On the problem of the correct interpretation of phason elasticity in quasicrystals

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Recently Francoual et al. \cite{1} claimed to have observed the dynamics of long-wavelength phason fluctuations in i-AlPdMn quasicrystals. We will show that the data reported call for a more detailed development of the elasticity theory of Jarić and Nelsson\cite{2} in order to determine the nature of small phonon-like atomic displacements with a symmetry that follows the phason elastic constants. At the end of our paper we present the reader with a discussion, where we rebut some recent objections.

Recently Francoual et al. \cite{1} claimed to have observed the dynamics of long-wavelength phason fluctuations in i-AlPdMn quasicrystals. These claims were based on the observation of very long relaxation times in the so-called speckle patterns of the diffuse scattering measured with coherent X-rays. These claims run contrary to the fact that the diffuse scattering and/or its kinetics cannot possibly correspond to the flipped tile configurations that occur in the Monte Carlo random tiling simulations.\cite{3,4} In fact, in this model the number of flipped tiles, and correspondingly the diffuse scattering intensity, should increase with temperature, while the experimental data exhibit precisely the opposite temperature dependence. The authors are aware of this: In reference\cite{5} they stated that the data obtained by tile flips, as the temperature dependence of the diffuse scattering measured with coherent X-rays, increases when the temperature is raised. This is model-independent factual information. If the diffuse scattering signal that corresponds to the tile flips increases when the temperature is raised. This is model-independent factual information. If the diffuse scattering observed by the authors were to correspond to tile flip kinetics it should follow the same temperature behaviour as in the neutron data rather than the opposite one.

Because the data actually contradict an interpretation in terms of a signal corresponding to structural disorder obtained by tile flips, as the temperature dependence of the data already mentioned clearly indicates. The authors explicitly announce their awareness of the fact that the word phason is ambiguous as it has been used with several different meanings, while it is the transgression of this very caveat that tacitly serves as a platform for their unjustified claims, by confusing two different meanings of the terminology phason: The existence of a terminology “phason elasticity” and the fact that their model can be called a “random tiling model” are used to suggest without any proof that what they observe would be phason flips. Rather than being able to prove the random tiling scenario the authors had great difficulties in saving the random tiling paradigm and were forced to introduce several ad hoc assumptions in order to achieve this. This rescue operation works only in the appearances. In fact, as we already indicated, the intensity of the quasielastic neutron scattering signal that corresponds to the tile flips increases when the temperature is raised. This is model-independent factual information. If the diffuse scattering observed by the authors were to correspond to tile flip kinetics it should follow the same temperature behaviour as in the neutron data rather than the opposite one.

Perhaps, this requires a more detailed discussion. If
one were able to diagonalize the huge jump matrix that describes the whole of the phason dynamics one would find a (very large) number of characteristic times, each leading to a Lorentzian signal with a dynamical structure factor. Such a jump matrix exists both for the coherent and for the incoherent scattering case. Such a theoretical treatment is beyond reach however, due to the sheer size and complexity of configuration space. The observed neutron scattering data correspond to the sum of coherent and incoherent scattering (contrary to the statements of Fracoual et al. that the neutron scattering signals would be incoherent). The long-time signals attributed to phason dynamics by Fracoual et al. would just correspond to some of these Lorentzians, with very long relaxation times. These long relaxation times are not elementary parameters of the jump model, but functions of more elementary jump times. These functions pop up as the inverses of the eigenvalues \( \lambda_j = f_j(\tau_1, \cdots, \tau_n) \) of the jump matrix that has been defined in terms of the few more elementary jump times, \( \tau_1, \cdots, \tau_n \), which are much faster. The Q-dependence of the intensities of all Lorentzians \( \Lambda_j \) is given by the corresponding structure factors. Any temperature dependence enters into the model through the temperature dependence of the elementary jump times in terms of activation energies. Through the functional dependence \( \lambda_j = f_j(\tau_1, \cdots, \tau_n) \) evoked, the temperature dependence of all Lorentzians is thus dictated by the temperature dependence of the elementary jump times. According to crude criteria such as increasing or decreasing of jump times or intensities, the long time dynamics should thus have the same temperature dependence as the short time dynamics, and any person who wants to formulate a claim that they could show opposite behaviour will have to work very hard to gain credibility for it.

But the experimental observation (from quasi-elastic neutron scattering) that the intensity, rather than the width of the fast signals increases with temperature is unusual. In a first approach, one might argue that it could be due to the finite energy resolution of the neutron scattering experiments: At low temperatures the dynamics are too slow to be resolved and appear as elastic. At higher temperatures they become resolved leading to the illusion that the intensity of the elastic peak decreases and the intensity of the quasielastic signals increases accordingly. But this is not what happens: The width of the quasielastic signals cannot be detected to change with temperature, while their intensities change drastically in a way that cannot be attributed to some broadening. One needs to introduce an assistance scenario to explain this very unusual behaviour.

But what Fracoual et al. observe and call the effect of an inverse Debye-Waller factor, is that the intensities (i.e. structure factors) of the very slow signals decrease while the temperature is raised, with the intensities being transferred to the Bragg peaks! If there were no assistance scenario in the jump dynamics, the intensity and its Q-dependences for a given Lorentzian \( \Lambda_j \) would remain the same at all temperatures. In fact, the structure factor of the Lorentzian \( \Lambda_j \) associated with \( \lambda_j \) is not changed by a speeding up of the dynamics (allowance made for the phonon Debye-Waller factor). At the very best, its intensity at a given Q-value would appear to be associated with a faster relaxation time, through the functional relationship \( \lambda_j = f_j(\tau_1, \cdots, \tau_n) \). If one wants to change \( f_j \) or the structure factors, rather than just \( \tau_1, \cdots, \tau_n \), one has to introduce special assumptions. The observation that the quasielastic neutron scattering intensity increases with temperature forced us to introduce such an assumption in the form of an assistance scenario, as even the elastic intensity is determined by the jump model: It corresponds to the eigenvalue 0 of the jump matrix, and hence its intensity or structure factor should normally not change with temperature. In other words: Allowing for the effect of the Debye-Waller factor due to the phonons, the ratios of the various structure factors, including the elastic one, should have remained the same. In the assistance scenario, the elastic intensity decreases with temperature, because one introduces long-lived excited states, whose population is governed by a Boltzmann factor with a large activation energy. What kind of most extraordinary ad hoc assumptions would have to be introduced into the jump model in order to obtain a decreasing diffuse intensity as observed by the authors, that could be attributed to phason jumps despite the fact that the quasielastic intensity corresponding to fast phason jumps has been observed to increase by neutron scattering?

To resume the situation: The number of tiles that flip increases when the temperature is raised. Therefore, the intensity of the signal that should betray the presence of these tile flips, e.g. off-Bragg-peak diffuse scattering claimed to correspond to the structural disorder produced by the flips, should also increase when the temperature is raised. Such a temperature dependence runs contrary to what the authors observe. They then decide to proceed by postulating an “alternative random tiling model”, wherein the diffuse scattering intensity decreases when the temperature is raised. Such an expedient does not change a iota to the fact that the diffuse scattering intensity cannot be attributed to structural disorder produced by tile flips as it has the wrong temperature behaviour. It follows that the diffuse scattering, which they call the “phason fluctuations” of the alternative random tiling model, must be dissociated from tiling disorder, i.e. the “phason fluctuations” are not tile flip kinetics.

But the authors just ignore this fact and introduce a new terminology “phason fluctuations” to suggest that the interpretation of the diffuse scattering in terms of tile flip kinetics would be saved by such an ad hoc swapping of models. This introduces several confusions. (1) Perhaps the random tiling philosophy can be saved by such
a swapping, but not the interpretation of the “phason fluctuations” in terms of tile flip kinetics. (2) The introduction of the new terminology “phason fluctuations” is also confusing. It works like a tacit to and fro swapping between two states of clarity about the validity of what is being claimed. As the temperature dependence shows, an interpretation of the data in terms of tile flip kinetics is clearly wrong. When the new terminology “phason fluctuations” is introduced, its exact meaning is not well defined, such that it is no longer clear what kind of interpretation for the data is being claimed. Our verdict about the validity of the interpretation is then in suspense: Perhaps the new terminology signals that the original scenario in terms of tile flip kinetics is being abandoned. When the presence of the word “phason” in the terminology is used to reintroduce the interpretation in terms of tile flip kinetics, we swap back to the context of the explicit original claims. Those remain wrong but the meandering path taken by the authors tends to leave the reader with the (false) impression that he no longer is able to be absolutely sure that the interpretation is in disagreement with the data. The inverse Debye-Waller effect can certainly not be just a matter of tile flips as the authors claim. The temperature dependence clearly shows that some other phenomenon must be responsible for the data, something that has nothing to do with the tile flip dynamics.

This is a towering microscopic-level objection against the phason interpretation of the specular signals. But the authors do not address these microscopic issues. By formulating their claims in a macroscopic language of phason elasticity, they dress a language barrier: Nobody understands how the macroscopic phason elasticity is supposed to relate to the microscopic-level tile flips, if it does at all. And therefore, nobody knows how the previously mentioned microscopic objections should be translated across this language barrier. Moreover, this phason elasticity scenario is presented as though it would be conceptually clear and self-evident while it is not. In Widom’s paper it is stated that on lowering the temperature the QC moves away from the ideal random tiling conditions and that this drives an elastic instability. It is not told how this should be described on the microscopic level. The elastic instability could e.g. correspond to a distortion of the tiles rather than to their mere flips. Widom’s paper talks about an inverse Debye-Waller effect on the elastic intensity. Why has this to apply for the diffuse scattering and not for the Bragg peaks, if it is true that the experimental data confirm this?

To save the interpretation of the data in terms of tile flips, the authors try to fall back onto critical fluctuations, whose microscopic description is again eluded. They do not address the question if after their 180 degrees turn in the interpretation of the data, phason elasticity can still be identified in a 1-1-way with a macroscopic description of tile flips with no other ingredient at all, like it appeared in the simple random tiling interpretation that was based on Monte Carlo simulation of purely entropic tilings. There is no elaboration of ideas or proofs in this at all. The authors just swap models in a tacitly assumed tertium non datur, while there is a very obvious alternative that would be worth investigating, viz. that the diffuse scattering intensity is not produced by tile flips.

The loophole of escape proposed by the authors cannot be correct. First of all, there is no evidence for the approach of a phase transition. In fact, one must introduce ad hoc assumptions in order to deny the clear experimental evidence that there is no phase transition. And secondly, we can state that in general, there is no guarantee for the attribution of a wavelength to the quantity \( q \) as the authors do. As there is no conclusive interpretation of the diffuse scattering, considerations about the nature of the ad hoc stipulated purely hypothetical transition (order-disorder, first or second order) cannot play a role at this stage. Consider thus the clear analogon of a (second-order) antiferromagnetic phase transition. (Note that the authors cite themselves the second-order phase transition in NaNO\(_2\) as an illustration of their views, in contradiction with their own claims that the transition should be first order). At approaching the Néel temperature from above, larger and larger antiferromagnetically ordered domains (or clusters) will occur that will take longer and longer times \( \tau \) to decay. This will show up as diffuse scattering intensity centered at the antiferromagnetic Bragg position, e.g. at \( \mathbf{Q} = \left[ \frac{1}{2}, 0, 0 \right] \frac{2\pi}{a} \) of the future low-temperature phase, where \( a \) is the lattice parameter of the high-temperature phase. The intensity at \( \mathbf{Q} + \mathbf{q} \) will have a characteristic decay time \( \tau \), which is a measure of how long an antiferromagnetically ordered cluster of size \( 2\pi/q \) will persist in time without being disrupted by the spin flip dynamics. We see that it is \( 2\pi/Q \) rather than \( 2\pi/q \) that characterizes the wavelength \( 2a \) of the spin wave that is being built up. The quantity \( 2\pi/q \) is not a long wavelength of some spin wave, but an instantaneous domain size, a coherence length of the short wavelength spin wave. The time \( \tau \) is not characteristic of the spin flips themselves (which are local), but of the absence of spin flips within a domain of size \( 2\pi/q \). These domain sizes increase when the spin flip dynamics slow down on approaching \( T_N \).

In this discussion, we use the phase transition only to illustrate a possibility of an interpretation. In the context outlined above, this possibility will remain valid in its general ideas, even if there is no phase transition at stake at all: \( q \) refers to a domain size, rather than to a wavelength. By analogy, we see that it is wrong in the quasicrystal, to associate \( 2\pi/q \) with some hypothetical long wavelength phason wave. Moreover, if there were some wavelength \( \lambda \) in the phason dynamics, diffuse scattering should build maxima at new Bragg peak positions at \( \mathbf{Q} \) with \( Q = 2\pi/\lambda \), or at satellites positions at
\[ Q = G + q \] rather than remaining smeared out over a continuum of positions \( G + q \) in a distribution centered on \( G \), with \( q = 2\pi/\lambda \) (if it is the signature of the mechanism behind the transition). As the diffuse scattering in QCs remains centered at the Bragg peaks of the high temperature regime and its maxima do not define new Bragg or satellite positions, the ad hoc interpretation in terms of critical scattering announcing a phase transition that would not be reached due to the slowing down of the phason dynamics, is wrong. Note that the slowing down of the spin flips is what triggers the antiferromagnetic phase transition rather than impeding it!

The battle horse of the authors to escape from these objections might well be the superstructure reported by Ishimasa, which shows both satellite peaks and diffuse scattering. However, for this exceptional observation there are many other ones where there is no phase transition at all. But even in the favorable case reported by Ishimasa, the dominant diffuse scattering maxima are centered on the Bragg positions of the QC, not on the satellites. The scenario is thus not one of diffuse scattering progressively building up at the future satellite positions, and eventually turning into satellite Bragg peaks.

Now that we have shown that both (quite opposite) random tiling scenarios do not agree with the data, we are left with the problem of providing their correct interpretation. This is not a logical necessity for establishing that the interpretation of the authors is wrong, but we fear that it might be argued that alternative interpretations that are not beset with similar errors are not at hand. In fact, the bold claims of the authors have installed a reversal of the charge of proof. The wrong interpretation and claims will keep hanging around until someone will have definitively solved the very hard problem of the correct interpretation of the diffuse scattering, and provided watertight proof for it, making cautiously allowance for all possible objections. While such a final, unambiguous solution is far beyond our possibilities we will nevertheless sketch a few arguments to convince the reader that an alternative interpretation is not at all impossible.

We should insist on the fact that an interpretation in terms of tile flips is a derived application of the elasticity theory, which is formulated in terms of a continuum of small atomic displacements rather than on a discrete set devoid of infinitesimals. The very definition of an elastic constant cannot be written down if we cannot assume that the atomic displacements explore a continuum. The validity of the derived application is not obvious, as on the microscopic level tile flips do not explore a continuum of atomic displacements. There is thus a priori no good theoretical rationale to explain the results of Tang except the post facto observation that it works despite such theoretical objections. To improve on this situation, Henley has proposed an argument in terms of coarse graining, but we find this rather vague and would prefer a more precise mathematical description. As a corollary, we think that it would be conceptually much more clear if even on the microscopic level we could have a continuum of small atomic displacements. In any case, it remains a cracking pass to generalize the finding by Tang in the sense that one takes it for granted that the only exclusive way to obtain such a dependence on the phason elastic constants would be the tile flips that are so improper for the first-hand application of the theory. Similarly, in Widom’s Landau-type theory it is not granted that the phason elastic constants can only correspond to tile flips: Even if some elastic instability were observed in diffraction experiments that completely tallied with his calculations, it would not yet prove the random tiling...
The situation with a physical theory is somewhat analogous to the one in analytical geometry. The geometrical information is coded by a 1-1-mapping into an algebraic formulation and the theorems are obtained by making the calculus and translating the final results backwards into geometry. Going backwards and forwards between the algebra and the geometry all along the development can be a very beautiful and revealing experience. In physics, we have a similar coding of the physical phenomena in the form of a calculus. The problem with the theory of Jarić and Nelsson is that it provides only the calculus and not the coding. It leaves the problem of cracking the code with the reader. Making good physical sense of the algebra is difficult, since the elasticity theory is a continuum theory, while the quasicrystal is a discrete set of atomic positions. What the microscopic interpretation of the continuum theory should be has never been very much debated, let alone that it would have been conclusively settled. Nonetheless, the authors tacitly introduce a very specific microscopic interpretation without any proof, and move on further as though it were self-evident, well established knowledge.

One way, admittedly not the most clever one, to crack a code is guessing. It is then necessary to check if the guess makes proper sense. Promoting the guess to dogma without checking will most of the time not lead anywhere. The authors' guess is that in a simplified picture, phason waves can be viewed as sine waves propagating in the perpendicular space. That guess sounds conceptually familiar and clear, but on checking if it makes physical sense (especially when no atomic displacements occur in between as in the picture of a wave with small amplitude and a long wavelength), it leaves the problem of cracking the code with the reader. Making good physical sense of the algebra is difficult, since the elasticity theory is a continuum theory, while the quasicrystal is a discrete set of atomic positions. What the microscopic interpretation of the continuum theory should be has never been very much debated, let alone that it would have been conclusively settled. Nonetheless, the authors tacitly introduce a very specific microscopic interpretation without any proof, and move on further as though it were self-evident, well established knowledge.

The “simplified” picture evoking a phason wave, is thus not at all as self-evident as suggested, and the misleading evocation of a pictorial simplicity helps the reader in accepting the introduction of an ill-defined, flawed concept rather than making sense of a real physical phenomenon. There exists no microscopic drawing in the literature showing the postulated simple picture of a phason wave in a quasicrystal. There also exists no schematic pictorial description of the diffusion kinetics of such a wave. There exists even less a rationale that would show how this diffusion would lead to the signals that are attributed to them. All this is not because these matters would be too trivial and self-evident to spend one’s time on explaining them, as one might infer from the tacit style of presentation. On the contrary, one runs into great difficulties when one tries to justify or make sense of the “simple picture”. The whole is just postulated, thereby transferring the charges of proof (that it cannot be true) and of creative thinking to those who wonder. (We will discuss a related problem below, viz. that reporting \( r \) for one selected set of \( (Q, q) \)-values has little physical meaning, and certainly does not correspond to the “simplified” picture of “phason wave” postulated by the authors. It can only be a Fourier component).

For phonons on a quadratic two-dimensional periodic lattice we can imagine four types of distinct phonon modes: Both the polarization and the propagation vector can be along the \( x \)- and the \( y \)-direction. One may guess that the analogon of this for the quasicrystal leads to four basic possibilities of propagation: \( \nu_{10} \sin(q_1 \cdot r_1) \), \( \nu_{10} \sin(q_1 \cdot r_1) \), \( \nu_{10} \sin(q_1 \cdot r_1) \), \( \nu_{10} \sin(q_1 \cdot r_1) \). But we must make a distinction between auxiliary and real physical quantities. At least in a first approach, the latter two possibilities can be disregarded, as in general, a small displacement along perpendicular space does not lead to any real-space atomic displacements, except for a few isolated atomic jumps. These phason jumps are the
exception rather than the rule with respect to the basic concept that a perpendicular space displacement should not lead to a visible displacement in real space. It would make thus much better sense that a phason wave would be of the second type, rather than of the third type as the authors claim, but we have to draw in still another consideration.

If this analogy with the phonons on a quadratic lattice were strict, \((r_1, r_\perp)\) would explore the set of nodes of the superspace hypercubic lattice. But QC's have the particularity that their atomic surfaces are not points but extended sets. This complicates the simple analogy with the square lattice developed above, since there can now also be a dependence of the amplitude of the displacements on \(r_\perp\) along the atomic surface, rather than just the \(r_\perp\)-coordinate of the node. Hence it is also possible to have e.g. \(u_0(r_\perp) = u_0 f(r_\perp)\), where \(f\) is a function on the atomic surface. In the continuum theory, all such detailed microscopic considerations are lost as one reasons on average atoms. The possibility \(u_0(r_\perp) = u_0 f(r_\perp)\) leads to real atomic displacements whose amplitudes can explore a continuum, rather than a discrete set, such that no linearization of the theory for small atomic displacements in the harmonic regime is feasible, even without going from the microscopic to the continuum regime. In conclusion, phason modes can be fields of small parallel-space atomic displacements whose amplitude is a function of the perp-space coordinate of the atomic position rather than its parallel-space coordinate as is the case for a phonon, e.g. \(u_0(r_\perp) = u_0 f(r_\perp)\), where \(f\) is an analytical function on the atomic surface, a linear one in the first order approximation.

In the further elaboration, this leads to further possibilities, e.g. \(u_0(r_\perp, r_\parallel) = u_0 f(r_\perp) \sin(q_\parallel r_\parallel)\). The latter is a wave propagating along parallel space, whose polarisation is a function of the perpendicular coordinates. The polarisation is of course along parallel space, as it should be. In the set of further possibilities, we now can recover the two possibilities \(u_{1,0} \sin(q_\parallel r_\parallel), u_{1,0} \sin(q_\perp r_\perp)\), which we \textit{a priori} had rejected, as they now lead in general to real-space displacements, since the introduction of \(f\) has introduced a 1-1-correspondence between the perpendicular and the parallel coordinates. Such a reintroduction of these two possibilities is however, a mere reformulation of the two more fundamental possibilities \(u_{0,0} \sin(q_\parallel r_\parallel), u_{0,0} \sin(q_\perp r_\perp)\), through the bias of the 1-1-correspondence introduced by \(f\). But due to this 1-1 correspondence, the word polarization can take now two quite different meanings: A derived one that refers to an undulation of the cut as suggested by the authors, and a more fundamental one that refers to an undulation of the atomic surfaces.\[20\] In the example of the Fibonacci chain, we could e.g. tilt all atomic surfaces over a small angle \(\alpha\). Such a displacement field would still lead to a diffraction pattern with the same Bragg peak positions. Only the intensities would be changed. If we imagine a fluctuating cut, we get a model that is very similar to the one that has been proposed by the authors, but that now contains small atomic displacements, and does not need to imply tile flips. From Tang’s random tiling simulations, we know that the cut can be a totally random function rather than a sine wave, and still lead to diffuse scattering at \(Q + q\), while \(q\) has nothing to do with a wavelength. If the assumptions of the authors are able recover all experimental characteristics (a)-(c) outlined above, then the same must be true for our model of small atomic displacements.

To be quite exact, we do not have to claim that our model is correct. But we do have proved that our model definitely excludes the model proposed by the authors from the list of possibilities. The essential point is that the real-space atomic displacements created by the fluctuation of the cut are much larger and not harmonic in the model of the authors. We think that our alternative leads to a less unphysical interpretation of the data, without a real necessity to invoke tile flips as the basic ingredient. The displacement fields are just like classical phonon displacement fields, except for the fact that they are parameterized by other, perpendicular space coordinates. We also want to stress that the procedure of tilting the atomic surfaces is only a first-order approximation to illustrate the idea. In reality, we should introduce a kind of devil’s stair case in order to account for far-away changes of configurations. Furthermore, we should modify the atomic surfaces in such a way that it does preserve the symmetry. Duneau has shown that in an admittedly wrong, polynomial approach for icosahedral symmetry, the minimal degree of the polynomials that comply with this condition is three. The idea of modulating the atomic surfaces finds its confirmation in numerical calculations of the dynamics, where it has to be introduced in order to relax the initial system. The idea of modulating the atomic surfaces is also present in a work of Steurer,\[22\] who calls it the IMS setting (as opposed to the QC setting).

It remains to explain how the diffuse scattering resulting from our alternative model could decrease when the temperature is raised, but there are many possibilities to do this. We have already stated that the data might show that there is some softening of the elastic constants. Widom’s instability, with tile-flip phason elasticity replaced by a phason elasticity based on small atomic displacements, would already to the job. But it is even not necessary to claim that the QC would not be stable. A mere softening of the elastic constants would do. And it is even not necessary to invoke a softening of the elastic constants. It could just be that the system acquires supplementary possibilities to reduce the strain. One possibility is e.g. that thermal vacancies contribute to the relaxation of the observed strain fields. It is quite plausible that their number becomes significant at the temperatures where the fluctuations observed by the authors set
in. Also fast phason hopping between two positions could help in relaxing strain fields. For the physical origin of the continuous displacement fields many causes could be invoked, e.g. chemical disorder, a domain structure as described in reference,\[21\] etc... It is in view of this profusion of alternative possibilities, the unspecific character of the data and the internal contradictions mentioned above that the high-profile claims of the authors are just not justified, especially as they are apt to profoundly bias the opinions on very crucial issues.

We may finally note that a linear relationship $\tau \propto 1/q^2$ certainly does not prove that the data are produced by a diffusion mechanism. The relevant parameter for the diffuse scattering is $1/q^2$, such that the first terms of the Taylor expansion for any possible underlying physics will lead to $\tau = C_1 + C_2(1/q^2)$. The authors have previously considered the relationship $\tau = C_1 + C_2(1/q^2)$ and this resulted in a much better fit of their data. Such a relationship is totally unspecific. In general, fits of the type $\Gamma = 1/\tau = \Gamma_0 + Dq^2$ (where $\Gamma_0 \neq 0$ is an indication for confined motion) are used to analyze data when we already know that they are produced by a diffusion mechanism, not to present the data as supplementary evidence that a diffusion mechanism would be at work.

But let us admit that the analysis of the authors in terms of a diffusion constant is correct. We want to point out how the use that the authors make of Lubensky’s statement that “phason modes are diffusive” is then still wrong and dangerously misleading, as it creates the false impression that the data analysis would contain further proof for their interpretations. The present author has tried to understand the origin of Lubensky’s statements, by tracing back the citations to ever earlier references, and ended up in specialized literature about liquid crystals. Just as with the problem of the microscopic interpretation of the hydrodynamical theory one feels thus being confronted with a black box. Perhaps, Lubensky’s statement means that the hydrodynamical mode corresponds to a diffusive type of dynamics. In any case it is clear that the concepts of dynamics and hydrodynamical modes should not be confused. In other words, the fact that both are qualified by the adjective “phason”, does not imply that “phason elasticity” has a 1-1-correspondence with “phason dynamics”. E.g. Huang scattering in standard crystals is traditionally described as a “frozen phonon”, but it has nothing to do with phonon dynamics. The kinetics of frozen phonons will lead to (very narrow) quasielastic scattering, while dynamical phonons correspond in general to non-zero frequencies. The kinetics of such frozen phonons shall be “diffusive” in many instances, although phonons are not qualified as diffusive by Lubensky. That the kinetics of the diffuse scattering is of the relaxational or even of the “diffusive” type is thus totally unspecific. This reveals an improper, verbalist way of using citations and homonyms, to validate personal interpretations of the terms ”diffusive” and “phason”.

These would be the essentials of our objections if it were not that the paper disseminates a number of confusions that are apt to interfere with our attempts of clarification. These confusions are centered on two main themes.

(1) Coherent scattering signals collect contributions from all particles of the system that have a non-zero coherent scattering amplitude. It is thus a many-particle signal. Despite all possible folk lore, this should not be identified with a “collective” signal or with a signal of some correlations, as the latter implies that the particles are no longer independent and would move in a concerted, correlated fashion, due to some coupling or interaction, as is e.g. the case for phonons. In fact the oppositions independent vs. not independent, coherent vs. incoherent, single-particle vs. many particle cannot be amalgamated.

(1a) Coherent scattering with a certain structure can also occur in a system wherein the dynamics of all particles are totally independent. A clear example of this are the Monte Carlo simulations of Tang et al. The tile flips are here completely random and independent, but they lead to a clear coherent signal that is actually very similar in its reciprocal-space properties to the one observed by the authors. Certainly, it can occur that locally, a tile flip only becomes possible after another one, and one could build a chain of such possibilities over a long distance. But many other tile flips can disrupt this chain, and such chains are certainly not the main contribution to the coherent scattering signal reported by Tang et al. What is the solution of the apparent paradox that the dynamics are independent, but nevertheless lead to highly structured diffuse intensity? In fact, totally uncorrelated jumps in this model will nevertheless give rise to strongly structured coherent signals, but this is due to the constraints of the random tiling model, rather than some correlations or lack of independence in the tile flips. We should thus not confuse the concepts of constraints and correlations: The jumps are totally uncorrelated within the given set of constraints dictated by the random tiling model. To give an analogon: For two completely independent walkers in a city where all streets run only either North-South or East-West, like New York (without Broadway), we might find a mysterious correlation in that they are found to walk always only in mutually perpendicular or parallel directions. This is not a mysterious correlation between the two independent walkers, but a constraint imposed by the city map of New York.

(1b) Coherent scattering signals can be obtained from the dynamics of a single particle, provided it is a coherent scatterer. This is independent by definition. Conversely, many-particle systems can give rise to incoherent signals, even if the dynamics are strongly correlated. It just suffices that the particles are incoherent scatterers.

(2) A second amalgamate that should be avoided is the
one between waves and Fourier components. QCs do not have translational invariance in the form of lattice periodicity. It follows that the Bloch theorem does not apply and the only Bloch wave for an eigenvalue problem on a QC is the trivial constant function. E.g. a phonon problem, the eigenvalue $\omega = 0$ gives rise to an eigenvector that takes the same values on all sites of the quasilattice. (But note that even this function does not lead to a periodic structure after its restriction to the quasicrystal lattice: Its Fourier transform is the diffraction pattern of the quasilattice). For $\omega \neq 0$ a $q$-value that one can read from the pseudo-dispersion curve merely defines a Fourier component of the eigenvalue $v_\omega$:

$$\forall r_j \in QC : v_\omega(r_j) = \int C(\omega, q) e^{i q \cdot r_j} \, dq, \quad (1)$$

with $C \in \mathbb{C}$. Experimentally, we measure $|C|^2$. For a periodic lattice, a dispersion curve is a convenient representation of the eigenvalues $\omega$ and their corresponding eigenvectors $v_\omega$ defined by $v_\omega(r_j) = e^{i q \cdot r_j}$, as knowing $q_\omega$ is sufficient to define the whole Bloch wave. For a QC this no longer true. Moreover, not also reporting $|C(\omega, q)|$ consists in a severe loss of information, even if it is true that the phase factor of $C(\omega, q)$ is not available anyway. It follows that phonons in QCs are not properly studied by making constant-$q$ scans and reporting the corresponding central value $\omega(q)$ on a pseudo-dispersion curve. One should rather make constant-$\omega$ scans and report $|C(q, \omega)|$ for all $q$-values that lead to the same value of $\omega$, such that a crude attempt to reconstruct $v_\omega(r_j)$ can be made (allowing for the fact that without modeling we can never have access to the information about the phases of $C(q, \omega)$). The quantity $e^{i q \cdot r}$ for just one of these $q$-values that define the Fourier decomposition of $v_\omega(r)$ has no physical meaning. Analogously, in the speckle pattern, for a given relaxation time $\tau$, it is $v_\tau$ that has a meaning and not a single component $e^{i q \cdot r}$ that is being picked. The quantity $e^{i q \cdot r}$ is thus not a wave with any particular physical meaning but just a mathematical auxiliary quantity, a Fourier component, and Fourier components can be calculated for mathematical functions that have nothing of a wave, e.g. a function that is only non-zero on a given interval. Moreover, such a Fourier component does not correspond to the “simplified picture” of a phason wave introduced by the authors, as the latter is not periodic. And components with the same value of $q$ but different values of $Q$ may not have the same relaxation time $\tau$.

In practice, the situation can be less bad. The restriction to a quasilattice of a periodic wave that defines small (parallel-space) atomic displacements, will lead to many Fourier components with wave vectors $Q + q$. One may argue that in the long-wavelength limit, the restriction of such a wave may well lead to an intensity pattern where $q$ remains almost constant when $Q$ runs through all the Bragg peaks. The Fourier reconstruction of the initial wave from the intensities while keeping $q$ rigorously constant, will then not be too bad. However, as in our reasoning we started from a continuous wave of small atomic displacements, we see once a again that one cannot take it for granted that the reconstruction of the intensity patterns observed by the authors would lead to a displacement field that consists uniquely of jumps.

One must make the distinction between a meaningful physical wave and a mere Fourier component of an instantaneous structural configuration. The difference is that a physical wave owes its pattern to interactions between the atoms, while a Fourier component can also be defined for a system where all atoms are mutually independent. We can thus encounter three possibilities: (a) a meaningful physical wave as e.g. a phonon in a crystal; (b) a Fourier component of a pattern that is nevertheless produced by some atomic interactions; and (c) a Fourier component of a pattern that comes about without interactions because all particles are independent. In the simulations of Tang et al. we are in case (c), while the diffuse scattering observed by the authors we are certainly in case (b) rather than in case (a) as is being claimed.

In this respect, it might be misleading that theoretical physicists also use the term elasticity for situations where there are no such interactions between atoms. E.g. in the simulations of Tang, the tile flips are totally independent, but still a “phason elasticity” can be defined to refer to an “entropic restoring force”. If this is not appreciated properly, it can lead to more confusion in terms of “elastic wave” pictures that do not apply.

(3) It is well known that a Katz-Kalugin transition in the phason dynamics is necessary to reach the full random-tiling regime. It is generally admitted that the few claims that this transition would have been observed are ill-founded.

In conclusion, we have shown that the claims of the authors are not justified. The claims are formulated in a terminology that sounds very familiar but introduces several confusions.

**Discussion**

We reproduce here verbatim two referee reports that were sent to us by the editorial board of Physical Review and used to thwart the publication of our work. We afterwards take their points one by one. This is perhaps an unusual procedure, but it is just too easy to play on the appearances by writing things that are very obviously wrong to an editor who is not going to understand the issues anyway. It is also just too easy on behalf of editors to “believe” such very obviously biased reports uncritically.
The work of G. Coddens is devoted mainly to the analysis of eventual mistakes in the the papers (cited as Ref. [1-2] in the MS) explaining diffuse scattering in quasicrystals (QC) by phason disorder.

From the very beginning I’d like to stress that Coddens’ arguments about the discrepancy in papers [1-2] seem to me not convincing enough. The arguments given in the actual version of the MS can permit simply to claim that there can exist mechanisms of diffuse scattering others than phason disorder.

The mechanism of diffuse scattering generation by small atomic shifts proposed by G. Coddens represents in its actual form an abstract scheme which is not developed at all. Maybe after a detailed development of these raw ideas, namely after a real derivation of the expressions for scattering and their real comparison with the experimental data this work will take a form suitable for publication in PRB. But I doubt if there exists any serious scientific review which would accept the MS in its actual form. G. Coddens does not perform the calculations to obtain expressions for diffuse scattering but proposes rather general considerations. The reader is invited to make the conclusion (which seems to me rather doubtful) that if one makes all necessary calculations the mechanism proposed by G. Coddens would lead to the same expression as in the classical model (Ref. [2] in the MS).

Let me also briefly review the criticism of the classical model done by the author of the MS. First of all this criticism is based on the idea that in the traditional model “the number of flipped tiles, and correspondingly the diffuse scattering intensity, should increase with temperature, while the experimental data exhibit precisely the opposite temperature dependence”. The situation is not exactly like this. In the framework of the traditional model, the diffuse scattering intensity should not necessarily increase with temperature. One should simply define this framework more carefully: At high temperatures the overdamped phason waves (elementary non-localized excitations or phason fluctuations with a polarization in the perpendicular space) can be in the thermodynamical equilibrium with the system. The average of each elementary wave of this type is $1/2KpT$. Each wave gives the contribution to the diffuse scattering amplitude proportional to the scalar product of the wave amplitude and the perpendicular component of the corresponding Bragg reflection index. Rather simple discussion of above items can be found, for example, in PRB 64, 144204 (2001), by S.B. Rochal. The results of Rochal are slightly different from those obtained for the first time in pioneering work [2] as a generalization of Huang effect for QC’s. Nevertheless, the difference between both works is not essential since the phonon elastic constants in icosahedral QC’s are much greater than the phason ones (a big number of publications prove this fact). Due to this fact, the amplitudes of phason fluctuations (and their contribution to the diffuse scattering) are much greater than the amplitudes of acoustic phonon fluctuations. Then neglecting the phonon contribution one easily obtains the well known expression which is used since at least ten years by many authors (including the authors of [1]) to fit the diffuse scattering spectra. It’s difficult to suppose that G. Coddens is unaware of this formula.

According to this expression the diffuse scattering intensity is surely proportional to the temperature, but it is also inversely proportional to the phason elastic constants. Thus, to explain “precisely the opposite temperature dependence” it is sufficient to suppose that the phason constants $K_1$ and $K_2$ increase with temperature faster than the first degree of temperature. The answer to the question why this growth is fast was given by Widom (Ref. [6] in the MS) and is cited by the author in the MS: “In Widom’s paper it is stated that on lowering the temperature the QC moves to ... an elastic instability”.

I’d like to add more comments (which constitute a not exhaustive list) on the MS:

1) The author tries to show that the phason waves represent a useless notion. Maybe it is the case of the irrelevant phason waves with a big amplitude considered by the author. However, the traditional model deals with the phason waves with a small amplitude.

In the second paragraph page 12, G. Coddens gives the arguments in favor of unphysical properties of these waves but he does not take into account the fact that doubling of the wave amplitude lead to a doubling of the switched atoms number and, consequently, to a doubling of the superstructure reflections amplitudes. I see nothing unphysical in the properties of these waves with the amplitudes proportional not to the atomic displacements but to the number of switched atomic positions.

In addition, phason waves are the solutions of the dynamic equations and this fact justifies their use in the theory.

2) According to the author, atomic jumps correlated in space or a diffusion correlated in space are impossible. But in this case the order-disorder phase transitions in solids are also impossible, which is in evident contradiction with all basic physical data. Making a comment on the consideration presented in the end of page 12, I’d like to note that the free energy of an order-disorder transformation begins with the quadratic terms (like the elastic phason energy in QC does) though “an atomic jump never explores the harmonic regime of the potential”.

3) The MS has no any structure. It seems to me that the only factor stimulating this work was “a denunciation” of the authors of [1]. 3/4 of the MS is devoted to this aim.

Finally, I think that in its present form the paper is unsuitable for publication. I propose to G. Coddens
to develop a constructive part of his theory. But I'd like to stress that the acceptable version of the MS should contain the expression for the diffuse scattering in this model and its justified derivation. Otherwise, my opinion on this work will be negative. If the author really tries to perform this essential calculation and if his final expression is different with respect to the classical model, it would be very interesting to see its comparison with the experimental data.

Report of the Second Referee

The manuscript submitted by G. Coddens does not meet any criterion for a publication in Phys. Rev. B.

- The manuscript is written in a very aggressive style. It is a long and badly written paper against the random tiling model rather than a critic of the paper by Francoual et al., whose results were published in the framework of the continuum hydrodynamic theory of quasicrystals.

I develop below some of the arguments given above.

(i) The first seven pages of the manuscript are a lengthy discussion on the interpretation of papers published 10 years ago. In short, Coddens accuses Francoual et al. to have built up an ad-hoc theory to interpret the temperature variation of the diffuse scattering (an “alternative random tiling model”, “180 degrees turn in data interpretation”). Unfortunately this point of view is wrong since the theory used by de Boissieu et al. in these papers is mainly the one of the continuum hydrodynamic theory, and the different temperature “scenarios” were available in published simulations or theoretical papers (some of them not even referred to by Coddens, as for instance the key simulation done by Dotera and Steinhardt, PRL, 1991).

Of course the question of the microscopical interpretation of the hydrodynamic theory is still an open question. However, this continuum theory is firmly established and has been published in many theoretical papers. In short, the temperature dependence of the diffuse scattering is related to the still going one controversy on the stabilising mechanism of quasicrystal i.e. energy versus entropy; two models have been proposed which predict a quite different behavior of the diffuse scattering as a function of the temperature: Coddens simply ignores these theoretical papers and prefers to criticize the probity of de Boissieu et al. who would have “made a 180 degrees turn in the interpretation”.

The “random tiling theory” is even not properly presented by Coddens. Contrary to what he writes the “random tiling” model hypothesis is fully explained in a long paper by Henley published in 1992: it is clearly stated that the quasicrystal is only stable at high temperature because of configurational entropy terms and that a transition toward a crystalline state should be observed. An “inverse” Debye-Waller factor is also predicted by Widom and Ishii in their study of the elasticity theory of quasicrystals. Moreover the author does not seem to have fully understood the meaning of these papers when for instance p.7 he writes “Widom’s paper talks about an inverse Debye-Waller .... Why has this to apply for the diffuse scattering and not for the Bragg peaks”: this is the well known some rule which implies that any diminution of the Bragg peak intensity (by the Debye-Waller) results in an increase of the diffuse scattering.

(ii) The next two pages are dedicated to an analogy with an order-disorder transition. Whereas it might be interesting to look for order-disorder transition, especially in metallic alloys, the arguments given by Coddens have little to do with the complexity of what is encountered in quasicrystals. Again, there are false assertions: Coddens states (p. 8 bottom) that a phason mode with wavelength \( \lambda \); should show up at a position \( Q = 2\pi/\lambda \); rather than at \( Q = Q_B + q \), where \( q \) is the wave vector of the phason mode and \( Q_B \) the corresponding Bragg peak position. Again this is wrong, and shows a deep misunderstanding of what is a phason mode. All theoretical papers dealing with phason modes clearly demonstrate, that equilibrium phason fluctuations are to be observed at \( Q = Q_B + q \). In complete analogy with thermal phonon fluctuations (references 12, in the PRL), and should display a continuous distribution of \( q \) wavevectors.

(iii) The remaining part of the manuscript comes, again and again, with repetitive arguments on the microscopical interpretation of the continuous hydrodynamic theory. A few pages are dedicated to an alternative interpretation. Unfortunately, Coddens failed to give any credible arguments in term of, for instance, a computation of the hydrodynamic matrix, or a simulation that would reproduce the observed diffuse scattering. Aware of this serious problem Coddens writes: “while such a final, unambiguous solution is far beyond our possibilities we will nevertheless sketch a few arguments to convince the reader that an alternative interpretation is not at all impossible”. It is probably not necessary to call on Karl Poper for assistance to show that this approach has little to do with a scientific discussion. Moreover, as for the other parts, many mistakes can be outlined:

- First there is a poor understanding of the hydrodynamic theory by Coddens, a point that he recognizes himself since he writes “The present author has tried to understand the origin of Lubensky’s statement.... And ended up in specialized literature about liquid crystals”. It is certainly useful to recall that the hydrodynamic theory has for basis the famous theory of “broken symmetry”, which by symmetry and order parameter arguments and analysis allows one to predict the long wavelength excitations that exist in a system. There are many references and even text book such the one of Chaikin and Lubensky, in which the theory is explained. Of course this theory has been applied in the field of liquid crystal, but also in many other condensed matter fields. We can
quote for instance: sound modes in condensed matter, spin waves in ferromagnets, second sound in superfluid Helium4, supra-conductors.... One of the core arguments of Coddens is a criticism of the “statement” of Lubensky (p.17 of the manuscript) that phason modes are diffusive. Unfortunately this is not a statement but a rigorous deduction from the broken symmetry and mode counting analysis in aperiodic crystal! A quite different story! This as such is enough to discredit the entire paper of Coddens.

- The analysis of modes in quasicrystal is wrong (p. 13 and following). Coddens affirm (without any proof) that a mode with a wavevector in parallel, physical space, and a polarization in the perpendicular should be discarded. This point has been discussed in details by Radulescu and Janssen in two papers: indeed such a mode has to be considered, both from an approach in term of the hydrodynamic theory and from simulations. Again, instead of going either in some detailed simulations, or rigorous demonstration Coddens prefers to stay on general assessments in a non scientific posture, without any critical reading of the published literature.

- Coddens propose that small parallel component to the atomic surfaces might be an alternative and that this might be related to phason elasticity. That some parallel components are necessary to fully explain the structure is well known both from the experimental (note quoted by Coddens) and simulation side. However this parameter can not couple to the phason elasticity as claimed by Coddens. Indeed the very essence of the “phason elasticity” comes from the invariance of the free energy of the system with respect to a rigid translation of the cut in the perpendicular direction: this is this degeneracy with respect to this degree of freedom that leads to phason modes. As shown by Ishii for instance, this implies that phason modes have a polarization along the perpendicular direction. Thus the small parallel shifts are not linked with the phason elasticity; they are just a necessary relaxation to minimize the energy of the system by minimizing the energy of the different local environment.

(iv) The conclusion of the manuscript is symptomatic of the only objective of Coddens.

The paper by Coddens should be rejected.

Is it true?

There are several points that illustrate the lack of objectivity of these referee reports. In fact, a referee report should also point out the parts that are correct. One such point which is without any appeal (see below) is that the diffuse scattering that de Boissieu observes cannot possibly correspond to the signal of tile flip disorder as he claims, because that is in contradiction with model-independent neutron scattering data. It is a point of major importance. A long discussion of the paper is devoted to this point, and all referees pass it under the greatest silence.

Another illustration of the lack of objectivity are attacks on issues, to which the answer is already clearly given and discussed in the paper. This way they present a very long list of virtual objections against my paper, although they know that the answers to them are already contained in the paper. The sheer length of this very efficiently creates the (false) impression that there is an enormous amount of problems with my paper, and that is of course extremely harmful and detrimental to me.

Let me first make some introductory remarks. The referee reports contain accusations that I would question (1) Lubensky’s hydrodynamical theory, (2) the theory of Jaric and Nelson, (3) the random tiling theory based on various papers. That is total misrepresententation of the issues and my paper.

There are two main issues in my paper.

(1) A theory might be very elegant and correct. In physics the idea is that it always must be validated by experimental data. That applies also to the random tiling model in quasicrystals. Contrary to what one would like to suggest, I have no pre-established judgement about the validity of that theory, and I totally subscribe the results of Lubensky and of Jaric and Nelson, on which the random tiling theory is built, because they are universally valid, independently of the validity of the random tiling model.

What I do have big trouble with is that in case of the random tiling model, the theoreticians take the work of the experimentalist (A) as a proof for the validity of the model (B), hence A → B, while simultaneously the experimentalist uses the starting ansatz that the random tiling model is correct to interpret his data, hence B → A. That is a vicious circle, and the reader who tries to make up his mind is kept running from Pontius to Pilatus. It is the task of the experimentalist to prove A ⇒ B, but the motivation of the papers has been largely dominated by B ⇒ A. This way, it has been claimed time and again that the random tiling model would have been proved by the experimental data, while these experimental data all are almost unspecific. It is totally premature to make such high-profile claims on the basis of such data. Once again, this does not mean that I claim that the random tiling model is wrong. I am just stating that it has not been proved, and that the statements that one encounters, that it would have been proved are falsehoods.

Physics is an inductive science, and it is well known that induction cannot logically justified in a watertight fashion. Logically spoken, induction is wrong. Hence, what one does to improve the credibility of an induction is in general discarding as many alternatives as possible. An interpretation must therefore often go with a lengthy discussion of alternative possibilities, trying to rule them out. There is very little of that in the claims A ⇒ B,
and when some of such subsidiary issues are debated, in general they are concerned with harmless, selected issues that are not crucial. While, following Popper, all issues should be examined. One single discrepancy, one single counter example is enough to condemn a theory, how sexy it might be. My viewpoint is not that the random tiling theory would be wrong. It is rather that it is still badly in lack of proof.

(2) de Boissieu has superposed on (a) his claims about the random tiling theory the tenet (b) that the diffuse scattering he observes is the diffraction signal of disorder produced by tile flips. For me, the issues (a) and (b) are totally disconnected, although de Boissieu presents them as a single one. Indeed, the quasi-elastic neutron scattering data show that the number of tile flips increases with rising temperature, while the diffuse scattering intensity decreases with rising temperature. The quasi-elastic data and their temperature behaviour are completely model-independent information. They show that (b) is wrong. Referee (2) tries to discredit me by suggesting that this implies that also (a) is wrong, and that the main contents of my paper would consist in challenging long-established theories, which is a total misrepresentation of the issues. There is a whole lot of such methodology of attacking my work on misrepresentations of the issues I raise in the report of referee (2), as we will see. We will come back of the origin of (b) below.

REFEREE 1.

(1) Referee 1 states “The mechanism of diffuse scattering generation by small atomic shifts proposed by G. Coddens represents in its actual form an abstract scheme which is not developed at all.” This remark can be classified under issue (2) above. It can be rejected on several grounds

⇒ I have stated that my quasielastic data are model-independent information that shows that de Boissieu is wrong on issue (2). I could have stopped here. I have no logical obligation to add anything further. The argument is clean and without any appeal.

⇒ de Boissieu also flagrantly contradicts himself when he admits that the microscopic origin of phason elasticity is not known, while with (b) he stipulates exactly the contrary, viz. that he perfectly does know what this origin is, specifying that the diffuse scattering corresponds to tile flip disorder.

⇒ I tried to provide some insight where de Boissieu took an unjustified leap in taking it for granted that the phason waves from the theory would correspond to tile flips (b), by giving a counter-example of suggesting an alternative possibility. According to this path of thought, de Boissieu has to prove that this alternative possibility is wrong in order to prove that he can maintain his claim that phason waves are tile flips, because it would be the uniquely possible interpretation. It is de Boissieu’s task to discard this possibility by a calculation (actori incumbit probatio) because he made the claim about the tile flips. The query of referee (1) that I should make the simulation is in this respect a reversal of the charge of proof. It tries to impose on me a task that would keep me busy for a long time, and that is just not fair. It is remarkable that the same task has not been forwarded to de Boissieu (see below), because what he claims without proof by identifying (a) and (b) is equally an abstract scheme that is not developed.

⇒ Nonetheless, I have very good reasons to believe that my alternative possibility is viable. In fact, I proposed a QC model wherein the atomic surfaces are tilted rather than perpendicular to the cut. That leads to diffraction patterns with the very same Bragg peak positions in both models, only the intensities are different. This is the only difference between the two models. They are both quasicrystals.

Now considerations about the precise outlook of the atomic surfaces do not enter into the theories (1)-(3). All one has to take care off, is to make sure that the detailed nature of the atomic surface obeys to symmetry constraints. It is in this respect that I cited a private communication by Duneau. As the issue if the atomic surfaces are tilted (in the Fibonacci chain) or perpendicular to physical space, does not enter into the considerations, the same theoretical machinery can be unleashed on both models. Hence, if there exists a detailed calculation that shows that de Boissieu’s phason waves (in the way he defines them) lead to the diffuse scattering with the properties he observes, then by a 1-1 mapping of the arguments, the very same calculation will show mutatis mutandis that my model leads to diffuse scattering of the same type. This argument is somewhat similar to the one of Poincaré when he showed that the parallels postulate in geometry is independent, by making a 1-1-mapping between the axioms of non-Euclidean geometry and Euclidean geometry. If de Boissieu is right, I am right as well.

⇒ As we will see below, by adding claim (b) de Boissieu is taking an element from an old version of the random tiling model that is incompatible with the version that is presently accepted on certain crucial temperature dependence issues.

In conclusion I would appreciate if referee (1) makes himself the calculation he tries to impose on me. There is a very important reason to do that. In fact, if one wants to maintain that issues (b) and (a) cannot possibly be disconnected, then the model-independent quasielastic neutron scattering data show that the random-tiling model is wrong. Rather than attacking the random tiling theory, as I am being accused of, I am trying to propose a scheme that perhaps could save the random tiling model from the verdict of these data. I could have left out this model, and it would have been much worse for the de-
fenders of the random tiling model to figure out a reply, because in my present understanding it is their firm belief that (b) must be part of this model. Perhaps, this may show that what I am interested in are not personal issues, as the accusations go, but in the truth.

(2) Referee 1 attacks me on the fact that “the traditional model, the diffuse scattering intensity should not necessarily increase with temperature”. This is a completely false presentation of the issues, and it contains the tacitly implied hint that I am so dumb that I would not even understand this trivial point. The whole paragraph that contains this statement and the next one are useless. They are very long, creating the impression that there is a whole lot wrong with my paper, but it is not about my paper. I already pointed out why above: I am relying on model-independent data and I am not attacking any theory. Moreover, the point is clearly stated in my paper, but the referee passes it under silence. My paper does not address the issues the referee tries to put on my back. I am only forced to cite them because of what de Boissieu writes.

⇒ First of all that statement comes from de Boissieu himself, as can be seen from his ISIS report.
⇒ Secondly, before Widom’s paper (Theory 2) was published, the random tiling theory already existed. Widom’s paper introduced new features, that were not accounted for in the pristine theory (Theory 1). Experimental data related to these new features would have not been accounted for by the pristine theory. In fact, while Theory 1 foresees that the diffuse scattering intensity should increase when the Temperature is increased\([x]\), Theory 2 states that the intensity can both increase\([x]\) or decrease\([y]\) when the temperature is increased. In this respect Theory 1 and Theory 2 contradict each other on issue \([y]\), because Theory 1 denies the possibility \([y]\). It is exactly to this point that de Boissieu’s statement refers, because his data clearly indicate that we are in the presence of \([y]\). Now referee 1 misrepresents the whole discussion, by pointing out that the opposition between \([x]\) and \([y]\) is meaningless within Theory 2, while it is perfectly meaningful between Theory 1 and Theory 2.

⇒ We may note that it is within the motivation of Theory 1 that the result of Tang has been derived. I emphasize on the motivation, because Tang’s result is model-independent. Tang has shown that tile flip disorder (phason1) leads to diffuse scattering of a type that is comparable to what can be deduced from a model with continuous phasons (phason2), following Jaric and Nelsson, while the tile flip disorder (phason1) is something entirely different from continuous phasons (phason 2). Hence:

\[\text{phason1} \Rightarrow \text{diffuse scattering (Tang)}\]
\[\text{phason2} \Rightarrow \text{diffuse scattering (Jaric and Nelsson).}\]

while not(\text{phason1} ⇔ \text{phason2}) (else Tang’s work would not have been necessary, because it could have been derived from the equivalence and the work of Jaric’ and Nelsson).

Due to the fact that

\[\neg (\text{phason1} ⇔ \text{phason2})\]

it is obvious that both

\[\text{diffuse scattering} ⇔ \text{phason1}\]
\[\text{diffuse scattering} ⇔ \text{phason2}\]

are logically wrong. Additional information is required in order to conclude what kind of “phasons” are signalled by the diffuse scattering. Nevertheless, de Boissieu claims without any proof or discussion that the diffuse scattering corresponds to phason1, which is his claim (b). He even claims that phason1 and phason2 are equivalent, because tile flip disorder would be waves of correlated atomic jumps.

The worst is that all this is perfectly present in the paper despite all conclusions one might be tempted to draw from the referee’s presentation.

(3) Referee 1 states: “The author tries to show that the phason waves represent a useless notion. Maybe it is the case of the irrelevant phason waves with a big amplitude considered by the author. However, the traditional model deals with the phason waves with a small amplitude”.

Again this does not be discussed, because it is perfectly present in the paper, when I point out that on going from 6D to 3D the wave character is lost. Here referee 1 persists in denying an obvious and trivial mathematical fact, viz. that the mapping that translates the 6D wave to a 3D atomic displacement field is not analytical. The effect of an infinitesimal variation of the 6D wave is not infinitesimal in 3D: it is either 0 or a finite number (the minimal phason jump).

What I maintain is that phason waves are a useless motion in the context of (b), i.e. that phason waves are a meaningless concept in (phason1), not in (phason2). Nevertheless, the referee uses (phason2) to attack me on statement that is within the context of (phason1). Again the assertion of the referee is not true, and again I have discussed it in the paper. And, as the reader can check, I have discussed both small and large amplitudes.

When the amplitudes are small, there will exist only a very tiny amount of flipped tiles, separated by big distances. That is not a physical wave: In a real wave there is some displacement amplitude in every lattice site of its extent. One can then understand that the displacement of a first atom, induces a displacement of a second atom, etc... And this way one can build a chain of cause and effect over large distances. That is not at all the case here: the atoms in between remain exactly where they were, there are large intermediate regions without any flip at all, and it is thus impossible to understand how the flip in the first position could have induced one in the remote second position, as there is no neighbour-to-neighbor transmission mechanism. There can thus be no force transmitted between such atoms that are separated by a large distance, with nothing in between.
The same displacement field could be obtained by a totally different perp-space function than the sine wave proposed. Moreover, the Fourier components in the diffraction pattern of such a displacement field will not correspond to the wave initially postulated. It is easy to draw of a small-amplitude sine-wave where there are no atomic flips over a whole period, and where one has to go out much further out in space to find the first next flip. The doubling of the amplitude of the 6D wave, will not lead to an exact doubling of the intensities of the Fourier spectrum, but add new Fourier components, etc... What the referee states: “but he does not take into account the fact that doubling of the wave amplitude lead to a doubling of the switched atoms number and, consequently, to a doubling of the superstructure reflections amplitudes” is rigorously wrong, because for an exact doubling of the Fourier amplitudes, one has to double the effect in direct space in exactly the same positions. Adding switched atoms in new positions is not such a doubling. And the doubling of the number of switched atoms is not rigorous.

He also states: “In addition, phason waves are the solutions of the dynamic equations and this fact justifies their use in the theory” This is a mere play with words, that consists in confusing the reader between (phason1) and (phason2). The microscopic interpretation of the phason waves that are the solutions of the dynamical equations (which yield (phason2)) is not clear, as de Boissieu states. Therefore it is not clear if these waves correspond to tile flips (phason1), as the author takes for granted by taking advantage of the fact that the word “phason” has been used with several different meanings. That is also clearly written in the paper, and again the referee prefers to act as though he has not seen it.

The phason waves of small amplitude the referee refers to are in the infinitesimal-amplitude limit, while there is even nothing that permits to think that in de Boissieu’s tile flip disorder scenario the amplitudes of the Fourier components of the function that describes the deformation of the cut remain small. There is no proof that the amplitudes in de Boissieu’s tile flip scenario are not large. And his data even do not correspond to the tile flip scenario. Finally, the problem is not if the displacement field proposed by de Boissieu is physical, but that it is not a wave, as he claims. His displacement field does not correspond to the wave theory he tries to invoke.

(4) referee 1 states: “But in this case the order-disorder phase transitions in solids are also impossible, which is in evident contradiction with all basic physical data.”

This is reasoning against obvious facts. What shall we think about a claim without any proof that in a metallic alloy, atomic jumps are correlated over large distances, e.g. 1000 or 10000 Angstroms. And what should we think about the reply that my objection would be mere speculation, when I am pointing out that postulating such coherent diffusion is a strange, exceptional claim, that, to use an euphenism, requires discussion and proof.

There is no prove for the existence of a phase transition in QCs. Let alone that it would be an order-disorder one. This is typical of a whole attitude of just layering one ad-hoc assumption on top of another one. There is no evidence for a phase transition in QCs, as is crucial for the random tiling model? Surely, it just is not observed due to the slowing down of the kinetics. There is no reason for believing that phason jumps are correlated over long distances in QCs? Surely there must be a order-disorder transition....

Let us ironize a little bit about the claim about long distance correlations. Let us consider two points A and B separated by a large distance of 1000 Angstroms. In point A we have a first jump. Due to the correlation invoked, then one of its neighbours will jump. Due to the correlation invoked, then one of the neighbours of the latter one will jump, etc... This way we build a whole domino game of correlated jumps diffusing from A to B. The whole chain of causes and effects arrives at B after about 100 seconds, inducing a jump at B. The problem is that the neutron and Mössbauer data show that at the temperature of 650°C of his experiment, the atomic jumps take place on the time scale between picoseconds and nanoseconds. Hence, during the 100 seconds time lapse de Boissieu is talking about, the atom in B will have jumped a 10^{11} to 10^{12} times that cannot be attributed to a correlation that would link a jump in B to a jump in A, by diffusing from B to A.

And as I pointed out under (3), when the waves de Boissieu stipulates have very small amplitudes, they have nothing to do with such a neighbour-to-neighbour transmission mechanism, because they contain large regions where there are no flips at all.

(5) referee 1 states: “I’d like to note that the free energy of an order-disorder transformation begins with the quadratic terms (like the elastic phason energy in QC does) though “an atomic jump never explores the harmonic regime of the potential””.

This is again reasoning contrary to obvious facts. The very nature of an atomic jump implies that it jumps in a double-well. Such a double well can never be described by a quadratic function. The atom may explore harmonic forces when it is at the bottom of one of the double wells, but not on the saddle point on its way to the other well. So, whatever his mental construction tries to prove, it runs contrary to very obvious facts.

(6) Referee 1 states: “It seems to me that the only factor stimulating this work was “a denunciation” of the authors of [1]. 3/4 of the MS is devoted to this aim”.

This is again a misrepresentation of the issues. He could also have written “a dissatisfaction with the arguments of [1]”, because all that counts is the validity of my scientific arguments, and the personal motivations he wants to accredit me with should not have any incidence on the judgement of my paper.
(7) referee 1 concludes: “I propose to G. Coddens to develop a constructive part of his theory. But I’d like to stress that the acceptable version of the MS should contain the expression for the diffuse scattering in this model and its justified derivation. Otherwise, my opinion on this work will be negative. If the author really tries to perform this essential calculation and if his final expression is different with respect to the classical model, it would be very interesting to see its comparison with the experimental data.”

This would just cripple my paper and conveniently hide a few very disturbing facts from the eyes of the community. What we can keep from it is that we can see that the referee admits that he has no arguments to claim it would be wrong.

REFEREE 2 is de Boissieu.

In this report there is a systematics of misrepresenting the issues I raise. Each time my issues are reformulated and denaturated in the form of an issue that is so very obviously wrong, that you could not possibly win, if you yielded to the temptation to get sidetracked on this false issue. Referee (2) advances a whole collection of such false issues and shows each time with pathos how ridiculous and incompetent they are. That creates a very bad impression about my paper (not to say me), but it all has nothing to do with the real contents of my paper. The bottom line of it is that we are confronted with one elusive move after another one, and that it appears impossible to pin him down on a discussion of the crucial real issues. This clearly shows that de Boissieu has no answer to the issues I am raising. The many ad hominem statements also attempt to elude a discussion of these issues on a scientific level, by having the paper rejected on the basis of the non-scientific issues.

(1) He states: “It is a long and badly written paper against the random tiling model rather than a critic of the paper by Francoual et al., whose results were published in the framework of the continuum hydrodynamic theory of quasicrystals.”

I have already stated that this is a misrepresentations of the issues above. I am not attacking the random tiling model. The words “in the framework” confirm, what I pointed out above, viz. that de Boissieu uses B ⇒ A. In fact de Boissieu works “in the framework of the random tiling model”.

(2) In the ISIS report de Boissieu admits that he would have expected the opposite temperature behaviour and that he had to shift to a more elaborated random-tiling model.

Afterwards this temperature behaviour has been used to claim that it proved the random tiling model. As the same could have been claimed with the opposite behaviour, this has no persuasive value at all. de Boissieu should have tried to prove that this temperature behaviour excludes all possible alternative models, which he did not. In stead of that he tacitly introduced a “tertium non datur” and went on claiming. As I explain in the paper most of the results he uses do not discriminate between the random tiling and alternative models at all, as they rely on Lubensky, and on Jaric and Nelsson, while these papers have a much larger scope of generality and remain perfectly valid in the context of all possible other models.

It has been claimed that the temperature behaviour would contradict the energetic stabilization scenario, which is really an oversimplification of the issues, by presenting it as though it could not be that the energetic stabilization scenario could be right, although it could be something totally different than the stability issue which is producing the effects observed in the data. That the defenders of the energetic scenario do not reply, is not because they could not possibly think of a scenario. It is because that there are so many scenarios, that it would be ridiculous to pick one and propose the one picked as the one. There is simply not enough information to allow picking one. The entropic stabilisation scenario has difficulties in its own right because it stipulates a periodic ground state, which is not observed, and then introduces the ad hoc assumption that the ground state is not reached because the kinetics slow down too fast. All this shows is that the whole issue of energetic against entropic scenario is far more complex than de Boissieu’s tries to suggest. He tries to impose that issue by brute force on his data suggesting that the mere temperature dependence of the diffuse scattering would be able to settle the issue. It is not because some data can be put in a given perspective (e.g. a stability issue) in one theory, that it must be put in the same perspective in a competing theory. They could address a totally different issue in the competing theory.

(3) It is then stated: “Coddens simply ignores these theoretical papers and prefers to criticize the probity of de Boissieu et al. who would have “made a 180 degrees turn in the interpretation”.”

Once more this has nothing to do with my paper, as my point is model-independent.

(4) It is stated: “Contrary to what he writes the “random tiling” model hypothesis is fully explained in a long paper by Henley published in 1992”.

The phrasing “Contrary to what he writes” is just a falsehood, and tries to put words into my mouth that I never said.

(5) Moreover the author does not seem to have fully understood the meaning of these papers when for instance p.7 he writes “Widom’s paper talks about an inverse Debye-Waller .... Why has this to apply for the diffuse scattering and not for the Bragg peaks”: this is the well known some rule which implies that any diminution of the Bragg peak intensity (by the Debye-Waller) results in an increase of the diffuse scattering.”
This is again a misrepresentation.

That the diminution of the Bragg peak in the data goes with the increase of the diffuse scattering is clear in the experimental data, and as such this is model independent. Contrary to what de Boissieu claims, I understand this perfectly, and it is even written in my paper, when I state that the intensity is transferred from the diffuse scattering to the Bragg peak.

A true Debye-Waller diminishes all the elastic intensity at the profit of the inelastic intensity. There is a sum rule between the elastic and the inelastic intensity. My point was that the Bragg peaks and the diffuse scattering intensities are both elastic intensities, such that they should be both affected the same way.

I have found the solution to that riddle myself in the mean time. What Widom calls the Debye-Waller factor in his paper is not the true Debye-Waller factor, but a theoretical auxiliary quantity that consists on integrating on only the very long-wavelength modes (i.e. on only an infinitesimal domain of q-vectors). It thus excludes the whole phonon density of states (as e.g. measured by Suck), except that infinitesimal part. Similarly, it excludes all the phason dynamics I have measured by TOF neutron-scattering, except an infinitesimal part. Within this long-wavelength approximation Widom then calculates his auxiliary quantity that indeed applies to the transfer of intensity between the Bragg peak which is elastic and the diffuse scattering which becomes inelastic in this approach. But it follows that the true Debye-Waller factor, obtained by including the rest of the full q-range, could again invert the tendencies described by Widom, i.e. some Bragg peaks could show the inverse effect, while others could show the normal effect.

(6) “The next two pages are dedicated to an analogy with an order-disorder transition. Whereas... should display a continuous distribution of q wavevectors.”

Again this is a total misrepresentation of what I am saying. de Boissieu is putting here words into my mouth that I never said. I have not written anything like that at all. As can be seen on the place he refers too, I was talking about spin waves. The context is totally different from what he tries to make us believe. I am adressing the point that according to the random tiling model there should be a low-temperature periodic phase, and that this phase has never been observed. The primordial claim of the random tiling, the low-T periodic phase has not been observed! The ad hoc assumption that has been used to talk this serious objection away is that the low temperature phase is not reached due to a quenching of the kinetics.

I inspect therefore if some observations could nevertheless be used to claim that a phase transition has indeed been observed. I see two possibilities: (a) a periodic phase like the rhombohedral microcrystalline approximant in AlCuFe; (b) the phase with the satellites observed by Ishimasa. First of all these are exceptions rather than the rule. For a slightly different concentration the phase transition is missed. Secondly, the rhombohedral phase has a large unit cell. Such large unit cells are hardly an improvement over the QC in the question on how they can possibly exist. Third, in Ishimasa’s phase we get sattelites, which means that we go to a modulated QC phase, which is in fact even more complicated than a periodic phase, and cannot serve as the periodic ground state, we are looking for. Finally, and this were de Boissieu totally misrepresents the issues, if the phonon waves are the unique mechanism that drive the phase transition to the periodic ground state, they should build up progressively intensity at the future Bragg peak positions of the periodic ground state, and no such tendencies can be observed in the data. The Q-values of these Bragg peaks have a physical meaning in the periodic low-T system. And the q values of intensity at positions q+Q, where Q is such a future Bragg peak, have also a physical meaning, with respect to the low-temperature phase. For sure, in the periodic phase, there are no phasons at all. When a phase transition takes place, we are entitled to relate at a certain stage of progress in the transition the Q-values to the frame of the periodic phase rather than to the frame of the quasiperiodic phase, and the interpretation of intensity must change from phason to non-phason.

de Boissieu tries by brute force to discredit my remarks by imposing the quasiperiodic reference frame, and imposing the framework of the random-tiling theory on top of that, while my remarks are in a different context, and not stupid as he would like us to believe. I have never stated that the distribution would not be continuous, as he tries to make us believe. I have only stated that it should contain local maxima, which are not observed.

I think my motivations were perfectly spelled out in the paper, but once again they have just been totally misrepresented.

(7) referee (2) states:

“Aware of this serious problem Coddens writes: “while such a final, unambiguous solution is far beyond our possibilities we will nevertheless sketch a few arguments to convince the reader that an alternative interpretation is not at all impossible’. It is probably not necessary to call on Karl Poper for assistance to show that this approach has little to do with a scientific discussion.” ”

As I pointed out above, I do not have to make this calculation to prove that his assertion (b) is wrong. He should have made this calculation to prove that assertion (b) is right (which it is not anyway) by eliminating the alternative.

(8) There is the passage: “ First there is a poor understanding of the hydrodynamic theory by Coddens, ... This as such is enough to discredit the entire paper of Coddens.”

This is again a misrepresentation of the issues. Lubensky’s presentation does not permit us to spot the rigorous definitions that would allow us to invalidate the use that
is made of the statement that phasons are diffusive. I am not at all questioning the symmetry arguments of Lubensky as de Boissieu wants us to believe. I am just pointing out that the statement that the phason modes are diffusive has been misused by de Boissieu, by using a play of words. It must be that two different meanings of the word ‘diffusive’ are identified, because diffuse Huang scattering scattering based on phonon rather than on phason elasticity, would also manifest itself as ‘diffusive’ (in the sense he uses it) in the type of experiment de Boissieu reports, while phonons are not diffusive in the sense of Lubensky. de Boissieu is going to extremely exotic situations (time scales of minutes) to claim that identification, while there are many other time scales where Lubensky’s theory should be right as well.

(9) “The analysis of modes in quasicrystal is wrong ... without any critical reading of the published literature.” is again a misrepresentation. The only thing I said was that once we project the physics onto 3D space (which one always has to do in the end), there must remain some polarization in the physical space, else the wave is physically irrelevant. de Boissieu uses the fact that I swap between a 6D mathematical and a projected 3D physical description to present my language in 3D as though it would be stupid language in 6D. The two contexts have to be clearly separated, which I do in the paper, but he mixes them up to discredit me.

(10) “Coddens propose that small parallel component ... energy of the different local environment.”

I have already given the explanation of my model above, showing that it is in 1-1-correspondence with his claims.

Finally, I would like to point out the reversal of rôles and denial of rights of recourse installed by the accusation that I would raise personal issues. For more than 12 years Janot, Dubois and de Boissieu systematically questioned my competence with an incessant series of far-fetched invalid criticisms on my work on quasielastic neutron scattering from quasicrystals (phason hopping):

(a) the quasielastic signal would not be due to atomic hopping but to localized vibrations from clusters.
(b) the quasielastic signal would not be due to phason hopping but due to preferential segregation of Cu into the grain boundaries.
(c) the quasielastic signals are not due to phason hopping but to rotating molecules.
(d) the quasielastic signals would be minuscule and could only be evidenced with the aid of a fit program.
(e) phason hopping is nothing special for quasicrystals.
(f) phason dynamics occurs also in periodic crystals.
(g) the quasielastic signals could be due to tunneling states.
(h) The important issue in phason dynamics is not the hopping but long-wavelength phason fluctuations.
(i) The first experimental evidence for phason hopping was obtained by Janot and published in ILL reports.

We submitted in 1994 a proposal to the ILL to measure phason dynamics. In the selection committee Dubois told the other committee members that the experiment had already been done by Janot, and therefore should not be awarded beam time. It was just not true. Our proposal was then rejected without even being discussed. When I objected, I was discredited, just like now, with the argument that I tried to question the probity of this group and of the entire ILL. A few months later Janot and de Boissieu did the experiment in our place in “test” beam time on IN16, but they melted their sample. This attempt is e.g. mentioned in reference [19] and the citation therein. Contrary to the self-acquitting claims in these papers, they had searched for the very same signal, in the same Q-range, in the same very narrow energy-range, within the same temperature range, on the same single-grain QC alloy, with the same type of instrument. They had these claims co-signed by two colleagues from my own lab, who discovered post factum that their request to remove the corresponding passages had been ignored. To prove that it was “different” they introduced the wrong alternative interpretation they wanted to give to the type of quasielastic signals we had measured, replacing the scientific issues, and shifting appreciations.

The undue confusion produced by (a)-(i) tends to ease the attempt to install this shift through reference [1]. Each time I had to discover these informal and damaging Comments (with their de facto denial of my rights of reply) as an accomplished fact in the published literature. To try to undo the damage I was forced to write a Comment with reversed rights of reply. Their replies contained then new invalid damaging statements, to which I was, as always, denied any possibility of recourse. I really do not see, why I should have to accept being framed up with such methods, and moreover being personally discredited on the basis of totally biased representations of the context and one-way readings of the rules, each time I try to defend myself against this.

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