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Friction in aperiodic crystals *

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Abstract

Aperiodic crystals may show low lying excitations related to the possibility of describing these structures in a higher-dimensional space. These phasons and their non-linear extensions are discussed. Conditions are given under which a sliding with low dissipation may occur.

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1 Introduction

Recent experiments have shown that the friction on the surface of a quasicrystal may be very low. A natural question then is what is the role of the aperiodicty in this phenomenon. This question leads back to properties of other aperiodic crystals where zero frequency modes have been reported besides the well known uniform acoustic modes ($\vec{k} = 0$). The additional zero frequency modes are strongly related to the possibility of describing aperiodic crystals in a higher-dimensional space. The zero frequency modes are similar to new hydrodynamic modes in this space.

An aperiodic crystal is defined as a structure that shows in its diffraction pattern sharp Bragg peaks on positions of a Fourier module, which is a

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generalization of the reciprocal lattice. The positions of the Bragg peaks are

$$\vec{k} \;=\; \sum_{j=1}^{n} h_j \vec{a}_j^* \qquad \text{(integer } h_j\text{)}. \tag{1}$$

Here the vectors $\vec{a}_j^*$ form a basis of the module. The minimum number of basis vectors n is called the rank of the module. If $n = 3$, the module is a reciprocal lattice but if $n > 3$, the structure does not have lattice periodicity. It is aperiodic. Examples of such structures are abundant: modulated crystal phases of minerals, intercalated compounds, inclusion compounds and quasicrystals. The positions of the atoms in a modulated crystal phase are given by

$$\vec{r}_{\vec{n},j} \;=\; \vec{n} + \vec{r}_j + \vec{f}_j(\vec{q}.\vec{n}), \tag{2}$$

where $\vec{n}$ is a vector of a 3-dimensional lattice, $\vec{r}_j$ is the position of atom j in the unit cell and $\vec{f}_j$ is a periodic function with the period 1. A composite structure has two (or more) subsystems which are modulated phases, such that the lattices are mutually incommensurate and the displacement function $\vec{f}$ of one subsystem has the periodicity of other subsystem(s).

Aperiodic crystals of a rank $n > 3$ may be embedded into a n-dimensional space such that the 3-dimensional aperiodic structure is the restriction of a periodic structure in n dimensions with the physical space. For this reason one considers the basis vectors $\vec{a}_j^*$ of the module as projections from n basis vectors $(\vec{a}_j^*, \vec{b}_j^*)$ of an n-dimensional reciprocal space:

$$\vec{k} \;= \pi \vec{k}_{\rm s} \;=\; \pi \sum_{j=1}^{n} h_j (\vec{a}_j^*, \vec{b}_j^*). \tag{3}$$

If the density of the aperiodic 3-dimensional structure is $\rho(\vec{r})$, then a periodic function in n dimensions is defined by

$$\rho(\vec{r}) = \int \hat{\rho}(\vec{k}) \exp(i\vec{k}.\vec{r}) {\rm d}\vec{k} \;\rightarrow\; \rho(\vec{r}, \vec{r}_{\rm I}) = \int \hat{\rho}(\pi\vec{k}_{\rm s}) \exp(i\pi\vec{k}_{\rm s}.(\vec{r}, \vec{r}_{\rm I})) {\rm d}\vec{k}_{\rm s}. \tag{4}$$

Point atoms in this approach are embedded as $(n-3)$-dimensional objects (called atomic surfaces) in n-dimensional space. A simple example is the embedding of the modulated phase, which becomes

$$(\vec{n} + \vec{r}_j + \vec{f}_j(\vec{q}.\vec{n} + t), \quad t).$$

This is a periodic array of lines left invariant by the lattice generated by the 4 vectors $(\vec{a}_j, -\vec{q}.\vec{a}_j)$ $(j = 1, 2, 3)$, and (0,1).

A similar embedding of a composite gives two arrays of lines,

$$\left(\vec{n} + \vec{r}_j + Z_1 t + \vec{f}_j(\vec{q}_2.\vec{n} + t,\ t\right)$$

for one subsystem and

$$(\vec{m} + \vec{r}_k - Z_2 t + \vec{g}_k(\vec{q}_1.\vec{m} - t), t)$$

for the other, where $\vec{n}$ and $\vec{m}$ are lattice vectors of the basic structures, and $\vec{q}_j$ belongs to the reciprocal lattice of subsystem j. The two arrays together have a lattice periodicity.

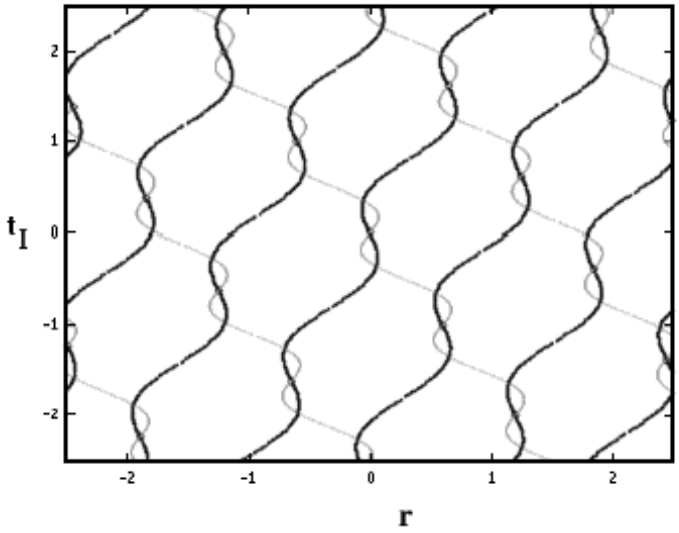

Figure 1: Embedding of the ground state of an incommensurate composite.

2 Phasons

The projection of the n-dimensional lattice on the additional space forms a dense set. Otherwise the 3-dimensional structure would be periodic. This means that there is a dense set of values of the argument t in the modulation functions for which all mutual distances of the atoms are the same. The ground state has an infinite degeneracy. If the modulation functions are continuous, the potential energy does not depend on the 'phase variable' t

and this, in turn, implies the existence of a zero frequency mode connected to this continuous degeneracy. Phonons that have such a character (with possibly slowly spacial variations) are expected to have a low frequency. Due to a possibility of describing them in terms of the phase oscillations, they are called phasons.

The frequency of the phonons, which can be considered as 'phasons', is zero. However, phonons are the solutions of the linear dynamical problem in the crystal. A phason is a shift of the modulation function for increasing amplitude implying also non-linear terms. The same holds for the sliding mode of an incommensurate composite as well. The question is whether there are large amplitude non-linear oscillations with a low frequency, just as there are low-frequency oscillation corresponding to other hydrodynamic, namely acoustic, modes. Below we will study linear and non-linear dynamics of quasiperiodic structures for two different models.

3 Phasons and phase waves in modulated crystals

A simple model for an incommensurate modulated phase is the discrete frustrated ϕ^4 (DIFFOUR) model [1]. We assume a tetragonal crystal with one particle per unit cell to have one degree of freedom for each atom, which is not necessarily a displacement. It has an on-site potential, harmonic interactions between first neighbours and harmonic interactions between second neighbours along the unique axis. The Hamiltonian is

$$H = \sum_n \left(\frac{p_n^2}{2} - a\frac{x_n^2}{2} + \frac{x_n^4}{4} + \sum_{n'} x_n x_{n'} + d\sum_{n"} x_n x_{n"} \right). \qquad (5)$$

Depending on the parameters a (characterising the depth of the double well at the site) and d (characterising the ratio between 1st and 2nd neighbour interaction), the ground state may be periodic $x_n = x_{n+N}$ or quasiperiodic $x_n = f(q.n)$. Typically, for a fixed d one finds a sequence of phases at the increase of a. For $a < a_i$ the solution is trivial ($x_n = 0$), for $a_i < a < a_c$ it is incommensurate, and for $a > a_c$ the solution is a superstructure (periodic with the period N). The wave number q of the modulation, generally, changes and acquires also commensurate values, for which one may calculate the phonons in the standard way. The first result is that, in general, there is a value a_d such that for $a_i < a < a_d$ there is a phonon with zero frequency and eigenvector proportional to the derivative of the modulation function. For $a_d < a < a_c$ there is a 'phason gap'.

The calculated modulation function is continuous for the values of a for which no phason gap exists. At $a = a_d$ the gap opens simultaneously with the appearance of discontinuities in the modulation function. This proves the first conjecture.

To check whether there are hydrodynamic waves, it is convenient to replace the non-linear equations of motion by their continuum approximation. The Lagrangian in this approximation is

$$L = \int \left(\frac{\dot{x}(z)^2}{2} + a\frac{x(z)^2}{2} - \frac{x(z)^4}{4} - \sum x(z)x(z \pm c) - \sum dx(z)z(z \pm 2c)\mathrm{d}z \right). \tag{6}$$

The Euler-Lagrangian equation for this Lagrangian has a solution $f(x_n) = f(nc - vt)$ for a small amplitude of the modulation function if

$$v^2 \; < \; -2 - 8d.$$

Whether this remains true for a discrete system, can be checked by solving the non-linear equations of motion taking as initial conditions the positions in the ground state and the velocities proportional to the derivative of the modulation function. The result is that for an initial speed below a critical value the speed remains constant, but when the speed exceeds this critical value, dissipation occurs [2].

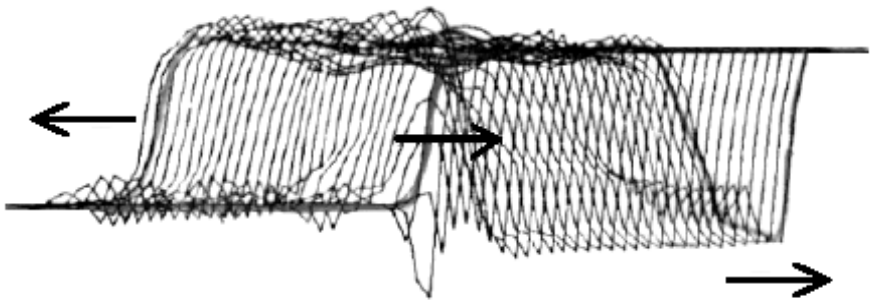

Figure 2: Moving domain wall in the DIFFOUR model for a high initial velocity. The domain wall (centre) starts and transforms into a domain wall doublet moving to the right and a single domain wall moving to the left.

Near the transition to the superstructure the modulation function is no longer of almost sinusoidal form. If we consider a transition at a_c to a structure with $N = 2$, the variable x_n can be written as the product

$x_n = (-1)^n Q_n$, where Q_n is a slowly varying function. One can also use a continuum approximation and derive a differential equation for the function $Q(z)$. It has a solitary wave solution

$$Q(z) = \sqrt{a+2-2d}\tanh\left((z-z_0-vt)\sqrt{\frac{a+2-2d}{4-8d-2v^2}}\right).$$

This solution having the shape of a domain wall. This solution is again used as initial configuration for the numerical solutions of the non-linear equations of motion. For small values of v there is, indeed, a motion without the loss of energy. For higher values of v energy is lost by creation of phonons, and at even higher values the domain wall may decompose into 2 walls moving in the original direction and one in the opposite direction. A speed range also exists, in which the dissipation is low. We note that the model is a Hamiltonian system with conserved energy. Dissipation here means the energy transfer from the initial mode to phonons.

4 Phasons and sliding in composites

A simple model for incommensurate composites, in which one can verify the conjectures concerning phasons, is the double chain model (DCM) [3]. It has two parallel chains with atoms at the positions x_n in the first chain, and y_m in the second one. The potential energy is

$$V = \sum_n V_1(x_n - x_{n-1}) + \sum_m V_2(y_m - y_{m-1}) + \lambda \sum_{nm} V_3(x_n - y_m). \quad (7)$$

Here the interaction potentials are the Lennard-Jones potentials. The lattice constant of the first chain for $\lambda = 0$ is a, that for the second chain is b. The ground state is formed by two modulated chains, with the modulation periodicity of the modulation of the first chain is b and that of the second chain is a.

For $\lambda < \lambda_c$ both modulation functions are continuous, for $\lambda > \lambda_c$ they are discontinuous. By taking commensurate approximants with lattice constants a_k and b_k such that $\lim_{k\to\infty} a_k/b_k (= L_k/N_k) = a/b$, phonons may be calculated as the limit of phonons of the approximants, which gives the following result. For $\lambda = 0$ there are two zero-frequency modes corresponding to linear combinations of the acoustic modes of the two chains. For $0 < \lambda < \lambda_c$ there are 2 modes with $\omega = 0$ as well, which are linear combinations of the mode where all atoms have the same displacement, and the

sliding mode in which the two chains move with respect to each other. For $\lambda > \lambda_c$ a gap between the two modes opens up. Therefore, there is a sliding mode for continuous modulated subsystems.

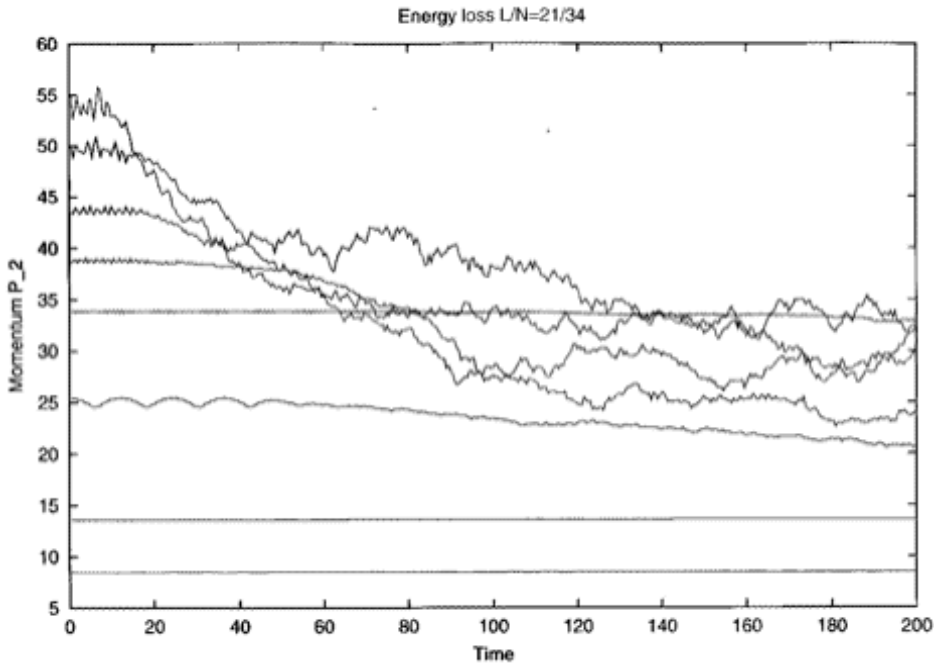

Figure 3: Momentum of one chain in the DCM as the function of time for various initial velocities.

The non-linear equations of motion may be integrated numerically. We give here a short overview of the results. In the regime $\lambda < \lambda_c$, where there is a sliding mode of zero frequency, integration of the non-linear equations of motion with the initial condition corresponding to a relative motion of the chains with a velocity $v < v_c$, results in a motion with little dissipation. The initial momentum is conserved with good accuracy, except for some cases. For the speed causing the frequency experienced by one chain moving over the other (the 'washboard frequency') to be equal to the frequency of a phonon with a wave vector belonging to the Fourier module, a resonance occurs. After initial oscillations, dissipation becomes important. For a speed exceeding v_c, dissipation sets in immediately. For $\lambda > \lambda_c$ there is no dissipationless regime [4].

5 Concluding remarks

Aperiodic crystals with a smooth embedding demonstrate zero frequency phason modes. In that case the phase waves may travel through the system with little dissipation, provided that the initial speed is below a critical value. For discontinuous embedding there is a phason gap and the critical speed is zero. Quasicrystals have disjunct pieces of embedding (atomic surfaces). Therefore, dissipation is always present and phasons will be strongly damped. A different situation may occur for a crystal moving over a quasicrystalline surface. Depending on the interaction between the crystal and the substrate, there may be a regime with little dissipation, i.e. with low friction. The situation for higher dimensions is more complicated, because the transversal and longitudinal motions may be coupled.. This has not been discussed here. Work on this, and other important features, such as the role of electrons and defects, is in progress.

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