matter what we pick since the 11th Fibonacci sequence will have the 10th embedded, etc. This properly is called self-similar and comes up in the study of fractals). Let the force constant between A and B be $K_{A,B} = K_{B,A}$ and between B and B be $K_{B,B}$. Notice that by construction there will never be AA sequence. The possible sequences of three we can have are $\{BBB,\ ABB,\ BAB,\ BBA\}$. Using the string count function in Mathematica the 24th Fibonacci chain contains the following distribution

BBB	BBA	BAB	BAA	ABB	ABA	AAB	AAA
10945	17711	17711	0	17711	0	0	0

.

Now let u_n represent the displacement of the nth particle in the Fibonacci chain (either $n = A$ or B) from its equilibrium position with corresponding mass m_n, and force $K_{n,n\pm1}$. So,

$$m_n \frac{\partial^2 u_n}{\partial t^2} = K_{n,n+1}(u_{n+1} - u_n) + K_{n,n-1}(u_{n-1} - u_n).$$

As before, we guess solutions of the form $u_n = \epsilon_n e^{-i\omega t}$. Our equation becomes,

$$m_n\omega^2\epsilon_n = (K_{n,n+1} + K_{n,n-1})\epsilon_n - K_{n,n+1}\epsilon_{n+1} - K_{n,n-1}\epsilon_{n-1}.$$

V. CLOSING REMARKS

Initially I wanted to do the analysis for an aperiodic lattice in 2D, however due to time constraints and debugging, I had very little time do do the analysis in 2D. However, the other problem I ran was in drafting solutions in 2D. While the constructions are ordered, but do not have transnational work and so we would have to calculate motion for patches of the surface since we can see that those patches do show periodically (see FIG. 10). I have included my code (Appendix A and B) to generate tiling on a Fibonacci sequence. If you are somewhat familiar with Mathematica, you should be able to modify to generate different tiling. In Appendix B, I modified my code to it to include particles of the form ABC by defining a Triboncacci sequence $F_n = F_{n_1} \bigoplus F_{n-2} \bigoplus F_{n-3}$.

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APPENDIX

Appendix A Code for Fibonacci sequence

The following is the code to generate FIG. 5 - FIG. 9 For particles that follow AB_2.

```
(*Here we define our Fibonacci sequence*)
Trib[1] := "A";
Trib[2] := "B";
Trib[n_] := Trib[n - 1] <> Trib[n - 2]
(*We want the qth sequence*)
q = 10;
a = StringLength[Trib[q]];
(*we want to create a grid that is mxm,
we don't want to overwork some toaster so we
will just stick to atmost 20x21 (mxm+1))*)
m = Min[a, 20];
(*Grid with the number of sequences of A–A,
A——B, B——A, B\[Equal]B*)

Grid[{{"AA", "AB", "BA", "BB"},
    {StringCount[Trib[q], "AA"],
        StringCount[Trib[q], "AB"],
        StringCount[Trib[q], "BA"],
   StringCount[Trib[q], "BB"]}},
        Frame -> All]
array[n_] := Drop[ToExpression[
   StringDrop[
    StringReplace[
        Trib[q], {"B" -> "{2,2}~Join~",
        "A" -> "{1}~Join~"}], -6]], n]
(*Now we create an cluster of arrays
    to plot*)
clusteraray = Table[Take[array[i], m],
    {i, m, 0, -1}];
ArrayPlot[clusteraray,
ColorRules -> {1 -> Pink, 2 -> Black}]
```

APPENDIX

Appendix B Code for Tribonacci Sequence

Modifying the code presented in Appendix A to consider particles that follow *ABC* (Fig 10)

```
(*Here we define our Tribocci sequence*)
Trib[1] := "A";
Trib[2] := "B";
Trib[3] := "C";
Trib[n_] := Trib[n - 1] <> Trib[n - 2]
<> Trib[n - 3]
(*We want the qth sequence*)
q = 11;
a = StringLength[Trib[q]];
(*we want to create a grid that is mxm,
we will just stick to atmost 20x20*)
m = Min[a, 30];
array[n_] := Drop[ToExpression[
   StringDrop[
    StringReplace[
        Trib[q], {"B" -> "{2,2}~Join~",
        "A" -> "{1}~Join~",
      "C" -> "{3,3,3}~Join~"}], -6]], n]
(*Now we create an cluster of arrays
to plot*)
clusteraray = Table[Take[array[i], m],
{i, m, 0, -1}];
ArrayPlot[clusteraray,
 ColorRules -> {1 -> Pink, 2 -> Black,
 3 -> Gray}]
```

Appendix C Tiles of Aperiodic Sequences

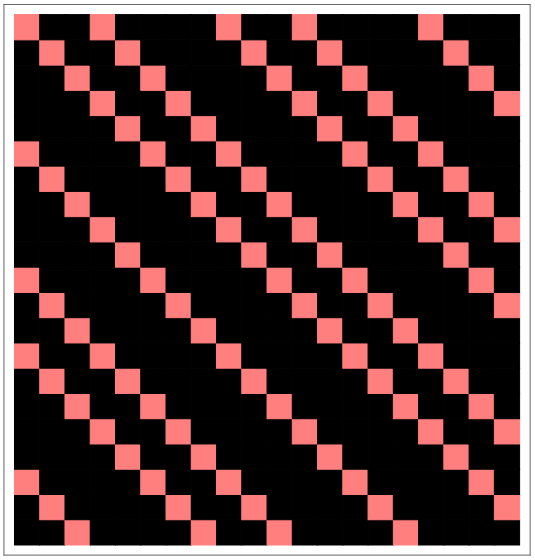

FIG. 5. 2D Tile constructed with first 30 atoms in the sequence of F_{10} with $F_1 = A$, $F_2 = B$ and B being twice the size of A.

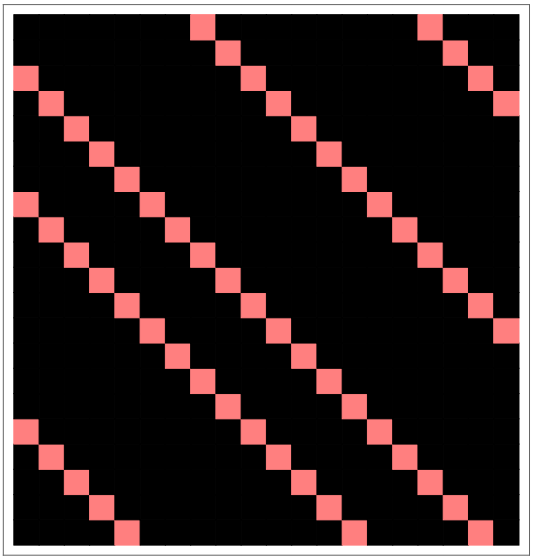

FIG. 6. 2D Tile constructed with first 30 atoms in the sequence of F_{10} with $F_1 = A$, $F_2 = BB$ and B being twice the size of A.

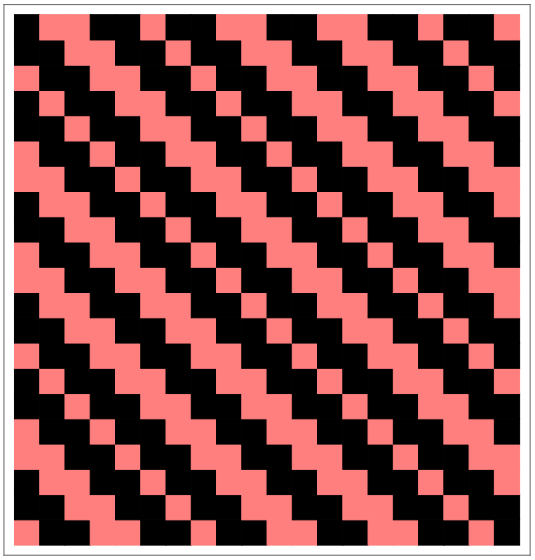

FIG. 7. 2D Tile constructed with first 30 atoms in the sequence of F_{10} with $F_1 = A$, $F_2 = AB$ and B being twice the size of A.

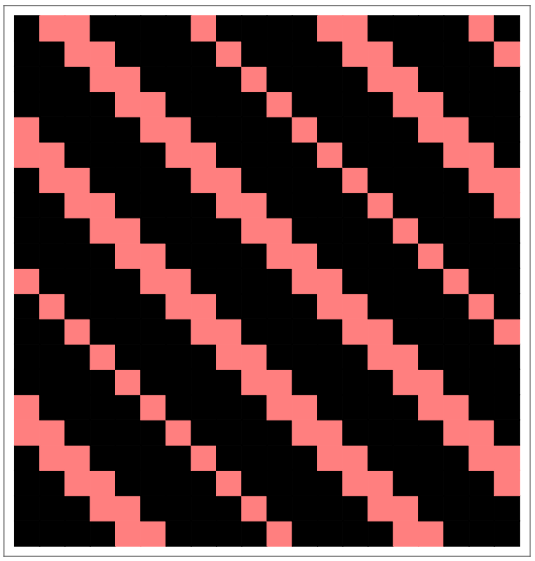

FIG. 8. 2D Tile constructed with first 30 atoms in the sequence of F_{10} with $F_1 = A$, $F_2 = BBA$ and B being twice the size of A.

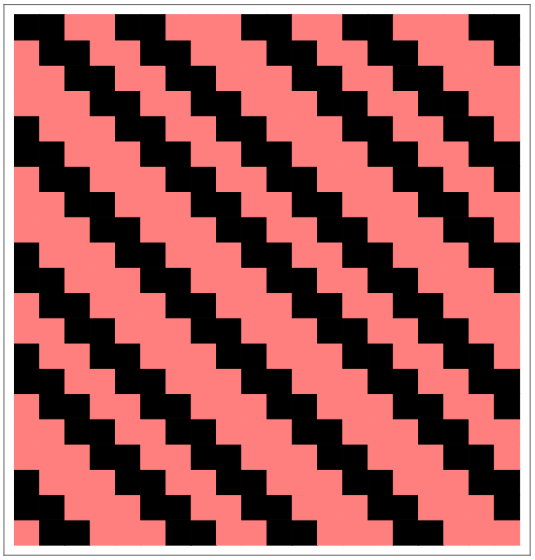

FIG. 9. 2D Tile constructed with first 30 atoms in the sequence of F_{10} with $F_1 = BA$, $F_2 = A$ and B being twice the size of A.

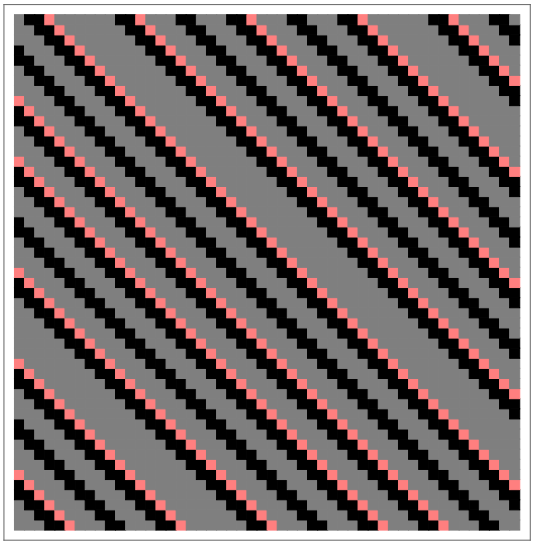

FIG. 10. 2D Tile constructed with first 50 atoms in the Tribonacci sequence of F_{10} with $F_1 = A$, $F_2 = B$, $F_3 = C$, B being twice the size of A and C being three times the size of A.

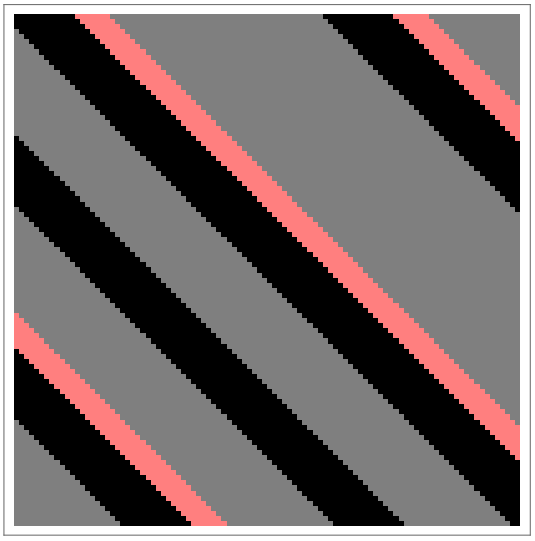

FIG. 11. 2D Tile constructed with first 100 atoms in the Tribonacci sequence of F_{10} with $F_1 = AAAAAAA$, $F_2 = BBBBBBB$, $F_3 = CCCCCCC$, B being twice the size of A and C being three times the size of A.