Phason disorder in 2D quasicrystals

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Equilibrium phason fluctuations in $2D$ quasicrystals stabilized by short-range forces are studied. Even if the quasicrystal is the ground state, the phason correlation function $\langle(\varphi(0)-\varphi(R))^2\rangle$ diverges, at arbitrarily low temperatures, no more slowly than as $\exp(-C\epsilon/T)\ln R$, where ϵ is a characteristic binding energy.

The model[1,2] of a quasicrystal described by a tiling of the space by two types of unit cells uses a special quasiperiodic alternation of these cells. If there is no regularity in this alternation, the model becomes that of a random quasicrystal. As it turns out, however, a random quasicrystal retains many features of a regular quasicrystal, in particular, singularities in the Fourier transform of the density (admittedly, these are power-law, rather than δ-function, singularities). The reason lies in the slow divergence of the phason correlation function[3,4]

$$\langle(\varphi(0)-\varphi(R))^2\rangle \sim \ln R. \qquad (1)$$

The phason coordinate φ is defined here in the same way as for a regular quasicrystal, through a rise into a multidimensional space.[3] This behavior of the correlation function corresponds to a contribution $\sim T(\nabla\varphi)^2$ to the free energy which is related to the phason gradient.

There can, however, be an intermediate situation: something which lies between a random quasicrystal and an ideal quasicrystal. Specifically, the alternation of unit cells in ideal quasicrystals can be carried out in accordance with local rules.[5,6] If we then assign a positive energy ϵ to each violation of the local rules, we see that the ground state in this model is an ideal quasicrystal. The region $T\gg\epsilon$ then corresponds to a completely random quasicrystal. In a situation of this sort a phason correlation function might assume a form at low temperatures which is different from (1). We will examine this point, making use of the circumstance that a plane quasicrystal may be thought of as a $2D$ section of a multidimensional crystal. If short-range forces stabilize an atomically smooth surface of an ordinary crystal at absolute zero, this atomic smoothness is retained over a finite temperature interval, up to the roughness transition.[7,8] In the case of a quasicrystal this result would mean that $\langle(\varphi(0)-\varphi(R))^2\rangle$ does not diverge even at nonzero temperatures. Our purpose in this letter is to demonstrate that this is not the case.

We begin by noting that the phason shift φ can be determined within an error $h\ll 1$ only within a region no smaller than $\sim h^{-1}$ in size (we are assuming the size of the unit cell to be 1). The reason is that the interchange of unit cells upon a uniform phason shift of h occurs on lines which are separated by a distance on the order of[5]

h^{-1}—this is a necessary condition for the existence of local rules. We will accordingly estimate a lower limit on the partition function of the defects which arise when there is a small phason gradient $\alpha = |\nabla \varphi|$. We can shrink the configuration space of the defects by requiring that this gradient be realized as a sequence of steps of height $h \ll 1$ which are separated by a distance h/α. We should accordingly choose $h/\alpha > h^{-1}$ or

$$h^2 > \alpha. \tag{2}$$

In this case the defects will lie at places where the steps intersect restructuring lines associated with the corresponding phason shift, i.e., at the boundaries of regions which have and have not become restructed (Fig. 1). Also requiring that the steps not be overly bent—e.g., requiring that they intersect straight lines running parallel to the restructuring lines only once—we find the following estimate of the partition function:

$$Z > \exp((-\epsilon/T)C'\alpha A)\zeta, \tag{3}$$

where A is the total area, C' is a number on the order of 1, and ζ is a combinatorial factor, i.e., the number of different arrangements of defects. The quantity $C'\alpha A$ limits the total number of defects in this case. The steps themselves are "observable" only in regions where they intersect restructuring lines, i.e., where the requirements of the local rules are not met, and a defect arises. Furthermore, the quantity ζ can also be estimated from

$$\zeta > \exp(s_0\alpha A)(1/h)^{C''\alpha A}. \tag{4}$$

The first term here gives us the number of topologically different positions of the steps among the restructuring lines, the second arises because for a given topology of steps

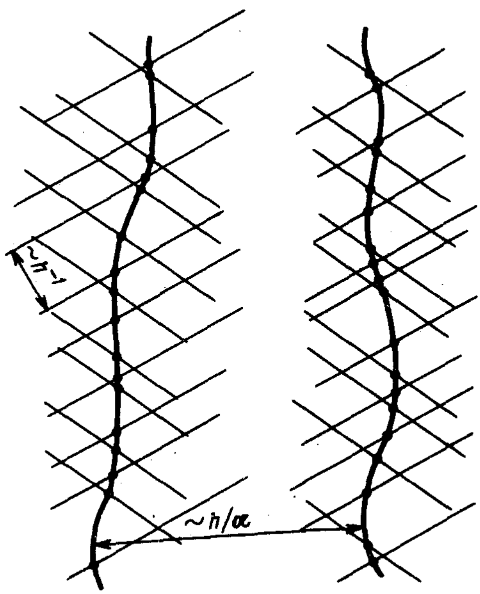

FIG. 1. Phason steps of height h and restructuring lines which arise upon a corresponding shift (only two families are shown). The circles show the positions of defects.

and restructuring lines each defect can independently assume $\sim h^{-1}$ positions (Fig. 1). We also note that the quantity s_0 is finite at $h/\alpha > h^{-1}$. Choosing h^2 to be greater than α by only a finite factor, we find

$$Z > \exp(\alpha A[(-C'\epsilon/T + s_0) + (C''/2)\ln\alpha]) \qquad (5)$$

or

$$F/A < \alpha[(\epsilon C' - Ts_0) - (TC''/2)\ln\alpha]. \qquad (6)$$

We thus see that at any arbitrarily low temperatures there are phason gradients $\alpha \sim \exp(-C\epsilon/T)$ of such a magnitude that the free-energy density is negative. The "typical" phason gradient in regions of size $\sim \exp(C\epsilon/2T)$ (or h^{-1}) should be on the same order of magnitude. Over distances much greater than h^{-1} the phason gradients fluctuate independently, since the interface between regions with different gradients does not correspond to any excess energy (there is nothing at all that sets this interface apart from others). Again, therefore, the problem takes the form of the problem of a totally random quasicrystal, with the one distinction that the smoothing begins at phason gradients on the order of $\exp(-C\epsilon/T)$. As a result, we find the following behavior for the phason correlation function:

$$\langle(\varphi(0) - \varphi(R))^2\rangle \sim \exp(-C\epsilon/T)\ln R/R_c, \quad R_c \sim \exp(C\epsilon/2T). \qquad (7)$$

In conclusion we need to comment on the nature of the defects which we have been discussing here. Expression (4) shows that most of the configuration space under consideration here is occupied by a region which satisfies the condition $h^2 > \alpha$ most poorly. This circumstance means that real defects do not correpsond to any stepped phason shift and are not line defects. If the defect density is low, each defect is capable of moving only along some restructuring line associated with it. This result means that defects are not point defects in the ordinary sense of the term. Despite these distinguishing features, which make a topological classification of these defects impossible, these defects are nonremovable.

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