On brillouin zones and related constructions

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In this paper we discuss the physical and geometrical content of the various equivalent definitions that have been given so far in the literature of a crystal's Brillouin zones. This serves as a motivation to introduce a computationally and conceptually simpler definition. Calculation of Brillouin-zone related properties in two-dimensional lattices is carried out as an illustration of the versatility of this new approach, particularly a count of the number of Landsberg subzones in these Bravais lattices is given, which could be of interest for theoretical physics and number theory.

Keywords: Bravais lattices; Landsberg subzones; reduced zone scheme.

En este trabajo se presenta una discusión sobre los contenidos físicos y geométricos de las diversas definiciones que se han propuesto hasta ahora para definir las zonas de Brillouin de un cristal. Con base en ello, se introduce una nueva definición, que es computacional y conceptualmente más sencilla. Para demostrar la conveniencia de esta nueva propuesta, se realizan cálculos de algunas propiedades relacionadas con las zonas de Brillouin de redes cristalinas bidimensionales; particularmente, se da un conteo del número de zonas de Landsberg en dichas retículas de Bravais, que puede ser provechoso para la física teórica y la teoría de números.

Descriptores: Redes de Bravais; subzonas de Landsberg; esquema de zona reducida.

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1. Introduction

Brillouin zones are introduced in the physics curriculum at the upper-undergraduate level, when there is need to delve into the physics of a wave or an electron in a perfect crystal. They are useful geometrical constructs that convey information about diffraction conditions, but also encode the notion of nth order neighbors (nearest, second nearest, etc.) to a lattice point. Their discussion, however, is usually centered on giving a historically relevant definition, not so much on explaining their intrinsic properties.

An atomic crystal can be mathematically modeled by defining a set of basic vectors, called lattice vectors, that upon linear combination generate a lattice. For example, given two vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, a lattice Λ is formed by taking all the possible combinations $n_1\mathbf{a}_1+n_2\mathbf{a}_2$, with $n_1, n_2 \in \mathbb{Z}$. As it turns out, a lattice may satisfy a certain number of symmetries depending on the lattice vectors. If in the above example we further specify $\mathbf{a}_1 \cdot \mathbf{a}_2 = 0$, and $|\mathbf{a}_1| = |\mathbf{a}_2|$, a so-called square lattice is formed; furthermore it is symmetrical (invariant) under a rotation of 90°. A lattice that satisfies a particular set of symmetries is called a Bravais lattice. Since the original physical motivation for introducing Brillouin zones was to study propagation in crystals it is only natural to make use of Fourier transforms. The Fourier transform of a crystal, also called reciprocal space, results in another, possibly different, Bravais lattice. It is in reciprocal space that wave propagation is analyzed and where Brillouin zones display their convenience.

The purpose of this paper twofold. The main purpose is to present an alternative definition of Brillouin zones that allows for a more tractable way of constructing them. As far as the author is aware of, there exist no methods for finding higher-order Brillouin zones in a general Bravais lattice since it has been cumbersome to take a region-oriented approach instead of a point-oriented one. The second purpose is to provide alternative geometrical pictures when trying to explain the idiosyncrasies of periodic lattices to junior physics students. Perhaps one way of thinking might have more appeal to a student over other ways of presentation, but we hope that by grasping onto different pictures a firmer understanding will be achieved.

In Sec. 2 we present and discuss the relationship between different but equivalent definitions of Brillouin zones. This serves as a motivation for introducing in Sec. 3 a new definition. In Sec. 4 we give examples of how we put our definition to computational use.

2. Discussion of previous definitions of Brillouin zones

Brillouin zones emerged as a useful concept for understanding the physics of waves within a crystal structure, and thus they encompass the various equivalent conditions that must be met in reciprocal space by a wave vector that undergoes diffraction from an atomic lattice. Each way of defining the zones corresponds to a different intuition, be it geometrical or physical, of the intrinsic characteristics of periodic lattices. Altogether, all the definitions involve a way of stating that constructive interference between to incoming plane waves scattering elastically takes place at boundaries of Brillouin zones. The traditional manner of defining them goes as follows. Let Λ be a Bravais lattice in reciprocal space, $\mathbf{L} \in \Lambda$

be a lattice vector of Λ, and call the perpendicularly bisecting plane of $\mathbf{L}$ a *Bragg plane*. Then the nth Brillouin zone taken with respect to an origin $\mathbf{0}$, $B_n(\mathbf{0})$, is defined as the set of points $\mathbf{k}$ such that one crosses at most n Bragg planes, and encounters at least n of them when going from the origin $\mathbf{0}$ to $\mathbf{k}$. We shall call this the von Laue definition, which is related to the diffraction condition

$$\frac{1}{2}L = \mathbf{k} \cdot \hat{\mathbf{L}}; \tag{1}$$

as expressed in Aschroft and Mermin, [4] with $\mathbf{k}$ representing a wave vector. What Eq. (1) means is that for an incident plane wave $\mathbf{k}$ and an outgoing plane wave $\mathbf{k}^{'}$, some lattice vector $\mathbf{L}$ is defined as $\mathbf{L} = \mathbf{k} - \mathbf{k}^{'}$, so that in the regime of elastic scattering the wave vectors of the incoming and outgoing waves must meet at Bragg planes for diffraction to take place.

We can analogously define Brillouin zones through another interpretation of the diffraction condition, in what we shall call the Ewald definition. Following Kittel, [5] by squaring $\mathbf{L} = \mathbf{k} - \mathbf{k}^{'}$ and imposing elastic scattering we may reexpress Eq. (1) as

$$L^2 = 2\mathbf{k} \cdot \mathbf{L}, \tag{2}$$

but this time we see it as the definition of a sphere of radius k, centered at $\mathbf{k}$, such that it touches a lattice point at a distance L from the origin — the equivalence of the physical content of the two equations is discussed in Ashcroft and Mermin [4]. Now let $C(\mathbf{k})$ be the number of lattice points on the surface of the sphere so defined, $N(\mathbf{k})$ be the number of lattice points in the interior of the surface, and $E(\mathbf{k}) = C(\mathbf{k}) + N(\mathbf{k})$. Then $B_n(\mathbf{0})$ is the set of points $\mathbf{k}$ such that $C(\mathbf{k}) < n \leq E(\mathbf{k})$.

Naturally, both the von Laue and the Ewald definitions are equivalent to Bragg's law of diffraction. But the intention here is to motivate a geometrical understanding of Brillouin zones through the physical phenomenon that brought them to life. We see that depending on view point, we can think about drawing planes or spheres in reciprocal space in order to find Brillouin zones. From here on we move onto purely geometrical considerations.

As has been pointed out elsewhere (see for example Veerman *et al.* [3]), the first Brillouin zone coincides with the definition of a *Voronoi cell* of the lattice [7], *i.e.* the set of points that are closer to the origin than to any other lattice point. The collection of Voronoi cells of a set of points is called a *Voronoi diagram*, which can be conceived in a conceptually simple manner [7]: at each point in the set define a sphere whose radius $r = r(t)$, $r(0) = 0$, grows with time. The Voronoi diagram of the set is given by the intersections of the spheres with their nearest neighbours as they expand. This parallel permits us to put forward an argument that bridges the von Laue and Ewald definitions of Brillouin zones, and leads to two other definitions. At each lattice point, let a sphere of radius given by a variable wave vector $|\mathbf{k}(t)|$ expand initially from $k(0) = 0$. Then the wave-vector spheres define the $B_n(\mathbf{0})$ as they sweep through the lattice in the manner of the Ewald definition, and the perpendicular bisectors of the von Laue definition are given by the first intersections of the growing spheres with the sphere centered at $\mathbf{0}$. This implies what we call the Jones definition — after G. A. Jones [1]: a point $\mathbf{k}$ is in $B_n(\mathbf{0})$ if the elements $\mathbf{L}_1, \mathbf{L}_2, \ldots$ of Λ can be ordered so that

$$|\mathbf{k} - \mathbf{L}_1| \leq |\mathbf{k} - \mathbf{L}_2| \leq \ldots \tag{3}$$

with $\mathbf{L}_n = \mathbf{0}$. Let us note that the Jones definition lessens the geometric importance of the point $\mathbf{0}$ as an origin for the lattice coordinate system, shifting instead its role to that of a "dummy" index that tells us how to choose an origin in order to fix $B_n(\mathbf{0})$. Furthermore, by establishing $\mathbf{L}_n = \mathbf{0}$ we automatically define the set of Bragg planes taken with respect to $\mathbf{0}$, let us call it $H_\Lambda(\mathbf{0})$, that yields the von Laue definition. But we can as well start by fixing $H_\Lambda(\mathbf{0})$, in which case we need to utilize the inequalities of Eq. (3) to our advantage.

3. A new definition

A remark about Brillouin zones is in order. We can think them as being composed of two elements, convex polygons whose vertices are defined by intersections of Bragg planes, and the interior regions enclosed by such polygons. In this picture Bragg planes — and thus also lattice points except the origin $\mathbf{0}$ — do not belong exclusively to one Brillouin zone because they represent the various possibilities of satisfying the diffraction condition. And of course not every polygon that can be drawn out between Bragg plane intersections will turn out to be the boundary of some Brillouin zone. But it is the case that there is a simple way of picking out the correct interior regions of Brillouin zones without having to worry about their boundaries. Therefore we may find Brillouin zones by taking the union of its interior regions, which we shall call b_n, with the set of Bragg plane segments that make contact with them.

On to the *definition of Brillouin zones by constraints*. Let $\mathbf{d_L} = \mathbf{L}/2$ be a point defined by the Bragg plane $H_\mathbf{L}(\mathbf{0})$, and let $D(\mathbf{k})$ be the number of constraints of the form $k > d_\mathbf{L}$, subject to $\mathrm{sgn}((\mathbf{k} - \mathbf{d_L}) \cdot \mathbf{d_L}) = 1$, satisfied by the point $\mathbf{k} \in \mathbb{R}^m - \{H_\Lambda(\mathbf{0})\}$. Then the set $b_n(\mathbf{0})$ of interior points to the nth Brillouin zone $B_n(\mathbf{0})$ is $b_n(\mathbf{0}) = \{\mathbf{k} | D(\mathbf{k}) = n\}$.

The above definition gives a rule for assigning the various regions enclosed by a set of Bragg planes $H_\Lambda(\mathbf{0})$ to their proper Brillouin zones. Plainly stated it says that a point is inside $B_n(\mathbf{0})$ if it "lies outside" n Bragg planes. The advantage of this approach is that it focuses on regions defined by constraints, instead of the previous point-oriented definitions. When finding Brillouin zones, however, we also need to find the set of Bragg planes $H_\Lambda(\mathbf{0})$. We may still use the constraint definition in a methodical manner to construct Brillouin zones for a given lattice point. The method consists of finding the half-distance $\mathbf{d}_{\mathbf{L}_i}$ of each lattice point $\mathbf{L}_i$ in order of increasing distance to $\mathbf{0}$, tracing the appropiate Bragg plane and updating the number of constraints satisfied by each newly formed region. We say that we have

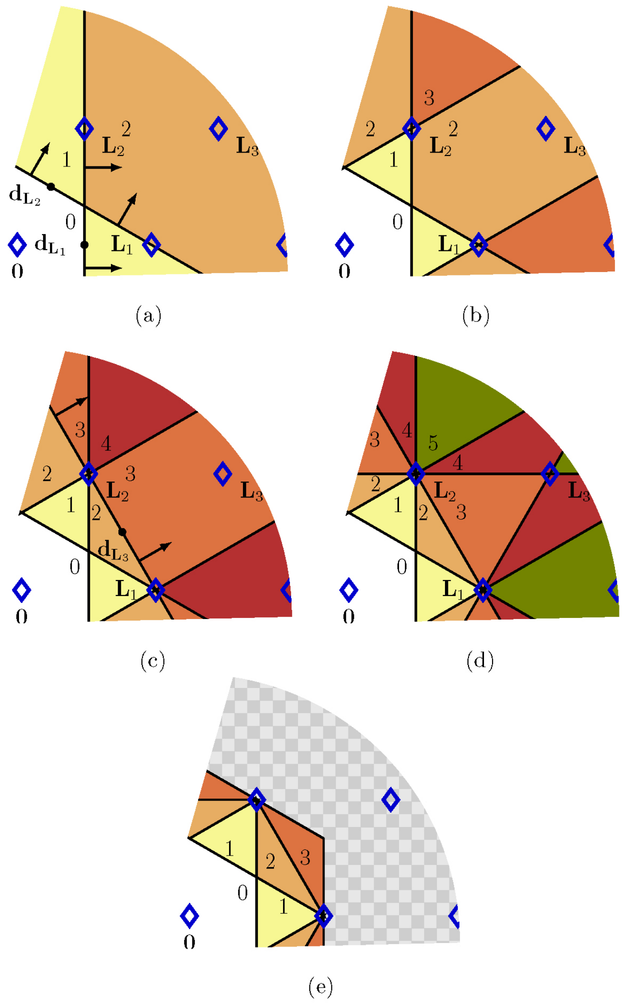

FIGURE 1. Finding the first three Brillouin zones in an hexagonal lattice by the constraint definition. For simplicity only a subset of reciprocal space is shown. The arrows attached to a Bragg plane indicate its outside region, or the direction of sweeping. $D(\mathbf{k})$ is identified by color and number; notice how with each successive Bragg plane reciprocal space is subdivided according to how they satisfy $k > d_{\mathbf{L}}$ while being outside of each corresponding Bragg plane. Fig. 1e shows the first three Brillouin zones.

found a Brillouin zone when no more Bragg planes cross through a region.

To clarify the application of the method, let us use it to find the first three Brillouin zones of an hexagonal lattice in $\mathbb{R}^2$. The process is illustrated in Fig. 1. First, we define an origin $\mathbf{0}$, and locate the (six) nearest points to it. We pick one of them, say $\mathbf{L}_1$, and trace its Bragg plane. Now we imagine the Bragg plane sweeping reciprocal space parallel to itself, and to the counter of every point touched by the plane in this fashion we add a 1. That is, for every point $\mathbf{k}^+$ outside of this Bragg plane, $D(\mathbf{k}^+) = 1$, whereas for every point $\mathbf{k}^-$ on the inside $D(\mathbf{k}^-) = 0$. Continuing in the same fashion with $\mathbf{L}_2$, we end up with three divisions, $D(\mathbf{k}) = 0, 1, 2$, depending on whether the point lies on the outside of two, one or none of the Bragg planes (Fig. 1a). After doing the same on all the nearest lattice points (Fig. 1b), we proceed to trace the Bragg planes of the second-nearest neighbors. We pick $\mathbf{L}_3$, trace its Bragg plane and sweep reciprocal space (Fig. 1c). In Fig. 1d we show how the regions look like after tracing all the Bragg planes of the second-nearest neighbors. After finishing

TABLE I. Number of Landsberg subzones in B_n. Due to low symmetry, extremely small Brillouin zones form in an oblique lattice, so we only provide a count up to B_{10}. For the other lattices the count can be continued to much higher orders, although only a sample is given here.

B_n	Square	Rectangular	Hexagonal	R. Centered	Oblique
0	1	1	1	1	1
1	4	4	6	6	6
2	8	10	6	8	12
3	12	12	6	14	18
4	20	18	12	22	24
5	20	26	18	24	28
6	12	30	30	28	36
7	12	34	30	36	42
8	20	38	18	44	48
9	28	42	18	48	54
10	44	48	36	52	60
11	48	50	42	52	...
12	48	58	54	62	...
13	64	68	54	70	...
14	60	76	42	72	...
15	52	72	66	76	...
16	60	78	72	80	...
17	52	86	72	88	...
18	40	88	96	88	...
19	52	96	84	102	...
20	72	100	72	102	...

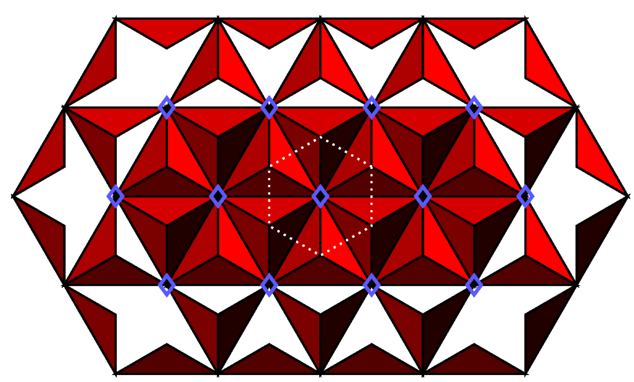

FIGURE 2. Construction of the reduced zone scheme for B_2 in an hexagonal lattice. Here we show $B_2(\mathbf{0}), B_2(\mathbf{L}_1), \ldots, B_2(\mathbf{L}_i), \ldots, B_2(\mathbf{L}_{12})$, with their corresponding lattice points. To show how they intertwine, the Landsberg subzones of each $B_2(\mathbf{L}_i)$ get darker counterclockwise. $B_0(\mathbf{0})$ is drawn with a dotted white line.

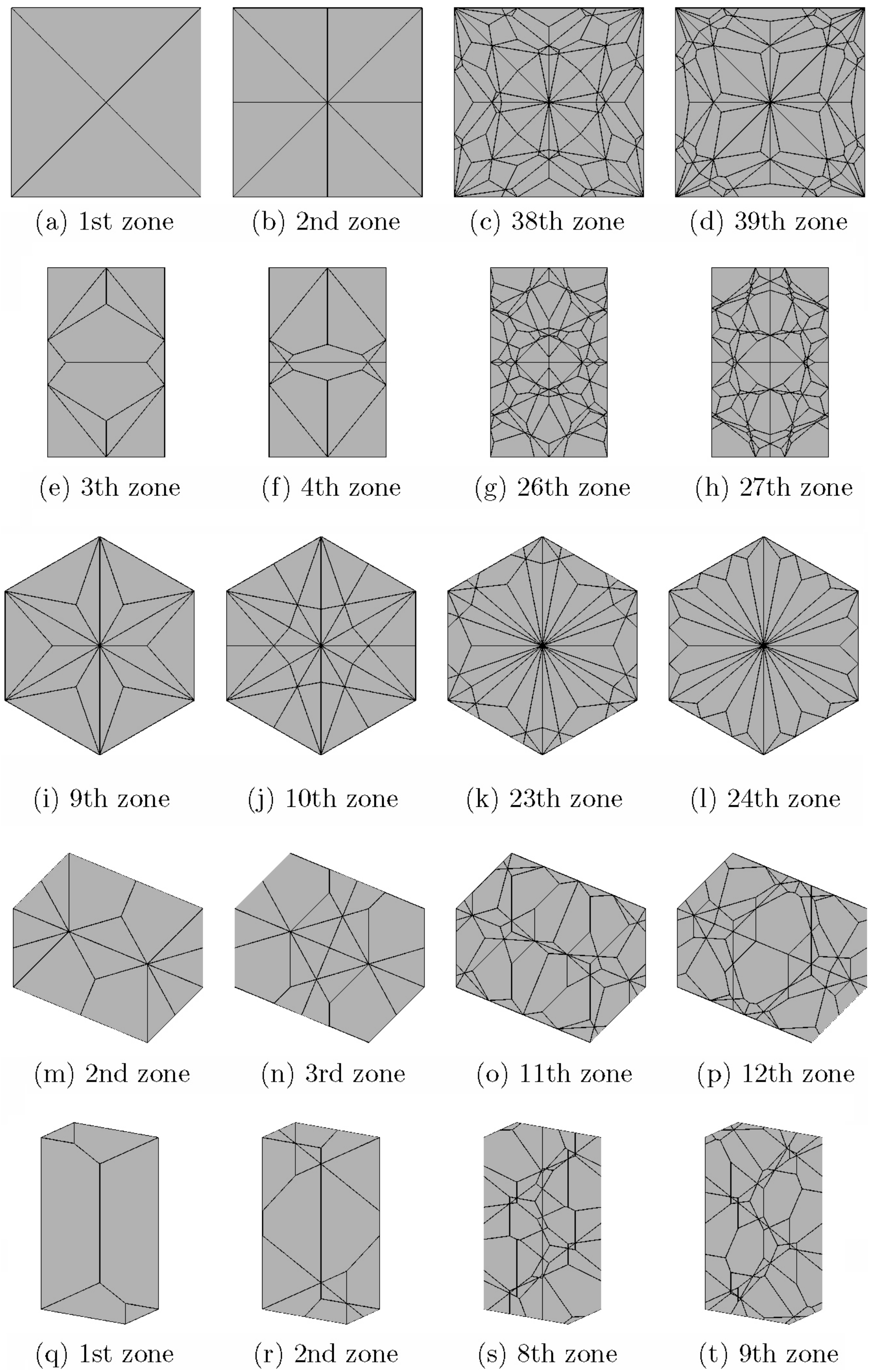

FIGURE 3. Various puzzle tessellations of B_0 for the five two-dimensional Bravais lattices, in top-down row order: square, rectangular, hexagonal, rectangular centered, oblique.

tracing and sweeping with the Bragg planes of the third-nearest neighbors, we may notice that no further Bragg planes will cut through $B_0(\mathbf{0}), B_1(\mathbf{0}), B_2(\mathbf{0})$, nor $B_3(\mathbf{0})$: we have thus found the first three Brillouin zones (Fig. 1e).

By taking into account symmetry it is possible to consider a smaller subset of $H_\Lambda(\mathbf{0})$ and still be able to construct all of B_n.

A dynamic geometrical picture of the method can be imagined. Instead of growing spheres from lattice points and following their intersections, or instead of counting plane crossings for every point in reciprocal space, as the Ewald and von Laue definitions require, we take only one expanding sphere centered at the origin $\mathbf{0}$, and as it reaches the various $\mathbf{d_L}$ we attach to it tangents planes at those points. Then we think of points in reciprocal space as initially empty bins and for each Bragg plane that passes by them, we add one to their counter. With the sphere sweeping through reciprocal space, different numbers are added to these bins as different constraints are satisfied, hence different Brillouin zones are created.

The idea of a growing sphere with Bragg planes being attached to it is supported by the fact that as $n \to \infty$, the B_n tend to a circular annulus shape [1]. To wit, more and more Bragg planes are added as tangents, so they intersect to n more rapidly and over a smaller radial interval.

4. Landsberg subzones and the reduced zone scheme

We shall now briefly illustrate how can the constraint definition enter in calculations related to Brillouin zones in two dimensions. First we sketch a method for counting the number of interior regions b_n, called Landsberg subzones, that make up B_n. Next we sketch how can one find the reduced zone scheme by tessellation. To the best of our knowledge, there exists no previous attempt at performing these calculations neither for high n nor for the less symmetrical lattices. Practical implementations require tuning that would distract from the main ideas.

4.1. Counting Landsberg subzones

The $b_n(\mathbf{0})$ that we have previously defined have a connection to number-theoretical properties of interest to mathematicians [2], and of possible theoretical use in physics [3]. We may take advantage of some tools of morphological image processing, (for further clarification see any standard text on digital image processing), namely, erosion and dilation of sets, and extraction of connected components. Shortly put, eroding (dilating) an image means making it smaller (larger) by erasing (drawing) along its border with a specified pen-element. After calculating b_n we perform on it an erosion followed by a dilation, which has the effect of rounding vertices and making the regions comprising b_n become practically disconnected. Then making use of standard algorithms for counting the number of disconnected sets we may find the number of Landsberg subzones that compose $B_n(\mathbf{0})$. This computations were done in MATLAB 7. The results are given in Table I. Due to the low symmetry of the oblique lattice, near-intersections of Bragg planes result in a substantial number of minute Landsberg subzones, so it was only feasible to count up to B_{10}.

4.2. Finding the Reduced Zone Scheme and Brillouin Zone Puzzles

It can be shown [3] that not only do Brillouin zones $B_n(\mathbf{0})$, $n = 1, 2, \ldots$, tessellate the plane, but this is also true of the $B_n(\Lambda)$ for a fixed n. From this we may find the reduced zone scheme by constructing $B_n(\Lambda)$ and looking at $B_0(\mathbf{0})$. In practice, a routine based on the aforementioned method for constructing Brillouin zones was used to calculate B_n at each lattice point. Then $B_0(\mathbf{0})$ was calculated. In Fig. 3 we show a number of *Brillouin zone puzzles*, which are constructed from various tessellations $B_n(\Lambda)$ with the boundary of B_0 superimposed [8]. These puzzle figures were done with MATLAB 7.

5. Final Remarks

In this paper we have elaborated on a geometrical interpretation of the diffraction condition in crystals, which we then combined with intution about Voronoi diagrams. This lead us to an insight of the more mathematically oriented definition used by Jones [1] and served to propose the constraint definition for finding the interior points of Brillouin zones. This definition depends upon a suitable notion of the "outside" of a Bragg plane; the interior of the nth Brillouin zone is then seen to lie outside n Bragg planes, so it may be further extended to non-euclidean metrics in lattices by re-stating it with an acceptable notion of the inside-outside of the Bragg planes.

Further intuition of Brillouin zones might stem from yet another approach inspired in computational geometry or digital image processing. As it stands, the method here proposed counts the number of constraints that a point satisfies for the outsides of Bragg planes, because of its convenience. But we can just as well change the definition to count to how many insides a point belongs, for a given subset of $H_\Lambda(\mathbf{0})$. This would give way for an analogy of the *backprojection method* of tomographic reconstruction if we think it in terms of the trace-and-sweep picture. An exploration of this topic might yield interesting results on the geometry of periodic lattices.

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7. The first Brillouin zone is also called the Wigner-Seitz cell in physics.
8. A technical point. The number puzzle pieces that appear in B_0 for a given tessellation $B_n(\Lambda)$ is the same as the number of Landsberg zones in B_n due to properties of periodic lattices. In Fig. 3, however, one should be aware that the Brillouin zone puzzles are comprised of *two* boundaries: B_n and B_0. This has the effect of seemingly "cutting" some pieces of B_n in a very few cases (B_2, B_3, and B_{20} in the hexagonal lattice, for example), but in no case does this imply that the reduced zone scheme "sees" more Landsberg zones than it should.