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SIMPLE POTENTIAL LANDSCAPE GENERATORS

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Dedicated to the memory of Professor Mitchell Jay Feigenbaum

ABSTRACT

Simple programs can generate great complexity, do not involve too much conceptual sophistication, and can also enrich a student's intuition on glass science. We proposed simple potential landscape generators, based on the ideas of the late American physicist Martin Goldstein (1919 - 2014), using elementary iterated functions proposed by the American electrical engineer and physicist Mitchell Jay Feigenbaum (1944 - 2019) that can produce non-periodic barriers, choosing any number between $0 < x < 1$. Other iterated functions can produce regular patterns, similar to the view of the Swiss physicist Felix Bloch (1905 - 1983) on periodic potentials of a crystal lattice.

Keywords: *Glass; Crystal; Energy Landscape*

1. INTRODUCTION

Everything is made of atoms. Atoms in a solid state are tightly bound to each other. Solid is one of the few fundamentals states of matter, basically separated in crystalline (*i.e.*, in a regular geometric lattice) or non-crystalline (*i.e.*, irregularly, as some amorphous or common window glasses), About the intrinsic nature of the glass transition temperature, T_g, Zanotto and Mauro proposed two definitions of glassy state.[1] The first one, simple and intuitive, is that "glass is a nonequilibrium, non-crystalline state of matter that appears solid on a short time scale but continuously relaxes towards the liquid state". An alternative, more detailed definition is that "glass is a nonequilibrium, non-crystalline condensed state of matter that exhibits a glass transition. The structure of glasses is similar to that of their parent supercooled liquids (SCL), and they spontaneously relax toward the SCL state. Their ultimate fate, in the limit of infinite time, is to crystallize".

Unlike a solid, the molecules in a liquid – that is another fundamental state of mater, have a much greater freedom to move, as a fluid. Some solid turns into a liquid for example when its temperature is raised to its melting point or *liquidus* temperature, T_m. Supercooling is the process of lowering the temperature of a liquid below T_m without it becoming a solid. One key to reach such condition is to freeze very fast a liquid, so the time control is important. A supercooled liquid is considered a metastable state of mater – this means that they eventually crystallize after a certain time. For example, glasses can crystallize under certain conditions, but at room temperatures and normal pressure conditions, they do not become a crystal at human time scale.[1] An important point is that glasses exhibit a T_g and amorphous solids do not. The change from supercooled liquid to glass depends on the rate process, thus T_g is not a well-defined temperature but can be considered a temperature interval.[2] The glass transition region appears also in organic glasses as copolymers and polymer blends, while various kinds of its dependence on concentration are known.[3]

The American chemistry educator and science writer Martin Goldstein (1919 - 2014) established a seminal work in the physics of viscous liquids and glasses writing a paper in 1969 on a glass potential energy barrier[4]. This potential depends on the spatial location for each of those *N* particles that composes a glass that, briefly speaking, is a supercooled liquid that is frozen at T_g, the glass transition temperature. According to Stilinger[5], conceptual precursors can be found at least ten years earlier[6,7].

Goldstein described his theory assuming that there is no unique structure of a liquid but a myriad. All liquids are randomly changing their configurations even when their physical properties as volume and energy, among others, do not change. According to Johari and Angell,[8] in Goldstein's picture, each of the minima separated by the barriers on a potential energy surface represents a specific 3D structure of a liquid. In other words, a liquid flows because its structure can migrate from one minimum potential to another, surpassing barriers without costs in terms of energy (or volume). This approach changed the comprehension of glass formation and the nature of the vitreous state, giving more insights. For example, scientists working in diverse topics and areas have applied the potential-energy landscape to illustrate structure fluctuations of new substances as hydrated proteins, and used to study on different problems as diffusion-controlled kinetics, nucleation and crystallization, rheology, aging of glass and nanoparticles. For the general reader, some characteristics, properties and historical overview of the glassy state can be found elsewhere.[9]

According to Mauro *et al*.,[10,11] the object of the landscape approach is related to a macroscopic system containing a large number ($N \sim 10^{23}$) of interacting atoms (or ions, or molecules). When associated with nonequilibrium statistical mechanics methods, the energy / enthalpy landscape picture allows for T_g modeling based exclusively on fundamental physics, with no use of empirical fitting parameters. Some techniques were proposed in these years,[4-5,11] one of them applied to a metallic selenium glass[10].

Goldstein's proposal can be considered as a complementary view (or at least was inspired by one), that follows the original idea of the Swiss physicist Felix Bloch (1905 – 1983, Figure 1*a*) on periodic potentials of a crystal lattice.[12] He was the first doctorate student[13] of the German physicist Werner Karl Heisenberg (1901 – 1976, Figure 1*b*), and his title thesis was on "The Quantum Mechanics of Electrons in Crystal Lattices" defended at the University of Leipzig in 1928. Bloch applied the same title to his famous publication,[11] treating the motion of the electrons in a tridimensional crystal lattice like that of most metals - not as free electrons, but modulated by a potential of the same periodicity as that of the crystal lattice structure.

In two dimensions, a crystal lattice corresponds to the tiling concept. A periodic tiling has a repeating pattern, with no overlaps and no gaps ,such as cemented ceramic squares or even hexagons, which also present translational symmetry. Thus, a tiling that lacks a repeating pattern and also presents no translational symmetry is named aperiodic. An aperiodic tiling example was proposed by the English mathematical physicist and philosopher of science Roger Penrose (*b*. 1931) in 1974, that is a structure that is ordered but not periodic.[14]

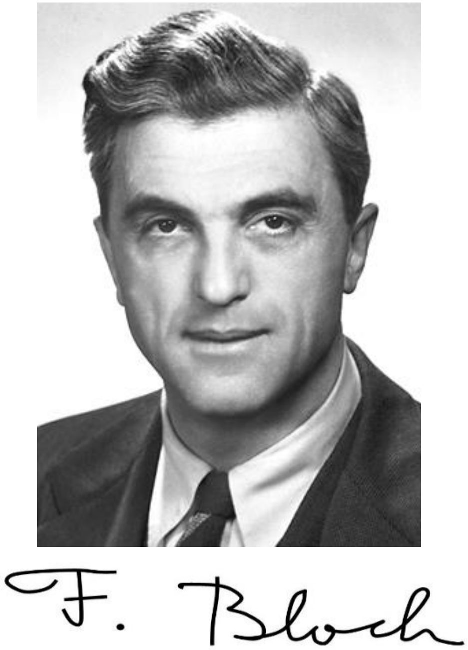

Figure 1a. Felix Bloch (1905 - 1983), Swiss physicist and laureate of the Nobel Prize in Physics (1952).

Figure 1b. Werner Karl Heisenberg (1901 - 1976), German physicist and laureate of the Nobel Prize in Physics (1932).

2. RESULTS

A simple picture of a regular periodic potential can be obtained by means of an elementary expression[15] given by the British mathematician Ian Nicholas Stewart (*b*. 1945, Figure 1*c*), for every positive number *n*:

$$x_{n+1}= x_n^2-1, \qquad (1)$$

and the concept of *iteration*. Choosing any initial number between $0 < x_1 < 1$, such as 0.54321, the result is $x_2 = -0.70492$ (considering just five decimal places in Eq. (1)). Replacing this last number in the expression, iterating over and over, there is a simple pattern, of zeros and minus ones (Figure 2*a*), like a Bloch's potential. This last result is expected because $0^2 - 1 = -1$ and $(-1)^2 - 1 = 0$. For sure, any other number, with a different quantity of decimals, would work.

But another simple expression, considering an integer $n > 0$:

$$x_{n+1}= 2x_n^2-1, \qquad (2)$$

shows a different result following the same premise, *i.e.*, choosing any initial number between $0 < x_1 < 1$. Starting with $x_1= 0.54321$, it results $x_2= -0.40984$ (considering five decimal places in Eq. (2)). Again, iterating such results over and over, another pattern rises (Figure 2*b*), between ones and minus ones, like a Goldstein's potential. Another special result is noticeable when choosing different x_1 starting values – even for small differences, as $x_1 = 0.54322$, a resulting non-periodic pattern arises. To visualize better such concepts in terms of a regular and non-regular structure, this was presented at the first time by the classical work[16] of the Norwegian-American physicist William Houlder Zachariasen (1906 - 1979), see Figures 3*a*,*b*. He was the first to propose correctly the structure of a glassy state by means of experimental X-ray diffraction data. An example of quasicrystal is presented in Figure 4.

X-ray diffraction has a long history since the discovery of X-rays by the German mechanical engineer and physicist Wilhelm Conrad Röntgen (1845 – 1923), the first Nobel Prize in Physics in 1901.[17] The most used technique was first proposed by the British physicists William

Henry Bragg (1862 – 1942) and his son William Lawrence Bragg (1890 – 1971) in 1913. Both were laureate of the Nobel Prize in Physics two years later.[18]

Historically, the basic idea behind iteratively replace of some function by another was proposed by the German mathematician and logician Ernst Friedrich Wilhelm Karl Schröder (1841 - 1902) in an 1870 seminal paper.[19] Just a century latter independent studies replacing x (between zero and one) by simple functions as $kx(1-x)$, with k around 3 gave the first insights of the new branch of chaos theory. The major contributions were done by the Australian biologist Robert McCredie May (*b*. 1936)[20] and the American electrical engineer and physicist Mitchell Jay Feigenbaum (1944 - 2019, Figure 1*d*).[21] Since 1975, Feigenbaum did his mathematical experiments on a pocket HP-65 programmable calculator, according to the British-American computer scientist Stephen Wolfram (*b*. 1959) notes.

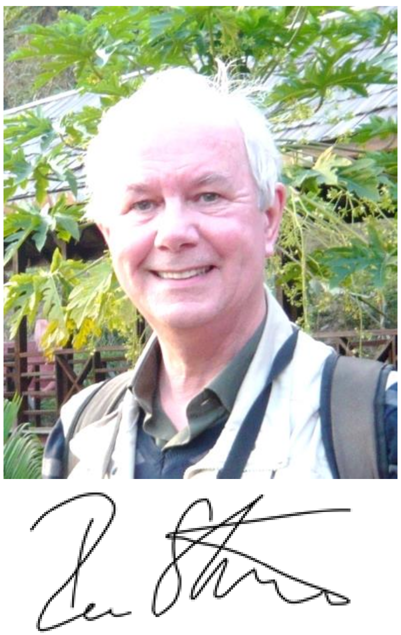

Figure 1c. Ian Nicholas Stewart (b. 1945), British mathematician and popular-science and Science-fiction writer.

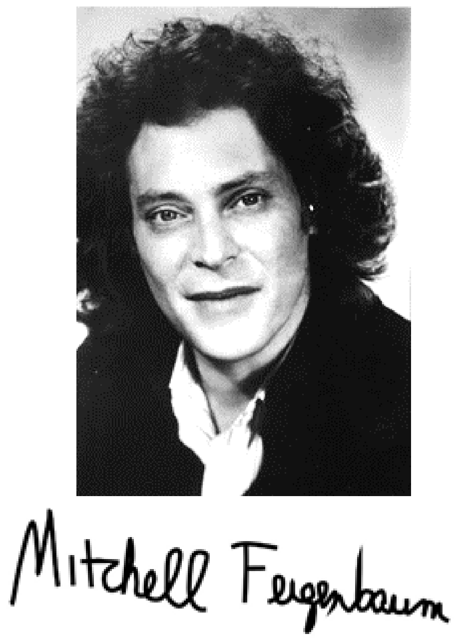

Figure 1*d*. Mitchell Jay Feigenbaum (1944 - 2019), American electrical engineer and physicist.

3 . DISCUSSION

In fact, the expression:

$$x_{n+1}= kx_n^2-1, \qquad (3)$$

is special in the sense that, choosing $k = 1$ and starting iterations choosing any initial number between $0 < x_1 < 1$ one gets a regular potential; and choosing $k = 2$, a non-regular one. More intriguing, choosing a number k between $1 < k < 2$ for Eq. (3), other interesting results take place: for example, when $k = 1.4$ a rather complicated cycle through sixteen different values arises for larger and larger iteration numbers. Higher values than $k = 1.5$ will present a more and more non-regular pattern.[15]

Such a simple computer experiment example[22] is now considered by Wolfram as a new revolution in mathematics, a paradigm shift so as the Goldstein's proposal in glass science. According to Wolfram, traditional intuition might suggest that to do more sophisticated computations would always require more sophisticated underlying rules. Despite the simplicity of these rules, the behavior of the iterations is far from simple, producing great complexity. More: due to this simplicity, no specialized scientific knowledge on physics, or about potentials, or even glass science is required. Wolfram presented another elementary way to elaborate a non-periodic pattern based on the concept of cellular automata: briefly speaking, just consider the decimals of successive powers of 3/2. Starting with $(3/2)^0 = 1.\underline{0}$, the successive numbers are: $(3/2)^1 = 1.\underline{5}$, $(3/2)^2 = 2.\underline{25}$, $(3/2)^3 = 3.\underline{375}$, $(3/2)^4 = 5.\underline{0625}$, $(3/2)^5 = 7.\underline{59375}$ and so on. Such decimals in sequence will present an *irregular* pattern[22] between 0 and 1 similar to Figure 2*b*. In the opposite view, another classical periodic (one dimensional) model of an infinite periodic array of rectangular potential barriers that was proposed by Ralph de Laer Krönig (German physicist, 1904 - 1995) and William George Penney (English mathematician, 1909 - 1991).[23]

4. CONCLUSION

In conclusion, we agree with May that the most important application of proposals like these is pedagogical[20] – especially considering the iterated functions presented above, for scientists and engineers. Certainly, there is an elegant body of mathematical concepts underlying these iterated functions first proposed by Feigenbaum, but as this study does not involve as much conceptual sophistication as does basic *calculus*, it would greatly enrich students' intuition about Bloch's potential and the Goldstein's energy landscape.

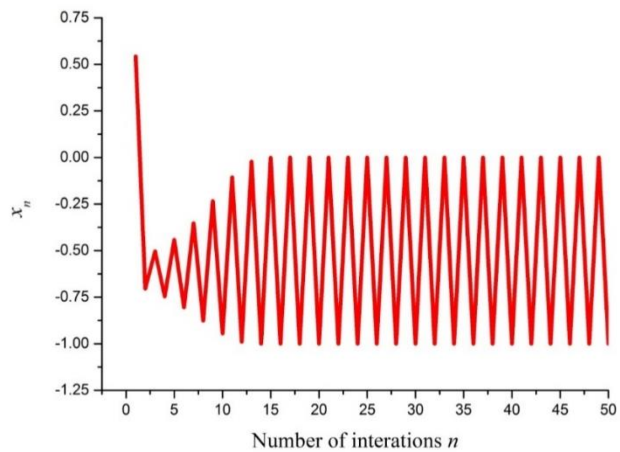

Figure 2*a*. Fifty iterations of $x_{n+1} = x_n^2 - 1$ leads to regular, periodic potential, considering any starting value between $0 < x_n < 1$ for $n > 0$. In this graph the value of x_n is plotted vertically, and the number of iterations runs horizontally. The resulting values are between zero and one. Minima correspond to a virtually perfect crystal, in Bloch's sense.

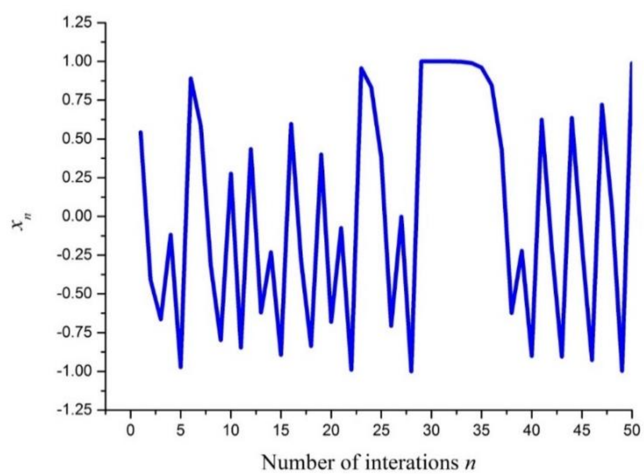

Figure 2*b*. Fifty iterations of $x_{n+1} = 2x_n^2 - 1$ leads to a non-regular potential, considering any starting value between $0 < x_n < 1$ for $n > 0$. The resulting values are between minus one and one. This simplified representation can be viewed as a glassy potential barrier landscape, where minima correspond to mechanically stable arrangements of N particles in space.

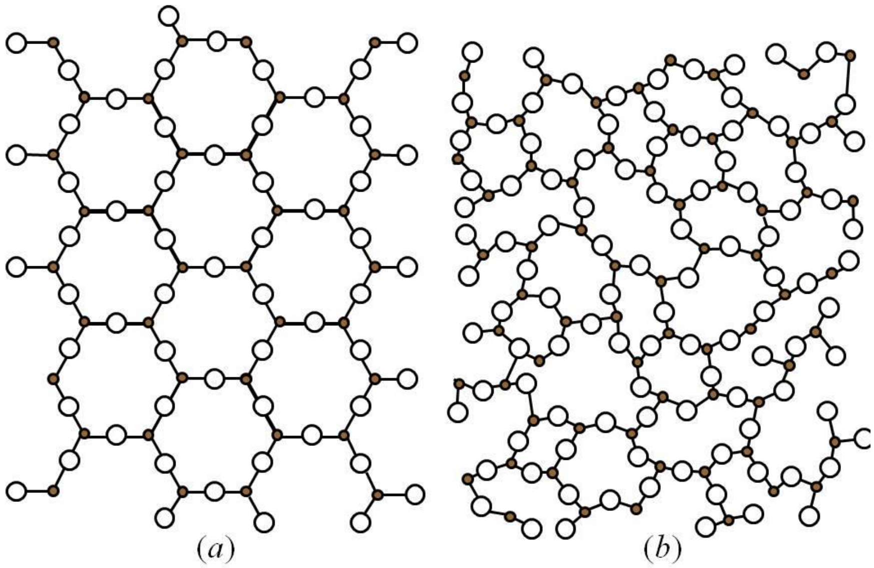

Figure 3. *a*) Schematics of a bidimensional molecular periodic arrangement of a crystal structure (a periodic tiling example) similar to B_2O_3, where B represents the small and O the large atoms. Note that borons are coordinated to three oxygens, and each oxygen to two borons at crystal phase, following a Bloch scheme.[12] *b*) The glassy counterpart of a crystal, showing a non-periodic structure, following Zachariasen's proposal.[16] This picture represents the structure of an idealized glass. Glasses cannot be defined in terms of a simple unit cell that is repeated periodically in space. In fact, from this simple example, some oxygens could be linked to only one boron in a glassy phase (that is called a nonbridging oxygen). Charge compensations can occur for example with an addition of alkali metal ions (not shown in figure).

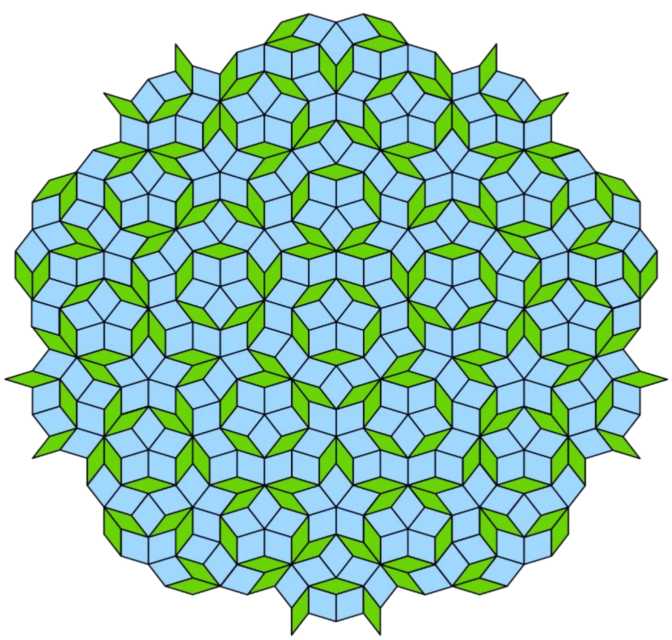

Figure 4. An aperiodic tiling, that is a bidimensional example of a quasicrystal (or quasiperiodic crystal). It is a structure that is ordered but not periodic. Such special tiling was proposed by the English mathematical physicist and philosopher of science Roger Penrose (*b*. 1931).

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