Quasicrystals: The Paradox of Long-Range Order and Aperiodicity

Elliot Kisiel[1]

[1]*Department of Physics, University of California at San Diego, La Jolla, CA 92093*

Quasicrystals exhibit long-range order while simultaneously lacking periodicity presenting a paradoxical material. While the natural algebraic objects for studying crystalline solids in 3 dimensions are groups and their 3-dimensional representations, quasicystals can be viewed as projections of $3+k$ dimensional representations of groups to 3 dimensions. We present this view of quasicrystals and briefly discuss their implications on the physical properties exhibited by this class of materials.

INTRODUCTION

One of the greatest success of quantum mechanics is its application to crystalline solids, particularly when applying Bloch's theorem to elucidate transport properties. Bloch's theorem relies heavily upon the regular periodicity of the lattice and associated potential. Additionally, crystals exhibit long-range order in their atomic positions as a result of the periodicity of the lattice. Compared with amorphous solids, which are both aperiodic and lack long-range order, crystalline solids have natural symmetries associate with them which give rise to a group theoretical description of crystalline solids In fact most modern density functional theory calculations rely on these group theoretic models of crystals and molecules to drastically reduce computation time [1]

Compared to crystals, quasicrystals exhibit aperiodic properties, yet have the paradoxical property of possessing long-range order [2]. The fact that these solids exhibit long-range means that their diffraction patterns are composed of discrete Bragg-peaks situated at integer multiples of a set of basis vectors. In contrast, the aperiodicity of the quasicrystal brings about a dense packing of these Bragg peaks along the basis vector sets [2]. Nevertheless, the long-range order that persists in these quasicrystals implies that there exists some finite basis elements which exist in an aperiodic manner throughout the crystal structure. Mathematically speaking, these quasicrystals lack translational symmetry in at least one of the dimensions of our crystal.

The question then becomes, what tools do we have to study these types of materials from a mathematical point of view if we are lacking translational symmetry in at least one direction? Groups will not be sufficient to study the properties of these materials in <3-dimensional space as the lack of translational symmetry in one of the dimensional will break the closed nature of the group. However if we expand our space to one which will allow the translational symmetries to exist by In this way, we can use groups to study the larger n-dimensional lattice in the hopes of elucidating properties about our lower dimensional quasicrystal. We investigate this method of studying quasicrystals and touch on both the strengths and limitations of viewing these materials from this viewpoint. Much of the discussion of this subject has been shortened from the master's thesis of Foger Ympa [3] and the paper by Ian Putnam [4]. References to these two papers are implied and other resources are directed as utilized.

MOTIVATING EXAMPLE

To get a grasp on this odd combination of aperiodicity with a long-range order, let us first investigate the following example which we will formalize afterwards. Consider the one-dimensional Fibonacci quasicrystal which first arose in the study of rabbit populations. We generate it as such:

*Start with a single mature rabbit and label it **L**. For every generation, each mature rabbit produces a smaller rabbit **S** to the right of it. Additionally, after each generation an **S** rabbit becomes an **L** rabbit. Performing this iteration yields an aperiodic crystal with long-range order.*

If we now look at this sequence, we get something that takes on the form.

LSLLSLSLLSLLSLSLLSLSL...

From this, we start to see regular long range orders appearing such as the **LSL** and **SL** terms, however they do not appear to be in any particular periodic order.

If we look at this space, we see that we are lacking the necessary dimensions to be able to describe the symmetries associated with this quasilattice. However, we can construct this lattice from a larger 2-dimensional space, by taking a cut from it and projecting it down to our 1-dimensional line. Let us see this procedure in action.

If we take the space $\mathbb{Z}\times\mathbb{Z}$, any rationally sloped line will regularly intersect with lattice points in a periodic fashion. If however, we take a slice of this space with an irrationally sloped line, we will never have an intersection of the line with a lattice site. But if we define "planes" (in this case another line) of these lattice points each corresponding to an x and y direction of that lattice site, then the intersection of our line with an x "plane" we can denote as S and an intersection of our line with a y "plane" we can denote as L. For our rabbit case above we can check that this is generated by the cut line with slope $\frac{1}{\tau}=\frac{2}{1+\sqrt{5}}$.

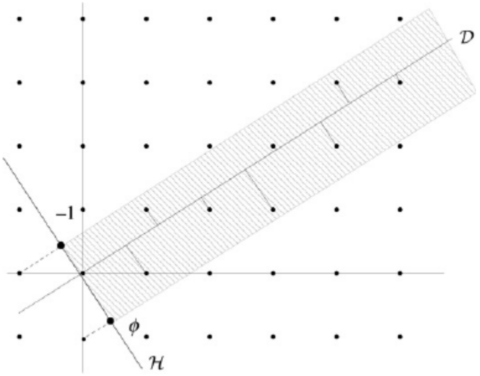

FIG. 1: The cut-and-project method for the Fibonacci quasicrystal with $\mathcal{D} = \mathbb{R}^{\parallel}$, $\mathcal{H} = \mathbb{R}^{\perp}$ and $W = \phi$ [5].

FORMALISM

From our example, what glimpses about the structure of the quasicrystal can we hope to gleam from this kind of construction particularly with respect to the types of Hamiltonians that occur. The rest of this paper will discuss the means by which we can construct quasicrystals from our projection method and the implications on the allowed Hamiltonians. We will start by defining a cut and project system.

Definition 1 *A **cut-and-project system** is a triple* $(\mathbb{R}^{\parallel}, \mathbb{R}^{\perp}, \mathcal{L})$ *with* $\mathbb{Z}^N = \mathcal{L} \subset \mathbb{R}^{\parallel} \times \mathbb{R}^{\perp} \cong \mathbb{R}^N$ *a lattice such that,*

- *The restriction of the projection operator* $\pi^{\parallel} : \mathbb{R}^{\parallel} \times \mathbb{R}^{\perp} \to \mathbb{R}^{\parallel}$ *to* $\mathcal{L}$ *is injective.*
- *The image of the projection operator* $\pi^{\perp}$ *of* $\mathcal{L}$ *is dense in* $\mathbb{R}^{\perp}$*.*
- *Additionally, if the restriction of the domain of* $\pi^{\perp}$ *to* $\mathcal{L}$ *is injective then the system is aperiodic.*

To start off, we have two mutually orthogonal spaces $\mathbb{R}^{\perp}$ and $\mathbb{R}^{\parallel}$ which are subspaces of a larger space $\mathbb{R}^{\parallel} \times \mathbb{R}^{\perp}$ and their projectors to their respective spaces, $\pi^{\parallel}, \pi^{\perp}$. Embedded in this larger space is a periodic lattice $\mathcal{L}$. When we "cut" our system into $\mathbb{R}^{\parallel}$ and $\mathbb{R}^{\perp}$, we only get a system which is a cut-and-project system if our $\mathbb{R}^{\parallel}$ is an irrational sloped hyperplane in at least one of the dimensions. This naturally leads us to our previous notion about quasicrystals which lack a translational symmetry in at least one of the spatial dimensions.

The "project" part of this construction comes when we consider a window $W \subset \mathbb{R}^{\perp}$ which is closed and compact. When we consider the space $\mathbb{R}^{\parallel} \times W$ and project all the points of this space which intersect with the lattice $\mathcal{L}$ down to $\mathbb{R}^{\parallel}$ we get an aperiodic lattice. Considering our case of the Fibonacci chain from before, 1 shows both the $\mathbb{R}^{\parallel}$ and the window W together with the projection of the lattice points to $\mathbb{R}^{\parallel}$.

This method actually lends itself to useful constructions of real quasicrystal. In real quasicrystals, movement of atoms in the crystal is achieved by means of phasons, namely a quasilattice phonon [6]. The means by which this is achieved mathematically is by shifting the window in $\mathbb{R}^{\perp}$ which has the effect that when a new lattice point enters into the window, another one leaves somewhere else in the quasilattice. Additionally, by shifting the window over a certain region in $\mathbb{R}^{\parallel}$ we can achieve the imposition of defects into our quasicrystal.

Now that we have established the method by which we can construct these quasicrystals, we are left with describing the physical properties of the crystal. To do so, we need to look at the set observables in the system which lend themselves to producing the physical properties. As all observable are self-adjoint, when we consider this set, we are led to these possessing certain properties with respect to their underlying structure. One such structure is the $C*-algebra$, which is an algebra, together with an involution $*$ and which is also a complete normed vector space. We formalize this with a definition.

Definition 2 *A **C*-algebra** is a Banach algebra together with an involution* $*$*.*

In the case we are considering, our involution is due to our self-adjoint operators and our Banach space is the set of bounded operators on our Hilbert space $\mathcal{H}$. Notice here that we actually can utilize much of the theory of representation that we have formulated about groups to these $C*-algebras$ in the sense that all bounded operators on a Hilbert space $\mathcal{B}(\mathcal{H})$ have a natural homomorphism to $GL(n, \mathbb{C})$ when $\dim\mathcal{H} = n$. Moving forward, we introduce one more definition which will allow us to consider tilings T as they relate to translations of the space.

Definition 3 *A **hull** of a tiling* T *is the completion of the metric space* $(T + \mathbb{R}^N, d)$*.*

While we have not defined the metric here, we will instead give an intuitive feeling to what this object is. In short, the hull is all of the translations of tilings $T + \vec{x}$ and those tilings which are close enough to a translation of of the tiling (i.e. within some ϵ ball). While there is a rich source of information and results from introducing this object, the main result we will use is that a tiling T is aperiodic if its hull consists only of non-periodic tilings. As it turns out, quasicrystal's hulls contain only non-periodic tilings.

Our final piece of information we need when considering the electronic properties of quasicrystals is a Hamiltonian. If we consider our system, we have a single Hamiltonian describing how an electron will move through the lattice. This Hamiltonian however possess none of the symmetries that will allow us to solve for the properties that we are interested in. To remedy this, we look at a single electron at the origin which observes an initial tiling T_0. Instead of letting the electron hop from lattice sites, we instead translate the lattice so that the electron remains at the origin and observes a new tiling $T = T_0 + \vec{x}$. With each of these "new" tilings, we have an associated operator describing the electrons motion, H_T, where we have the association between two operators as,

$$\mathcal{T}(x) H_T \mathcal{T}(x)^{-1} = H_{T+x} \tag{0.1}$$

Now we can use this aperiodic tiling and its hull, together with a set of operators $\{H_T\}_{T \in hull}$ associated with a $C*-algebra$ to discuss the spectrum of the $C*-algebra$. One of the main results from the paper is the following

Theorem 1 *Given a certain translationally invariant probability measure, μ, on our hull, the spectral projection of H_T up to a finite value E is continuous and bounded on the spectrum of H_T if and only if E is not in the spectrum of H_T.*

This essentially tells us that for the measure that we defined, our projection onto the spectrum of H_T up to a value of E is well understood and behaved as long as our value E lives in a gap of the spectrum. Leading from this then, we have the resolution that the spectrum of almost any H_T is equal to the spectrum of our original Hamiltonian H. Without addressing many of the nuances and details involved in showing these results, the main takeaway from this is that when certain symmetries begin to fail in our models we must start branching out to other non-group theoretic methods to explain our results.

CONCLUSION

Quasicrystals were only first observed naturally in the 1980s and since then the mathematical framework to describe this class of materials has grown significantly [7] These first observations relied on the fact that no crystal can possess 5-fold rotational symmetry or any n-fold rotational symmetry when $n > 6$. Some of the first methods to bring these materials into mathematical description was through the cut-and-project method as discussed before. While this process was great for constructing these lattices, it gave little insight into the properties of the materials. With that, a further investigation into the topologies, algebraic structures and representations of these quasicrystals arose.

The discussion of quasicrystals naturally brings to light the failings of group theory's capabilities. While symmetries exists throughout many facets of nature, there are still sections which lend themselves to breaking and avoiding these symmetries. This leads us to develop new techniques which are more powerful and able to handle the subtleties that occur when our symmetries fail. In a further more in depth conversation of the failings of group theory, especially when discussing quasicrystals, we might encounter certain non-commutative topologies, groupoids and K-theory. All have their merits in discussions surrounding quasicrystals with groupoids relaxing conditions of closure and K-theory establishing topological invariants associated with the space of the $C*-algebras$. All in all, while we look deeper into the underlying structures of nature, we require mathematical tools which are equally robust and intricate as the instruments we use to probe.

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