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Average lattice and the long-wave length behavior of quasicrystals

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Abstract

Using the generalized dual method, close analytical expressions for the coordinates of the quasiperiodic lattice are given. This allows to define the lattice as an average plus a fluctuation part. The average is a superposition of crystalline lattices, and the dynamical structure factor or the diffraction pattern of the quasiperiodic structure can be expressed in terms of the average plus the fluctuation part. The average lattice dominates the response for long-wave modes of a probe particle or field, which is relevant in some recent application of quasiperiodic structures. The method can be extended for quasiperiodic grids, and is a very efficient algorithm to perform calculations in quasicrystals. Finally, the present approach can be used to define a Brillouin zone without ambiguities in the reciprocal space.

Keywords: Quasicrystals; Dynamic structure factor; Average lattice

Although quasicrystals are materials with a new kind of order, intermediate between periodic and disordered, many of their physical properties are not intermediate. In some cases, they behave as periodic systems, and in others as amorphous ones [1]. However, it is now clear that the electronic stabilization via the Hume–Rothery mechanism is fundamental in understanding the physics behind quasicrystals [2]. Within this mechanism, electrons are diffracted because the Fermi surface touches the Brillouin zone boundary—usually called Jones zone in a quasicrystal or disordered material—and a deep pseudo-gap is open at the Fermi energy [1]. In quasilattices, the problem arises when we try to define the first Brillouin zone, since formally the basis of the reciprocal space can only be established up to a scale factor [3]. Thus, this zone is defined in an empirical way by considering the most intense peaks in the diffraction pattern. Moreover, the importance of the Fourier space of quasilattices has been recently stirred after the advent of experiments on photonic band gaps in quasiperiodic arrangements of dielectric cylinders or holes drilled in a dielectric plate [4,5]. It is interesting to stress that in band gap experiments the first band gap appears when the wave-vector reaches the boundary of the first Brillouin zone (i.e. the wavelength is equal to twice the lattice parameter), consequently the main effect can be studied under a long-wave approximation. The importance of the diffraction pattern has been recognized even before the discovery of quasicrystals, and De Bruijn developed the so-called multigrid method to generate Penrose pattern vertex coordinates that further developments allowed to find the diffraction pattern of quasiperiodic lattices [1]. The multigrid method was later generalized to arbitrary quasilattices and was called *generalized dual method* (GDM) [6,7]. Although the ideas behind the computation of the lattice and its diffraction pattern were presented in many works [8,9], the determination of the points to be projected and their diffraction pattern are generally achieved numerically, since analytical expressions were not available [10]. The problem resides in the determination of the points that are inside the band, and in the determination of the Fourier transform of these called ‘acceptance domain’ (the projection of the strip onto the perpendicular space), which is a polytope in a space of more than three dimensions. As it will be shown, the method developed here allows us to unambiguously define a basis for the reciprocal space of the quasilattice, and is highly simplified under a long-wave approximation (which in our case requires wavelengths larger than the lattice parameter). It is also very useful for determining the response of a quasicrystal in an inelastic scattering experiment (dynamical structure factor). In some sense, the

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average lattice is a generalization of the observation made for the one-dimensional Fibonacci chain, where the positions can be written as an average lattice plus a fluctuation part [11], and in fact for 1D, Wolny independently developed the concept of an average unit cell of a quasiperiodic sequence, plus a fluctuation given in a probabilistic sense [12].

In the GDM, a quasiperiodic structure is obtained by the following steps [6,7]: construct a star of N basis vectors $\bar{e}_i$ which contains the rotational symmetry of the lattice to be constructed, build a set of parallel planes perpendicular to each of the star vectors, to obtain a grid. These planes satisfy:

$$\bar{r}\cdot\overline{e_i} = n_i + \alpha_i$$
$$\bar{r}\cdot\overline{e_j} = n_j + \alpha_j$$
$$\bar{r}\cdot\overline{e_k} = n_k + \alpha_k$$

where i, j and k are three different vectors, $\bar{r}$ is a vector in 3D, n_i, n_j and n_k are three arbitrary integers and the α's are real phases. The grid divides the space in open regions limited by planes. Each point in these spaces are indexed by a set of integers corresponding to its ordinal position in the grid (given by n_i) for each of the N directions defined by the star vectors. The regions generate N ordinal coordinates $(k_1,k_2,\ldots,k_N)$. A point in the quasilattice $(\bar{t})$ is obtained by making a dual transformation that maps each open region to a point in the quasiperiodic packing [6],

$$\bar{t} = \sum_{j=1}^{N} k_j\bar{e}_j$$

The problem of building the lattice is thus reduced to find the allowed combinations of the k_i. To solve this problem, we look at each of the possible solutions of the set of equations of the planes. Each solution, is a point where three planes intersect. Using the Kramer's rule, these solutions are of the form,

$$\bar{d}_{sjk} = (n_s + \alpha_s)\bar{u}_s + (n_j + \alpha_j)\bar{u}_j + (n_k + \alpha_k)\bar{u}_k$$

where the vectors u are defined as,

$$\bar{u}_{sjk} = \frac{\bar{e}_j \times \bar{e}_k}{\bar{e}_s\cdot(\bar{e}_j \times \bar{e}_k)} = \frac{\bar{e}_j \times \bar{e}_k}{V_{sjk}}$$

and V_{sjk} is the volume of a rhombohedra with sides $\bar{e}_s$, $\bar{e}_j$ and $\bar{e}_k$. Around this intersection, there are eight regions with ordinal coordinates that share the same ordinal positions with respect to the other grids different from s, j and k. These ordinal positions are given by the integer part (denoted by $\lfloor x \rfloor$) of the intersection point and the star vector,

$$k_l = \lfloor \bar{d}_{sjk}\cdot\bar{e}_l \rfloor + 1$$
$$= \left\lfloor (n_s + \alpha_s)\frac{V_{lsj}}{V_{sjk}} + (n_j + \alpha_j)\frac{V_{ljk}}{V_{sjk}} + (n_k + \alpha_k)\frac{V_{slk}}{V_{sjk}} \right\rfloor + 1$$

By using this result for making the dual transformation, we arrive at the following analytical expression for one of the vertices of a rhombohedra (where s, j and k take values from 1 to N),

$$\bar{t} = \sum_{n_s,n_j,n_k}\left(n_s\bar{e}_s + n_j\bar{e}_j + n_k\bar{e}_k + \sum_{l\neq s\neq j\neq k}(\lfloor \bar{d}_{sjk}\cdot\bar{e}_l \rfloor + 1)\bar{e}_l \right)$$

The other seven vertices are,

$$\bar{t}+\bar{e}_s, \bar{t}+\bar{e}_j, \bar{t}+\bar{e}_k, \bar{t}+\bar{e}_s+\bar{e}_j, \bar{t}+\bar{e}_s+\bar{e}_k, \bar{t}+\bar{e}_j+\bar{e}_k, \bar{t}+\bar{e}_s+\bar{e}_j+\bar{e}_k$$

Using these expressions, we can define an average lattice since the integer part satisfy the identity $x = \lfloor x \rfloor + \{x\}$, where $\{x\}$ is the fractional part of the number x. The advantage of this approach is that the fractional part is bounded and periodic with period one. As a result, we can define the quasilattice as the sum of an average lattice,

$$\langle \bar{t} \rangle = n_s\bar{a}_{sjk} + n_j\bar{a}_{jks} + n_k\bar{a}_{ksj} + \bar{R}$$

where $\bar{R}$ is a vector that shifts the lattice, and the basis vectors a are defined as,

$$\bar{a}_{sjk} = \bar{e}_s + \sum_{l\neq s\neq j\neq k}\frac{V_{lsj}}{V_{sjk}}\bar{e}_l$$

$$\bar{a}_{jks} = \bar{e}_j + \sum_{l\neq s\neq j\neq k}\frac{V_{ljk}}{V_{sjk}}\bar{e}_l$$

$$\bar{a}_{ksj} = \bar{e}_k + \sum_{l\neq s\neq j\neq k}\frac{V_{slk}}{V_{sjk}}\bar{e}_l$$

for each combination of s, j and k. The corresponding fluctuation part is,

$$\bar{f} = \sum_{l\neq s\neq j\neq k}\left(\frac{1}{2} - \{\bar{d}_{sjk}\ \bar{e}_l\}\right)\bar{e}_l$$

The importance of this development is seen when one calculates the response of the system to a probe particle or field with wave-vector $\bar{q}$ and frequency w, which is contained in the dynamic structure factor, defined as [13],

$$S(\bar{q},w) = -\frac{1}{N}\sum_{\bar{r},\bar{r}'} e^{i\bar{q}(\bar{r}-\bar{r}')}\,\mathrm{Im}\,G_{\bar{r},\bar{r}'}(w^2)$$

where $G_{\bar{r},\bar{r}'}(w^2)$ is the Green's function of the quasicrystal at sites $\bar{r},\bar{r}'$. By decomposing $\bar{r}$ as an average part, plus fluctuations, the exponential that contains the bounded fluctuations can be expanded in powers of $\bar{q}$,

$$S(\bar{q},w) = -\frac{1}{N}\sum_{\bar{r},\bar{r}'}\left(1 + i\bar{q}(\bar{f}-\bar{f}') - \frac{(\bar{q}\cdot(\bar{f}-\bar{f}'))^2}{2} + \cdots\right)$$
$$\times\, e^{i\bar{q}(\langle\bar{t}\rangle - \langle\bar{t}'\rangle)}\,\mathrm{Im}\,G_{\bar{r},\bar{r}'}(w^2)$$

The dominant response comes from the term of order zero, in which the average lattice gives the main contribution. Observe that the Green's function is still a function of $\bar{r}$, however, the small fluctuations are only shifts of the atom's equilibrium positions and for low frequencies, we expect to have a small impact in the dynamics of the system, which is governed by the Hamiltonian. As an example, the above statements indicate that the dispersion relation and the sound velocity for acoustic modes depends mainly on the average lattice parameters, defined by the basis vectors a. In this point it is worthwhile mentioning that in the 1D Fibonacci lattice, the speed of sound depends only on the average spacing between sites and the elastic constants [11].

The same approach can be used for elastic scattering experiments, like in a diffraction experiment. If we put a delta potential at each vertex of the quasicrystal, the structure factor is the Fourier transform of this potential, and using the concept of average lattice,

$$F(\bar{q}) = \sum_{\bar{r}} e^{i\bar{q}\bar{r}} = \sum_{\langle \bar{t} \rangle + \bar{f}} e^{i\bar{q}(\langle \bar{t} \rangle + \bar{f})}$$

Again we can expand the fluctuation term as a series in $\bar{q}$ or a Fourier series. However, in any case, the dominant response comes from the average lattice. Since this lattice is a superposition of crystalline lattices, this can serve as a definition of a Brillouin zone due to the periodicity of the exponential factor of the average. The most intense peaks in the diffraction pattern are given by the condition $\bar{q}(\langle \bar{t} \rangle) = 2\pi s$, where s is an integer. Another sets of peaks with less intensity are obtained when other powers of the wave-lengths and the fluctuations are considered. In conclusion, the average lattice is a useful tool in the long-wave length approximation, and allows to define a first Brillouin zone, and can be extended in a natural way to quasiperiodic grids that are used by the GDM, where the Fourier transform is not known.

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