Superspace description of quasiperiodic structures and the nonuniqueness of superspace embedding

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Some of the features of the superspace description of quasiperiodic structures, of the so-called superspace embedding, can be arbitrarily chosen. The superspace approach is reviewed in such a way that these particular features, which are not intrinsic to the theory, are explicitly indicated and separated from the fundamental formalism. Although the superspace density as a scalar function of n variables is uniquely defined, the embedding is only fully determined once the internal subspace is chosen. As the internal subspace is usually represented perpendicular to the ''parallel'' subspace, the different possible embeddings can be considered as different choices for the metric associated with the superspace and, therefore, for the n-dimensional representation of the superspace density. This freedom on the superspace description of a quasiperiodic system is discussed and interpreted through the following examples: a modulated incommensurate structure, a composite incommensurate structure, the Fibonacci chain, and an icosahedral quasicrystal. For each case, the standard embedding usually considered in the literature is compared with other possible alternative choices. In general, the standard embedding is clearly distinguished by the greater simplicity it conveys. However, there are cases where a unique ''better'' embedding choice does not exist. The composite incommensurate structures and the Fibonacci chain are two clear examples of this fact. A particular superspace embedding implies a particular election for the so-called *phason* degrees of freedom in the system. The existence of different equivalent superspace embedding evidences the impossibility in these cases of totally determining the phason modes from purely static considerations. [S0163-1829(96)06241-8]

I. INTRODUCTION

The description and analysis of experimental quasiperiodic structures, such as incommensurate systems and quasicrystals, are being done very successfully using the so-called *superspace* approach, where the structure is *embedded* in an n-dimensional superspace and is interpreted as a section of an n-dimensional *superspace density*. This approach is based on the uniqueness of the indexation of the diffraction diagram with a basis of n vectors (n being larger than the dimensionality of the system). The experimental Fourier amplitudes indexed with n indices are then interpreted as the Fourier components of an n-dimensional periodic structure (the superspace density). The uniqueness of the indexation guarantees that there is a one-to-one relation between the so-defined superspace density and the experimental quasiperiodic structure. Hence the problem of describing the quasiperiodic structure is transformed into the description of an n-dimensional periodic structure. Indeed, the symmetry of a quasiperiodic structure can be interpreted as the n-dimensional space group of the corresponding superspace density.

The superspace formalism is specially powerful in direct space as a sort of ''bookkeeping'' of the *aperiodic* but *ordered* atomic positions in the structure. Every atomic position in real space is associated with a certain point within the n-dimensional unit cell of the superspace density. The superspace description would be of no use if one needed to specify one by one all these points. Fortunately, they seem to form in experimental cases closed and dense domains in the superspace,[1] the so-called *atomic surfaces*, which can in principle be described with a few parameters. Then the description of the quasiperiodic structure reduces to a crystallographic problem in n dimensions, where the position, form, and composition of the atomic surfaces in a single n-dimensional unit cell determine the whole structure.

Despite its success, one should not forget the purely mathematical meaning of the superspace construction and overcome the temptation of giving much physical meaning to the additional dimensions introduced when describing the structure in the superspace. In fact, Mermin and co-workers,[2–4] have demonstrated that the Fourier spectrum and the superspace groups of quasiperiodic systems can be described in real physical space, without the need of an n-dimensional formalism. The abstract features of the superspace construction imply some intrinsic ambiguity on the superspace embedding. The superspace density is uniquely defined as a scalar function of n variables, but the geometrical meaning of these variables in an n-dimensional *superspace* is undefined and open to any choice. Hence the superspace embedding of a quasiperiodic structure is not fully determined until a definite metric is introduced in the superspace. Because of historical reasons and, also, because some particular choices of metric are simpler and natural for certain type of systems, the superspace formalism is usually introduced with an implicit metric for each type of structure.[5–7] This has led to the

widespread erroneous belief that these particular embeddings are unique or have in general some absolute physical meaning. This fact has been pointed out for some particular systems as the Fibonacci chain[7] and incommensurate composite structures,[8] but, as shown below, has general validity. In the present work, we consider the nonuniqueness of the superspace embedding in a general context and show that it is a rather general property of any quasiperiodic structure.

First, we review the superspace approach[9–11] in such a way that particular metric features which are not intrinsic of the theory are explicitly indicated and separated from the fundamental formalism.[12] Then, by means of examples, ranging from a modulated incommensurate structure to an icosahedral quasicrystal, the freedom on the superspace image of a quasiperiodic system is discussed and interpreted.

II. SUPERSPACE DESCRIPTION OF A QUASIPERIODIC STRUCTURE

By definition, the vectors for which the Fourier transform of a quasiperiodic system is nonzero can be indexed with a finite set of rational independent vectors $\mathbf{k}_i$:

$$\mathbf{H}=\sum_{i=1}^{n} h_i\mathbf{k}_i, \tag{1}$$

with h_i representing integers and $n>d$ (d being the dimension of physical space). The quasiperiodic structure is then given by a density $\rho(\mathbf{r})$:

$$\rho(\mathbf{r})=\sum_{\mathbf{H}} F(\mathbf{H})\exp\left(2\pi i\sum_{i=1}^{n} h_i\mathbf{k}_i\cdot\mathbf{r}\right), \tag{2}$$

where $F(\mathbf{H})$ is the structure factor for the diffraction vector $\mathbf{H}$. Being $n>d$, $\rho(\mathbf{r})$ is not in principle lattice periodic. However, a related ''superspace density function'' can be defined as

$$\rho_s(\theta_1,\theta_2,\ldots,\theta_n)=\sum_{\mathbf{H}} F(\mathbf{H})\exp\left(2\pi i\sum_{i=1}^{n} h_i\theta_i\right), \tag{3}$$

which is periodic in its n variables. The relation between both functions is simply

$$\rho(\mathbf{r})=\rho_s(\mathbf{k}_1\cdot\mathbf{r},\mathbf{k}_2\cdot\mathbf{r},\ldots,\mathbf{k}_n\cdot\mathbf{r}). \tag{4}$$

Hence the physical density is given by a three-dimensional ''cut'' of the n-dimensional superspace density. All the information about the structure is in the function $\rho_s(\theta_1,\ldots,\theta_n)$. Once the basis $\{\mathbf{k}_i\}$ has been chosen, the indexation (1) is unique, and, therefore, by definition, there is a one-to-one relation between both functions, i.e., the function ρ_s is fully determined by the physical density ρ and vice versa. In principle, there is no need for a geometrical picture of the abstract superspace density $\rho_s(\theta_1,\ldots,\theta_n)$. The embedding of the real space structure within the superspace density, defined in Eq. (3), is independent of any geometrical meaning we may associate to the variables $\theta_1,\ldots,\theta_n$ in an n-dimensional ''superspace.'' These variables are, in fact, adimensional and do not have *a priori* a geometrical meaning.[13] They can be interpreted as the phases of the modulation waves associated with the wave vector basis $\mathbf{k}_i$.[10,11]

In order to work with a fixed reference frame in physical space, we choose within it an arbitrary vector basis $\{\mathbf{a}_j\}$ and its reciprocal basis $\{\mathbf{a}_j^*\}$, so that any generic vector in real space can be described by

$$\mathbf{r}=\sum_{j=1}^{3} x_j\mathbf{a}_j, \tag{5}$$

while the n wave vectors $\mathbf{k}_i$ in Eq. (1) can be expressed in terms of the reciprocal basis

$$\mathbf{k}_i=\sum_{j=1}^{3} \alpha_{ij}\mathbf{a}_j^*, \quad i=1,\ldots,n. \tag{6}$$

According to Eqs. (4) and (6), a vector $\mathbf{r}$ in real space (5) corresponds to a superspace point $\theta=(\theta_1,\theta_2,\ldots,\theta_n)$ satisfying

$$\theta_i=\sum_{j=1}^{3} \alpha_{ij}x_j, \quad i=1,\ldots,n. \tag{7}$$

We can, therefore, define a linear coordinate transformation in superspace with the subspace associated to the real space being given by the three first coordinates:

$$\theta_i=\sum_{j=1}^{3} \alpha_{ij}x_j+\sum_{j=1}^{n-3} \gamma_{ij}x_{Ij}, \quad i=1,\ldots,n. \tag{8}$$

The x_i coordinates generate the so-called ''parallel'' space, and the set $\{x_{Ii}\}$ generates the ''internal'' or ''perpendicular'' space. The internal coordinates x_{Ij} ($j=1,\ldots,n-3$) are defined in such a way that the section $x_{Ij}=0$ ($j=1,\ldots,n-3$) of the superspace density represents the density in real space as a function of the coordinates x_i ($i=1,\ldots,3$), with respect to the chosen basis in Eq. (5). This property of the defined coordinates x_{Ij} ($j=1,\ldots,n-3$) is independent of the actual values of γ_{ij} in Eq. (8). These values are, in fact, arbitrary, except for the condition of linear independence of the set of n equations. The transformation (8) can be abbreviated as

$$\hat{\theta}=\mathbf{A}\hat{x}=\mathbf{A}\begin{pmatrix}\mathbf{x}\\ \mathbf{x}_I\end{pmatrix}, \tag{9}$$

with $\hat{\mathbf{x}}=(x_1,x_2,x_3,x_{II},\ldots,x_{In-3})$, $\hat{\theta}=(\theta_1,\ldots,\theta_n)$, $\mathbf{x}=(x_1,x_2,x_3)$, $\mathbf{x}_I=(x_{II},\ldots,x_{In-3})$, and

$$\mathbf{A}=\begin{pmatrix}\alpha_{11} & \alpha_{12} & \alpha_{13} & \gamma_{11} & \cdots & \gamma_{1n-3}\\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\ \alpha_{n1} & \alpha_{n2} & \alpha_{n3} & \gamma_{n1} & \cdots & \gamma_{nn-3}\end{pmatrix}. \tag{10}$$

The first three columns of the matrix $\mathbf{A}$ are fixed once we have chosen the $\{\mathbf{a}_i\}$ basis in physical space and the n vectors $\{\mathbf{k}_i\}$ to index the diffraction pattern, while the remaining $(n-3)$ columns are arbitrary, except for the condition that the determinant of $\mathbf{A}$ should be nonzero. Therefore, $n(n-3)$ parameters can be, in principle, arbitrarily chosen when defining the internal space.

If we call $\{\hat{e}_i\}$ the basis in superspace corresponding to the coordinates θ_i, the matrix $\mathbf{A}$ in Eq. (9) represents a transformation to a new basis $\{\hat{\varepsilon}_i\}$ so that

$$\hat{\varepsilon}_i=\sum_{j=1}^{n} A_{ji}\hat{e}_j, \quad i=1,\ldots,n. \tag{11}$$

The first three vectors $\{\hat{\varepsilon}_1,\hat{\varepsilon}_2,\hat{\varepsilon}_3\}$ generate the parallel space representing the real space as explained above, and the rest $(n-3)$ $\{\hat{\varepsilon}_i\}$ $(i=4,\ldots,n)$ generate the complementary internal space. It should be noted that no scalar product, and therefore no metric, has been yet introduced in the superspace. It is important to stress that for practical purposes as, for instance, the calculation of the structure factors, atomic positions in real space, etc., the specific metric attributed to the superspace is irrelevant: All these quantities can be obtained from expressions like Eqs. (3), (4), and (5), and no particular superspace metric is needed. However, for the sake of concreteness, it is convenient to develop a simple graphical picture of the superspace density and its relation with the actual structure in real space. For this purpose, a metric is being usually introduced for the vectors $\{\hat{\varepsilon}_1,\hat{\varepsilon}_2,\hat{\varepsilon}_3\}$ equivalent, except for a scale factor, to the one of the $\{\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3\}$ vectors in physical space:

$$\hat{\varepsilon}_i\cdot\hat{\varepsilon}_j=c\mathbf{a}_i\cdot\mathbf{a}_j,\quad (i,j=1,2,3), \tag{12}$$

where c is an arbitrary constant. For completeness, and introducing no essential restriction, the rest of basis vectors $\hat{\varepsilon}_i$, $i=4,\ldots,n$, vectors are normally considered to be mutually orthogonal and also perpendicular to the first three:

$$\hat{\varepsilon}_i\cdot\hat{\varepsilon}_j=\delta_{ij},\quad i=1,\ldots,n,\quad \text{and}\quad j=4,\ldots,n. \tag{13}$$

In the following, we will assume this condition for the working basis which decomposes the superspace in their parallel space+internal space components. This is the usual assumption in most of the works on the subject. Thus, the actual metric of the superspace is then defined by Eqs. (12) and (13) and the matrix **A**, the partial arbitrariness of the matrix **A** allowing different equivalent metrics in the superspace. Different choices of the coefficients γ_{ij} in **A** represent alternative geometrical images of the superspace density, i.e., alternative *embeddings*. A unique choice for the superspace embedding can only result from some additional requirements which are not essential within the formalism. For instance, as discussed below, the requirement of a simplified expression for the algebraic equations describing the rotational symmetry properties of the system can be used for this purpose and sometimes is a sufficient condition for reaching, in practice, a unique embedding choice.

One could rightly argue that the introduction of a metric in the superspace is a step not essential in the superspace description and can be avoided. As stressed above, the n-dimensional geometrical picture of the superspace density is irrelevant, and indeed, all experimental quantities can be expressed in terms of the superspace density as a unique well-defined scalar function of n variables. But, in this case, the freedom on the choice of the transformation matrix **A** can be interpreted as an ambiguity on the definition of the internal subspace. Indeed, from a structural viewpoint, the matrix **A** defines the coordinate system, under which the superspace density is to be described. According to the formalism, the superspace density within the unit cell can be considered as a set of atomic surfaces centered at different points,

$$\rho_s(\hat{\theta})=\sum_{\mu}\rho_s^{\mu}(\hat{\theta}-\hat{\theta}_{\mu}) \tag{14}$$

and the structure factor of the real space structure is equal to the structure factor of the superspace density:

$$F(\mathbf{H})=\sum_{\mu}G_{\mu}(\mathbf{H})\exp(2\pi i\hat{h}\cdot\hat{\theta}_{\mu}), \tag{15}$$

with $G_{\mu}(\mathbf{H})$ being the scattering form factors of the corresponding atomic surfaces:

$$G_{\mu}(\mathbf{H})=\int d\hat{\theta}\;\rho_s^{\mu}(\hat{\theta})\exp(2\pi i\hat{h}\cdot\hat{\theta}), \tag{16}$$

where $\hat{h}\cdot\hat{\theta}$ represents $\Sigma_{i=1}^{n}h_i\theta_i$ $(h_1,\ldots,h_n)=\hat{h}$ being the indices used in the indexation (1). In practice, the θ-coordinate system is not used for the calculation of the form factors $G_{\mu}(\mathbf{H})$. According to the superspace formalism, a cut of the atomic surfaces along the parallel subspace must consist of a peak of atomic density centered at some point in parallel space. Therefore, in general, the atomic surfaces can be expressed by functions of the form

$$\begin{aligned}\rho_s^{\mu}(\hat{\theta})&=\rho_{\mu}(\mathbf{x}-\mathbf{u}_{\mu}(\mathbf{x}_I)),\quad \mathbf{x}_I\in S_{\mu},\\ \rho_s^{\mu}(\hat{\theta})&=0,\quad \mathbf{x}_I\notin S_{\mu},\end{aligned} \tag{17}$$

where, according to Eq. (9), $(\mathbf{x},\mathbf{x}_I)=\mathbf{A}^{-1}\hat{\theta}$, $\rho_{\mu}(\mathbf{r})$ is the real space density associated to the atom represented by the atomic surface, and $\mathbf{u}_{\mu}(\mathbf{x}_I)$ is the position of the center of the peak density, which depends on the value of $\mathbf{x}_I$. S_{μ} is the domain in internal space occupied by the atomic surface. Using Eq. (17), the integral (16) transformed into the coordinate system $(\mathbf{x},\mathbf{x}_I)$ leads to the expression which can be used in practice:

$$G_{\mu}(\mathbf{H})=\frac{1}{|\mathbf{A}|}f_{\mu}(\mathbf{H})\int_{S_{\mu}}d\mathbf{x}_I\exp\{2\pi i[\mathbf{h}_I\cdot\mathbf{x}_I+\mathbf{h}\cdot\mathbf{u}_{\mu}(\mathbf{x}_I)]\}, \tag{18}$$

where $|\mathbf{A}|$ is the absolute value of the determinant of **A** and $(\mathbf{h},\mathbf{h}_I)=\mathbf{A}^T\hat{h}$.

The logical choice of the transformation **A** should, therefore, be one where the functions $\mathbf{u}_{\mu}(\mathbf{x}_I)$ in Eq. (17) are as simple as possible, and this can depend, in principle, on the form of the atomic surfaces.

III. ROTATIONAL SYMMETRY

The symmetry of a quasiperiodic structure can be defined as the set of rotational (proper and improper) operators in real space **R**, such that the structure factor in Eq. (2) satisfies, for any **H**;

$$F(\tilde{\mathbf{R}}\mathbf{H})=F(\mathbf{H})\exp(-2\pi i\hat{h}\cdot\hat{t}), \tag{19}$$

where $\hat{h}\cdot\hat{t}$ represents $\Sigma_{i=1}^{n}h_it_i$, with $(t_1,\ldots,t_n)=\hat{t}$, a set of n numbers which depend on the operation **R** and the indexation basis used. The set of elements $\{\mathbf{R}|\hat{t}\}$ form a group, the so-called superspace group, that describes the symmetry of the structure. Expression (19) implies that the diffraction diagram should have the point group symmetry corresponding to the set of rotations $\{\mathbf{R}\}$ in the superspace group, the observed extinction rules being related to the nonprimitive ''translations'' $\hat{t}$ of some elements.

The symmetry relation (19) is difficult to visualize in physical space; it means that the rotation $\mathbf{R}$ transforms the structure $\rho(\mathbf{r})$ in a new atomic configuration that is physically indistinguishable from the original one.[2–4] But it has a simple interpretation for the superspace density if an integer $n\times n$ matrix $\hat{\mathbf{R}}$ is defined with its coefficients r_{ij} being given by the transformation of the indexation basis vectors $\mathbf{k}_i$ through $\mathbf{R}$:

$$\tilde{\mathbf{R}}\mathbf{k}_i=\sum_{j=1}^{n} r_{ij}\mathbf{k}_j, \quad r_{ij}: \text{ integers}; \quad i=1,\ldots,n. \tag{20}$$

From Eqs. (3), (19), and (20), it is straightforward to demonstrate that the superspace density defined in Eq. (3) satisfies

$$\rho_S(\hat{\mathbf{R}}\hat{\theta}+\hat{t})=\rho_S(\hat{\theta}), \tag{21}$$

in which $\hat{\mathbf{R}}\hat{\theta}$ is the point in superspace with coordinates $\Sigma_{j=1}^{n} r_{ij}\theta_j$. Hence the set of operations $\{\hat{\mathbf{R}}|\hat{t}\}$ form a n-dim space group describing the symmetry of the superspace density in the basis $\{\hat{e}_i\}$.

From its definition, it can be easily seen that the parallel subspace is invariant for any superspace transformation $\hat{\mathbf{R}}$ included in the superspace group. Hence, in general, the form of the rotational symmetry elements $\hat{\mathbf{R}}$ in the basis $\{\hat{\varepsilon}_i\}$ is

$$\mathbf{A}^{-1}\hat{\mathbf{R}}\mathbf{A}=\begin{pmatrix}\mathbf{R} & \mathbf{R}_M\\ 0 & \mathbf{R}_I\end{pmatrix}, \tag{22}$$

where $\mathbf{R}$ is the 3×3 matrix associated (in the $\{\mathbf{a}_i\}$ basis) with the corresponding three-dimensional rotation in physical space.

In general, the internal subspace is not invariant for the rotational symmetry elements. The set of integer matrices $\hat{\mathbf{R}}$ is a representation of a point group and this representation is, in general, reducible.[14] The γ_{ij} can be chosen so that $\mathbf{R}_M=0$ while both $\mathbf{R}$ and $\mathbf{R}_I$ in Eq. (22) become orthogonal transformations in parallel and internal subspaces, respectively. The internal subspace becomes also invariant for the high-dimensional rotational transformations. This is very convenient to simplify the algebra: The symmetry relations among the atomic surfaces and their consequences in expressions like Eq. (15) are especially simple. This is the usual choice and in the case of icosahedral and polygonal quasicrystals is enough for fixing the embedding, except for trivial degrees of freedom (scale, etc.).

IV. EXAMPLES OF ALTERNATIVE SUPERSPACE EMBEDDINGS OF QUASIPERIODIC STRUCTURES

The possibility of making different superspace embeddings of the same quasiperiodic structure was pointed out previously for two specific cases: the Fibonacci chain[7] and incommensurate composite structures,[8] but as seen above, this ambiguity is general for all quasiperiodic systems, including incommensurate materials and quasicrystals. There is, in many cases, a type of embedding which is simpler and the obvious choice, but we do not know of any physical reason which privileges this choice from any other possible one. In this section, we apply the general arguments presented above in a unified context to four different examples of quasiperiodic structures, including the particular cases considered.[7,8]

A. Incommensurate modulated structure with one modulation vector

As a first example, let us consider an incommensurate modulated structure with a single modulation vector along the z axis. Three vectors ($\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_3$) index the main reflections and are the reciprocal vectors of those that define the unit cell of the average structure. A fourth vector, say, $\mathbf{k}_4=\alpha\mathbf{k}_3$, is necessary to index the remaining reflections of the diffraction pattern, i.e., the satellite reflections. Following the prescription of the previous sections, we choose as basis of the reciprocal space the first three vectors:

$$\mathbf{a}_i^*=\mathbf{k}_i, \quad i=1,2,3. \tag{23}$$

The matrix $\mathbf{A}$ in Eq. (9) can then be written as

$$\mathbf{A}=\begin{pmatrix}1 & 0 & 0 & \gamma_1\\ 0 & 1 & 0 & \gamma_2\\ 0 & 0 & 1 & \gamma_3\\ 0 & 0 & \alpha & \gamma_4\end{pmatrix}, \tag{24}$$

where still the coefficients of the last column are to be chosen. As $\mathbf{k}_3$ and $\mathbf{k}_4$ are collinear, according to Eq. (20), the form of the $n\times n$ $\mathbf{R}$ matrices corresponding to the structure superspace group are necessarily of the form

$$\hat{\mathbf{R}}=\begin{pmatrix}r_{I1} & r_{12} & 0 & 0\\ r_{21} & r_{22} & 0 & 0\\ 0 & 0 & r_{33} & 0\\ 0 & 0 & 0 & r_{44}\end{pmatrix}, \tag{25}$$

with $r_{33}=r_{44}=\pm1$; i.e., the subspaces generated by $\hat{e}_3$ and $\hat{e}_4$ have the same transformation properties, being both invariant. The invariance of the subspace generated by $\hat{e}_3$ is forced (and, hence, that of the second subspace) by the existence of a single rationally independent modulation wave vector in the structure. Any rotation $\mathbf{R}$ satisfying Eq. (19) and transforming $\mathbf{k}_3$ into a linear combination containing $\mathbf{k}_1$ and/or $\mathbf{k}_2$ would also imply the existence of a second rationally independent modulation wave vector $\mathbf{R}\mathbf{k}_4$.

From the general form (25) of the matrices $\hat{\mathbf{R}}$ in the basis $\{\hat{e}_i\}$, the requirement on the transformation $\mathbf{A}$ to keep $\hat{\mathbf{R}}$ in a block-diagonal form, with the internal subspace invariant, is not enough to fix the fourth column in Eq. (24). γ_1 and γ_2 must be zero, but γ_3 and γ_4 can take any value with the only requirement that $\gamma_4-\alpha\gamma_3\neq0$. As by definition the vectors $\{\hat{\varepsilon}_i\}$ are orthogonal, an arbitrary choice of (γ_3,γ_4) implies in general that $\hat{e}_3$ and $\hat{e}_4$ have an oblique relative orientation. The usual choice[5,6] is ($\gamma_3=0$, $\gamma_4=1$), so that $\hat{e}_4$ and $\hat{\varepsilon}_4$ coincide, and $\hat{e}_3\cdot\hat{e}_4=-\alpha$. The first three vectors $\{\hat{\varepsilon}_i\}$ define the average unit cell in parallel space, while the fourth one represents the phase of the modulation. A typical example under this embedding corresponding to a structure with a unit cell containing only one atom and a sinusoidal modulation is shown in Fig. 1(a) within the plane (x_3,x_{I1}). The modulation is described by one ''atomic surface'' repeated in superspace according to the lattice periodicity given by the cell vectors $\hat{e}_3$ and $\hat{e}_4$. The coordinates x_3 in Eq. (5) of the atomic posi-

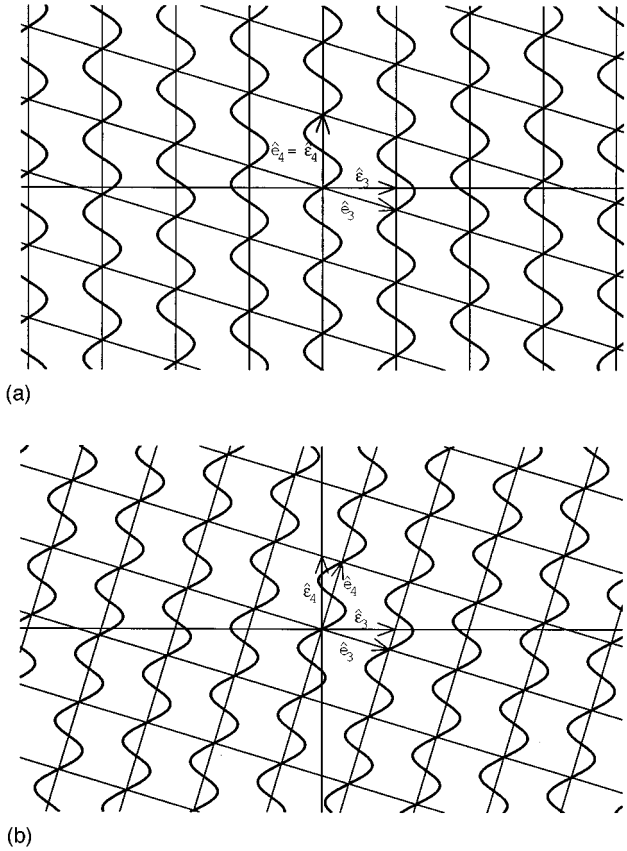

FIG. 1. Section, parallel to the direction of the modulation and the internal subspace, of the superspace embedding of an incommensurate structure with one atom per unit cell. (a) Usual embedding. (b) Alternative embedding described by Eq. (27).

tions are the intersections of the atomic surfaces with the plane $x_{I1}=0$. The curve describing the atomic surface associated to cell ''zero'' is given by a sinusoidal function

$$x_3=x_3^0+f\ \sin(2\pi x_{I1}). \tag{26}$$

Instead of this embedding, we could choose infinitely many others, for example, the one given by the following matrix **A**:

$$\mathbf{A}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -\alpha \\ 0 & 0 & \alpha & 1 \end{pmatrix}. \tag{27}$$

This choice means a square lattice for the superspace density, i.e., $|\hat{e}_3|=|\hat{e}_4|$ and $\hat{e}_3\cdot\hat{e}_4=0$, while the $\hat{\varepsilon}_4$ vector is no longer parallel to $\hat{e}_4$. The result is shown in Fig. 1(b). The modulated structure given by the section $x_{I1}=0$ is the same as in Fig. 1(a), but the superspace density is rather different. The two superspace densities can be considered to be related by a deformation that keeps undeformed the section associated to the parallel space. The atomic ''surface'' cannot be described in this embedding by Eq. (26). Taking into account Eqs. (8) and (26), the equation describing the form of the atomic surface in the θ-coordinate system is

$$\theta_3=x_3^0+f\ \sin[2\pi(\theta_4-\alpha\theta_3)]. \tag{28}$$

This expression can be then transformed to any particular x_i, x_{1i} system, once the matrix **A** has been chosen. For instance, for the choice given by Eq. (27), it becomes

$$x_3=x_3^0+\alpha x_{I1}+f\ \sin[2\pi(1+\alpha^2)x_{I1}]. \tag{29}$$

In order to have simple block-diagonal forms for the four-dimensional $\hat{\mathbf{R}}$ matrices, we have restricted γ_1 and γ_2 to be zero. However, in principle, a more general matrix could be chosen. In such case, the function that describes the atomic surfaces would mix the coordinates x_1 and x_2 with x_3 and x_{I1}. Obviously, such choice would complicate unnecessarily the description, i.e., the expression for the atomic surfaces, but in principle is also mathematically valid.

B. Incommensurate composite structure

We consider now a composite structure consisting of two periodic monatomic substructures with two common periods, while the third one along a common direction is mutually incommensurate. Also, in this case, the superspace is fourth dimensional and the atoms are represented by one-dimensional functions. The usual description of this type of structures is similar to the one of an incommensurate modulated structure. The reflections due to the average reciprocal lattice of one of the substructures are taken as the ''main'' reflections and the rest as ''satellites.'' The choice of superspace embedding is given by the same matrix **A** as in the modulated case:

$$\mathbf{A}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & \alpha & 1 \end{pmatrix}, \tag{30}$$

with α being the factor relating the incommensurate cell parameters of both subsystems: $\mathbf{a}_3^{*(2)}=\alpha\mathbf{a}_3^{*(1)}$. In Fig. 2(a) an example of this type of structures is depicted under this standard choice of embedding. The picture represents the plane containing the direction of the parallel space in which both superstructures have incommensurate periodicities and the internal direction x_{I1}. The physical structure is again given by the section $x_{I1}=0$. Obviously, one should consider that the two independent sets of one-dimensional atomic surfaces have different positions along the directions not included in the figure so that the atoms at $x_{I1}=0$ are never too close. In general, each subsystem is modulated with the periodicity of the other one. For simplicity, the two modulations have been taken in the figure sinusoidal, so that the atomic surfaces at the ''zero'' cell associated to the two subsystems are given by the functions

$$\begin{aligned} x_3^{(1)}&=f^{(1)}\sin(2\pi x_{I1}), \\ x_3^{(2)}&=-\frac{x_{I1}}{\alpha}-f^{(2)}\sin\left(\frac{2\pi x_{I1}}{\alpha}\right), \end{aligned} \tag{31}$$

for subsystems 1 and 2, respectively. Note that the atomic surfaces repeat according to the lattice periodicity:

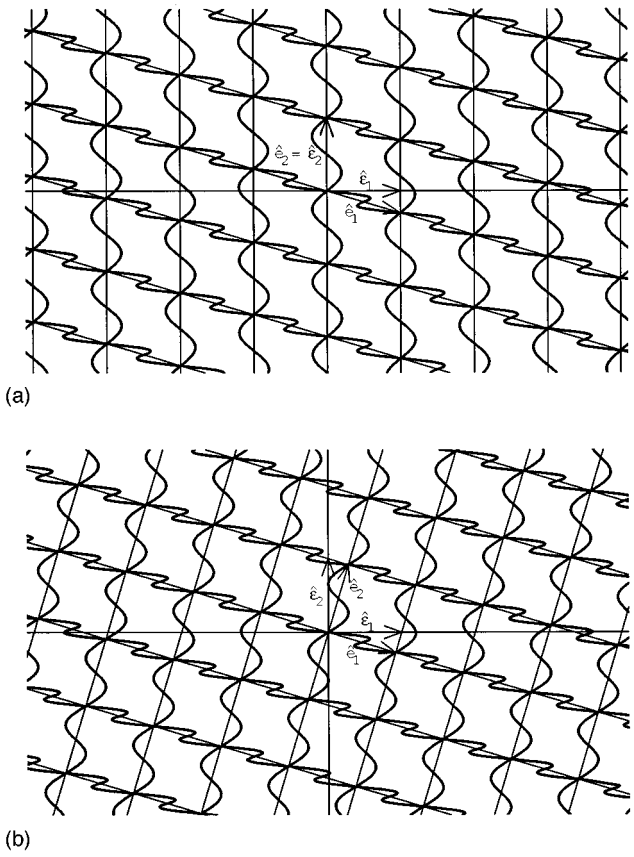

FIG. 2. Section, parallel to the direction of the modulation and the internal subspace, of the superspace embedding of a composite structure with two subsystems. (a) Usual embedding with subsystem 1 privileged. (b) Alternative embedding with square unit cell.

$$x_3^{(1)}(n_3)=n_3+f^{(1)}\sin[2\pi(x_{I1}+n_3\alpha)],$$
$$x_3^{(2)}(n_4)=-\frac{x_{I1}-n_4}{\alpha}-f^{(2)}\sin\left(\frac{2\pi(x_{I1}-n_4)}{\alpha}\right), \tag{32}$$

where n_3 and n_4 are integers. The atomic positions along the direction z are then given by the values of the functions (32) at $x_{I1}=0$, that is

$$x_3^{(1)}(n_3)=n_3+f^{(1)}\sin(2\pi n_3\alpha),$$
$$x_3^{(2)}(n_4)=\frac{n_4}{\alpha}+f^{(2)}\sin\left(\frac{2\pi n_4}{\alpha}\right). \tag{33}$$

Thus, if we take into account that $|\mathbf{a}_3^{(1)}|$ is being used as length unit and that in these units $|\mathbf{a}_3^{(2)}|=1/\alpha$, Eqs. (33) describe a configuration where atoms 1 are quasiperiodic, with period $|\mathbf{a}_3^{(1)}|$, plus a sinusoidal modulation with wavelength $|\mathbf{a}_3^{(2)}|$, while atoms 2 are quasiperiodic with period $|\mathbf{a}_3^{(2)}|$ plus a sinusoidal modulation of wavelength $|\mathbf{a}_3^{(1)}|$.

The embedding described in Fig. 2(a) privileges subsystem 1, in the sense that it is taken as a reference for the second one; i.e., a translation along the internal coordinate x_{I1} (the famous phason degree of freedom) represents a translation of the subsystem 2 with respect to the subsystem 1, which is kept at rest. Obviously, as stressed by Yamamoto,[8] the roles of the two subsystems can be interchanged. In our notation, this corresponds to the choice of the matrix **A** in the form

$$\mathbf{A}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&1\\0&0&\alpha&0\end{pmatrix}. \tag{34}$$

Note that this inversion of the roles of the two subsystems does not require to change the reference reciprocal basis vectors in Eq. (6), which are still the reciprocal cell vectors of subsystem 1. As in the previous example, in order to express the atomic surfaces (32) in this alternative embedding, it is convenient to express them in the invariant form given by the variables θ_i:

$$\theta_3=n_3+f^{(1)}\sin[2\pi(\theta_4-\alpha\theta_3+n_3\alpha)] \quad \text{for subsystem 1,}$$
$$\frac{\theta_4}{\alpha}=\frac{n_4}{\alpha}-f^{(2)}\sin\left(2\pi\,\frac{(\theta_4-\alpha\theta_3-n_4)}{\alpha}\right) \quad \text{for subsystem 2,} \tag{35}$$

which with the use of the matrix (34) can be put in the form adequate for the new embedding:

$$x_3^{(1)}=n_3-x_{I1}-f^{(1)}\sin[2\pi\alpha(x_{I1}-n_3)],$$
$$x_3^{(2)}=\frac{n_4}{\alpha}+f^{(2)}\sin\left[2\pi\left(x_{I1}+\frac{n_4}{\alpha}\right)\right]. \tag{36}$$

It is easy to check that the atomic positions along the axis x_3 are again given by Eq. (33), so that the ''real'' structure is the same as the one represented in Fig. 2(a). The internal coordinate x_{I1}, however, represents now a translation of the subsystem 1 in the reference frame of subsystem 2.

Between these two embeddings, an infinite set of equivalent ones can be used. For instance, one can introduce a square lattice for the superspace lattice as in Fig. 2(b), which corresponds to a choice of the matrix **A** as

$$\mathbf{A}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&-\alpha\\0&0&\alpha&1\end{pmatrix}, \tag{37}$$

with the atomic functions becoming more complex:

$$x_3^{(1)}=n_3+\alpha x_{I1}+f^{(1)}\sin\{2\pi[(1+\alpha^2)x_{I1}+n_3\alpha]\},$$
$$x_3^{(2)}=\frac{n_4}{\alpha}-\frac{x_{I1}}{\alpha}-f^{(2)}\sin\left(2\pi\,\frac{(1+\alpha^2)x_{I1}-n_4}{\alpha}\right). \tag{38}$$

C. Fibonacci chain

The Fibonacci chain is a one-dimensional quasiperiodic structure. Two types of elementary cells are arranged in a quasiperiodic form along the space. The ratio of the lengths of the two segments is the ''golden mean'' $\phi=(\sqrt{5}-1)/2=1/\tau$. If the two segments are a_1 and a_2, the diffraction pattern of that structure can be indexed by means of two one-dimensional ''vectors'' $k_1=1/a_1$ and $k_2=1/a_2$, so that $k_2=\phi k_1$. The superspace is then two dimensional, and if we

take as real space bases in Eqs. (5) and (6) the parameters a_1 and $a_1^*=k_1$, respectively, then the general form of the matrix **A** is

$$\mathbf{A}=\begin{pmatrix} 1 & \gamma_1 \\ \phi & \gamma_2 \end{pmatrix}. \tag{39}$$

As the only possible ''rotational'' operations in one dimension are reduced to the identity and the inversion, the requirement that the symmetry elements (22) have a block-diagonal form does not restrict the possible values of the γ_i parameters in Eq. (39). The usual superspace embedding of the Fibonacci chain introduces a square lattice ($|\hat{e}_1|=|\hat{e}_2|$ and $\hat{e}_1\cdot\hat{e}_2=0$). This corresponds to the choice $\gamma_1=-\phi$ and $\gamma_2=1$. The atomic surfaces are parallel to the internal space and are the projection on this subspace of the unit cell. In the θ-coordinate system, the atomic surface at the origin is the segment joining the points

$$\left(\frac{\phi^2}{1+\phi^2},-\frac{\phi}{1+\phi^2}\right) \quad \text{and} \quad \left(-\frac{\phi}{1+\phi^2},\frac{1}{1+\phi^2}\right). \tag{40}$$

As an alternative embedding to Eq. (39), we can consider, for instance, the typical one for an incommensurate modulated structure:

$$\mathbf{A}=\begin{pmatrix} 1 & 0 \\ \phi & 1 \end{pmatrix}. \tag{41}$$

The segment that defines the atomic surface in the θ-coordinate system is still described by its two extreme points given by Eq. (40), but the meaning of the internal space is changed, as shown in Fig. 3(a). The atomic surfaces are no longer parallel to the internal space, and the unit cell takes the typical form of the one used for an incommensurate modulated structure. The atomic surfaces are rather characteristic, since the modulation functions are two valued within some intervals of the internal coordinate, but this is no obstacle for interpreting the structure as modulated. In fact, there are experimental structures which have been worked out as incommensurately modulated, where this type of two-valued modulation functions have been observed.[15]

However, we can even find a matrix **A** which produces an embedding typical of a modulated structure with single-valued modulation functions:

$$\mathbf{A}=\begin{pmatrix} 1 & 1 \\ \phi & -1 \end{pmatrix}. \tag{42}$$

With this choice, the superspace structure becomes that of Fig. 3(b). The unit cell of the superspace lattice in this figure can be changed to $\hat{e}_1'=\hat{e}_2$ and $\hat{e}_2'=\hat{e}_1-\hat{e}_2$. This would correspond to an alternative choice of the indexing vectors $\mathbf{k}_i$ in Eq. (1): $\mathbf{k}_1'=\mathbf{k}_1+\mathbf{k}_2$ and $\mathbf{k}_2'=\mathbf{k}_1$. With this unit cell, the superspace picture of the structure depicted in Fig. 3(b) can be fully identified with a modulated structure, with the modulation of the atomic positions having a sawtooth form. This fact was already pointed out by Janssen.[7]

D. Icosahedral quasicrystal

The diffraction pattern of an icosahedral structure can be indexed by means of six vectors pointing to six vertices of a regular icosahedron. If we take an orthonormal basis $\{\mathbf{a}_i^*\}$, the α_{ij} parameters in Eq. (6) can be chosen in the following way:

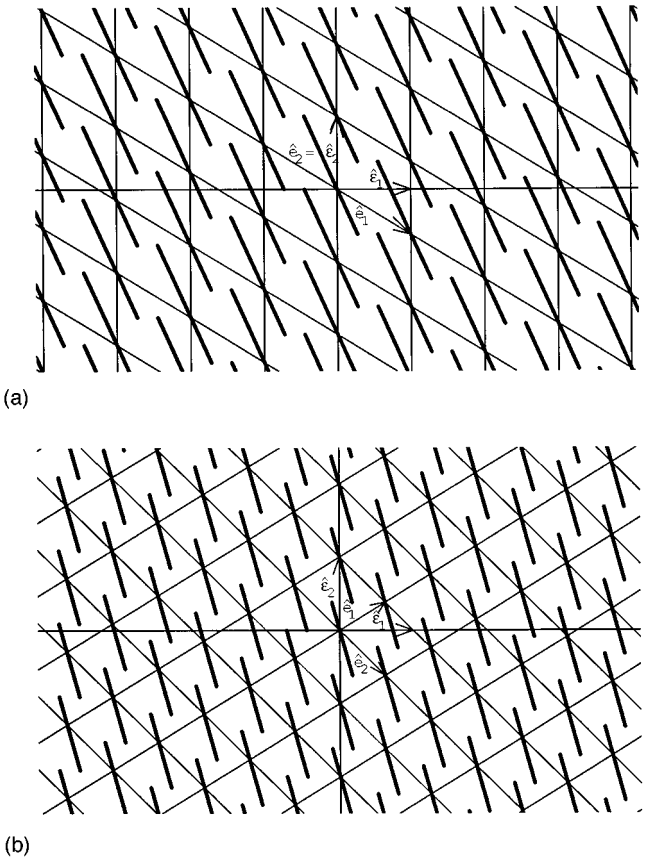

FIG. 3. Embedding of a Fibonacci chain in (a) incommensurate-type description with double-valued functions as atomic surfaces. (b) Incommensurate description with single-valued functions as atomic surfaces.

$$(\alpha_{11},\alpha_{12},\alpha_{13})=\left(0,0,\frac{1}{\sqrt{2}}\right),$$

$$(\alpha_{i1},\alpha_{i2},\alpha_{i3})=\left(\frac{2}{\sqrt{10}}\cos\frac{2\pi i}{5},\frac{2}{\sqrt{10}}\sin\frac{2\pi i}{5},\frac{1}{\sqrt{10}}\right) \tag{43}$$

$$\text{for } i=2,\ldots,6.$$

The usual requirement of a block-diagonal form for the symmetry rotational operators ($\mathbf{R}_M=0$ in Eq. (22)] strongly restricts in this case the possible choices for the matrix **A**. The internal subspace is uniquely determined, and the remaining arbitrariness on the coefficients γ_{ij} corresponds to the trivial freedom on the choice of the coordinate system within this internal subspace. If we want a coordinate system in the internal subspace which makes the $\mathbf{R}_I$ in Eq. (22) to be orthogonal, with the orientation of the symmetry elements in internal subspace being given by expressions analogous to those in parallel space (for the basis $\mathbf{a}_i$ used), the choice of the coefficients γ_{ij} is reduced to

$$(\gamma_{11},\gamma_{12},\gamma_{13})=\left(0,0,\frac{1}{\sqrt{2}}\right),$$

$$(\gamma_{i1},\gamma_{i2},\gamma_{i3})=\left(-\frac{2s}{\sqrt{10}}\cos\frac{4\pi i}{5},-\frac{2s}{\sqrt{10}}\sin\frac{4\pi i}{5},-\frac{s}{\sqrt{10}}\right)\quad\text{for } i=2,\ldots,6, \tag{44}$$

where only a single scale factor s remains arbitrary. The metric implicit on this choice is such that the moduli of all vectors $\{\hat{e}_i\}$ are equal, but their relative orientation, being in general oblique, depends on the scale factor s. The usual (standard) embedding considers $s=1$, which makes the vectors $\{\hat{e}_i\}$ mutually orthogonal, i.e., an orthonormal basis. Although an hypercubic unit cell in superspace may be esthetically appealing, it is fully irrelevant and does not introduce any further simplification of the algebra. In fact, it is conceptually misleading, and can be seen, for instance, in the custom of measuring in Å the distances in the internal subspace, when in fact this space is adimensional.

Let us consider, now, an imaginary monatomic icosahedral quasicrystal with a single atomic surface per unit cell centered at the cell origin, perpendicular to the parallel subspace and with its boundaries in the internal subspace of the standard embedding given by the projection of the six-dimensional unit cell onto this subspace. The form of a single atomic surface is then a rhombic triacontahedron.[16] Figure 4(a) represents a section of the corresponding superspace density within the standard (hypercubic) embedding. This section contains the vectors $\hat{e}_2-\hat{e}_3$ and $\hat{e}_4-\hat{e}_6$, and it includes one direction in parallel space and another one of internal space (horizontal and vertical axes, respectively, in the figure). The sections of the triacontahedra are linear segments parallel to the internal space forming a structure analogous to that of the Fibonacci chain. The exact squarelike lattice in Fig. 4(a) is an artifact of the standard hypercubic embedding, with no special meaning. As stressed above, the scale of the internal subspace is arbitrary and independent of the one used for the parallel subspace. In a more general embedding, but standard in the sense of maintaining the block-diagonal form of the rotational operations, the length of the ''sticks'' in the pattern can be made to have any value, with the unit cell sections becoming an oblique parallelogram. Only relative volumes and relative lengths in internal space have any physical meaning. This rather trivial scale arbitrariness within the superspace embedding in icosahedral quasicrystals, already pointed out in previous literature,[9] is at odds with the persistent custom of giving to the atomic surfaces of experimental quasicrystals ''Angstrom-like'' sizes in internal space.[17–19]

We can make more radical changes in the embedding chosen, but in this case at the cost of having to use nondiagonal block matrices for the rotational operators. For example, as in the Fibonacci chain, we can find a matrix **A** which produces an embedding typical of a modulated structure, at least in three directions:

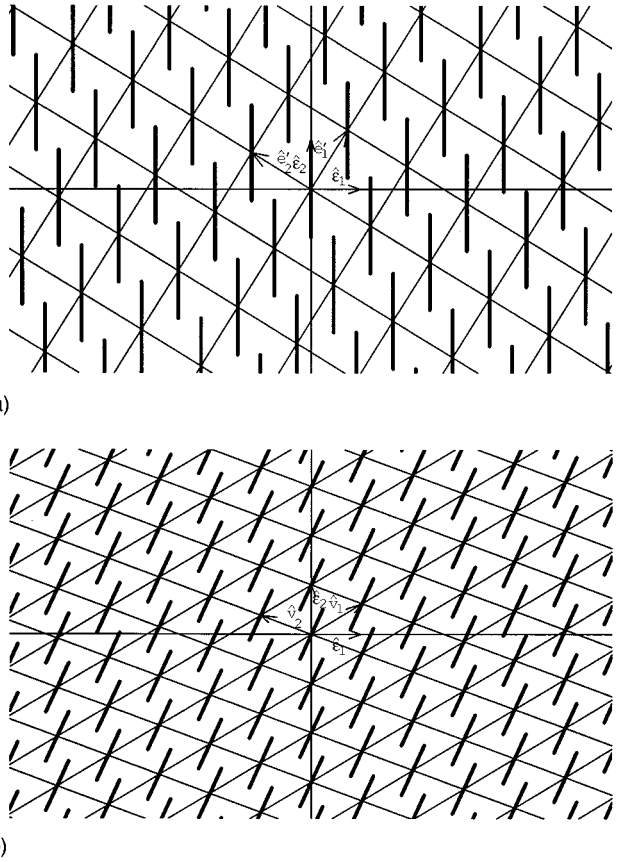

FIG. 4. (a) Planar section parallel to $\hat{v}_1\equiv\hat{e}_2-\hat{e}_3$ and $\hat{v}_2\equiv\hat{e}_4-\hat{e}_6$ of the imaginary icosahedral structure described in the text in the usual, hypercubic, description. (b) The same section of (a) in an incommensurate-type embedding.

$$\begin{pmatrix}\gamma_{11}&\gamma_{12}&\gamma_{13}\\ \gamma_{21}&\gamma_{22}&\gamma_{23}\\ \gamma_{31}&\gamma_{32}&\gamma_{33}\\ \gamma_{41}&\gamma_{42}&\gamma_{43}\\ \gamma_{51}&\gamma_{52}&\gamma_{53}\\ \gamma_{61}&\gamma_{62}&\gamma_{63}\end{pmatrix}=\begin{pmatrix}1&1&0\\ -1&1&1\\ -1&1&-1\\ -1&-1&1\\ -1&1&0\\ -1&-1&-1\end{pmatrix}. \tag{45}$$

Figure 4(b) depicts the same section of Fig. 4(a), but in this alternative embedding that describes the system as a modulated structure. The atomic surfaces remain flat, but they are not parallel to the newly defined internal (perpendicular) space, and can now be viewed as forming a specific modulation function $\mathbf{u}(x_{11},x_{12},x_{13})$ with sawtooth sections. Under this embedding, there are three periodic directions $\hat{e}_2-\hat{e}_3+\hat{e}_4-\hat{e}_6$ [vertical direction in Fig. 4(b)], $\hat{e}_1-\hat{e}_2-\hat{e}_3-\hat{e}_4-\hat{e}_5-\hat{e}_6$, and $\hat{e}_1+\hat{e}_2+\hat{e}_3-\hat{e}_4+\hat{e}_5-\hat{e}_6$, which have no component in parallel subspace, so that their reciprocal ones lie in the parallel-reciprocal subspace. In this description, these three reciprocal vectors can be viewed as the basis for indexing the set of ''main'' reflections, the rest being ''satellites.'' Obviously, icosahedral symmetry operations will relate ''satellite'' and ''main'' reflections, as the corresponding 6-dim matrices have not a block diagonal form, but, in principle, the description is perfectly valid, and only requires a scarcely more complex algebraic treatment of

the rotational symmetry, when describing the symmetry relations among the atomic surfaces.

V. CONCLUSIONS

Some of the features of the superspace description of quasiperiodic structures, of the so-called superspace embedding, can be arbitrarily chosen. The superspace density, as a scalar function of n variables, is uniquely defined, but its practical description in terms of atomic surfaces requires a transformation into a coordinate system that separates the so-called parallel subspace, isomorphous to real space, and its complementary, the so-called internal subspace. Part of the transformation matrix defining this coordinate system is arbitrary. The different embeddings materialized in different choices for this matrix can be interpreted as different choices for the internal subspace. As the internal subspace is usually represented as being perpendicular to the parallel subspace, the different embeddings imply different metrics associated to the superspace and, therefore, different geometrical representations of the superspace density. Under this viewpoint, the superspace densities of two different embeddings are in general related by an n-dimensional strain that keeps undeformed the parallel subspace.

In practical terms, a choice of embedding represents a specific coordinate system to be used for the description of the atomic surfaces forming the superspace density. Through the examples discussed above, it is clear that the description of simple atomic surfaces can be rather complex in the original ''periodic'' coordinates, while the standard embeddings for the different cases correspond to a transformation into a coordinate system where, in general, the description of the corresponding atomic surfaces is particularly simple. Thus, the more adequate embedding and, therefore, more adequate definition of the internal subspace depend in general on the form of the atomic surfaces. In the case of highly symmetric quasicrystals, the rotational symmetry strongly restricts the form of the atomic surfaces, and the simplest embedding is then essentially determined by this symmetry. There are other cases, however, where a unique choice is not obvious. For instance, in composite incommensurate structures each substructure is simpler under a different embedding, and so there is no clear unique choice. In fact, each substructure can be in practice considered under its own embedding. In the case of the Fibonacci chain, the embedding usual for modulated structures yields a description of the atomic surfaces so simple as the usual ''quasicrystalline'' embedding. In this sense, the Fibonacci chain can be considered an incommensurate modulated structure with a specific type of modulation function.

From a physical viewpoint, the internal subspace is identified with the so-called phason degrees of freedom in the structure, which correspond to modes that, although involving local rearrangements of the atoms, have null-energy cost. One could then think that this physical property could be used for obtaining an absolute definition of the internal subspace and, hence, of the superspace embedding. Indeed, in the case of incommensurately modulated structures, the standard embedding corresponds to choosing the phase(s) of the structural modulation as the degrees of freedom corresponding to the internal subspace. As seen in the first example, a nonstandard embedding in the incommensurately modulated structures implies, in general, nonbounded displacements of the atomic positions when moving along the internal space, i.e., an undesired translational component in the definition of the internal coordinate(s). However, the other examples demonstrate that this criterion is not valid for a general case. Up to our knowledge, there is no absolute general criterion for ''orthogonalizing'' the phason degrees of freedom with respect to the translational modes. Contrary to previous statements in the literature,[10] phason modes, in general, shift the mass center of the system, both locally and globally. So this property cannot be used to distinguish the internal subspace. The example of the Fibonacci chain demonstrates how two different definitions of the phason mode can be equally valid. In fact, the actual structure of the phason modes as dynamical degrees of freedom and the weight of the translational modes on them will depend on their coupling at finite wavelengths and, therefore, cannot be determined *a priori* by purely static arguments.

ACKNOWLEDGMENTS

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[1] The theoretical possibility of more complex nondense domains, as fractals, has been pointed out. In any case, one expects that the atomic domains can be described by a simple algorithm, i.e., a few parameters.

[2] D. S. Rokhsar, N. D. Mermin, and D. C. Wright, Acta Crystallogr. A **44**, 197 (1988).

[3] D. S. Rokhsar, N. D. Mermin, and D. C. Wright, Phys. Rev. B **37**, 8147 (1988).

[4] N. D. Mermin, in *Methods of Structural Analysis of Modulated Structures and Quasicrystals*, edited by J. M. Perez-Mato, F. J. Zuñiga, and G. Madariaga (World Scientific, Singapore, 1991), pp. 129–184.

[5] P. M. de Wolff, Acta Crystallogr. A **30**, 777 (1974).

[6] A. Janner and T. Janssen, Phys. Rev. B **15**, 643 (1977).

[7] T. Janssen, Phys. Rep. **168**, 55 (1988).

[8] A. Yamamoto, Acta Crystallogr. A **48**, 476 (1992).

[9] T. Janssen, Acta Crystallogr. A **42**, 261 (1986).

[10] P. Bak, Phys. Rev. B **32**, 5764 (1985).

[11] P. Bak, Scr. Metall. **20**, 1199 (1986).

[12] L. Elcoro, J. M. Perez-Mato, and G. Madariaga, Acta Crystallogr. A **50**, 182 (1994).

[13] The definition of the superspace density is also valid in the case of a normal crystal, where the rank n coincides with the dimension of the physical space, and the three coordinates θ_i, according to Eq. (4), can be identified with the relative coordinates of a point $\mathbf{r}$ in physical space with respect to the reciprocal basis of $\{\mathbf{k}_i\}$.

[14] T. Janssen, Acta Crystallogr. A **47**, 243 (1991).

[15] V. Petricek, Y. Gao, P. Lee, and P. Coppens, Phys. Rev. B **42**, 387 (1990).
[16] V. Elser, Acta Crystallogr. A **42**, 36 (1986).
[17] M. de Boissieu, P. Stephens, M. Boudard, C. Janot, D. L. Chapman, and M. Audier, J. Phys. Condens. Matter **6**, 10725 (1994).
[18] C. Janot, M. de Boissieu, and M. Boudard, in *Proceedings of the International Conference on Aperiodic Crystals: Aperiodic '94*, edited by G. Chapuis and W. Paciorek (World Scientific, Singapore, 1996), pp. 491–504.
[19] S. Y. Qiu, C. R. Rowell, and M. V. Jaric, Comput. Phys. **10**, 154 (1996).