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Quasiperiodic packing densities

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The problem of the packing density on quasiperiodic lattices is discussed in a systematic way using projection techniques. For compact domains a direct construction is presented using a Voronoi construction on a quasilattice in perpendicular space defined by the forbidden volume of the packed objects. A generalized inflation law, valid for arbitrary shapes of the acceptance domain using the properties of linear mappings of the hyperlattice on itself which commute with the symmetry group, is used to show that the packing densities and the whole structure of the projected quasilattice are periodic under scale transformations. We find the optimal compact acceptance domains and packing densities for several icosahedral problems. For the packing of spheres on the primitive lattice, an icosahedron and the truncated triacontahedron give equal densities but different quasilattices. For the packing of icosahedra one finds only the second lattice and a very high density. For the fcc and bcc lattices the maximum density acceptance domain is a triacontahedron and the densities are considerably lower. The results of Henley for including correlations to increase the density are reformulated in terms of a graph problem in perpendicular space. Including only the graphs equivalent to his, we find the same packing density for the two primitive and for the fcc lattice. It is shown that a generalization leads to an interesting and very complex problem in graph theory which we are unable to solve.

I. INTRODUCTION

An interesting aspect of quasicrystalline ordering is the question of the packing densities associated with such arrangements. In essence this is also the zero-order approximation for the structural stability problem. The problem is nontrivial because different atomic sites have different environments and a considerable variety of (nearest-neighbor) Voronoi polyhedra, even for the simplest case of single-species undecorated quasicrystals. When one considers a quasicrystal as a projection of a periodic hyperlattice in a higher-dimensional space,[1,2] one finds that the quasiperiodic arrangement of projected points depends not only on the chosen hyperlattice but also on the shape of the acceptance domain used for the projection. The packing density one can achieve then depends both on the point density of the quasicrystal and on the size of the largest objects of a given shape which can be placed at all these points. In particular, for a packing of spheres this depends on the smallest nearest-neighbor distances in the quasilattice. Clearly the largest spheres one can pack cannot have a diameter larger than this distance. Henley[3] has recently discussed the icosahedral quasiperiodic packing of spheres using several shapes for the acceptance domain. Using the techniques developed by Elser[4] one can determine the point density and other properties, like the distribution of nearest-neighbor distances, from the volume and shape of the acceptance domain. Our purpose here is to develop a systematic approach for this problem.

In Sec. II we show how one can calculate packing parameters and the conditions for the appearance of the various separation vectors between the projected lattice points from the structure of the acceptance domain. Our considerations in this section are very similar to those of Elser,[4] and most of the results we derive are not new. The essential point is that the volume of the acceptance domain (in perpendicular space) is proportional to the density of the projected points. Thus one has to maximize this volume subject to the constraints imposed by the packing conditions.

In Sec. III we use these results to develop a systematic procedure for maximizing the packing density, on the quasilattice, for objects of arbitrary shape and size. The procedure only assumes that one wants to place the *same* object at all the points of the quasilattice. The shape and size of the object define an excluded volume in parallel (physical) space. No other (quasi)lattice points are allowed within this volume around any occupied point. This excluded volume, considered as an acceptance domain, defines a quasilattice in perpendicular space consisting of the projections of all the hyperlattice vectors which are *forbidden.* One is looking for the largest acceptance domain (in perpendicular space) which excludes all these vectors around any accepted point. For compact acceptance domains the density is maximized by a Voronoi cell around the origin of this quasilattice in perpendicular space.

We then prove that the packing density is periodic in the size of the packed objects. To prove this we use a generalized form of inflation, based on the properties of linear operators which map the hyperlattice on itself while they remain simple scale transformations in both parallel and perpendicular space separately. The existence of such operators, their relation to inflation, and their mathematical context were discussed recently by

Ostlund and Wright.[5] Our derivation is different. For the icosahedral group the definition of these operators is essentially unique and their construction is straightforward. The scale factors are τ^3 and τ^{-3}. The shrinking of any acceptance domain by τ^3 will give a quasicrystal identical to the original one except for a τ^{-3} scale transformation. The result for the packing densities follows. This is the context of Sec. IV.

These results are applied to the packing of spheres on undecorated icosahedral quasilattices in Sec. V. We derive the acceptance domains which maximize the density for all three lattices. We find two acceptance domains for the primitive lattice, a truncated triacontahedron discussed already by Henley[3] and an icosahedron, and for both the fcc and the bcc lattice a triacontahedron. The maximum packing densities for compact acceptance domains are 0.56 for the primitive (sc) lattice for both acceptance domains, 0.30 for the centered icosahedral (or bc) lattice and 0.48 for fc. We also give results for the distributions of neighbor distances for the icosahedral acceptance domain supplementing the results of Henley[3] for the truncated triacontahedron. For the packing of icosahedra[6] we find that the acceptance domain is the truncated triacontahedron and the packing density is extremely high (0.62), much higher than any of the results of Ref. 6.

The Voronoi construction maximizes the density for compact acceptance domains. It was noted by Henley[3] that one can obtain considerably higher densities if one allows for correlations in the quasilattice. This results in an acceptance domain which has a larger volume but is no longer simply connected. Using the results derived earlier we reformulate this problem as a condition on the acceptance domain. We show that the terms considered are only the simplest, and can, at least formally, be generalized. One ends up with a very interesting problem in graph theory—namely the minimal number of points needed to decompose a graph formed by the vectors of the forbidden quasilattice, and the shape of the acceptance domain which corresponds to this decomposition. This problem turns out to be completely intractable even as a computational problem as soon as one includes anything beyond the smallest vectors (the Henley approximation). Thus all we were able to show was that higher densities are probably possible. We also apply the lowest-order corrections to the sc lattice with an icosahedral acceptance domain and to the fcc lattice, and find in both cases a density equal to that achieved by Henley (0.62).

II. DENSITIES AND THE ACCEPTANCE DOMAIN

Consider a lattice (L^D) in D-dimensional space (R^D) consisting of the vectors

$$R_D = \sum_i n_i \mathbf{e}_i \; , \tag{1}$$

where the $\mathbf{e}_i$ are linearly independent. We decompose R^D into two mutually orthogonal subspaces $R^{\parallel}$ and $R^{\perp}$. A general vector $\mathbf{r}_D$ in R^D can then be decomposed into its parallel and perpendicular components $(\mathbf{r}_{\parallel};\mathbf{r}_{\perp})$. A projected (quasi) lattice $L^{\parallel}$ in $R^{\parallel}$ is defined by

$$\mathbf{R}_{\parallel} \in L^{\parallel} \quad \text{if} \quad \mathbf{R}_{\perp} \in S^{\perp}(\mathbf{r}_{\perp}) \quad \text{and} \quad \mathbf{R}_D = (\mathbf{R}_{\parallel},\mathbf{R}_{\perp}) \in L^D \; , \tag{2}$$

where the acceptance domain $S_{\perp}(\mathbf{r})$ is some region in $R^{\perp}$. This is equivalent to the projection of a slice of L^D of "width" $S_{\perp}(\mathbf{r}_{\perp})$ in $R^{\perp}$ on $R^{\parallel}$. $L^{\parallel}$ is a "lattice plane" of L^D (and therefore a periodic lattice in $R^{\parallel}$) if all its direction cosines with the $\mathbf{e}_i$ [Eq. (1)] are rational. Otherwise it is a quasiperiodic quasilattice. Quite generally one has for the volumes

$$V_D = V_{\parallel} V_{\perp} \; , \tag{3}$$

where V_D is the volume of a region in R^D and $V_{\parallel}$ and $V_{\perp}$ are the volumes of the projections of this region on $R^{\parallel}$ and $R^{\perp}$, respectively. Thus if the volume of the elementary unit cell of L^D in R^D is 1, then

$$v_{\parallel} S_{\perp} = 1 \quad \text{and} \quad \rho_{\parallel} = 1/v_{\parallel} = S_{\perp} \; , \tag{4}$$

where $S_{\perp}$ is the volume of the acceptance domain $S_{\perp}(\mathbf{r})$ in $R^{\perp}$, $v_{\parallel}$ is the volume per point, and $\rho_{\parallel}$ the density of the points in $L^{\parallel}$. These relations, which are always true on the average (when one averages over the positions ($\mathbf{r}'$) of the acceptance domain $S_{\perp}(\mathbf{r}-\mathbf{r}')$ with respect to the projection of the origin [in Eq. (1)] on $R^{\perp}$) become *independent* of the position of $S_{\perp}(\mathbf{r}-\mathbf{r}')$ when $R^{\perp}$ contains no lattice vectors of L^D. We shall assume this implicitly in the following. The considerations become a little more complex when this does not hold even when $L^{\parallel}$ is still a quasilattice—as for the projections of the Penrose tiling from five dimensions.[7] This is proven in great detail by Elser.[4]

While the density $\rho_{\parallel}$ depends only on the *volume* of the acceptance domain, other properties depend also on its shape. Thus a separation $\mathbf{R}_{\parallel}$ between two points in $L^{\parallel}$ can appear only when two points separated by the corresponding perpendicular projection ($\mathbf{R}_{\perp}$) can both fall simultaneously into $S_{\perp}(\mathbf{r}_{\perp})$. The density of such pairs in $L^{\parallel}$, $\rho_{\parallel}(\mathbf{R}_{\parallel})$, is then given by the volume $S_0(\mathbf{R}_{\parallel})$ of the overlap region $S_0(\mathbf{r}_{\perp};\mathbf{R}_{\parallel})$

$$\rho_{\parallel}(\mathbf{R}_{\parallel}) = S_0(\mathbf{R}_{\parallel}) \quad \text{when} \quad S_0(\mathbf{r}_{\perp};\mathbf{R}_{\parallel}) = S_{\perp}(\mathbf{r}_{\perp}) \cap S_{\perp}(\mathbf{r}_{\perp}+\mathbf{R}_{\perp}) \; ; \quad \mathbf{R}_D = (\mathbf{R}_{\parallel},\mathbf{R}_{\perp}) \in L^D \; , \tag{5}$$

where the two regions $S_{\perp}(\mathbf{r})$ and $S_{\perp}(\mathbf{r}+\mathbf{R}_{\perp})$ are shifted by $\mathbf{R}_{\perp}$ with respect to each other.

Most of our considerations below will use this relationship or its analogs. In particular, it follows that $\mathbf{R}_{\parallel}$ will not appear for acceptance domains such that the overlap [Eq. (5)] is empty. As stated in the Introduction these results are in the main equivalent to those of Elser.[4]

III. THE VORONOI CONSTRUCTION

It is clear from the above that the packing density for objects of a given shape will depend on the shape of the acceptance domain. If, for example, we want to pack spheres of diameter d then the largest spheres compatible with a given acceptance domain will have a diameter equal to the smallest nearest-neighbor distance allowed. This is, according to Eq. (5), the smallest $R_{\parallel}$ for which $S_0(\mathbf{R}_{\parallel})$ defined in Eq. (5) does not vanish. For spheres of diameter d we therefore need an acceptance domain $S_\perp(\mathbf{r};d)$ such that

$$S_0(\mathbf{R}_\parallel)\equiv 0 \quad \text{if} \quad R_\parallel < d \; . \tag{6}$$

To maximize the packing density one needs the acceptance domain which satisfies Eq. (6) and has the largest volume.

It is evident that the vectors $\mathbf{R}_\perp$ for which Eq. (6) holds, form a quasilattice $L^\perp$ in perpendicular space ($R^\perp$) with the spherical acceptance domain (in $R^\parallel$) $R_\parallel < d$:

$$\mathbf{R}_\perp \in L^\perp \quad \text{if} \quad R_\parallel < d \quad \text{and} \quad \mathbf{R}_D = (\mathbf{R}_\parallel, \mathbf{R}_\perp) \in L^D \; . \tag{7}$$

Thus the acceptance domain for the quasicrystal we want to construct must exclude all the vectors ($\mathbf{R}_\perp$) belonging to $L^\perp$. The condition is obviously that Eq. (5) will give $S_0=0$ for all these vectors. If we want a compact domain the largest volume for which this holds is given by a Voronoi construction. One draws the planes bisecting all the vectors $\mathbf{R}_\perp$ of $L^\perp$. The region defined by this construction around the origin is the largest compact acceptance domain which excludes all vectors $\mathbf{R}_\perp$. It is the Voronoi polyhedron of the origin on the quasilattice $L^\perp$ defined (in $R^\perp$) by Eq. (7).

The maximum volume packing density (c) for these spheres is then given by

$$c = \rho_\parallel(d) v = S_\perp(d) v \; , \tag{8}$$

where $S_\perp(d)$ is the volume of the Voronoi cell defined by the above construction and v ($=\pi d^3/6$) the volume of the packed spheres.

There are now two complications.

(a) It is evident that this acceptance domain will not change smoothly as a function of the sphere diameter (d). The Voronoi polyhedron is determined by a small number (usually one or at most two) of stars of the quasilattice. They change only for certain discrete values of d. These special values of d obviously give the maximum (volume) packing density for a given acceptance domain. One also finds that, in general, not all vectors of $L^\perp(\mathbf{R}_\perp)$ play a role. As the diameter is increased, and as a result $L^\perp$ changes as new vectors are added (or some vectors are subtracted), only certain special vectors ever show up as those determining the acceptance domain (i.e., the Voronoi polyhedron of the origin).

(b) The second problem is more delicate. In general one can obviously vary d through the whole range $0<d<\infty$. There is no way one could check this whole range directly. We solve this problem by showing that the packing density is periodic in the scale. For the icosahedral quasicrystals we show that spheres of radius d and of radius $\tau^3 d$ always have identical packing fractions. We shall do this by proving a generalized inflation rule for lattices generated by arbitrary acceptance domains.

Finally, we note that the procedure we have discussed above can obviously be generalized to calculate the packing density of objects of arbitrary shape. The only difference is that the forbidden excluded volume in $R^\parallel$ around any lattice point of $L^\parallel$, which defines the quasilattice $L^\perp$ in $R^\perp$, will then not be spherical. It will have a different shape and the Voronoi construction has to be implemented for the resulting quasilattice. Also, in calculating the packing density through Eq. (8), we have to use the correct volume v of the packed objects.

We shall first prove the generalized inflation rule in the following section and then proceed to calculate the relevant acceptance domains and packing fractions for the icosahedral lattices.

IV. INFLATION FOR GENERAL ACCEPTANCE DOMAINS

A general vector of L^D can be written in terms of its components in Eq. (1) [$\mathbf{R}_D=(n_1,n_2,\ldots,n_D)$]. We note that this description is not necessarily orthogonal in R^D [if the vectors $\mathbf{e}_i$ in Eq. (1) do not form an orthonormal set]. Assume for simplicity that the lattice is primitive[8] (i.e., there are no restrictions on the n_i). The lattice is then mapped on itself by the D dimensional matrices M with integral elements. If, in addition, $\det\|M\|=\pm 1$ then M has an integral inverse and the mapping is one to one. The matrices K for which this holds form a group $[K]$. A general transformation K in this group is a linear affine transformation of R^D on itself which conserves volume. For completeness we note that when $R^\perp$ contains lattice vectors it is useful to use a more general definition of $[K]$ because an infinite number of different points in L^D then have the same $\mathbf{R}_\parallel$ but different $\mathbf{R}_\perp$. The generalization is straightforward[7] but in the following we assume, for simplicity that this is not the case.

Let the lattice L^D be invariant under some point group G. It is then always possible to represent the operations of G in the form K and this defines a unique subgroup $[G]$ of $[K]$.[9] $[G]$ describes the way G acts on the lattice vectors of L^D but also the way the operations of G act on the whole space R^D when they act at the origin of L^D and leave this origin invariant. The cases of interest are those in which these representations of G are reducible. They can then be reduced[10] to a form in which they act separately in n irreducible, mutually orthogonal, subspaces of $R^D - R^1, R^2, \ldots, R^n$. One of these would be $R^\parallel$. It is then possible to find a subgroup of $[K]$, $[K^\circ]$, of operators which commute with $[G]$. These operators define inflations of $L^\parallel$ which can be obtained by suitable scale transformations of the (arbitrary) acceptance domain in each of the subspaces R^i orthogonal to $R^\parallel$ separately. The existence of these operators, their relevance to the description of inflation, and many of their mathematical properties were recently discussed by Ostlund and Wright.[5]

We notice that any matrix which, when reduced, is a constant (scale factor) λ_1 in each subspace R^i separately will commute with $[G]$. Among these there are obviously matrices whose determinant is one. The demonstration that the λ_i can always be chosen so that one obtains integer representations which belong to $[K]$ is a little more complex, but elementary. We omit the demonstration here. A much more sophisticated proof is given in Ref. 5. We construct the operators explicitly for the icosahedral lattices below.

It is simplest to see why operators of the group $[K^\circ]$

define an inflation when $R^{\parallel}$ and $R^{\perp}$ are both irreducible. Let the two scale factors obtained when the matrix is reduced be $\lambda_{\parallel}$ and $\lambda_{\perp}$ where obviously $(\lambda_{\parallel})^{d_{\parallel}}(\lambda_{\perp})^{d_{\perp}}=1$ and we can assume $\lambda_{\parallel}>\lambda_{\perp}$ (otherwise we look at the inverse matrix).

Consider now what the transformation does. It transforms the set of vectors in the original projected slice $\{\mathbf{R}_D\}$ with projections $\{\mathbf{R}_{\parallel}\}$ and $\{R_{\perp}\}$ into a new set of vectors of L^D: $\{\mathbf{R}'_D\}$ with scaled projections $\{\mathbf{R}'_{\parallel}\}=\lambda_{\parallel}\{\mathbf{R}_{\parallel}\}$ and $\{\mathbf{R}'_{\perp}\}=\lambda_{\perp}\{\mathbf{R}_{\perp}\}$. Obviously, the projected lattice $L^{\parallel'}$ is simply the lattice one would obtain from L^D by using an acceptance domain scaled by $\lambda_{\perp}$ but of the same shape as the original acceptance domain. The result $L^{\parallel'}$ is identical to $L^{\parallel}$—point by point—except for a scale factor $\lambda_{\parallel}$. The transformation is thus equivalent to a projection of the same lattice with an acceptance domain reduced by a factor $\lambda_{\perp}$ leading to a scaled version (by $\lambda_{\parallel}$) of $L^{\parallel}-L^{\parallel'}$. The points of $L^{\parallel'}$ all belong to $L^{\parallel}$. At the same time they can also be tiled in the same way as $L^{\parallel}$ but with larger, scaled, tiles. The relation to standard geometric definitions of inflation is obvious. The advantage of our procedure is that it holds for arbitrary shapes of the acceptance domain and defines an inflation for any arbitrary form of tiling one may choose.

In the following we illustrate this for projections of icosahedral lattices from six dimensions. We choose an orthonormal set of vectors $\mathbf{e}_i$ in R^6 as a basis set and choose Y so that each of these axes is invariant under one of the fivefold rotations. Any matrix M of the form

$$M=\begin{bmatrix} m & n & n & n & n & n \\ n & m & n & -n & -n & n \\ n & n & m & n & -n & -n \\ n & -n & n & m & n & -n \\ n & -n & -n & n & m & n \\ n & n & -n & -n & n & m \end{bmatrix} \quad (9)$$

then commutes with $[Y]$. It is easy to see that the eigenvalues of these matrices are $\lambda_{\pm}=m\pm n\sqrt{5}$. They therefore belong to $[K]$ (and then obviously also to $[K°]$) only when $m^2-5n^2=\pm 1$. The smallest eigenvalue (larger than one) is $2+\sqrt{5}(\tau^{-3})$ for $m=\pm 2$ and $n=\pm 1$.

For the packing density of spheres it follows that it is therefore sufficient to investigate the range

$$1\le d\le \tau^{-3}=2+\sqrt{5}\ . \quad (10)$$

Any possible packing density must also show up in this range for any shape of the acceptance domain. This is the result for the primitive (sc) lattice. Clearly all powers of this scale factor are also allowed.

For the two other lattices it is convenient to take the size of the cubic cell as one so that points with half integral indices appear. It can thus be seen that half integral values of m and n are allowed in the matrices M which otherwise still have the form given in Eq. (9). The smallest eigenvalues appear for $2m=\pm 1$, $2n=\pm 1$ giving a scaling factor $\lambda_{\pm}=(1\pm\sqrt{5})/2=\tau^{\pm 1}$ for both these lattices.

We note that the reflection of these inflation rules in the Fourier spectrum were already noticed by Elser[4] and are discussed in detail by Ostlund and Wright.[5]

TABLE I. The small index vectors with projections closest to the origin. We give the six-dimensional description, the lengths of the two projections, and the number of vectors in the icosahedral stars.

	Vector						$r_{\parallel}$	$r_{\perp}$	n
1	1	0	0	0	0	0	1	1	12
2	1	1	0	0	0	0	1.47	1.35	30
3	1	−1	0	0	0	0	1.05	1.7	30
4	−1	0	1	0	1	0	0.56	2.38	20
5	1	−1	1	−1	0	0	0.63	2.74	

V. THE OPTIMAL COMPACT ACCEPTANCE DOMAINS FOR THE ICOSAHEDRAL LATTICES

The results of constructing the acceptance domains according to these prescriptions are shown in Tables I–IV. In Table I we list some of the lattice vectors with small indices which are useful in this context. We also give the number of vectors in the icosahedral star to which these vectors belong and their parallel and perpendicular projections.

In Table II we give the results for the primitive (sc) lattice. We find two acceptance domains which give equal densities. One is an icosahedron (with 20 faces) and the other a truncated triacontahedron. The latter domain is also mentioned by Henley.[3] The icosahedral acceptance domain has not been discussed before. Both acceptance domains give an optimal volume packing density of $c=0.56$. The two quasilattices are however quite different in detail. This can be seen by comparing the distribution of neighbor environments for the icosahedral domain given in Table IV with the corresponding results of Henley[3] for the truncated triacontahedron.

TABLE II. Determining vectors, their projected lengths, and the resulting packing densities for the sc lattice. It can be seen that one obtains two types of Voronoi cells which repeat periodically as the scale is changed.

	Vector						$r_{\parallel}$	$r_{\perp}$	f	Stars	n
1	1	0	1	−1	0	0	0.563	2.38	0.55	1	20
2	1	0	0	0	0	0	1	1			12
3	1	−1	0	0	0	0	1.7	1.05	0.55	2,3	30
4	1	0	1	1	0	0	2.38	0.563	0.55	4	20
5	1	−1	−1	1	2	1	4.22	0.236	0.55		12
6	0	−3	−2	2	3	0	7.2	0.248	0.55	5,6	30

TABLE III. Same as Table II but for the fc lattice.

	Vector						$r_{\parallel}$	$r_{\perp}$	f	s
1	0	1	1	0	1	1	0.63	2.76	0.48	30
2	1	−1	0	0	0	0	1.05	1.7	0.48	30
3	1	1	0	0	0	0	1.7	1.05	0.48	30
4	0	1	1	0	−1	−1	2.76	0.63	0.48	30

Even more striking is their role when one tries to pack other objects. We have constructed the excluded volume and Voronoi cells for the packing of icosahedra, a problem studied in great detail in Ref. 6. One only finds the truncated triacontahedron as acceptance domain. The icosahedral Voronoi cell does not appear at all in this packing problem. Since the volume of the accommodated icosahedra is larger than that of the spheres, for the same point density, one obtains a very high-volume density of 0.65. This is much higher than the densities found in Ref. 6 for the same problem using other techniques. On the other hand, only the icosahedral acceptance domain appears for the packing of objects with the shape of the truncated triacontahedron.

For fc we find a triacontahedron as the only shape of the acceptance domain and the density is 0.48. This is described in Table III. In both tables we have retained some redundancy to illustrate the scaling periodicity discussed in Secs. III and IV above. For the centered bcc lattice the maximum density is 0.3 but we do not give the details of the construction.

VI. HIGHER DENSITIES AND COMPLEX ACCEPTANCE DOMAINS

A. The Henley acceptance domain

Henley[3] first noted that the packing density can be increased considerably if one allows for more complex correlations in the positions of the accepted sites. The argument is simple, at least in principle. The Voronoi construction assumes a compact domain. Any point *inside* the domain excludes all regions of $R^{\perp}$ which are closer to it than any of the forbidden vectors $\mathbf{R}_{\perp}$ in the quasilattice $L^{\perp}$ defined in Sec. III. This can be quite inefficient when some regions in the compact acceptance domain are responsible for the exclusion (from the domain) of several regions of equal volume which are outside. The density (that is the volume of the acceptance domain) can then be increased by punching a hole into the original domain and adding to it the regions which are forbidden by the projections of lattice sites in the hole. In physical space this amounts to a rearrangement of some configurations in a way which will allow the accommodation of more spheres (this is the argument used in Ref. 3). The simplest correlations are those related directly to the forbidden vectors for which $R_{\perp}$ is smallest. Henley[3] noticed that they show up in the form of chains and the density can be increased for chains with an odd number of vertices. This allowed him to increase the packing density considerably—from 0.56 to 0.62. We want to put this in a more general and systematic context.

In Sec. III we defined an acceptance domain so that it does not contain any vectors with a short parallel projection (smaller than d). This led to the Voronoi construction. Assume now that we expand this domain somewhat and check if we can somehow find a larger volume within this larger trial region.

The expansion of the acceptance domain will result in the appearance of "connected points"—meaning points in the expanded domain which are connected by "forbidden" vectors with a short parallel component. At least one of these points is always inside the original acceptance domain, because that is the way it was constructed. If only points connected to a single other point appear then we cannot gain anything. Replacing the original point in the compact region by its partner (or more accurately interchanging the two regions associated with the two ends inside the expanded domain) will change the shape of the acceptance domain but not its volume. If, on the other hand, we find chains of connected points we may be able to increase the total acceptance volume by disconnecting these chains in a different way. For example, a chain of three in the expanded domain with its central point inside the original domain can be disconnected by removing the center. This procedure will result in an acceptance domain full of holes but with a larger volume. Starting with the Voronoi cell one can continue expanding the acceptance domain in this way until it becomes so large that new (and larger) forbidden vectors belonging to $L^{\perp}$ begin to appear. This happens when the boundaries of the expanded domain reach those of the second Voronoi cell around the origin. Until that point only the Henley[3] chains show up and they can be disconnected efficiently in a trivial way. This procedure is in essence equivalent to that of Henley[3] if the rearrangements in real space, which he carries out, are done with sufficient care so as not to destroy the quasiperiodicity. Our procedure obviously assures the quasiperiodicity automatically and the volume of the corrected domain gives the new density.

TABLE IV. Distribution of numbers of near neighbors for the primitive (sc) quasilattice obtained with the icosahedral acceptance domain of Table II. n is the number of neighbors and the frequency of sites with this number of neighbors given for the shell at 1, for the shell at 1.05, and for both shells combined (that is the density of sites having this number of neighbors in both shells together).

n	$r=1$	$r=1.05$	$1+1.05$
0	0	0.051	0
1	0.007	0.046	0
2	0.013	0.03	0
3	0.033	0.119	0
4	0.316	0.093	0
5	0.26	0.36	0
6	0.252	0.212	0.007
7	0.02	0.093	0
8	0.046	0	0.046
9	0.007	0	0.44
10	0	0	0.1
11	0	0	0.36
12	0.044	0	0.04

Explicitly the procedure amounts to the following. One starts out with the "second" Voronoi cell of the origin in $L^{\perp}$ which includes all the forbidden vectors responsible for the boundaries of the "first" Voronoi cell discussed in Sec. III but no larger forbidden vectors. One can then construct chains from these forbidden vectors inside the trial region. The chains are disconnected in the most efficient way by punching holes. We shall call the resulting acceptance domain the Henley domain.

We have constructed acceptance domains in this way for both the sc and the fc lattice. For sc we confirm Henley's result and obtain an increase in packing density from 0.56 to 0.62. Somewhat surprisingly the correction for fc is much larger. The Voronoi construction gave only 0.48 in this case but the corrected density is the same, 0.62. This is of course close to the densities of random close packing.[11]

B. The general problem

If we generalize these results the question of higher densities for projected quasilattices is formally well defined. We can go on increasing the region we investigate in $R^{\perp}$. When we cross the boundaries of the second Voronoi cell new vectors $\mathbf{R}_{\perp}$ and therefore new and much more complex forbidden graphs appear. The problem reduces to a problem in graph theory of finding a minimal separating set for these graphs. Since the complexity of these graphs increases very rapidly and one even encounters infinite graphs very soon, this problem is far from being trivial either formally or as a computational problem. Since the complexity of the graphs increases very rapidly naive approaches are useless. In particular, it is not known whether one can construct a systematic iterative procedure for successive corrections.

At this stage we do not even know for sure if there are higher quasiperiodic densities than those found by Henley,[3] though one obviously expects this. It is also not clear if the addition of successively larger stars (in $R^{\perp}$) and therefore of more complex graphs, results in a systematic iterative procedure for the quasiperiodic packing. It is possible that the whole acceptance domain may have to be redesigned at each successive stage when a new star is added but this would contradict our expectations. Somehow one would hope that successive rearrangements would involve more complex and rare local environments and smaller gains in the total density. It is, however, by no means evident that this is indeed the case.

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[8] For nonprimitive lattices some M may map the lattice on a different lattice of the same structure and special fractional values of the elements can appear. This is illustrated by the discussion of the two nonprimitive icosahedral lattices at the end of this section.

[9] In general $[K]$ will have more than one subgroup isomorphic to G. $[G]$ is, however, determined uniquely by the geometrical interpretation of G in R^{D}.

[10] This can be achieved by a coordinate transformation in R^{D}.

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