Impossibility of continuous deterministic phasons in octagonal quasicrystals

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It is shown that quasicrystals with octagonal symmetry do not admit continuous deterministic phasons. This rules out the possibility of finding a dynamical model of the Frenkel-Kontorova type for this simplest class of quasicrystals.

I. INTRODUCTION

In the past, all the known quasicrystals had phasons present merely as a frozen-in disorder: their dynamics were irrelevant on experimental time scales.[1] Since then, a class of quasicrystals with *dynamical* phasons was discovered by Bancel.[2] He interpreted his results via phason relaxation times on the order of minutes. In his case, phasons most likely have some sort of diffusive dynamics, which can be accomplished by the hopping motions of the atoms. This experimental discovery provides an added incentive to study an even more "pristine" possibility: phasons with nonrelaxational dynamics, under which the atoms move continuously in a predetermined way. In the one-dimensional (1D) case, this situation is exhibited by the Frenkel-Kontorova model.

It was shown in[3] that, in the case of quasicrystals, there exist rather nontrivial constraints that are absent in 1D. These constraints can *a priori* jeopardize the very existence of the Frenkel-Kontorova type models for quasicrystals. Before such a model is even written down, we require its solutions to satisfy a *symmetry* requirement (e.g., icosahedral, decagonal, octagonal, etc.) and the topological requirement of *continuity* of atomic motions.[3] When combined with several other general physical restrictions (a precise formulation is in the next section), it turns out that these conditions may be incompatible with each other in some situations.[3-6] Even when they are compatible, they can severely limit the allowed solutions.

Given the nontriviality of constraints posed by symmetry and continuity, much effort has been directed towards the classification of the geometric structures corresponding to continuous phasons. Luckily, the most physically interesting icosahedral symmetry turned out to be compatible with continuous phasons, and some progress has been made towards the goal of a complete classification of the possible solutions in this case.[4,5,7] However, until recently, the two-dimensional quasicrystals have received little attention. We now know that pentagonal quasicrystals in two dimensions do not admit continuous phasons.[4] This work is devoted to proving a similar result for octagonal quasicrystals. As explained, this unfortunately rules out the possibility of constructing a Frenkel-Kontorova-type model for this simplest class of quasicrystals.

While quasicrystals with octagonal symmetry may appear to be a somewhat academic case, we would argue against such a viewpoint. As we emphasized above, the classificational studies of the *geometric* structures admitting continuous phasons are a very important step, but finding a *dynamical* model (whose solutions would of course correspond to these geometric structures) might be of even greater physical significance.[8] From the viewpoint of inventing such a model, one may be better off exhausting the two-dimensional possibilities before addressing the more complicated icosahedral case. The lower-dimensional situations are easier to visualize, and this would be of help in the search for the model.[9]

We now turn to formulating the problem in a more precise fashion, and then, to the proof of impossibility of continuous phasons in the octagonal case.

II. FORMULATION OF THE PROBLEM

Since the general formulation of the problem has appeared before,[3-5] we choose brevity over detail in this section. The quasicrystal structures we consider are obtainable as cuts in higher-dimensional spaces[10] (hyperspaces). One defines a subspace, or a plane, in this hyperspace. This subspace has the same dimensionality as the quasicrystal under consideration and is called a physical space. A maximal subspace orthogonal to the physical space is called a normal space. One introduces a set of atomic surfaces, whose intersections with the physical plane determine the locations of the atoms comprising a quasicrystal. This set of surfaces is invariant under a specified space group acting on the hyperspace. The physical plane is chosen in such a way that any element of this group of symmetry operations preserves its overall orientation in the hyperspace. (This automatically preserves the orientation of the normal space as well.) While the *overall* orientation of the physical space is preserved, these symmetry operations can still induce the motions of the atoms *within* the physical space.

Moving the physical plane along itself induces trivial translations of the atoms in it. Moving the physical plane in the direction perpendicular to itself corresponds to far less trivial rearrangements of atoms corresponding to the phason degrees of freedom. We are interested in studying continuous deterministic phasons. This implies further restrictions on the atomic surfaces, besides the symmetry restriction already mentioned. These surfaces have to be continuous, if atoms are to move continuously in the physical plane in response to the displacements of the physical plane. Furthermore, they cannot have holes. We do not want atoms appearing and disappearing or jumping under phason degrees of freedom. Finally, one imposes a physical requirement that no two atoms can get too close to each other. These conditions are formally summarized as follows (cf. Ref. 3).

Condition 0: Determinism. The atomic positions are defined by intersecting a d-dimensinal physical plane, whose precise location is determined by $\mathbf{x}_0^\perp$, its point of intersection with a normal plane, with a D-dimensinal surface.

Condition 1. Periodicity. The atomic surface is periodic in $D>d$ dimensions.

Condition 2. Conservation of atoms. Under changes in $\mathbf{x}_0^\perp$, atoms are never created or destroyed.

Condition 3. Smoothness. The atomic positions are a continuous function of $\mathbf{x}_0^\perp$.

Condition 4. Hard cores. Atoms cannot get closer than a minimum distance r.

It had been shown[3] that these conditions result in another important property of the atomic surfaces: each of them is "plane-like", i.e., each stays within a finite distance of a plane of dimensionality $d_\perp = D-d$, and these "approximating planes" are rational within the hyperspace.

This property is at the root of difficulties in finding the structures that obey both continuity and symmetry. If condition 1 is supplemented with a requirement that a set of atomic surfaces is not merely invariant under a group of translations in the hyperspace, but rather, under a space group that includes rotations as well, contradictions can result. Rotating an atomic surface results in a surface with a differently oriented approximating plane. Indeed, two planes of different orientations, whose dimensionalities add up to (or exceed) the dimensionality of the hypersurface, will generically intersect. The same applies to the *continuous* surfaces they approximate. Intersections mean that two atoms can get arbitrarily close to each other when the physical plane comes near the intersection, which violates condition 4. Only if the two approximating planes are oriented in a nongeneric way, such that they share a common direction (more precisely, if the totality of vectors from both planes do not plan the full hyperspace), can one avoid intersections.

If one starts from some generically oriented atomic surface, acting on it with rotations from our symmetry group will typically produce surfaces whose approximating planes are oriented in a way that intersections cannot be avoided. Only if *every* single plane that results under every single symmetry operation acting on the initial plane shares a common direction with it can we hope to obey all of our conditions. If one cannot find a plane with the needed orientation, one need look no further: a continuous deterministic quasicrystal will not exist for that particular symmetry group. We claim that one cannot find such a plane in the octagonal case.

III. PROOF

We now prove our assertion that there are no continuous deterministic phasons in the case of octagonal quasicrystals.

Theorem. Conditions 1–4 are incompatible with octagonal symmetry.

Proof. We first review some geometric facts about the eightfold quasicrystals. A 2D quasicrystal with an eightfold symmetry is realized as a 2D cut in a 4D space. The physical 2D plane in the 4D space can be based, for example, on tangent vectors

$$\mathbf{t}_1=(1,2^{1/2},1,0)\ ,\qquad \mathbf{t}_2=(-1,0,1,2^{1/2})\ , \tag{1}$$

and the normal space can then be based on

$$\mathbf{n}_1=(2^{1/2},-1,0,1)\ ,\qquad \mathbf{n}_2=(0,1,-2^{1/2},1)\ . \tag{2}$$

It is easily checked that the following rotation of the 4D space leaves the physical and normal spaces invariant:

$$R=\begin{bmatrix} 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ -1 & 0 & 0 & 0\end{bmatrix}\ . \tag{3}$$

The physical and normal spaces rotate within themselves in an eightfold fashion (i.e., $R^8=E$). In the physical space the corresponding rotation is by 45°. A set of rotations R^k, $k=0,\ldots,7$, form a group.

As explained before, in order for a smooth deterministic eightfold quasicrystal to exist, there should exist a rational 2D plane p in the 4D space, such that for any element of the eightfold rotation group R^k, p and R^kp do not add up to a full 4D space. In other words, p and R^kp should always share at least a common direction. We will show that the only 2D spaces satisfying this property are the physical and normal spaces. These are not rational, therefore, this will mean no such structures are possible. The proof now proceeds in several steps.

(1) First we formalize the statement that p and R^kp share a common direction. Let p be spanned by two tangent vectors:

$$\begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix}=\begin{bmatrix} x_1 & x_2 & x_3 & x_4\\ y_1 & y_2 & y_3 & y_4\end{bmatrix}\ . \tag{4}$$

Then Rp is spanned by $(R\mathbf{x},R\mathbf{y})$. The fact that p and Rp do not span the full 4D space can be expressed as $\det(\mathbf{x},\mathbf{y},R\mathbf{x},R\mathbf{y})=0$, or

$$\begin{vmatrix} x_1 & x_2 & x_3 & x_4\\ y_1 & y_2 & y_3 & y_4\\ (Rx)_1 & (Rx)_2 & (Rx)_3 & (Rx)_4\\ (Ry)_1 & (Ry)_2 & (Ry)_3 & (Ry)_4\end{vmatrix}=0\ . \tag{5}$$

Substituting various R^k for R, we get a system of equations that, in principle, determines a set of possible $(\mathbf{x},\mathbf{y})$, i.e., a set of all planes p. These equations are hard to solve both due to the redundancy of such characterization of p and, also, due to the noninvariance of characterizing two-plane p by two arbitrary vectors from p.

(2) We now describe an invariant way of characterizing

2D subspaces of the 4D space. The 2×4 matrix

$$\begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix}=\begin{bmatrix}x_1 & x_2 & x_3 & x_4\\ y_1 & y_2 & y_3 & y_4\end{bmatrix} \tag{6}$$

is clearly not invariant under the replacements of $\mathbf{x}$ and $\mathbf{y}$ by their linear combinations. Consider, however, a set of six 2×2 determinants,

$$\Delta(12)=\begin{bmatrix}x_1 & x_2\\ y_1 & y_2\end{bmatrix},\quad \Delta(13)=\begin{bmatrix}x_1 & x_3\\ y_1 & y_3\end{bmatrix},\ \cdots . \tag{7}$$

These are essentially all the 2×2 minors of the 2×4 matrix above.

It is easy to see that all the six determinants $\Delta(ij)$ are only multiplied by a common scale factor under the replacements

$$\mathbf{x}=\alpha\mathbf{x}'+\beta\mathbf{y}' ,\qquad \mathbf{y}=\gamma\mathbf{x}'+\delta\mathbf{y}' , \tag{8}$$

and this factor is simply

$$\det\begin{vmatrix}\alpha & \beta\\ \gamma & \delta\end{vmatrix} .$$

The set of six $\Delta(ij)$ is thus similar to a set of direction cosines for a 1D line.

We now study the inverse problem of identifying a 2D plane from a set of $\Delta(ij)$. Suppose $\Delta(12)\neq0$. Then we can choose for tangent vectors,

$$\begin{bmatrix}\mathbf{x}\\ \mathbf{y}\end{bmatrix}=\begin{bmatrix}1 & 0 & x_3 & x_4\\ 0 & 1 & y_3 & y_4\end{bmatrix} . \tag{9}$$

This implies $\Delta(12)=1$, which sets the scale for $\mathbf{x},\mathbf{y}$. Then we obtain

$$\frac{\Delta(13)}{\Delta(12)}=y_3 ,\quad \frac{\Delta(14)}{\Delta(12)}=y_4 ,\quad \frac{\Delta(23)}{\Delta(12)}=-x_3 ,\quad \frac{\Delta(24)}{\Delta(12)}=-x_4 . \tag{10}$$

We note that $[\Delta(34)/\Delta(12)]$ is redundant, since we have

$$\frac{\Delta(34)}{\Delta(12)}=\frac{-\Delta(23)\Delta(14)+\Delta(24)\Delta(14)}{[\Delta(12)]^2} \tag{11}$$

or

$$\Delta(12)\Delta(34)-\Delta(24)\Delta(13)+\Delta(23)\Delta(14)=0 . \tag{12}$$

This last relation is invariant under the scale transformations of $\Delta(ij)$ and is generally more valid than the coordinate-dependent derivation given above. Finally, we note that this relation is analogous to the more familiar relation $\cos^2+\cos^2\beta+\cos^2\gamma=1$, for direction cosines of a 1D line in 3D.

For future reference, we now calculate the sets of $\Delta(ij)$ for the physical and normal spaces. For the physical space of Eq. (1), we obtain

$$\Delta(12)=2^{1/2},\ \Delta(13)=2,\ \Delta(14)=2^{1/2} ,\quad \Delta(23)=2^{1/2},\ \Delta(24)=2,\ \Delta(34)=2^{1/2} , \tag{13}$$

and for the normal space of Eq. (2) we obtain

$$\Delta(12)=2^{1/2},\ \Delta(13)=-2,\ \Delta(14)=2^{1/2} ,\quad \Delta(23)=2^{1/2},\ \Delta(24)=-2,\ \Delta(34)=2^{1/2} . \tag{14}$$

(3) We now derive a set of equations determining the allowed two spaces p in terms of $\Delta(ij)$. We basically reexpress the determinental Eq. (5) in terms of $\Delta(ij)$. First, we count our equations, however. Observe that $R^4=I$, where I is inversion [note that $\det(I)=1$ in 4D]. Inversion I does not change any linear vector subspace of 4D. Thus, only the determinantal equations for R, R^2, and R^3 need to be considered. We further notice that the equations for R and R^3 are really identical in our case. Indeed, $R^3=R^{-1}R^4=R^{-1}I$. Since I leaves a two-space p invariant, to say that p and R^3p do not add up to a 4D space is the same as saying that p and $R^{-1}p$ do not add up to a 4D space. Since p is arbitrary, we can replace $p\rightarrow Rp$. This results in a statement that Rp and p do not add up to a 4D space. Thus R^3 is indeed redundant.

So, we need only consider the equations for R and R^2, which are

$$\det\begin{vmatrix}x_1 & x_2 & x_3 & x_4\\ y_1 & y_2 & y_3 & y_4\\ -x_4 & x_1 & x_2 & x_3\\ -y_4 & y_1 & y_2 & y_3\end{vmatrix}=0 \tag{15}$$

and

$$\det\begin{vmatrix}x_1 & x_2 & x_3 & x_4\\ y_1 & y_2 & y_3 & y_4\\ -x_3 & -x_4 & x_1 & x_2\\ -y_3 & -y_4 & y_1 & y_2\end{vmatrix}=0 . \tag{16}$$

We expand each of these determinants via the Laplace theorem in terms of the minors of the first two and the last two lines. We obtain two equations,

$$[\Delta(12)]^2+[\Delta(14)]^2+[\Delta(23)]^2+[\Delta(34)]^2-2\Delta(13)\Delta(24)=0 \tag{17}$$

and

$$\Delta(12)\Delta(23)+\Delta(12)\Delta(14)+\Delta(23)\Delta(34)+\Delta(34)\Delta(14)-[\Delta(13)]^2-[\Delta(24)]^2=0 . \tag{18}$$

Equations (17) and (18), together with Eq. (12), constitute a set of three equations to be solved.

(4) We now solve these equations. Consider the following linear combinations of the three equations: Eq. (17) plus two times Eq. (18) plus two times Eq. (12); Eq. (18) minus two times Eq. (12); Eq. (17) minus two times Eq.

(18) plus two times Eq. (12). These lead to the following three equations:

$$[\Delta(12+\Delta(14)+\Delta(23)+\Delta(34)]^2 - 2[\Delta(13)+\Delta(24)]^2=0 , \quad (19)$$

$$[\Delta(12)-\Delta(34)]^2+2[\Delta(14)-\Delta(23)]^2=0 , \quad (20)$$

and

$$2[\Delta(13)-\Delta(24)]^2 + [\Delta(12)+\Delta(34)-\Delta(14)-\Delta(23)]^2=0 . \quad (21)$$

Equations (20) and (21) imply

$$\Delta(12)=\Delta(34)=\Delta(14)=\Delta(23)=x , \quad \Delta(13)=\Delta(24)=y , \quad (22)$$

where x, y are some real numbers to be determined. Equations (19) and (22) then result in $2x^2-y^2=0$, which is solved as

$$y=\pm 2^{1/2}x . \quad (23)$$

Substituting this answer in Eq. (22), we can see that these two solutions just correspond to the physical and normal spaces, for which the sets of $\Delta(ij)$ were given in Eqs. (13) and (14). These are the only two solutions to our equations, and thus, no rational solutions exist. Thus we cannot have a smooth deterministic octagonal quasicrystal.

IV. CONCLUSIONS

We have shown that octagonal quasicrystals will not admit structures with continous phasons. This means that there can be no model of the Frenkel-Kontorova type for these quasicrystals. We note that a similar result has been previously shown for pentagonal quasicrystals.[4] In light of these two results, it is tempting to conjecture that twelvefold quasicrystals will also not admit continous phasons,[11] and if that is true we may well have to contend with the icosahedral case in our search for a dynamical model exhibiting continuous phasons (barring the more complicated 2D space groups that, unlike the fivefold, eightfold, tenfold, and twelvefold cases, are not based on quadratic irrationalities).

There is of course another possibility; it is conceivable that this "no-go" theorem is flawed because some subtle *physical* property has been missed in what appears as a mathematically rigorous formulation of the relevant physics. Perhaps a different formulation of the idea of continuous deterministic phasons would allow us to escape the current constraints. To the best of our knowledge, this has not yet been shown to be the case.

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