common for 1-periodic quasicrystals, which makes this classification particularly interesting. We have tried to express everything in a geometrically natural basis, in order to facilitate the determination of an experimentally observed space group by means of the extinction pattern, and we hope that the tables given in this paper will prove useful for the determination of experimentally observed space groups.

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EXACT EXPRESSION IN TERMS OF ELEMENTARY FUNCTIONS FOR A QUASICRYSTALLINE DIFFRACTION PATTERN

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ABSTRACT: We use a modified version of the usual "strip" projection method in order to obtain a simple and short derivation of the diffraction pattern for a three dimensional quasicrystal. We obtain the location and amplitude of the diffraction peaks using exact expressions in terms of elementary functions.

Three-dimensional icosahedral quasilattices can be obtained by intersecting a three-dimensional hyperplane with a six-dimensional cubic lattice.[1] By appropriate atomic decorations, i.e. by placing atoms at and around the quasilattice sites, one can obtain a quasicrystal. de Bruijn[2] first proposed this projection method in the context of two dimensional Penrose lattices. He intersected a five-dimensional simple cubic lattice with a two-dimensional plane and then projected the centers of the intersected cubes onto the plane.

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Diffraction patterns of icosahedral quasilattices have been studied by several authors.[3-9] The most widely used method is the so-called "strip" or "corridor" method which invokes a sharp cutoff. This method projects the points of $\mathbf{Z}^6$ ($\mathbf{Z}^5$) which are located inside a strip surrounding a 3(2)-dimensional plane. Here, $\mathbf{Z}$ denotes the set of integers. The usual choice for the particle density is given by a superposition of delta functions,[3-7] each one located at the vertices of an hypercube.

Here we use a finite Gaussian strip as a replacement of the usual finite strip method in order to obtain a very brief and simple derivation of the diffraction pattern. The peak locations and amplitudes are exactly expressible as elementary functions. This derivation is made for an arbitrary number of dimensions. To choose a Gaussian window with a delta function-type density is related to using Gaussian densities and taking a sharp cutoff.[9]

We denote by $\mathbf{R}$ an r-dimensional simple cubic lattice and by $\vec{n} = (n_1, n_2, \ldots, n_r)$, where each n_i is equal to an integer, an element of $\mathbf{R}$. Let $\mathbf{S}$ be an s-dimensional subspace of $\mathbf{R}$ spanned by the orthonormal basis $\vec{a}_{(i)}, i = 1, \ldots, s$. We assume that the subspace $\mathbf{S}$ passes through a given point $\vec{\gamma}$ in $\mathbf{R}$ (See Fig. 1).

The distance d from a point $\vec{x}$ in $\mathbf{R}$ to its projection u on $\mathbf{S}$ is given by

$$d^2 = |\vec{x} - \vec{\gamma}|^2 - \sum_{i=1}^{s} u_i^2 \tag{1}$$

with

$$u_i(\vec{x}) \equiv \vec{a}_{(i)} \cdot (\vec{x} - \vec{\gamma}) \tag{2}$$

where u_i describes the coordinates on $\mathbf{S}$ defined by the unit vector $\vec{a}_{(i)}$.

Instead of the usual strip-type projection methods, we now associate with each lattice point $\vec{n}$ in $\mathbf{R}$ a projection site u_i on $\mathbf{S}$ with an appropriate amplitude

$$\rho(\vec{n}) = \exp\left\{-\beta\left[(\vec{n} - \vec{\gamma})^2 - \sum_{i=1}^{s}\left(\vec{a}_{(i)} \cdot (\vec{n} - \vec{\gamma})\right)^2\right]\right\} \tag{3}$$

where $\beta^{-1/2}$ is a measure of the effective width of the gaussian corridor. The overall distribution is given by the sum of $\rho(\vec{n})$ over $\vec{n}$ with their locations at $\{u_i\}$. Unlike the usual projection methods, we now have an infinite number of projection sites $\{u_i\}$ in any finite region. Out of these infinite number of points, only a small number of them are of significant amplitude. Indeed, if we choose β appropriately, and ignore points with sufficiently small amplitude, we obtain a projected distribution very similar to those generated by the strip method.

The structure factor of the lattice points is obtained by taking the Fourier transform of $\rho = \sum_{\vec{n}} \rho(\vec{n})$, i.e.

$$\begin{aligned} A(\{k_i\}) &\equiv \sum_{\vec{n}} \rho(\vec{n}) \; e^{ik_m u_m} \\ &= \sum_{\vec{n}} \exp\left\{-\beta\left[(\vec{n} - \vec{\gamma})^2 - \sum_{i=1}^{s}\left(\vec{a}_{(i)} \cdot (\vec{n} - \vec{\gamma})\right)^2\right]\right\} e^{ik_m u_m(\vec{n})} \end{aligned} \tag{4}$$

where repeated indices indicate a sum, $u_i(\vec{n})$ is the coordinate of the projection of $\vec{n}$, and $\vec{k}$ is the wave vector. Using Poisson's summation formula,

$$\sum_{\vec{n}} g(\vec{n}) = \sum_{\vec{m}} \int_{-\infty}^{\infty} d^r\phi \;\; e^{-i2\pi\vec{m}\cdot\vec{\phi}} \; g(\vec{\phi}), \tag{5}$$

we can rewrite $A(\{k_i\})$ as

$$\begin{aligned} &\sum_{\vec{m}} \int_{-\infty}^{\infty} d^r\phi \; e^{-i2\pi\vec{m}\cdot\vec{\phi}} \\ &\quad \exp\left\{-\beta\left[(\vec{\phi} - \vec{\gamma})^2 - \sum_{i=1}^{s}\left(\vec{a} \cdot (\vec{\phi} - \vec{\gamma})\right)^2\right] + ik_m\vec{a}_{(m)} \cdot (\vec{\phi} - \vec{\gamma})\right\}. \end{aligned} \tag{6}$$

Replacing $\phi - \gamma$ by a new variable ϕ, we have

$$\begin{aligned} A(\{k_i\}) &= \sum_{\vec{m}} e^{-i2\pi\vec{m}\cdot\vec{\gamma}} \int_{-\infty}^{\infty} d^r\phi \\ &\quad \exp\left\{-\beta\left[\vec{\phi}^{\,2} - \sum_{i=1}^{s}(\vec{a}_{(i)} \cdot \vec{\phi})^2\right] + ik_m\vec{a}_{(m)} \cdot \vec{\phi} - i2\pi\vec{m} \cdot \vec{\phi}\right\}. \end{aligned} \tag{7}$$

To carry out (7), we introduce additional unit vectors $\vec{a}_{(j)}$, $j = s+1, \ldots, r$, which, together with $\vec{a}_{(i)}, i = 1, 2, \ldots, s$, form a complete set of orthonormal basis in $\mathbf{R}$. In the following, we denote $\vec{a}_{(i)} \cdot \vec{\phi}$ by ϕ_i, $\vec{a}_{(j)} \cdot \vec{\phi}$ by

ϕ_j, etc., where index i always runs from 1 to s and j from $s+1$ to r. Then, we have

$$\vec{\phi}^{\,2} - \sum_i (\vec{a}_{(i)} \cdot \vec{\phi})^2 = \vec{\phi}^{\,2} - \sum_i \phi_i^2 = \sum_j \phi_j^2,$$

$$\vec{m} \cdot \vec{\phi} = \sum_i m_i \phi_i + \sum_j m_j \phi_j,$$

$$d^r \phi = \prod_i d\phi_i \prod_j d\phi_j.$$

The integration over ϕ_i leads to a set of δ-functions, and the integration over ϕ_j leads to a gaussian in $\vec{m}$, giving

$$\begin{aligned} A(\{k\}) &= \sum_{\vec{m}} e^{-i2\pi\vec{m}\cdot\vec{\gamma}} \int \prod_i d\phi_i \prod_j d\phi_j \\ &\exp\left\{ -\beta \sum_j \phi_j^2 + ik_i\phi_i - 2\pi i(m_i\phi_i + m_j\phi_j) \right\} \\ &= \left(\frac{\pi}{\beta}\right)^{\frac{r-s}{2}} \sum_{\vec{m}} e^{-i2\pi\vec{m}\cdot\vec{\gamma}} \prod_i 2\pi\delta(k_i - 2\pi m_i) \exp\left\{ -\frac{\pi^2}{\beta} \sum_j m_j^2 \right\} \\ &= \left(\frac{\pi}{\beta}\right)^{\frac{r-s}{2}} \sum_{\vec{m}} e^{-i2\pi\vec{m}\cdot\vec{\gamma}} \prod_i 2\pi\delta(k_i - 2\pi\vec{a}_{(i)} \cdot \vec{m}) \\ &\exp\left\{ -\frac{\pi^2}{\beta} \left[\vec{m}^2 + \sum_i (\vec{a}_{(i)} \cdot \vec{m})^2 \right] \right\}. \end{aligned} \tag{8}$$

The location of the diffraction pattern spots is determined by the delta-functions, and the amplitude is a superposition of gaussians whose intensity depends on the distances from the $\vec{m}$'s to the projection space. Note that the diffraction pattern is, of course, independent of the initial $\vec{\gamma}$. The width of the dual (Fourier space) lattice corridor is inversely proportional to the width of the original lattice corridor. In Fig. 2, we have plotted a typical difraction pattern.

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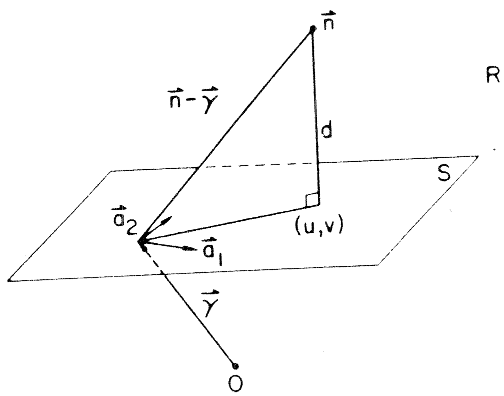

Figure 1: Schematic representation of the space **R** and its subspace **S** spanned by the orthonormal basis $\vec{a}_{(i)}$. The contribution of the point $\vec{n}$ to the intensity in **S** is proportional to $\exp(-\beta\, d^2)$, where d is the distance of $\vec{n}$ to the plane.

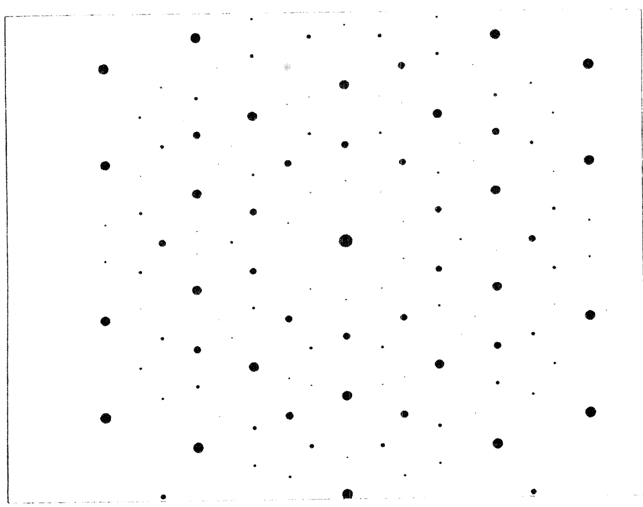

Figure 2: Diffraction pattern obtained from equation (8). The peaks above a given threshold are represented by circles with radii proportional to their amplitudes.

The Vertices of the Ideal 3-D Icosahedral Quasicrystal

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Abstract

The 24 possible vertex types of the ideal 3-D icosahedral quasicrystal are derived from the 6-D hypercubic lattice by dualization and klotz construction. We give a complete list of the vertices in an algebraic way as well as in the form of Schlegel diagrams.

Since the work of Shechtman et al. [15] the existence of quasicrystals has well been established. Therefore, it is of physical interest to study possible methods for the generation of quasiperiodic patterns.

In contrast to the situation in lattices or periodic packings, the local geometric structures of quasiperiodic patterns cannot be determined by just analyzing a fundamental domain. However, the more complex situation in a quasicrystal, if it is derived from a higher-dimensional lattice, can still be discussed completely.

One method for the generation of quasiperiodic patterns from higher dimensions is the procedure of dualization and klotz construction [13,12]. This method seems to be quite general in order to achieve a common framework in which one can hope to describe all relevant quasiperiodic scenarios. Furthermore, the dualization method provides the information encoded in the perpendicular space, especially the statistics for all objects in the quasiperiodic pattern.

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