Rules for Computing Symmetry, Density and Stoichiometry in a
Quasi-Unit-Cell Model of Quasicrystals

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The quasi-unit cell picture describes the atomic structure of quasicrystals in terms of a single,
repeating cluster which overlaps neighbors according to specific overlap rules. In this paper, we
discuss the precise relationship between a general atomic decoration in the quasi-unit cell picture
atomic decorations in the Penrose tiling and in related tiling pictures. Using these relations, we
obtain a simple, practical method for determining the density, stoichiometry and symmetry of a
quasicrystal based on the atomic decoration of the quasi-unit cell taking proper account of the
sharing of atoms between clusters.

I. INTRODUCTION

Quasicrystals are solids with quasiperiodic translational order and rotational symmetry that is dis-
allowed for periodic crystals, such as ten-fold symmetry in the plane or icosahedral symmetry in three
dimensions [1]. This paper focuses on decagonal quasicrystals that are quasiperiodic in the xy-plane and
periodic along the z direction [2, 3]. The atomic structure has conventionally been described as a periodic
stacking of quasiperiodically ordered layers each of which can be interpreted as a Penrose tiling formed
from two tile shapes. The two tiles correspond to two different atomic clusters which join to form the
layer.

We have proposed an alternative picture in which the quasicrystal structure is described in terms of
a single repeating unit called a “quasi-unit cell [4, 5, 6]”. For ten-fold symmetric layers, the quasi-unit
cell is typically chosen to be a decagon, corresponding to a decagonal atomic cluster. The tiling picture
and the quasi-unit cell picture are mathematically equivalent, but the latter has numerous advantages.
First, the quasi-unit cell picture encodes the entire structure, both the symmetry and the detailed atomic
decoration, within the single decagonal cluster. This simplifies the problem of finding the atomic
structure based on empirical data. Secondly, the quasi-unit cell suggests simple energetics that may
explain why quasicrystals form [4, 5, 8].

A key difference between quasi-unit cells and tiles is that the quasi-unit cells overlap. The overlap
corresponds physically to the sharing of atoms by neighboring decagonal clusters, a feature which is
observed in real quasicrystals [9, 10, 11]. The overlaps are restricted to certain relative positions and
orientations of the quasi-unit cells according to “overlap rules.” The overlap rules replace the Penrose
rules for joining tiles. In real quasicrystals, these overlap rules are automatically enforced by the atomic
decoration which only permits sharing corresponding to the allowed overlaps. For the decagonal case,
this means that the decoration breaks 10-fold symmetry.

The purpose of this paper is to discuss the precise relationship between atomic decorations in the
quasi-unit cell and the rhombus Penrose tiling pictures, which is rather subtle, and to present a method
for computing the density and stoichiometry of a quasicrystal given the atomic decoration of the quasi-
unit cell. The latter is a simple but powerful tool for comparing data to proposed atomic structural
models. For periodic crystals, the analogous calculation is trivial since the density and stoichiometry are
the same as that of the unit cell because the unit cells join face-to-face. The technical complication for
quasicrystals is finding a method that properly accounts for the overlap and avoids double-counting or
under-counting. This paper presents a straightforward method for handling the problem that has already
been used in analyzing data [7].

Section 2 discusses the relationship between the overlapping decagon quasi-unit cell picture, the rhom-
bus Penrose tiling and related tilings as ideal geometrical constructions (without atomic decoration).
Section 3 discusses the relationship between their atomic decorations. Section 4 discusses how this rela-
tion can be used to construct a method for computing the density and stoichiometry based on the atomic
decoration of a quasi-unit cell. Section 5 discusses an interesting subclass of quasi-unit cell decorations,
“Almost Occupied Decoration” (AOD) for which we have a very simple method of computing density
and stoichiometry. Section 6 discusses how to classify the symmetry of the atomic structure based on the
decoration of the quasi-unit cell.
II. RELATION BETWEEN DECAGON TILINGS AND PENROSE TILINGS

Figure 1 shows the overlap rule introduced by P. Gummelt which forces a perfect quasicrystalline structure with a single, repeating, decagonal quasi-unit-cell, the marked decagon shown in (a). The overlap rule allows two decagons to overlap only if the shaded regions overlap and if the overlap area is greater than or equal to the hexagon overlap region of Fig. 1(b). This permits five types of pairwise overlaps, four types of $A$-overlaps and one type of $B$-overlap as shown in (b). The two types of overlaps correspond to two separations between clusters whose ratio is the golden ratio. An infinite arrangement of decagons according to the above rule is called the decagonal “covering,” to distinguish it from a “tiling” in which the units join edge-to-edge without overlap. The covering can be mapped into a conventional edge-to-edge tiling in at least three ways:

- Convert the covering to a rhombus Penrose tiling by dividing up central area of each decagon into a Jack (known in the Penrose tiling literature to mean 5 fat and 2 skinny rhombi surrounding a Jack vertex). This construction leaves three skinny rhombus-shaped regions inside the decagon. When neighboring decagons overlap, these regions are filled in by skinny Penrose tile or a fraction of two fat Penrose tiles joined together, depending on the overlap. See Fig. 2(a).

- Convert the covering to a three-tile “core-area tiling” using the core area assignment. The core areas correspond to an area assigned to a given decagon in a decagon covering according to whether there are $A$ or $B$ overlaps on the sides. The core area tiling is useful in various computations with overlapping decagon tilings and is a quasiperiodic tiling in its own right. The fundamental decagon of Fig. 1(a) is marked with two “rocket”-shapes and one “star”-shape. The three types of core-area tiles are determined by the overlaps of the star-shaped region. They are a large rhombus (corresponding to two $B$-overlaps), a trapezoid (a $B$-overlap on one side and an $A$-overlap on the other), and a large kite (corresponding to two $A$-overlaps). See Fig. 2(b). If we draw only the long edges of the core areas, we get a hexagon-boat-star tiling.

- Convert to the original Penrose tiling consisting of star, ship, pentagon, and rhombus tiles by joining the centers of decagons. See Fig. 2(c).

The mapping can be reversed to produce a decagonal covering from a conventional tiling. The equivalence between the lattice structures of the decagonal covering and those of Penrose tiling has been shown explicitly. However, the relationship between the atomic models constructed by the quasi-unit-cell decorations and those obtained by Penrose tile decorations is a different issue and has not been carefully investigated previously. We will call the former atomic models as decagonal quasi-unit-cell models and compare them with the latter Penrose-tile models. For Penrose-tile models, we will consider rhombus Penrose-tile decorations.

III. ATOMIC DECORATIONS OF QUASI-UNIT CELLS AND PENROSE TILES

We define a Penrose atomic model to correspond to decorating each fat rhombus identically, each skinny rhombus identically, and then joining them to form a Penrose tiling. A quasi-unit-cell model corresponds to decorating a fundamental decagon and then covering the plane with the identical decorated decagon according to the overlap rule. The decoration must satisfy the condition that, where two atoms overlap, they are the same atom type. The rule is that this represents a single atom shared by the two decagon clusters. (There can be more than two overlaps, too, in which case one atom is assigned to be shared by 3 decagons.) If an atom in one decagon overlaps an unoccupied site in a neighbor site, the atom is still assigned to the spot and shared. For any given site, the associated “image” sites are positions in the fundamental decagon which can overlay that site when decagons are joined according to the Gummelt overlap rules. The number of image sites varies, depending on where the original site is in the fundamental decagon.

One might suppose that atomic decorations of the quasi-unit-cell models form a subset of the Penrose-tile models due to there being a single unit and its being subject to overlap decoration constraints. On the contrary, as we will show next, the set of atomic decorations of the decagonal quasi-unit-cell models is greater than the set of atomic decorations of a Penrose tiling model with the same edge length.

Lemma I: Every rhombus Penrose-tile model is equivalent to a decagonal quasi-unit-cell model with the same edge length.
Proof: A fundamental decagon can be subdivided into a Jack configuration of fat and skinny rhombi plus 3 skinny-shaped rhombus areas surrounding. Decorate each fat and skinny rhombus in the Jack according to the Penrose decoration. Place no atoms in the 3 skinny-shaped rhombus areas surrounding. This defines a decoration of the fundamental decagon. When the decagons are joined by the overlap rules, the Jacks join to form a full Penrose tiling with no gaps or overlaps. This result comes from the proof of equivalence between Penrose tiling and decagon tiling in Jeong and Steinhardt [8]. (The skinny outlying regions are always overlapped by Jack regions of neighboring decagon and thereby resolve into a skinny rhombus or parts of a pair of fat rhombi.) Hence, the Decagon decoration of the fundamental decagon obtained by this construction produces the same result as the Penrose decoration obtained by joining identically decorated fat and skinny Penrose tiles.

**Lemma II:** Some decagonal quasi-unit-cell models are not equivalent to rhombus Penrose-tile model with the same edge length.

Proof: This Lemma asserts that the converse of Lemma I is not true. Consider a configuration obtained by placing one atom at the center of the fundamental decagon as shown in Fig. 3(a). When the decagon is resolved into a Jack, one fat rhombus has an atom whereas the other four do not. When the decagons are joined to form an overlap tiling, many obtuse rhombi remain unoccupied despite the overlap (see the upper part of Fig. 3(a)). Hence, the decagon decoration is not equivalent to a Penrose-tile decoration based on these fat and skinny rhombi with the same edge length.

We have shown that the atomic decorations of decagons is strictly greater than the set of atomic decorations of Penrose tiles of *identical* edge length. However, the relationship between the two is more subtle than one might suppose. Let us next compare the atomic decorations of the decagons to decorations of *inflated* Penrose tiles whose edge length is greater than that of the decagons. For example, the quasi-unit-cell model of Fig. 3(a) is not a Penrose-tile model with the same edge size but it is a Penrose-tile model with the (single) inflated rhombi as shown in the lower part of Fig. 3(a). Each inflated fat rhombus is decorated identically and so is each inflated skinny rhombus. Is this true for a general atomic decoration of the quasi-unit-cell model? The answer is no, as can be seen from the example of Fig. 3(b). The inflated fat rhombi at the right upper corner are decorated with zero, one or two atoms depending on the context. Neither doubly (at the middle of the panel) nor triply (at the bottom of the panel) inflated Penrose rhombi are decorated identically. For example, some triply inflated fat tiles have six atoms while some others have five. Therefore, the quasi-unit cell decoration is not generally equivalent to a Penrose tiling even when one considers Penrose tiling edge lengths which are $\tau^3$ times that of the decagon.

However, an equivalence does emerge if one considers a Penrose-tile model with fourfold inflated Penrose tiles as shown in Fig. 3(c). (This result is surprising at first and hard to imagine since the fourfold inflated rhombus tiles, whose edge is $\tau^4$ times longer than the edge of the quasi-unit decagon, have scores of original decorated decagons. There are nine different types of decorations of the original (uninflated) decagons in general due to the nine different configurations of overlapping decagons in its neighbor as shown in Fig. 3(a). In spite of this large number of different decorations, the decagons at the equivalent positions in all fourfold inflated rhombus tiles turn out to be the same type. Therefore, the fourfold inflated tiles of the same shapes are decorated identically. The rigorous proof for this and the inflation rules for the decorated decagons will be published elsewhere. The right-lower panel of Fig. 3(b) illustrates our claim in a finite part of decagon covering. We put the overlap-type of each decagon in a decagon covering and overlay them with the inflated fat tile. We see that the decagon arrangement of all inflated tiles of the same shapes are identical but their types are not identical for doubly and triply inflated tiles. However, for the quadratically inflated fat tiles, we see that the types of decagons are identical as shown in the right-lower panel.

This relationship gives a precise quantification of the degree to which the quasi-unit cell picture simplifies the problem of defining (and finding) atomic structures of quasicrystals. That is, the quasi-unit cell description and the Penrose tiling description (allowing for fourfold inflation) are equivalent mathematically, but the quasi-unit cell has an area which is $1/\tau^2 \approx 0.1$ times smaller and, hence, defines the structure using $1/\tau^3$ times fewer atoms on average.

**IV. COMPARING DENSITY AND STOICHIOMETRY IN QUASI-UNIT-CELL AND TILING MODELS**

We define the number density of $\chi$-type atom, $n_\chi$, as the *average* number of atoms of type $\chi$ per unit volume in the model where $\chi = \alpha, \beta, \gamma, \cdots$ represents the atomic type of interest. (Greek letter, $\alpha, \beta, \gamma, \cdots$ signifies the different atom types.) For the purposes of this discussion, we will mod out the...
periodic direction in 3D decagonal quasicrystals which can be handled trivially. Therefore, \( n_\chi \) can be considered as the average number of \( \chi \)-type atoms per unit area in the quasicrystalline plane. In this plane, we take the edge of the decagonal quasi-unit-cell as the unit length.

Note that the number density of \( \chi \)-type atoms in any finite region is, in general, different from \( n_\chi \) due to the quasiperiodicity of the quasicrystalline lattice. We define \( n_{(\chi,C)} \) as the number density of \( \chi \)-type atom in a finite-area \( C \) for a given local context. For example, \( n_{(\chi,C_i)} \) represents the number density of \( \chi \)-type atom in the core-area (Fig. 2(b)) of the decagon at the center of the \( i \)th decagon configuration (Fig. 4(a)) where \( i = 1, \ldots, 9 \). The stoichiometry of \( \chi \)-type atom, \( s_\chi \) is the ratio of the \( \chi \)-type atoms to the total number

\[
s_\chi = \frac{n_\chi}{n} = \frac{n_\chi}{\sum n_\chi}, \quad (1)
\]

where the total number density \( n \) is

\[
n = \sum_{\chi \in \{\alpha, \beta, \gamma, \ldots\}} n_\chi. \quad (2)
\]

Analogously, the mass density \( \rho_\chi \) of the \( \chi \)-type atom with atomic mass \( m_\chi \) is is \( \rho_\chi = m_\chi n_\chi \) where \( \rho = \sum_\chi m_\chi n_\chi \) is the total mass density.

To compute the number density in a decagon tiling, we can first convert to a conventional tiling, where the calculation is trivial because tiles join edge-to-edge. The only complication for tilings is for atoms at the boundaries where the conventional approach works. Namely, if each boundary atom is treated as a disk with small finite radius, the atoms at the boundaries are assigned a fractional weight according to the fraction of the disk that lies within the tile.

In the previous section, we show that a quasi-unit-cell model is a rhombus Penrose-tile model with edge length \( \tau^4 \). Each fourfold inflated fat (\( F_4 \)) and skinny (\( S_4 \)) tile is decorated identically. Therefore, in principle, we can calculate the number density of \( \chi \)-type atom \( n_\chi \) in a quasi-unit-cell model in the following way. First, find the decorations of \( F_4 \) and \( S_4 \) which are equivalent to the given quasi-unit-cell model. Then, count the number of \( \chi \)-type atoms in a \( F_4 \), \( N_{(\chi,F_4)} \) and in a \( S_4 \), \( N_{(\chi,S_4)} \) including the fractional atoms at the boundaries. Since the area of \( F_4 \) and \( S_4 \) are \( A_{F_4} = \tau^8 \sin\left(\frac{4\pi}{5}\right) \) and \( A_{S_4} = \tau^8 \sin\left(\frac{2\pi}{5}\right) \) respectively, the number density of \( \chi \)-type atom in \( F_4 \) and \( S_4 \) are given by

\[
n_{(\chi,F_4)} = \frac{N_{(\chi,F_4)}}{A_{F_4}}/\tau^8 \sin\left(\frac{2\pi}{5}\right) \quad (3)
\]

\[
n_{(\chi,S_4)} = \frac{N_{(\chi,S_4)}}{A_{S_4}}/\tau^8 \sin\left(\frac{2\pi}{10}\right). \quad (3)
\]

The number density of \( \chi \)-type atom in the model \( n_\chi \) is now obtained by considering the fractional area occupied by \( F_4 \) and \( S_4 \) tiles:

\[
n_\chi = \frac{N_{F_4}A_{F_4}n_{(\chi,F_4)} + N_{S_4}A_{S_4}n_{(\chi,S_4)}}{N_{F_4}A_{F_4} + N_{S_4}A_{S_4}} = \frac{\tau^2 n_{(\chi,F_4)} + n_{(\chi,S_4)}}{\tau^2 + 1}, \quad (4)
\]

where \( N_{F_4} \) and \( N_{S_4} \) are the numbers of \( F_4 \) and \( S_4 \) tiles in the tiling and we used the fact that both \( N_{F_4}/N_{S_4} \) and \( A_{F_4}/A_{S_4} \) are \( \tau \).

Another way to calculate the density and stoichiometry is using core areas \( \mathbb{3} \), which have the advantage that they are not so large. We first assign the core-tile to each decagon in the decagon covering as described in Fig. 2(b) and then work out how the decagon decoration translates into a decoration of core-area tiles. In general, the same shaped core-area tiles can be decorated differently due to the overlap. There are nine different decorated core-area tiles due to the nine different ways of surrounding a decagon of Fig. \( \mathbb{3} \)(a).

The computational method is to determine the number density for each of the nine configurations and then use the density of each nine decagon-surrounding configurations in a decagon Penrose tiling. Using the per-space \( \tau \)-map volume, one can calculate the density of each nine configurations;

\[
\rho_1 = \tau^{-2} \rho_0, \quad \rho_2 = \tau^{-5} \rho_0, \quad \rho_3 = \tau^{-5} \rho_0, \quad \rho_4 = \tau^{-6} \rho_0, \quad \rho_5 = \tau^{-5} \rho_0,
\]

\[
\rho_6 = \tau^{-6} \rho_0, \quad \rho_7 = \tau^{-6} \rho_0, \quad \rho_8 = \tau^{-6} \rho_0, \quad \rho_9 = \sqrt{\tau} \rho_0,
\]

where \( \rho_0 = 1/(3\tau + 1) \) and \( \rho_i \) is the density of the \( i \)th configuration of Fig. \( \mathbb{3} \)(a). If \( N_{(\chi,C_i)} \) represents the
number of atoms of type $\chi$ lying within the core-area tile of the $i$th configuration, the number density for atom type $\chi$ is:

$$n_\chi = \sum_{i=1}^{9} \rho_i N(\chi, C_i)$$

(5)

and the ratios of $n(\chi)$ give relative stoichiometry.

V. SIMPLE COMPUTATION OF DENSITY AND STOICHIOMETRY

In the previous section, we presented two methods for calculating the density and stoichiometry for general quasi-unit cell models. However, both methods are somewhat cumbersome to use in practice. To calculate the density and stoichiometry for a given quasi-unit cell decoration using the first method, we must figure out the atomic decorations of the fourfold inflated fat and skinny tiles. The second method requires the atomic decoration of the center decagon in each of the nine different configurations of nearest-neighbor, overlapping decagons. A computer code is necessary to do the bookkeeping.

However, there is a subclass of decorations which includes the cases of most practical interest which can be calculated by hand. This class, which we call the “almost occupied decoration (AOD),” encompasses all decorations where core areas are decorated the same for any of the nine-configurations, so we can forego treating each of the nine separately. This class includes most decorations with physically reasonable densities. It is still includes and is larger than the Penrose tile decorations (with same edge length).

First, let’s consider the even simpler “fully occupied decoration (FOD)” in which overlap does not add any atoms to the core areas:

**Definition:** fully occupied decoration (FOD) — A single decagon decoration is a fully occupied decoration if, for every atom in the decagon, the image sites lying within the “big kite” core area are all occupied by the same atom type.

Here, the “big kite” core area is the kite core area shown in Fig. 5(a). Note that images outside the big kite core area may be unoccupied. The special property of FOD is that overlaps can be ignored in computing stoichiometry. The big kite core area is the largest of the core areas and all other core areas are subregions. If the decoration is fully occupied, then every atom anywhere in the decagon has all occupied image sites inside the big kite (and, therefore, inside each of the core areas). Therefore, overlapping neighbor tiles does not add any new atoms inside core areas in any case. Therefore, the stoichiometry can be computed by considering only three core-area types.

Let three Roman letters $A$, $B$, $C$ will signify the three types of decagons:

- $A =$ decagons with two $A$-overlaps,
- $B =$ decagons with two $B$-overlaps,
- $C =$ decagons with one $A$- and one $B$-overlap.

Here, we refer only to overlaps on the two sides of decagon. (In Fig 5, the center decagons in the configurations 1 and 2 are $A$ type, 3 – 6 are $C$ type and 7 – 9 are $B$ type.) Associated with each type of decagon above, we can assign a “core area” of the decagon.

- $A$: kite shape
- $B$: rhombus shape
- $C$: trapezoid shape

as shown in Fig. 2(b) and these core areas join to completely cover the plane with no gaps.

Let $N(x, X)$ represent the number of atoms of type $\chi$ lying within the core area of an $X$ decagon where $X = A, B,$ and $C$. Note that $N(x, X)$ can be counted directly from the fundamental decoration (the decagon decoration before overlap) since overlaps with the neighbor decagons do not add any new atoms inside core areas. The number density $n_\chi$ for atom type $\chi$ is now given by

$$n_\chi = \rho_A N_{(\chi, A)} + \rho_B N_{(\chi, B)} + \rho_C N_{(\chi, C)},$$

(6)

where, $\rho_A = 2\tau^{-3}\rho_0$, $\rho_B = \tau^{-3}\rho_0$, and $\rho_C = 2\tau^{-4}\rho_0$. 

Equivalently, we can divide the fundamental decagon into regions and assign the weight for each region as shown in Fig. 5(b). Since the the core area $A$ (kite shape) and $C$ (trapezoid) include the core area $B$ (rhombus shape), the atoms in the region I should be counted fully when we calculate the number density. Region II does not belong to the core area $B$ but 50 percent of it belongs to the core area $C$ and the whole area belongs to core area $A$. Therefore, the number density weights, $\rho_I$ and $\rho_{III}$ assigned to regions I and II are given by

$$
\rho_I = \rho_A + \rho_B + \rho_C = \rho_0
$$

$$
\rho_{III} = \rho_A + \frac{1}{2}\rho_C = \tau^{-1}\rho_0.
$$

(7)

Now, we introduce the AOD class models, for which the same shape of core areas are decorated identically as for the FOD class models but the core area decoration (after overlap) may be different from that of the fundamental decoration (before overlap).

**Definition:** almost occupied decoration (AOD) — A single decagon decoration is an almost occupied decoration if, for every atom in the decagon outside of the “tiny central kite” area shown in Fig. 5(c), the image sites lying within the “big kite” core area are all occupied by the same atom type.

**Lemma IV:** All core areas of the same shape have the same decoration after overlap.

This Lemma means that, as with the FOD, we do not have to consider each of the nine local arrangements of decagons separately. Proof: For an FOD class model, the same shape of core areas have the same decoration since the overlap does not bring any new image atoms to the core areas. For an AOD class model, new image atoms may exist in the tiny central kite area. However, due to the way the decagons overlap, the image atom arrangements in the central kite are the same for each type of core areas as shown in Fig. 5(d). When the central core area is the big kite shape (Conf.-1 and 2), overlapping decagons cannot add any images on the central kite area. Therefore, the big kite-shaped core areas (for both Conf. 1 and 2) have the same images. When the central core area is the rhombus shape (Conf.-7, 8 and 9), there are two neighboring decagons overlap with the tiny central kite area. For all three configurations, the relative position and the direction of the overlapping decagons are the same. Therefore, the image sites in the tiny central kite area are the same for all three cases. Finally, When the central core area is the trapezoid shape (Conf.-3, 4, 5, and 6), only one neighboring decagon can overlap the tiny central kite area. The position and the direction of the overlapping decagons are the same for the same orientation of the trapezoid (Conf.-3 and 4, and Conf.-5 and 6 are the same orientation respectively). Therefore, the trapezoid-shaped core areas with the same orientation have the same images. Altogether, the image sites in the tiny central kite area is the same decoration for the same shape of core areas.

Since the same shaped core areas are decorated identically, the number density $n_x$ for an AOD model can be calculated from Eq. (6) provided that $N_{(x,X)}$ is the number of atoms in the the core area $X (X = A, B, C)$ including image atoms. We can divide the fundamental decagon into regions with the weight for each region for AOD case too as shown in Fig. 5(d). Here, the atoms in the region III may bring new image atoms in the tiny central kite area and hence must be taken into account for the number density of the atoms. As mentioned, region III does not add any image atoms to the tiny central kite area for the A-decagons (Conf.-1 and 2) but always adds images for the B-decagons (Conf.-7, 8, and 9) and 50 percent for the C-decagons (Conf.-3, 4, 5 and 6). Therefore, the number density weights are given by

$$
\rho_I = \rho_0
$$

$$
\rho_{III} = \tau^{-1}\rho_0
$$

$$
\rho_{III} = \rho_B + \frac{1}{2}\rho_C = \tau^{-2}\rho_0
$$

(8)

for the AOD class models. Note that the overlap does not add the new image atom if there was an atom at the image site in the tiny central kite area of the fundamental decoration. Therefore, the weight $\rho_{III}$ should be assign to the atoms in the region III only if their images sites (in the tiny central area) are unoccupied. Also, it is possible that the image sites from the left and the right part of region III coincide as in the case of the mirror symmetric decoration. For these atoms, we should count them only once for
the type-B decagons and, therefore, we should assign
\[ \rho'_{III} = \frac{1}{2}(\rho_B + \rho_C) \]
\[ = \frac{1}{2}(\tau^{-3} + \tau^{-4})\rho_0 \] (9)
to the atoms in the regions III (whose image sites in the tiny central area are unoccupied).

While the description above may seem complex, a brief study will show that it is straightforward to apply the method using the back of an envelope for a wide class of useful decorations.

V. SYMMETRY OF A QUASI-UNIT-CELL MODEL

The unit cell construction in periodic crystals is used not only to determine the density and stoichiometry, but also to classify the symmetry. In this section, we analyze the symmetry of quasi-unit-cell models for decagonal quasicrystals whose atomic sites can be interpreted as projections from the higher dimensional hypercubic lattices. In general, the atomic positions in the fundamental decagon can be in any location as long as they satisfy the overlap decoration rule. However, here we only consider the fundamental decagon decorations whose atomic positions, relative to the position of a vertex of the decagon, are given by
\[ \vec{r} = \sum_{k=0}^{4} m_k \hat{e}_k, \] (10)
where \( m_k \) is an integer and \( \hat{e}_k = \cos(\frac{2k\pi}{5})\hat{x} + \sin(\frac{2k\pi}{5})\hat{y} \) is a unit vector in the physical space. Mathematically speaking, this quasilattice of points is a set of measure zero compared to the entire 2d interior of the decagon, but this does not impose any practical restriction on constructing physical atomic models since the quasilattice points are dense everywhere due to the irrationality between the basic vectors \( \hat{e}_k \)s.

For these models, atoms can be lifted to the five dimensional hypercubic lattice points and the information on the correlations between positions of atoms in the model can be encoded into the geometry of the perp-space images which is the set of points given by
\[ \vec{r}^\perp = \sum_{k=0}^{4} m_k \hat{e}_k^\perp, \] (11)
where \( \hat{e}_k^\perp = \cos(\frac{4k\pi}{10})\hat{x}^\perp + \sin(\frac{4k\pi}{10})\hat{y}^\perp \) is a unit vector in a plane perpendicular to the physical space. When the perp-space images of two models have the same geometrical shape, they are indistinguishable \[16\] since the correlations between atomic positions are fully determined by the shape of the perp-space image. Following Mermin \[16\], we call an operation \( g \) a symmetry operation if the state after the operation is indistinguishable from the state before the operation. That is, if \( g \) is a symmetry operation for a model with density function \( \rho(\vec{r}) \) then \( \rho(\vec{r}) \) and \( \rho'(\vec{r}) := \rho(g^{-1}\vec{r}) \) should have the identical correlation functions. Therefore, an operation \( g \) represented by
\[ g\hat{e}_k = \sum_j g_{jk} \hat{e}_j \] (12)
is a symmetry operation if the corresponding perp-space operation \( g^\perp \) given by
\[ g^\perp \hat{e}_k^\perp = \sum_j g_{jk} \hat{e}_j^\perp. \] (13)
preserves the geometry of perp-space images.

As one can see from the definition of \( \hat{e}_k \) and \( \hat{e}_k^\perp \), \( \frac{4\pi}{10} \) rotation in the real space corresponds to \( \frac{4\pi}{10} \) rotation in the perp-space since it is equivalent to \( \hat{e}_k \rightarrow \hat{e}_{k'} \) with \( k' = k + 1 \) (mod 5). A tenth of \( 2\pi \left( \frac{8\pi}{10} \right) \) rotation in the real space is equivalent to \( \hat{e}_k \rightarrow -\hat{e}_{k'} \) with \( k' = k + 3 \) (mod 5) and therefore corresponds to \( \frac{4\pi}{10} \) rotation in the perp-space. Since the \( \frac{4\pi}{10} \) rotation (with the modulus \( 2\pi \)) generates all ten integer multiples of \( \frac{2\pi}{10} \), the quasi-unit cell model has ten-fold symmetry if and only if the perp-space image has...
ten-fold symmetry. Also, the quasi-unit cell model has reflection symmetry to an \( \hat{e}_n \)-axis if and only if the perp-space image has reflection symmetry to the \( \hat{e}_n \)-axis. This is because the the reflection to the \( \hat{e}_n \)-axis in real space corresponds to the reflection to the \( \hat{e}_n \)-axis in the perp-space. They are equivalent to \( \hat{e}_k \rightarrow \hat{e}_{k'} \) or \( \hat{e}_{k'} \rightarrow \hat{e}_k \) with \( k + k' = 2n \) (mod 5) in both real and perp spaces.

The geometry of the perp-space image for a quasi-unit-model can be obtained from the perp-space image of the atoms in the fundamental decagon. Let us first consider a simple case where the fundamental decagon is decorated with only one atom. In this case, the perp-space image of the atoms in the decagons with a certain direction is a simply connected triangle shape. (The Gummelt decoration of a decagon breaks the 10-fold symmetry of the decagon. We can define the “direction” of a (Gummelt decorated) decagon from this. In Fig. 7(b) we define the direction of a decagon along the mirror symmetry line, from the intersection of two “rockets” to the center of the “star.” The decagon in a Gummelt covering has 10 different possible directions and the perp-space image of the Jack vertices in the decagons with the same direction is the triangle shown in Fig 7(b).) The perp-space images of all atoms in the model is then given by the union of ten triangles of ten different directions. Figure 7(a) shows such simple decoration of fundamental decagonal which is equivalent to a Penrose lattice decoration where atoms decorate each Jack vertex. The perp-space image of this quasi-unit-cell model is simply the perp-space occupation domain of Jack vertices \( \bar{J}_0 \) and given by Fig. 7(b). Here \( J_m \) and \( J_n \) represent the perp-space image of Jack vertices in the \( \hat{e}_k \) direction and the \( -\hat{e}_k \) direction respectively. Since the perp-space image has 10-fold symmetry and the mirror symmetry, the quasi-unit-cell model with the fundamental decoration of Fig. 7(a) has \( D_{10} \) symmetry.

The symmetry for a general fundamental decoration can be obtained similarly. If the relative position (from a Jack vertex) of a decorated atom is given by \( \vec{r} = \sum_{k=0}^{4} m_k \hat{e}_k \), then the perp-space image from the decagons with the \( \hat{e}_0 \) direction will be the triangle given by the \( \vec{r}_k = \sum_{k=0}^{4} m_k \hat{e}_k \) translation of the \( J_0 \) triangle. The perp-space image from the decagons with the \( \pm \hat{e}_0 \) direction will be obtained by rotating the \( \hat{e}_0 \) direction triangle by the angle that the \( \hat{e}_0 \) and \( \hat{e}_0 \) axes make. The perp-space image of all decagons is the union of these 10 triangles and always has 10-fold symmetry. Therefore we can conclude that all quasi-unit-cell models have 10-fold symmetry.

How about the mirror symmetry? The quasi-unit-cell model with the fundamental decoration of Fig 7(b) has the the mirror symmetry as well as the 10-fold symmetry. Is the mirror symmetry also general for quasi-unit-cell models? The answer is no, as one can see from the example of Fig. 8(b). In this example, the perp-space image has no mirror symmetry axis. Then when does the perp-space image have the mirror symmetry? From the fact that the reflection transforms the base vectors in the perp-space equivalently to the transform of base vectors in the real space, we can say that the perp-space image has the mirror symmetry if the decoration of fundamental decagon has the mirror symmetry. However, the converse is not true. Some asymmetric decorations of the fundamental decagon can produce a quasi-unit-cell model with the mirror symmetry as shown in Fig. 8(c) and (d).

In sum, a quasi-unit-cell model has the 10-fold symmetry. If the decoration of fundamental decagon has a mirror symmetry, then the quasi-unit-cell model has a mirror symmetry as well as the 10-fold symmetry.

VII. CONCLUDING REMARKS

We have shown that a Penrose-tile model is a quasi-unit-cell model with the same edge size and a decagonal quasi-unit-cell model is a Penrose-tile model with the quadratically inflated rhombi. This means the set of all decagonal quasi-unit-cell models is the same as the set of all rhombus Penrose-tile models. However, mathematical equivalence between the two sets does not imply that they are physically equivalent in constructing atomic models for quasicrystals. We need only one kind of atomic clusters as a building unit in quasi-unit-cell models while at least two basic building units are needed in Penrose-tile models. Furthermore, the building unit size is much smaller for quasi-unit-cell models. For a general quasi-unit-cell decoration, the corresponding Penrose tiles, whose decorations are identical, have scores of original quasi-unit-cell. In other words, we have to look for more and larger building units when we use Penrose tile models.

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Figure Captions

Fig. 1: Marked decagon and overlapping rules which force a quasiperiodic tiling. (a) Marked decagon can force a quasiperiodic tiling when it is arranged by the Gummelt overlapping rules. (b) Gummelt overlapping rules demand that two decagons may overlap only if shaded regions overlap and if the overlap area is no smaller than the hexagon overlap region in A.

Fig. 2: Decagon covering can be mapped into a conventional tiling by decorating decagon properly. (a) Rhombus Penrose tiling by dividing up central area of decagon into Jack. (b) Three-tile core-area tiling using the core area assignment of Jeong and Steinhardt [5]. (c) Original Penrose tiling [13] of 4-tile tiling by joining the centers of decagons.

Fig. 3: Quasi-unit-cell models and Penrose-tile models. (a) Decagon decoration at the top is not a decoration of original Penrose tile (upper part) but a decoration of single inflated tiles (lower part). (b) This decagon decoration is not a decoration of original (upper left) Penrose tile, nor single inflated (upper right) tile. Neither doubly (middle) nor triply (bottom) inflated Penrose tiles are decorated identically. (c) Decagon decoration of (b) is a Penrose decoration of quadratically inflated Penrose tiles.

Fig. 4: (a) Nine ways of surrounding a decagon found in a Gummelt decagon covering [14]. The numbers represent the surrounding configuration types. (b) Typed decagon arrangements in the decagon covering. The decagon arrangements in all inflated tiles of the same shapes are identical but their types are not identical for doubly and triply inflated tiles. For the quadratically inflated fat tiles, the types of decagons are also identical as shown in the right-lower panel.

Fig. 5: (a) The big kite for FOD. For an FOD model, image sites lying in the shaded big kite region must be fundamentally decorated. (b) The regions for the number density weights for the FOD models. Weights $\rho_I = \rho_0$ and $\rho_{II} = \tau^{-1} \rho_0$ are assigned to the atoms in the regions I and II respectively. (c) The big and the tiny kites for AOD. For an AOD model, image sites lying in the shaded region must be fundamentally decorated. (d) The regions for the number density weights for the AOD models. The region II is the same as in (b). Weights for the region I and II are the same as the FOD case. For atoms in the regions III, weight 0, $\rho_{III}$, or $\rho'_{III}$ can be assigned (see text for detail).

Fig. 6: Overlaps between the core area of the central decagon and the surrounding decagons. The region III in Fig. 5(d) can overlap with the tiny central kite area of the central decagon for Conf.-3, ..., 9.

Fig. 7: A decoration of the fundamental decagon and the perp-space image of the resulting quasi-unit-cell model. When the decagon covering is converted to the rhombus Penrose tiling by dividing up central area of decagon into a Jack, the decorated atom position corresponds to the Jack vertex. In the perp-space image, $J_k$ and $J_k'$ represent the perp-space image of Jack vertices in the $\hat{e}_k$ direction and the $-\hat{e}_k$ direction decagons respectively.

Fig. 8: (a) A decoration of the fundamental decagon which results in a quasi-unit-cell model with no mirror symmetry. Both Fundamental decoration and the perp-space image have no mirror symmetry axis. (b) An asymmetric decoration of the fundamental decagon which results in a quasi-unit-cell model with the mirror symmetry. Although the fundamental decagon is decorated asymmetric, decagons in the covering are decorated with the mirror symmetry due to the overlap and their perp-space image has the mirror symmetry.
(a)

(b)

FIG. 4:
FIG. 7:

FIG. 8: