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Phasons, sliding modes and friction

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Abstract. Aperiodic crystals may have additional low frequency modes related to the possibility to describe them in a higher-dimensional space. Dynamics associated with these degrees of freedom is called phasonic, but there are very different phenomena of this type. A discussion is given of the use of the term. The relation between phason modes, the crystal structure, and the modulation and sliding modes is discussed. Finally a relation with frictionless motion is studied.

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1 Introduction

Quasiperiodic crystals are systems with sharp diffraction spots on the positions of a Fourier module: its wave vectors $\mathbf{k}$ satisfy

$$\mathbf{k} = \sum_{i=1}^{n} h_i \mathbf{a}_i^*, \tag{1}$$

where h_i are integers. The vectors $\mathbf{a}_i^*$ span the physical reciprocal space. If the minimal value of n is larger than the physical dimension the structure is aperiodic. n is the rank of the module.

Such quasiperiodic structures can be seen as intersections of periodic structures in n dimensions and physical space. The periodic structure is constructed as follows. Consider every vector $\mathbf{k}$ of the Fourier module as the projection of a reciprocal lattice vector $\mathbf{k}_\mathrm{s} = (\mathbf{k}, \mathbf{k}_\mathrm{I})$ in n dimensions into physical space. The components $\mathbf{k}_\mathrm{I}$ belong to the internal or perpendicular space. If $\hat{\rho}(\mathbf{k})$ is the Fourier transform of the density of the system, the density function

$$\rho_\mathrm{s}(\mathbf{r}, \mathbf{r}_\mathrm{I}) = \sum_{\mathbf{k}} \hat{\rho}(\mathbf{k}) \exp\left(\mathrm{i}(\mathbf{k}\cdot\mathbf{r} + \mathbf{k}_\mathrm{I}\cdot\mathbf{r}_\mathrm{I})\right) \tag{2}$$

is lattice periodic in n dimensions with as lattice Σ the direct lattice associated with the reciprocal lattice Σ^* of vectors $(\mathbf{k}, \mathbf{k}_\mathrm{I})$. Notice that $\rho_\mathrm{s}(\mathbf{r}, 0)$ is the density in the physical space. The information about the structure in the aperiodic crystal is mapped into the unit cell in n dimensions, but the information is exactly equivalent with that in physical space.

Examples of aperiodic crystals are incommensurate modulated structures, incommensurate composites and quasicrystals. If one constructs the embedding as mentioned above, the atom positions in physical space correspond to points of $(n-3)$-dimensional objects in the n-dimensional unit cell (or in the periodic n-dimensional structure). These objects are called atomic surfaces.

The projection of the n-dimensional lattice Σ of the periodic structure on the internal space is dense. If $(\mathbf{a}, \mathbf{a}_\mathrm{I})$ belongs to the lattice this implies

$$\rho_\mathrm{s}(\mathbf{r}, \mathbf{r}_\mathrm{I}) = \rho_\mathrm{s}(\mathbf{r} + \mathbf{a}, \mathbf{r}_\mathrm{I} + \mathbf{a}_\mathrm{I}) \tag{3}$$

for a dense set of vectors $\mathbf{a}_\mathrm{I}$. This means that a shift of $\mathbf{a}_\mathrm{I}$ in internal space gives the same density function in physical space shifted over a vector $\mathbf{a}$. Generally, the length of $\mathbf{a}$ is large for small values of $\mathbf{a}_\mathrm{I}$, but the result is just a shift of the whole crystal which leaves all distances invariant, and consequently the energy does not change. Therefore, the ground state of the aperiodic crystal is infinitely degenerate. Because the internal space for modulated structures corresponds to the space of phases of the modulation function(s) such a displacement in internal space is often called a phase mode. If the atomic surfaces are smooth the shifts in atomic positions for such a displacement are continuous which implies that an infinitesimally slow phase motion does not cost energy. This means that there is a zero frequency excitation. For a smooth modulation function the eigenvector of the corresponding mode is given by the derivative of the modulation function. It is sometimes called a phason.

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In this paper the following points will be discussed:

1. The term 'phason' is often used in an indiscriminate way. Can a more precise terminology be used?
2. The relation between phase modes of zero frequency and the continuity of the embedded structure in higher dimensions.
3. A zero frequency acoustic mode may have an arbitrary amplitude. Does the same hold for the zero frequency phase modes?

In Section 2 phason modes in incommensurate phases and composites are introduced. In Sections 3 and 4 the linear phasons and the ground state are studied on the so called DIFFOUR model. In Section 5 the non-linear phason dynamics for this model is discussed. In Sections 6 and 7 the linear and non-linear dynamics for composites is discussed in the framework of a double chain model (DCM). The results remind those of the DIFFOUR model, but the situation is more complicated. In Section 8 it is argued that the phason dynamics of quasicrystals is similar to that of incommensurate composites when the atomic surfaces are disjoint. In all systems phasonic motion occurs, and the term is used in various ways. This is discussed mainly in Sections 2 and 8. Finally a discussion is given in Section 9.

2 Phason modes

The zero frequency excitations besides the acoustic modes can be considered as uniform fluctuations in the additional space. One may describe them as well in physical three-dimensional space. We make a distinction between modulated crystal phases, composites and quasicrystals. A displacively modulated crystal is obtained from a lattice periodic structure by a periodic static displacement wave. In a one-dimensional system the positions of the atoms in the ground state are given by

$$x_{n,j} \;=\; x_0 + r_j + na + f_j(x_0 + r_j + na), \qquad (4)$$

where r_j gives the positions in the unit cell of the basis structure, a is the lattice constant of the basic structure, and f_j is a periodic displacement function with a period b that is incommensurate with a. Such a structure may have two zero frequency modes. One is the acoustic mode given by the displacement

$$x_{n,j} \to x_{n,j} \;+\; \delta, \qquad (5)$$

and the other is due to the incommensurability. It is given by

$$x_{n,j} \to x_{n+p,j} - pa \;\approx\; x_{n,j} + \epsilon f_j'(x_0 + r_j + na), \qquad (6)$$

where $pa - qb = \epsilon$ is a small integer combination of a and b, such that the fraction p/q is an approximant of the irrational number b/a. If the derivative of the modulation function exists, the motion does not require energy and the excitation has zero frequency.

Composite structures consist of two or more modulated subsystems with mutually incommensurate basic structure. For the case of 2 subsystems in one dimension the positions are given by

$$x_n = x_0 + na + f(x_0 + na), \qquad f(x) = f(x+b) \quad (7)$$
$$y_m = y_0 + mb + g(y_0 + mb), \qquad g(y) = g(y+a). \quad (8)$$

Here we consider for simplicity the case that each chain has only one atom per unit cell of length a, respectively b. Also in this case there may be two zero frequency modes. One is given by the displacements

$$x_n \to x_n + \delta, \qquad y_m \to y_m + \delta, \qquad (9)$$

and the other by

$$x_n \to x_{n+p} - pa \approx x_n + \epsilon f'(x_0 + na) \qquad (10)$$
$$y_m \to y_{m+q} - pa \approx y_m - \epsilon(1 + g'(y_0 + mb)). \quad (11)$$

Again the integer combination $\epsilon = pa - qb$ in the latter can be chosen to be (arbitrarily) small because of the incommensurability. The zero frequency mode corresponding with this has the same character as a phason mode and exists if the functions f and g are smooth, as will be discussed in the sequel. Because one subsystem moves with respect to the other it is also sometimes called a sliding mode. The two modes (acoustic and phason) are degenerate.

A zero frequency mode is a linear combination with arbitrary values of δ and ϵ. Among all possibilities we choose to call a mode the phason mode if it conserves the centre of gravity according to

$$\delta = \frac{\rho_2}{\rho_1 + \rho_2}\epsilon,$$

where ρ_i is the mass density of the ith subsystem. The uniform displacement and the phason mode are perpendicular with respect to the usual metric imposed by the dynamical matrix.

For quasicrystals there is also the same degeneracy: the energy is invariant under a rigid displacement in both physical and the additional (perpendicular) space. However, a zero frequency mode does not exist because the motion in additional space is associated with finite jumps in physical space, to be compared with the finite jumps occurring when a discontinuous modulation wave moves through a modulated or composite structure.

The acoustic modes and phason modes discussed so far correspond to rigid translations in physical space and in additional space, respectively. If the displacements depend on the physical coordinate as plane waves the phonons and phasons get a finite wave vector. For modulated crystals

$$x_{n,j} \to x_{n,j} + \epsilon(kna) f_j'(x_0 + r_j + na), \qquad (12)$$

and for composites

$$x_n \to x_n + \delta(kna) + \epsilon(kna) f'(x_0 + na) \qquad (13)$$
$$y_m \to y_m + \delta(kmb) - \epsilon(kmb)(1 + g'(y_0 + mb)), \qquad (14)$$

for slowly varying periodic functions ϵ and δ with period 1. The frequency then, generally, depends on that

wave vector and this dependence is given by the dispersion relations $\omega(k)$. The branches starting from zero then are also called acoustic modes and phason modes, respectively. They can be seen in the dynamical structure factor [1]

$$S(\mathbf{q},\omega) \sim \sum_{\text{modes } \nu} \exp(-W_\nu(\mathbf{q})) \times \sum_{n,j} |\mathbf{q}\cdot\mathbf{e}(\nu,n,j)| \exp\left(\mathrm{i}\mathbf{q}\cdot\mathbf{n}\right). \quad (15)$$

Here $\mathbf{e}(\nu,n,j)$ is the component of the eigenvector of the mode ν corresponding to particle j in unit cell n. In lattice periodic crystals the dispersion curves are seen as emanating from all (evenly spaced) Bragg peaks. In aperiodic (quasiperiodic) crystals the Bragg peaks occur on a dense set. Although the Bragg peaks form a dense set, and from each Bragg peak emerge two branches, the intensities of these two branches strongly depend on the crystallographic indices. Thus, phonon branches are visible only on a discrete set of peaks. The relation between intensities of branches and crystallographic indices can be used to assess the type of interaction and eventually distinguish between various classes of aperiodic crystals [2].

Here we call "phasons" elementary excitations of low or even zero frequency with eigenvectors that locally can be seen as a displacement in perpendicular space. Just as phonons these may be extended or localized, and they may be damped.

3 Phasons in modulated phases

Elementary excitations in quasi-periodic crystals can be studied in simple models. Crystals with competing interactions may show a soft mode with incommensurate wave vector, and the appearance of an incommensurate modulated phase. Models for such incommensurate phase transitions are the DIFFOUR (discrete frustrated ϕ^4) models [3]. The simplest one is a linear chain of particles with displacements x_n from an equidistant array na, with potential energy given by

$$V = \sum_n \left(\frac{A}{2}x_n^2 + \frac{1}{4}x_n^4 + Bx_nx_{n-1} + Cx_nx_{n-2} \right). \quad (16)$$

The ground state of such a system is given by the solutions of

$$\frac{\partial V}{\partial x_n} = Ax_n + x_n^3 + B(x_{n-1}+x_{n+1}) + C(x_{n-2}+x_{n+2}) = 0. \quad (17)$$

For high enough values of A the only solution is the unmodulated chain with $x_n = 0$. For this solution small deviations from equilibrium give phonons with a dispersion relation

$$m\omega^2 = A + 2B\cos(ka) + 2C\cos(2ka) \quad (18)$$

which has a minimum for

$$\cos(k_\mathrm{i}a) = -B/4C, \quad (19)$$

provided $|B/4C| \leq 1$. Otherwise, the minimum is at $k_\mathrm{i} = 0$ or $k_\mathrm{i} = \pi/a$. In general the value of k_i is incommensurate. The value of ω_k^2 at the minimum becomes zero for a critical value A_i given by

$$A_\mathrm{i} = 2C + B^2/(4C). \quad (20)$$

For values $A < A_\mathrm{i}$ the trivial solution is unstable and there appears a new ground state which is a modulated phase with wave vector equal to k_i, generally in an incommensurate position in the Brillouin zone. For values of A just below A_i this modulation function is smooth.

The soft modes at $\pm k_i$ are degenerate. For $A < A_\mathrm{i}$ they combine into two new excitations called the amplitude and the phase mode, or amplitudon and phason. The latter has the character described by equation (12). In the region with smooth modulation function the phason mode has an eigenvector that is the derivative of the modulation function, and its frequency is zero. This is connected with the degeneracy of the ground state: the phase of the modulation function is free. Therefore, a motion of the modulation function with respect to the lattice with infinitesimal speed will not cost any energy.

We check this numerically. An appropriate re-scaling of the coordinates and the energy leads to the potential energy

$$V = \sum_n \left(\frac{x_n^4}{4} - \frac{cx_n^2}{2} + (x_n - x_{n+1})^2 + d(x_n - x_{n+2})^2 \right), \quad (21)$$

where c and d are the new model parameters. For negative values of d the ground state of the system may be incommensurate. The basic structure has a lattice parameter equal to a. Notice that the change of parameters from A, B, C to c, d is such that A and c have opposite sign.

For the numerical study chains with 557 particles were used for several values of c and for $d = -0.4$. Periodic boundary conditions were taken. In the first step, the minimal-energy configuration was determined. It is a modulated structure with a period $b = 557a/79 \approx 7.05$ atoms.

The spectrum of the elementary excitations is given by the eigenvalues $\lambda_j = m\omega_j^2$ of $\partial^2 V/\partial x \partial x$. The lowest frequency $\omega_0 \approx 10^{-5}$ for $c < 0.5$ is small but non-zero because of the finite size. The corresponding eigenvector is proportional to $f'(x)$. Figure 1 shows the initial part of the spectrum. At $c = 0$ and $c = 0.5$ the dispersion is linear. However, the density of states is higher at $c = 0.5$. The value of $\int f'(z)^2 \mathrm{d}z$ is larger and the phason velocity smaller. At the critical value of c the modulation function becomes discontinuous, and the phason velocity vanishes. A gap forms at larger c, as illustrated in Figure 1.

4 The discommensuration transition

The discussed transition from a continuous to a discontinuous modulation function implies that the atomic surfaces

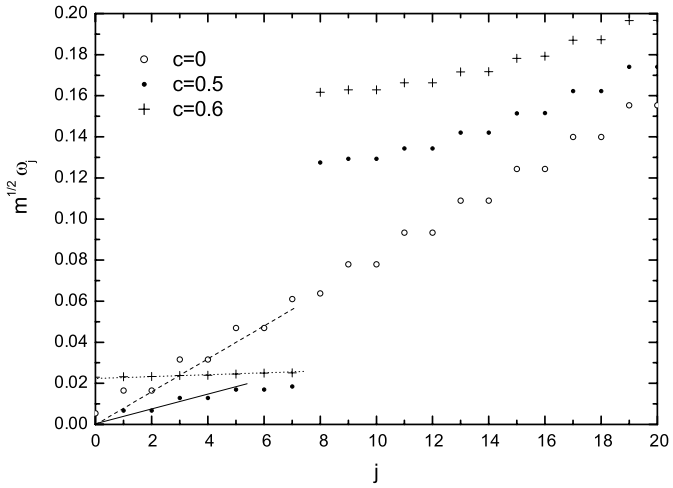

Fig. 1. The frequencies of the lowest modes in the DIFFOUR model for 3 values of the parameter c: 0, 0.5 and 0.6. For $c = 0.6$ there is a phason gap.

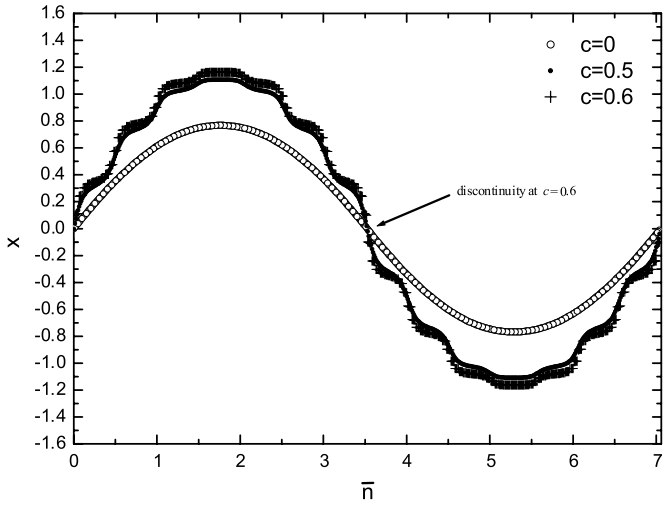

Fig. 2. Modulation function for the DIFFOUR model (Eq. (25)) for the same 3 parameter values as in Figure 1. For $c = 0.6$ the modulation function is discontinuous.

are no longer smooth. This may happen in modulated phases and in composites. In quasicrystals the atomic surfaces are generally discrete bounded objects. Therefore, the positions of the atoms are not continuous functions of the internal coordinate. For the two other classes of quasiperiodic systems these functions depend on the external parameters like temperature and pressure.

In incommensurate modulated crystals the modulation usually sets in at a second-order phase transition. Close to the phase transition the amplitude of the modulation is small and the function is smooth. However, further away from the transition line a transition to a discontinuous modulation function may take place. In the structure these discontinuities correspond to domain walls between domains with a structure that is close to a commensurate superstructure. The walls are called discommensurations and the transition may be called *discommensuration transition*. In the literature it is also known as the transition by breaking of analyticity [4]. This transition has particularly well been studied for the incommensurate version of the Frenkel-Kontorova (FK) model [5–7]. This model consists of a harmonic chain on a periodic substrate. Its potential energy is

$$V = \sum_n \left(\frac{\alpha}{2}(x_n - x_{n-1} - a)^2 + \frac{\lambda b}{2\pi} \cos(2\pi x_n/b + \phi) \right). \tag{22}$$

The ground state for this model has positions in the chain satisfying

$$\alpha(2x_n - x_{n-1} - x_{n+1}) - \lambda \sin(2\pi x_n/b + \phi) \;=\; 0. \tag{23}$$

For small values of λ the solution is $x_n = f(nq + \psi)$ where f is a smooth periodic function. For values of λ larger than a critical value λ_c the function f shows discontinuities.

Analogous transitions appear in other models for aperiodic systems, like modulated crystal phases and incommensurate composites. For modulated crystal phases the transition has been studied numerically in the discrete frustrated ϕ^4 (DIFFOUR) model.

Using the same values of the parameters c and d as in the previous section the shape of the modulation function was calculated. Figure 2 shows the displacements x_n plotted as function of the reduced number na mod b. This is the graph of the modulation function f. It is almost sinusoidal for $c = 0$, but less regular (although still continuous) for $c = 0.5$. At $c = 0.6$ the continuity of f breaks down, and for larger values of c the continuity is broken at several points. The transition from a smooth to a discontinuous modulation function occurs at the same value of c for which the phason gap opens. This is the discommensuration transition.

For incommensurate composites a similar transition occurs. This will be discussed using the double chain model (DCM) in Section 6. In all the cases we shall call this transition the discommensuration transition.

5 Modulation function displacements: non-linear dynamics

The phason frequencies are solutions of the eigenvalue problem of the dynamical matrix, *i.e.* solutions in a harmonic approximation. For displacements that are no longer infinitesimal non-linear terms become important. Although the displacement still connects degenerate ground states, there is no a priori reason that the phason would not couple to other modes for non-zero velocities. We consider the case that the phason is excited such that the amplitude is no longer infinitesimal. This would correspond to non-linear, large amplitude modes. Then the motion can be considered as a displacement of the modulation function $f(kna)$ with respect to the lattice. In the calculation particle n is given an initial speed proportional to the eigenvector u_n of the phason, *i.e.* equal to $\epsilon\, f'(kna)$.

For a sinusoidal modulation function $U\cos(kna)$ this velocity is

$$v = \epsilon\sqrt{2a/L}\sin(kna)$$

if $L = Na$ is the length of the normalization domain: $\sum_n |u_n|^2 = 1$. This can be compared to the phason velocity v_f, the slope of the phason branch which in the model is equal to $\sqrt{1/d - 16d}$. The motion of the excitation then is governed by non-linear equations. It is no longer a harmonic excitation, and we call it a phase wave.

We study the dynamics of phase waves in the incommensurate phase using the DIFFOUR model. Although we deal with a 1D system, the picture would not be very different in higher dimensions, because we shall not be concerned with (strongly dimension-dependent) fluctuation phenomena.

In the parameters c and d the Lagrange function has the following form.

$$\mathcal{L} = \sum_n \Bigg(\frac{m\dot{x}_n^2}{2} - \frac{x_n^4}{4} + \frac{cx_n^2}{2} - (x_n - x_{n+1})^2 - d(x_n - x_{n+2})^2 \Bigg). \quad (24)$$

Here x_n and $\dot{x}_n$ are the displacements and velocities of the particles of mass m, whereas c and d are model parameters.

Let us first consider a wave propagating in a system at zero temperature. The ansatz for the dynamics of the particles is that they move according to a wave traveling through the crystal, This means

$$x_n(t) = f(na - vt), \quad (25)$$

where v is the velocity of the wave, and the envelope f is a periodic function with some irrational period b, just as a moving modulation wave. For a non-zero velocity the modulation function should be continuous for the validity of the calculation that follows here. A further condition is that it has finite second derivative to ensure that the acceleration remains finite. With equation (25) substituted in equation (24) the Lagrangian function becomes

$$\begin{aligned}\mathcal{L} = \sum_n \big(& mv^2 f'(na - vt)^2/2 - f^4(na - vt)/4 \\ & + cf^2(na - vt)/2 - (f(na - vt) - f((n+1)a - vt))^2 \\ & - d(f(na - vt) - f((n+2)a - vt))^2 \big). \end{aligned} \quad (26)$$

All arguments of the periodic function f can be reduced to the first period: $f(z) = f(\bar{z})$ with $\bar{z} = z \bmod b$. Since b is irrational, the reduced arguments fill the range from 0 to b uniformally. For a smooth function f this allows to replace the sum by an integral over the first period.

$$\mathcal{L} = \frac{N}{b}\int_0^b \Bigg(\frac{mv^2 f'(z)^2}{2} - \frac{f^4(z)}{2} + \frac{cf^2(z)}{2} - (f(z) - f(z+a))^2 - d(f(z) - f(z+2a))^2 \Bigg) \mathrm{d}z, \quad (27)$$

where N is the total number of particles.

The equations of motion are satisfied if the action is extremal. In our problem the extremum is a maximum as one sees as follows. From the static case ($v = 0$) the potential energy takes a minimal value in the ground state. From the last formula it follows that $\mathcal{L}$ does not depend on time. Therefore, $\mathcal{L}$ is maximal in our case. The shape and period of f should fulfill this requirement. In general, they depend on the velocity of the wave because v enters equation (27).

For the trial function $f = f_0 \sin kz$ one obtains that

$$\left(\frac{c}{4} - 1 + \cos ka - d + d\cos 2ka + \frac{mk^2v^2}{4} \right) f_0^2 - \frac{3}{8} f_0^4 \quad (28)$$

is maximal, which gives a transcendental equation for k. It has non-trivial solutions $\pm k_0$ only if

$$2 + 8d + mv^2 < 0. \quad (29)$$

The quantity f_0 has a non-zero value only if

$$\frac{c}{4} - 1 + \cos k_0 a - d + d\cos 2k_0 a + \frac{mk_0^2 v^2}{4} > 0. \quad (30)$$

These conditions determine the possible speed of the wave. They are valid if the modulation function f is close to a sinusoidal function. This holds for small amplitude f_0, *i.e.* if the left hand side is small. This shows, under the given conditions, the existence of a travelling wave solution to the equations of motion in the continuum approximation. The solution has the character of a solitary wave.

For zero temperature the wave solution is a solution of the equations of motion in the continuum approximation. This means that the wave may propagate for a very long time without energy loss. An important question is whether a finite temperature would introduce friction or not. Numerical calculations show that for small velocities the wave still moves with very low dissipation.

We argue here that, at least for small velocities, the friction is almost absent if defects are neglected. The main reason is that the low-lying excitations show a linear dispersion law if (and only if) the modulation function is continuous. Although the criterion for superfluidity [8] fails in a crystal structure we expect low friction for a linear dispersion. To illustrate this statement, let us consider the spectrum of the elementary excitations. As one can see, the low-lying excitations are associated to long-periodic shifts of the modulation. We neglect here fluctuations of the amplitude of the modulation. Denote the slowly varying profile of the shift as $F(n,t)$. Then

$$x_n = f(na + F(n,t)). \quad (31)$$

In leading order the kinetic energy of the chain is

$$\sum_n \frac{mf'(n)^2}{2}\left(\frac{\mathrm{d}F}{\mathrm{d}t}\right)^2 \approx \frac{m}{2b}\int_0^b f'(z)^2 \sum_n \left(\frac{\mathrm{d}F}{\mathrm{d}t}\right)^2 \mathrm{d}z. \quad (32)$$

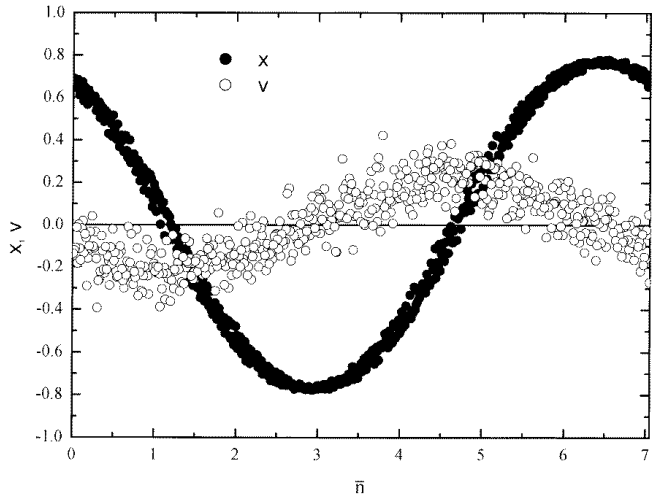

Fig. 3. The modulation function and the reduced velocity function after many time steps in the equations of motion. The spread is caused by a small random noise.

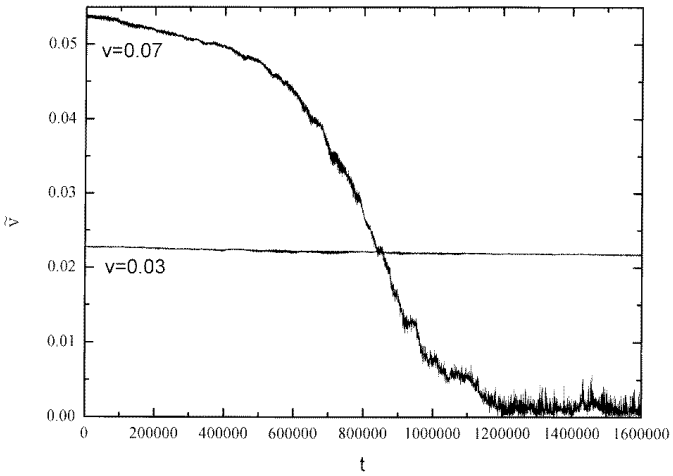

Fig. 4. The speed of the traveling solitary phase wave as function of time for two initial velocities: 0.3 and 0.7. For the higher speed the kinetic energy is distributed over all phonon modes.

In the last transition we took an average over the modulation period, as F is supposed to be a slowly varying function.

The inhomogeneous shift produces a change of the local period: $b_{\rm loc} = b(1 + {\rm d}F/{\rm d}n)$. Although the homogeneous shift of the modulation does not cost potential energy, the change of the local period does so. As the period b corresponds to the energy minimum, the change of the potential energy is quadratic in the change of $b_{\rm loc}$. Therefore, the part of the Lagrange function is associated with the long-period shift F, and is of the form

$$\sum_n \left(\frac{m}{2b} \int_0^b f'(z)^2 \left(\frac{{\rm d}F}{{\rm d}t} \right)^2 - \epsilon_p \left(\frac{{\rm d}F}{{\rm d}n} \right)^2 \right), \qquad (33)$$

where ϵ_p is a positive constant. In the case of a continuous f this leads to a linear dispersion. On the other hand, if f is discontinuous, the integral $\int f'(z)^2 {\rm d}z$ diverges, indicating that the dispersion is no longer linear. However, for linear dispersion we expect a low friction. We shall check this numerically.

When the ground-state properties are determined, we switch to a system with a propagating wave. The initial configuration was taken to be that of the stationary configuration. The velocities were set according to

$$v_i = v f'(x_i), \qquad (34)$$

where v is a small constant. Then the equations of motion

$$m\ddot{x}_n = a x_n - x_n^3 - 2(2x_n - x_{n+1} - x_{n+1}) - 2d(2x_n - x_{n-2} - x_{n+2}) \qquad (35)$$

were integrated numerically using a fourth order Runge-Kutta method with time step 0.03. In equation (35) no explicit damping term has been taken into account. Of course, there will be, in a real system, damping. However, transfer of energy to the phonons is possible in the model, because of the non-linear term. Additional damping then comes from defects. These have not been considered, because we want to know the intrinsic contribution to the damping. The question was, is there a propagating phase wave in an ideal aperiodic crystal?

In each integration step an additional term wr_i was added, where w is a small number, and r_i is a random number in the range from -0.5 to 0.5. The term mimics a non-zero temperature for the system. Figure 3 shows a typical profile of x_n and v_n after a large number of integration steps. The shape of the modulation function has not changed which means that the wave moves without distortion.

To study the loss of energy we calculate the average velocity as a function of time. The value of $\bar{v}$ is equal to the velocity of the solitary phase wave for the case of an exactly sinusoidal modulation function. In the general case, $\bar{v}$ is proportional to the velocity of the solitary phase wave. The data for $m = 1, c = 0, d = -0.4, v = 0.03, w = 0.04$ are presented in Figure 4. The value of $\bar{v}$ stays almost unchanged for a long time, reflecting the absence of friction. The few percent drop is probably due to the finiteness of the chain. An increase in v and w destroys the frictionless motion. As an example the curve for $v = 0.07, w = 0.04$ is given in Figure 4 as well. In this case, the phase velocity goes to zero after some time.

This motion without coupling to the phonon bath has been found also for the solitary wave excitations in the low-temperature commensurate phase in the DIFFOUR model [9]. For speeds lower than the phason velocity (the slope of the phason branch) the solitary wave moves without energy loss. For higher speeds there is energy loss to the phonon bath, and at sufficiently high speeds the wave may decay into two solitons and an anti-soliton.

6 Phasons and sliding modes in incommensurate composites

A model for incommensurate composites is the DCM (double chain model). It is a one-dimensional model with 2 parallel chains with particles at positions x_n in one chain and y_m in the other, and with potential energy

$$V = \sum_n V_1(x_n - x_{n-1} - a) + \sum_m V_2(y_m - y_{m-1} - b) + \frac{1}{2}\sum_{nm} W(x_n - y_m). \quad (36)$$

The intra-chain potentials V_i can, for example, be chosen as

$$V_(x) = \alpha x^2/2, \qquad V_2(y) = \beta y^2/2, \quad (37)$$

and the inter-chain potential W as a Lennard-Jones potential. If the distance between the (parallel) chains is d the latter potential is given by

$$W(r) = \lambda\left(\left(\frac{\sigma^2}{r^2+d^2}\right)^3 - \left(\frac{\sigma^2}{r^2+d^2}\right)^6\right). \quad (38)$$

The ground state follows by minimizing V with respect to $\{x_n\}$ and $\{y_m\}$ and the eigenvibrations from the eigenvalue problem for the dynamical matrix. In the incommensurate case a/b is an irrational number. In the calculations this is replaced by a rational approximant such that $Na = Lb$ is the unit cell of the periodic solution. In this approximation the eigenfrequencies follow from the eigenvalues ω^2 of the $(N+L)\times(N+L)$ dynamical matrix.

The ground state of the system has positions

$$x_n = x_0 + na + f(na+\phi),\ y_m = y_0 + mb + g(mb+\psi), \quad (39)$$

where f is a periodic function with period b and g a periodic function with period a. The character of the functions f and g depends on the value of the interaction parameter λ. For small values of λ both functions are smooth, but for λ above a critical value the modulation functions become discontinuous, just as, *e.g.*, in the incommensurate FK model. The change of the modulation function f with varying values of the coupling parameter λ is given in Figure 5. The change in g is similar. Both functions become discontinuous for the same value of λ.

For $\lambda < \lambda_c$ there are two eigenmodes with zero frequency (in the incommensurate case). One is the acoustic displacement mode, the other the shift mode describing the displacement of one chain with respect to the other. This is not a rigid displacement, because the distances between particles change when the chains move with respect to another. In the commensurate approximant the first still has zero frequency, but the second is separated from the first by a gap that goes to zero in the incommensurate limit. In the commensurate approximant two phonon

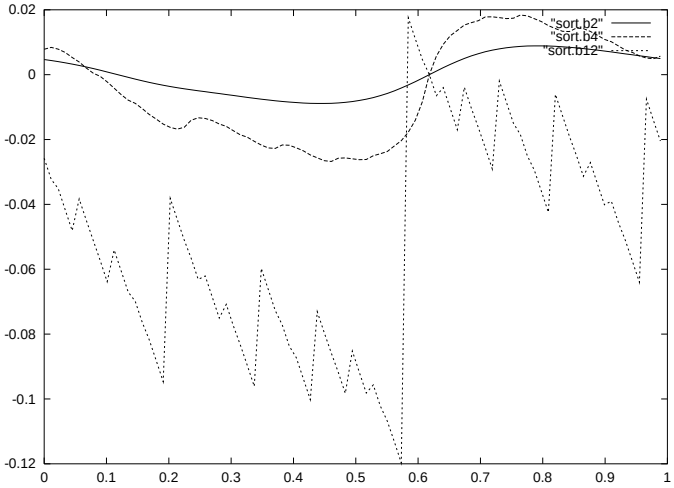

Fig. 5. The modulation of one chain in the DCM, for varying values of the inter-chain coupling. The dotted curve is the modulation function for a value for which there is a phason gap.

branches emanate from the origin in the Brillouin zone. The eigenvector of the second mode is the derivative of the modulation function. Because it corresponds to an infinitesimal shift of the phases of the modulation function, it can be called the phason mode, and the corresponding branch is the phason branch.

If λ exceeds the critical value the modulation functions are discontinuous, the only zero frequency mode is the acoustic mode, the other mode (previously the phason mode) gets a non-zero frequency and its eigenvector is no longer the derivative of the modulation function [10,11]. The modulation function tends to a piece-wise linear function. The jumps in the function correspond to discommensurations and the eigenvector of the second excitation corresponds to vibrations of these discommensurations. For still higher values of λ the frequency of the mode rises sharply and it is no longer the second mode that has the character of a sliding mode. From this point on the sliding mode can not unambiguously be identified. The definition used is then the following. Consider the (normalized) eigenvectors of the phonons: $\epsilon(k,i)$ $(i = 1, \ldots L+N)$. We take as definition that the phason mode is the vibration for which

$$\left|\frac{1}{N}\sum_{i=1}^{N}\epsilon(0,i) - \frac{1}{L}\sum_{i=N+1}^{N+L}\epsilon(0,i)\right|$$

has the maximal value.

The DCM has essentially 2 parameters: $\kappa_1 = \lambda/\alpha$ and $\kappa_2 = \lambda/\beta$. As discussed in [10], and [11] there exists in the $\kappa_1 - \kappa_2$ plane a line separating the domain with smooth modulation and zero frequency phason from that with a discontinuous modulation and phason gap. An incommensurate solution of the DCM can be embedded in two-dimensional superspace as follows.

$$x_n \to (x_0 + na + f(x_0 + na + t),\quad t) \quad (40)$$
$$y_m \to (y_0 + mb + t + g(y_0 + mb + t),\quad t).$$

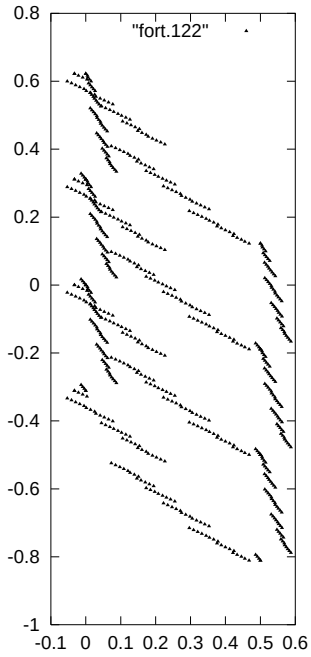

Fig. 6. Embedding of the ground state configuration of the DCM in two-dimensional superspace for the DCM with discontinuous modulation function.

An example is given in Figure 6 for a discontinuous modulation function. Notice the similarity between the latter and the embedding of a quasicrystal, i.c. a Fibonacci chain which consists also of disjoint bounded atomic surfaces.

It is the term t in the first component of $y_m(t)$ that is at the origin of the sliding character of a phason. A change in internal variable t shifts the 2 subsystems with respect to each other. This is different from incommensurate displacively modulated crystals, where a phason is not a sliding motion.

7 Sliding dynamics in incommensurate composites

For an incommensurate composite with a smooth modulation function the ground state is degenerate. The reason for this is that the structures obtained for 2 parallel shifted physical spaces are the same, up to a translation, if there is a lattice translation in superspace that connects them. Since the projection of lattice points on internal space is dense, the positions of the physical space with essentially the same configuration (*i.e.* differing only by a translation) are dense in internal space. For smooth atomic surfaces this means that a shift in an internal direction does not change the potential energy. A consequence of this is the absence of a phason gap if the inter-system interaction is weak enough. However, this does not mean that a motion of one subsystem with respect to another does not couple to phonons, or does not loose energy. This is a problem of non-linear dynamics in incommensurate composites.

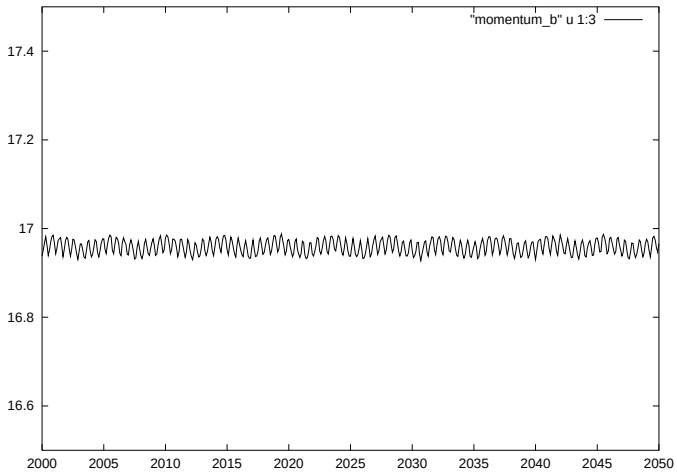

Fig. 7. Momentum of chain 2 of the DCM at $v = 0.5$ as a function of time in the case that the modulation function is smooth. The system continues without change till at least $t = 10,000$.)

To study sliding modes beyond the harmonic approximation we integrate numerically the equations of motion.

$$\begin{aligned} m_1\ddot{x}_n = &- \alpha(2x_n - x_{n+1} - x_{n+1}) \\ &+ \sum_m W'(x_n - y_m) - \gamma_1\dot{x}_n + F_1 \qquad (41) \\ m_2\ddot{y}_m = &- \beta(2y_m - y_{m+1} - y_{m-1}) \\ &- \sum_n W'(x_n - y_m) - \gamma_2\dot{y}_m + F_2. \end{aligned}$$

Here F_i is an external force on chain i and γ the friction coefficient due to additional effects, like damping caused by defects. Just as in the case of the modulated phase, we shall consider here only the intrinsic terms and take γ equal to zero. Also F_i is taken to be zero. As initial configuration $x_n(0), y_m(0)$ is chosen the static equilibrium configuration. The initial velocities are a (small) factor times the eigenvector components of the sliding mode. The difference of the velocities of the centers of mass of the two chains $(P_2 - P_1)$ is plotted as function of time.

For the case of a smooth modulation function examples are given in Figures 7 and 8. For small initial momentum for chain 2 and zero initial momentum for chain 1, the momentum of the first oscillates lightly around a constant value. However, for higher speed the energy of this mode decreases and is distributed to the phonon bath. The system is Hamiltonian, but the Poincaré recurrence time for recovering the centre of mass energy is presumably very large. This energy is practically lost to the phonon bath and we may thus speak of damping. One can conclude that there is a dynamic transition from a situation with zero or very low energy dissipation in the internal degrees to a situation (at higher velocities) where the center of mass energy is rapidly transferred to the internal degrees of freedom, the CM-motion remaining is due to the partioning of the energy over the modes.

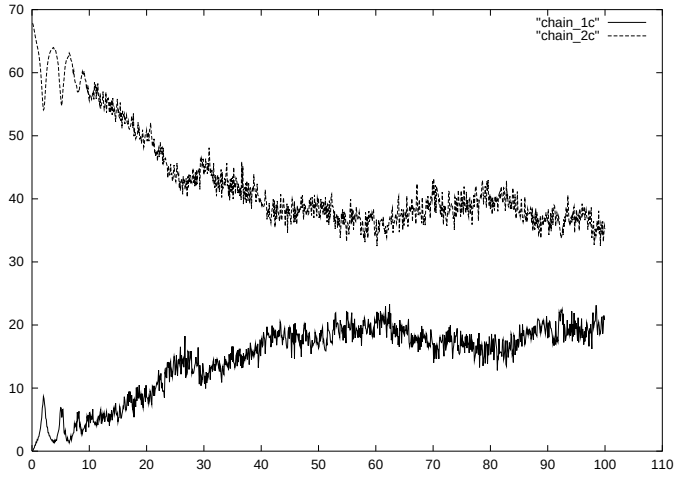

Fig. 8. The kinetic energy of both chains in the DCM as a function of time, for the same interchain coupling as in Figure 7, but for $v = 1.5$. The kinetic energy per particle tends to the same value in both chains.

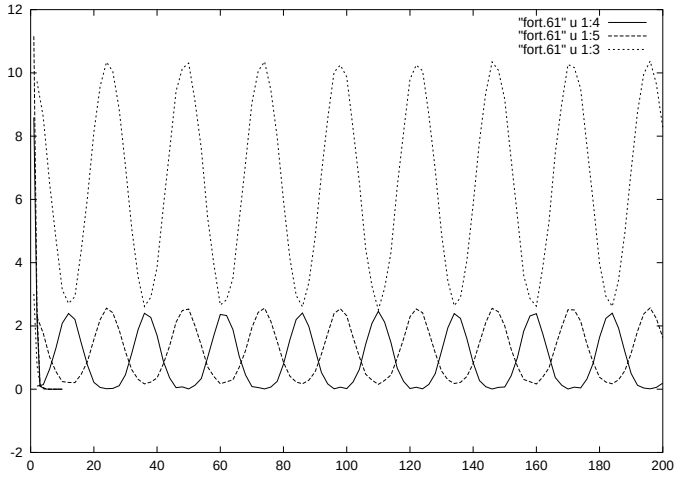

Fig. 9. Exchange of kinetic energy between both chains in the DCM for a coupling which gives a discontinuous modulation function, at low speed. Solid and dashed curves: kinetic energy of the two chains, dotted curve: momentum of the second chain.

A similar coupling is present in the case of a discontinuous modulation function. Starting with initial momentum P for chain 1 and zero for chain 2, the first decreases and starts oscillating. There is an exchange of kinetic energy between the two chains, as illustrated in Figure 9. When the inital velocity exceeds a critical value sliding occurs, but this is damped.

Recently the dynamics and damping of modes in incommensurate composites was studied in [12]. There the damping was put in by hand, and its consequences were studied. In the present paper there is no damping factor (γ in Eq. (41) is zero), and only intrinsic damping can occur. It is shown that for weak inter-chain coupling this intrinsic damping vanishes. This means that the damping considered in [12] has its origin in other sources, like the coupling to defects.

Figures 7 and 8 show that also in this case the sliding mode may move over distances beyond the harmonic approximation with very little energy loss if the initial velocity is small enough. The physical explanation of the low coupling to the phonon modes will be studied in a separate paper, because in the process the particular structure of composites, and not the general properties of aperiodic crystals plays a role.

8 Phasonic degrees of freedom in quasicrystals

In this section we compare the internal degrees of freedom in modulated and composite incommensurates with those in quasicrystals. We review some results from the literature. The fact that the atomic surfaces of quasicrystals are disjoint means that in the dynamics they will be comparable to incommensurate composites. In particular, it means that phason motion is strongly damped or even diffusive. However, in this field the word 'phason' has been used in again a different fashion. We briefly discuss the terminology here.

Quasicrystals can be embedded into a higher-dimensional space, because they are quasiperiodic. Also in this case motion in the internal space is related to motion in physical space. In the quasicrystal community the word phason is used in at least three different ways. Although often it is clear what is meant, this situation may easily lead to confusion.

If the physical space is moved parallel to itself in superspace intersections of atomic surfaces with physical space, which determine the positions of the atoms, will vanish and new intersections will appear. This means a finite jump of a particle from one site to another. This is called a *phason flip or jump*. The density of these jumps will increase with increasing shift of the physical space. Therefore, these phason jumps can be considered as local jumps. Because a jump will change the local configuration, the distances will change and other particles may come in a position favourable for a phason jump. So the phason jump may diffuse. This process of self-diffusion has been studied by Kalugin and Katz [13]. When the phason jumps are independent, they contribute to the diffuse scattering.

A collective motion occurs if a wave propagates along the physical space with displacement in the internal direction. This would be a propagating *phason*. In the long-wavelength limit these can be described as elastic waves connected with the phason components of the generalized elastic tensor ϵ. The generalized elastic tensor has phonon-phonon, phason-phason and phason-phonon components. respectively $\epsilon^{EE}, \epsilon^{II}$ and ϵ^{EI}. An elastic wave with polarisation in the internal space is

$$u_\mu(\mathbf{r}, t) \;=\; u^0_\mu \exp\left(\mathrm{i}(\mathbf{k}\cdot\mathbf{r} - \omega t)\right), \qquad (42)$$

where u_μ satisfies the eigenvalue equation

$$\rho\omega^2 u^0_\mu \;=\; \epsilon^{II}_{\mu j \nu \ell} k_j k_\ell u^0_\nu. \qquad (43)$$

Here $k, \ell = 1, 2, 3$ and $\mu, \nu = 4, \ldots, n$ in n-dimensional superspace. In general, these phasons are coupled to phason flips and usually overdamped. The theory of generalized elasticity is essentially that of the new hydrodynamical modes, associated with the degeneracy of the ground state. (*Cf.* [14].)

Finally, locally a quasicrystal structure may experience a deformation towards a locally periodic structure. Eventually, this may lead to an approximant. The associated picture in superspace is the tilting of the physical space. A static deformation of this type is called *linear phason strain* and may be characterized with a strain tensor [15]. Such a phason strain is observable in high-resolution electron images or in the diffraction pattern.

Very often the word phason is used for all three kinds of phenomena, but it would be better to make a distinction, keep the phason just for the propagating wave, and use otherwise phason flip and (linear) phason strain.

Although there are no propagating phason modes of zero frequency for quasicrystals, the question whether sliding modes exist may be asked for the situation where there is a lattice periodic crystal on a quasicrystalline substrate. This problem has been studied for a generalized Frenkel-Kontorova model with aperiodic substrate in [16]. The potential energy for this generalized FK-model is given by

$$V = \sum_n \Big(\frac{\alpha}{2}(x_n - x_{n-1})^2 + \lambda \left(\sigma \cos(2\pi x_n/b_1) + (1-\sigma)\cos(2\pi x_n/b_2) \right) \Big) . \quad (44)$$

If the length scales a, b_1, and b_2 are mutually incommensurate the structure of the ground state is, generally, of rank three. Another model for a two-dimensional lattice moving over an aperiodic substrate, is specified by the substrate potential

$$V(r) \;=\; \sum_{j=1}^{5} \lambda \cos(k_j r), \quad (45)$$

where the 5 vectors k_j in the plane may angles of $2\pi/5$ between them.

The generalized FK-model (44) has a quasiperiodic ground state that can be embedded as a periodic structure in 3 dimensions. Hence atomic surfaces are 2D. This implies that a discontinuity in the modulation functions does not necessarily yield a disconnected atomic surface. For strong interactions this will be the case, but there is an intermediate coupling range where the atomic surfaces are multiply connected. This may have an influence on the phason gap as well. For the 2D model (Eq. (45)) the dimension of the atomic surface is four, and there may be similar phenomena. Still another feature of the model of equation (45) is the coupling between motion along the x- and the y-axes. Since this goes beyond the questions we have asked here, these models will be discussed elsewhere.

9 Discussion and conclusions

In quasiperiodic systems particular dynamical phenomena occur related to the motion of the crystal in internal space. Because for incommensurate modulated crystals the internal space can be interpreted as the space of the phases of the modulation waves, it has become custom to call these motions phason motions. The name, however, refers to very different situations.

In incommensurate modulated phases a harmonic excitation may occur with an eigenvector that corresponds to an (infinitesimal) shift of the modulation wave with respect to the crystal. For small modulation amplitude, when the the modulation function is smooth, the frequency of this excitation is zero. In commensurate approximants of high order, *i.e.* where the modulation wave vector has as reciprocal lattice coordinates fractions with a (relatively) large denominator, the frequency of the excitation is still very low, but non-zero.

Starting from the equilibrium state with an initial velocity that is proportional to the eigenvector of the excitation, the modulation wave moves with a non-zero velocity with respect to the crystal. Below a critical speed the dissipation is zero although the motion is no longer harmonic. If the speed exceeds a critical value dissipation sets in, and energy is transferred to other phonon modes.

If the modulation function is discontinuous, which occurs far from the transition to the incommensurate state, still an excitation can be found with eigenvector corresponding to a shift of the modulation wave, but its frequency is non-zero. Giving the modulation wave a non-zero velocity the motion is pinned for low enough initial speeds. When the initial speed exceeds a critical value dissipation sets in.

For a crystal on a rigid periodic substrate there is also a harmonic excitation with zero frequency when the crystal and the substrate are incommensurate and the interaction between crystal and substrate below a threshold value. In this case the crystal is modulated with a smooth modulation function. The eigenvector of the harmonic excitation corresponds to a shift of the crystal with respect to the substrate. When the crystal is given an initial speed the coupling with the phonons in the crystal is small and the energy dissipation is low. In this case the motion can be called a sliding mode.

When the interaction is larger than the threshold value the modulation function becomes discontinuous. In this case the crystal is pinned for small velocities and dissipation *via* the phonons occurs for larger speeds.

For an incommensurate composite crystal the situation is very similar to that for a crystal on a rigid substrate. A sliding mode exists for small interaction between the subsystems. For larger values of the interaction the modulation function becomes discontinuous, corresponding to discommensurations. Motion of one subsystem with respect to the other goes *via* jumps of the particles from one discommensuration domain to the next.

In quasicrystals the motion in internal space induces jumps between almost degenerate positions of the particles. This motion does not have a range where there is a zero frequency mode. The system immediately is in a state comparable to the discommensuration region for incommensurate modulated and composite crystals.

The phenomena studied in this paper all are related to motions in aperiodic crystals that can be described with displacements in the additional internal space, if one uses the superspace description. Because this degree of freedom for an incommensurately modulated crystal can be seen as the phase of the modulation, it has become custom to call these phenomena 'phasons'. One should, however, keep in mind that very different phenomena have been called by the same name.

In incommensurate modulated crystals a shift of the modulation wave with respect to the crystal is an excitation that may have zero frequency. Then there is a zero frequency phason excitation. The excitations that are local phase shifts depending on the position in physical space and belong to a branch for which the frequency tends to zero in the long-wavelength limit are propagating phason modes. However, when these excitations are no longer harmonic, but non-linear, motions described as a shift of the phase of the modulation may still occur. Here they have been called modulation waves.

In incommensurate composites there are d acoustic modes (d is the space dimensionality) with frequency going to zero for the wavelength tending to infinity, and there may be harmonic modes described as the (possibly local) relative motion of the subsystems. Low-frequency modes of this kind with a long wave length are sometimes called sliding modes. If the amplitude is not infinitesimal these motions are no longer harmonic and could be called sliding motions. When one of the subsystems is rigid, as mimicked by FK models, the acoustic modes with zero frequency are no longer present.

For quasicrystals the word 'phason' is used in at least three different ways. The motion of atoms that can be described as a local shift in perpendicular space are actually phason jumps. Besides there may be propagating or diffusive modes corresponding to shifts in perpendicular space. These are directly comparable with phasons in modulated crystals and composites with discontinuous modulation functions. Finally the linear strain that (locally) changes the quasiperiodicity of the crystal is called phason strain if it corresponds to components in the generalized elastic tensor that involve internal degrees of freedom. Such strains occur in modulated crystals as well.

If an external stress changes the modulation wave vector, this change may be described as a phason strain. However, in the community of crystallographers dealing with modulated structures this terminology is never used.

In this paper the harmonic and the non-linear phason modes of the 3 classes of aperiodic crystals have been considered and compared. The equations of motion were Hamiltonian. The total energy of the system is conserved. Nevertheless, we can give a meaning to friction as a (practically irreversible) energy transfer from the centre of mass to the internal phonon degrees of freedom (*cf.* Refs. [17,18]). The goal was to study the intrinsic friction. For a realistic study of linear and non-linear modes the temperature and the dissipation due to defects should be taken into account as well. Only in that context it makes sense to distinguish between propagating and diffusive modes.

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