Ferroelectrics, 305: 199–202, 2004

ISSN: 0015-0193 print / 1563-5112 online
DOI: 10.1080/00150190490462775

Phason Coherency in Real Space

GERARDO G. NAUMIS[1] and J. L. ARAGÓN[2]

[1]*Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000, México D.F.*
[2]*Centro de Física Aplicada y Tecnología Avanzada, Universidad Nacional Autónoma de México, Apartado Postal 1-1010, 76000 Querétaro, México*

(Received 2 September 2003; accepted 8 October 2003)

By considering fluctuations of a random phason field, we show that phasons defects are correlated in real space. This produces regions of the quasicrystal that are more stable than others against phason disorder. Analytical formulae for the stable and unstable parts of a quasilattice are provided, and a discussion about the physical consequences of this phenomenon is made.

Keywords Quasicrystals; phasons; cut and projection; thermal phasons

1. Introduction

Since a quasicrystal (QC) is obtained by projecting an hyperlattice in D dimensions into a real d dimensional space, the Fourier transform contains more reciprocal basis vectors than the dimension of the space, and there are extra $D - d$ degrees of freedom. A change in d of these phases produces phonons, while a change in the remaining phases produces local rearrangements of some atomic sites called phasons [1], which are diffusive modes with very large diffusive times [2]. As hydrodynamic modes, phasons are low-energy excitations. But also phasons correspond to rearrangements of sites that require jumps over local energy barriers (E_v), which can be large (nearly the energy for creating a vacancy). Although this seems to be contradictory, the picture depends upon the scale; at small scales, phasons are local jumps, but at macroscopic scales, symmetry and conservation laws determine the dynamics [1]. From the atomic point of view, phasons in real space should be considered as local defects with short-distance correlations. The hydrodynamic picture, however, suggests long-distance correlations, and if this is the case, the use of a hyperlattice description can be controversial [3]. In this work, we show that a random phason field produced in a hyperlattice can lead to a certain spatial correlation in the QC and, consequently, some parts of the QC are more unstable against phason disorder.

2. Regional Stability and Phasons

The main idea of the work can be easily explained by considering the Fibonacci chain (FC). In Fig. 1 we show the cut-and-projection scheme: a line $E^{\parallel}$ with irrational inclination $\alpha = (\sqrt{5} - 1)/2$ crosses a square lattice and the FC is obtained by projecting, onto $E^{\parallel}$, the points falling inside a band of width L. As usual, the space is subdivided into $E^{\parallel}$ and its orthogonal complement $E^{\perp}$, such that any point $\mathbf{r}$ is written as $\mathbf{r} = \mathbf{r}^{\parallel} + \mathbf{r}^{\perp}$. The coordinates of the FC are given by $x = \mathbf{r}^{\parallel} W(\mathbf{r})$, where $W(\mathbf{r}) = 1$ if $\mathbf{r}$ is inside the band and 0 otherwise. A

Address correspondence to Gerardo G. Naumis, Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000, México D.F. E-mail: naumis@fisica.unam.mx

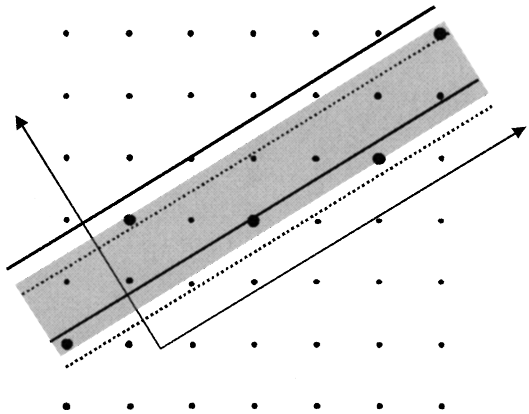

FIGURE 1 Schematic illustration of the cut and projection method. The strip (grey) is displaced along $E^{\perp}$ in two different directions: $+A$ (solid lines) and $-A$ (dashed lines). Unstable sites are represented by larger dots.

phason field is introduced by displacing the band along $E^{\perp}$ at each point $\mathbf{r}$, as shown in Fig. 1. The effect of this field in the coordinates of the FC can be written as: $x = \mathbf{r}^{\parallel} W(\mathbf{r} + \eta^{\perp}(\mathbf{r}))$, where $\eta^{\perp}(\mathbf{r})$ is the displacement of the band along $E^{\perp}$. The points where $\mathbf{r}^{\perp} \approx 0$ or $\mathbf{r}^{\perp} \approx L$ are closer to the limits of the band since $W(\mathbf{r} + \eta^{\perp}(\mathbf{r})) = W(\mathbf{r}^{\parallel} + \mathbf{r}^{\perp} + \eta^{\perp}(\mathbf{r}))$. These points are "unstable" under phason disorder since they can be dropped out the band even for a small $\eta^{\perp}(\mathbf{r})$. This observation holds for any phason field. For a slowly varying field the result is a modulation of a quasicrystal, but the most interesting effect is obtained when $\eta^{\perp}(\mathbf{r})$ is a random function. For example, if $\eta^{\perp}(\mathbf{r}) = A\chi(\mathbf{r})$, where A ($<1/2$) is the amplitude of the phason field, and $\chi(\mathbf{r})$ is a random variable uniformly distributed between $[-1/2, 1/2]$, the points with $\mathbf{r}^{\perp} \approx (L/2) \pm A$ are stable against this perturbation. This result has physical consequences since the thermal noise produces random fluctuations of the band and thus, at a certain temperature, there are always some lattice sites more stable than others (A should be of order $\bar{\lambda} \exp(-E_{\nu}/kT)$ where $\bar{\lambda}$ is the average separation of atoms). This example also suggests that a way to obtain the most stable lattice is by superposing the quasilattice with two displaced versions: one displaced by A, and the other one by $-A$. The stable points, under this perturbation, are those with the same coordinates in the three quasilattices. For the FC, the coherency of the unstable points can then be obtained as follows. The coordinates of the n-th vertex of the FC are given by [4]:

$$x_n = nL - (L - S)\lfloor n\alpha \rfloor = n\bar{\lambda} - (L - S)\{n\alpha\},$$

where $n \in \mathbf{Z}$, $\bar{\lambda} = (1 + \alpha)L - \alpha S$ is the average lattice parameter [4], L and S are the two possible separations of the quasilattice points, and $\{z\}$ is the fractional part of z. Since the saw-tooth function $\{n\alpha\}$ has period one if we apply a phason field, phasons are produced when

$$x_n' - x_n = (L - S)(\{n\alpha \pm A\chi((n, \lfloor n\alpha \rfloor))\} \mp A - \{n\alpha\}) = \pm(L - S).$$

The stable points satisfy $\{n\alpha \pm A\} = \{n\alpha\} \pm A$, or $A < \{n\alpha\} < 1 - A$. For the unstable points we have $\{n\alpha \pm A\} = \{n\alpha\} \pm A \pm 1$, that is, $0 \leq \{n\alpha\} \leq A$, and $1 - A \leq \{n\alpha\} \leq 1$. If $A \to 0$, the most unstable points satisfy $\{n\alpha\} \approx 0$ or 1, that is, $n\alpha \approx \lfloor n\,\alpha \rfloor$. If we approximate the golden mean as $\alpha \approx P/Q$, these points are obtained for $n = mQ$, $m \in \mathbf{Z}$. Thus, the unstable points are separated by Fibonacci numbers. In the general case $A \neq 0$, and for a uniform distribution of the random field in the unstable region, we have $p_{ph} = \left(|\{n\alpha\} - 1/2| - 1 + A\right)/A$, since $\|\mathbf{r}^{\perp}\|$ is the distance between the point $(n, \lfloor n\alpha \rfloor)$ and the line $y = \alpha x$.

The generalization to higher dimensions is straightforward by using the analytical formulae for quasilattices already reported [5]. To detect the stable sites, we should apply shifts A_l for each quasilattice direction. To simplify the expressions, however, we consider a uniform shift $\pm A$ of the window function. The coordinates of a three-dimensional QC, generated by the vectors $\mathbf{e}_l$, where $l = 1, \ldots, N$, with a shift in the window function, are given by

$$\mathrm{t} = \sum_{k<j<s}^{N} \left(\sum_{\gamma,\delta,\varepsilon=0}^{1} \sum_{n_s,n_j,n_k}^{\infty} ((n_s + \gamma)\mathbf{e}_s + (n_j + \delta)\mathbf{e}_j + (n_k + \varepsilon)\mathbf{e}_k \right.$$
$$\left. + \sum_{l \neq j \neq k \neq s}^{N} \left(\left\lfloor x_{n_s} \frac{V_{lsj}}{V_{sjk}} + x_{n_j} \frac{V_{ljk}}{V_{sjk}} + x_{n_k} \frac{V_{slk}}{V_{sjk}} - \alpha_l \mp A \right\rfloor + 1 \right) \mathbf{e}_l \right) \Bigg), \quad (1)$$

where l, j, k, s, n_s, n_j and n_k are integers, V_{lsj} is the volume defined by $V_{sjk} = \mathbf{e}_s \cdot (\mathbf{e}_j \times \mathbf{e}_k)$, α_l are real numbers that define a phase in each direction of the star vectors [5] and x_{n_s} is an abbreviation for $x_{n_s} = n_s - \alpha_s \pm A$. As in the one-dimensional case, the condition for the unstable points is inferred from (1) through an analysis of the floor function. After some algebra we get

$$\{R(n_s, n_j, n_k) \mp A\} = \{R(n_s, n_j, n_k)\} \mp A \pm 1,$$

where,

$$R = x_{n_s} \frac{V_{lsj}}{V_{sjk}} + x_{n_j} \frac{V_{ljk}}{V_{sjk}} + x_{n_k} \frac{V_{slk}}{V_{sjk}} - \alpha_l.$$

Thus $p_{ph} = (\{R(n_s, n_j, n_k)\} - 1/2 - (1 - A))/A$ is the probability of making a phason. By using 0, 1 to indicate the two different probabilities, we have that the unstable points satisfy

$$x_{n_s} \frac{V_{lsj}}{V_{sjk}} + x_{n_j} \frac{V_{ljk}}{V_{sjk}} + x_{n_k} \frac{V_{slk}}{V_{sjk}} - \alpha_l \approx \alpha_{n_s} \frac{V_{lsj}}{V_{sjk}} + \alpha_{n_j} \frac{V_{ljk}}{V_{sjk}} + \alpha_{n_k} \frac{V_{slk}}{V_{sjk}} - \alpha_l + 0, 1,$$

for the directions defined by $\mathbf{e}_s$, $\mathbf{e}_j$, with respect to the direction $\mathbf{e}_l$. These equations define "worm" planes, as they were called in plane tilings [6].

In conclusion, we have shown that even a random phason field produces a certain correlation in a QC, and the lattice is divided in stable and unstable regions. From the physical point of view, this fact has many consequences. For example, since the unstable regions sizes depend on the temperature, is clear that as we heat the quasicrystal, the structure of the stable regions is revealed. A similar effect has been observed in recent experiments [7], where well-correlated localized vibrations were observed in the real space of a decagonal quasicrystal. Also, since the worm planes are the natural channels to have diffusion, when the temperature is raised, the diffusion will increase due to the changes in the width of the channels. It also has implications ranging from the growth of the QC phase to the degree of structural refinement expected from the FT at a certain temperature, as we will show in future works.

Acknowledgment

We would like to thank DGAPA project IN-108502-3 for financial help.

References

1. P. J. Steinhardt and S. Ostlund, *The Physics of Quasicrystals*, World Scientific, Singapore (1987).
2. T. C. Lubensky, S. Ramaswamy, and J. Toner, *Phys. Rev. B* **32**, 7444 (1985).
3. D. M. Frenkel, C. L. Henley, and E. D. Siggia, *Phys. Rev. B* **34**, 3649 (1986).
4. G. G. Naumis, Ch. Wang, M. F. Thorpe, and R. A. Barrio, *Phys. Rev. B* **59**, 14302 (1999).
5. G. G. Naumis and J. L. Aragón, *Z. Kristallogr.* **218**, 397 (2003).
6. J. E. S. Socolar, T. C. Lubensky, and P. J. Steinhardt, *Phys. Rev. B* **34**, 3345 (1986).
7. E. Abe, S. J. Pennycook, and A. P. Tsai, *Nature* **421**, 347 (2003).