DO THERE EXIST TURBULENT CRYSTALS ?

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Abstract. We discuss the possibility that, besides periodic and quasiperiodic crystals, there exist turbulent crystals as thermodynamic equilibrium states at nonzero temperature. Turbulent crystals would not be invariant under translation, but would differ from other crystals by the fuzziness of some diffraction peaks. Turbulent crystals could appear by breakdown of long range order in quasiperiodic crystals with two independent modulations.

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It is known that the normal periodic structure of crystals is, in some cases, modulated incommensurably *). Four basic spatial frequencies may be present instead of three, so that a quasiperiodic structure arises. When a suitable thermodynamic parameter is varied (the temperature, say), frequency locking may occur, leading to a periodic structure, usually with large unit cell (supercell). Quasiperiodicity and frequency locking are reminiscent of the behaviour of differentiable dynamical systems, used in general to study time evolution rather than space translations. In hydrodynamics in particular, steady states, periodic and quasiperiodic time evolutions are observed, and also turbulent evolutions associated with strange attractors (see Lorenz [12], Ruelle and Takens [17]). Turbulent time evolutions are characterized by sensitive dependence on initial condition. The transition from quasiperiodicity to turbulence is visible in the frequency spectrum : the original sharp peaks are widened, and at the same time a continuous spectrum appears.

In view of the above, it is natural to propose that crystals may, in some cases, develop a turbulent structure (see Ruelle [16]). Some sharp spatial frequencies would then become fuzzy, and this broadening would be visible in X-ray or neutron diffraction patterns. The proposed turbulent crystals would be in thermodynamic equilibrium, and would not be invariant under the Euclidean group (or even translations). They would thus differ from a fluid phase or a non-equilibrium amorphous state. Non invariance under rotations would be easy to detect. In fact a turbulent crystal would still look like a crystal, but with a structure modulated in a non quasi-periodic manner, corresponding to fuzzy spatial frequencies in a diffraction

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*) See Janner and Janssen [9] for a review and for references (in particular to the work of de Wolff and coworkers).

pattern. Evidence that one is dealing with an equilibrium state could be provided by reversible transformation into an ordinary crystal (periodic or quasiperiodic) when a suitable thermodynamic parameter is varied. According to the analogy with time evolutions, one would expect that a crystal with five spatial frequencies, i.e., two independent incommensurable modulations would readily become turbulent (see Ruelle and Takens [17], Newhouse, Ruelle and Takens [13]). There are other pathways to turbulence (Feigenbaum [5], [6], [7] , Pomeau and Manneville [14], Eckmann [4]).

Models for modulated crystals are easily obtained in one dimension at temperature $T = 0$. They lead to differentiable dynamical systems (area preserving maps of the plane in examples studied by Aubry [1] and Janssen and Tjon [10]). This gives an interpretation of quasiperiodicity and frequency locking, and supports the idea that turbulent crystals may exist. The interest of one dimensional models is limited by the fact that crystal structure is washed out at temperatures $T > 0$ (for short range forces). In two dimensions also, crystal structure seems to disappear for $T > 0$, in the sense that there is no positional long range order (there may be long range order for the orientation). One believes of course that crystals exist in three dimensions for $T > 0$, but this has not been rigorously established from the general principles of statistical mechanics.

It should be pointed out here that states with $T > 0$ always exhibit fluctuations. Related to this is the fact that a diffraction pattern (for a crystal or a fluid) always exhibits a <u>continuous spectrum</u> (to which a discrete contribution of sharp peaks may or may not be added). The frequency spectrum for the time evolution of a hydrodynamical system behaves quite differently : in the periodic or quasiperiodic regime, only sharp peaks are present, and the appearance of continuous spectrum coincides with the broadening of the peaks. To clarify matters, we shall now discuss in more details the behaviour of statistical mechanical states under the Euclidean group. We shall thus be able to define precisely the periodic, quasiperiodic, or turbulent crystals. The existence of these structures will of course remain open (even the existence of periodic crystals has not been proved).

For simplicity we shall discuss classical systems (quantum systems could be handled in the same manner). An infinite configuration of a classical system consists of the positions of infinitely many atoms in $\mathbb{R}^3$. We may assume that these atoms belong to finitely many species. It is technically convenient to assume that the distances between atoms are $\geq R_0 > 0$ (a hardcore condition) so that the space K of infinite configurations is compact (see Gallavotti and Miracle [8]). Notice that the Euclidean group acts on K . A <u>state</u> of the system is a probability measure on K . If the interatomic interactions are invariant under the Euclidean group G , and the chemical potentials and temperature are fixed, and <u>equilibrium state</u> ρ is determined (invariant under G by definition). The <u>Gibbs phase rule</u> implies that this state is, in general, unique and ergodic (i.e., it cannot be written as $\frac{1}{2}\rho_1 + \frac{1}{2}\rho_2$ where ρ_1 and ρ_2 are distinct G-invariant states). While the equilibrium state ρ is Euclidean invariant, the states observed experimentally are <u>Gibbs states</u> which are often not invariant (see Dobrushin [2], [3], Lanford and Ruelle [11]). A Gibbs state is defined to be such that every subsystem contained in a bounded region of space is in equilibrium with the system outside this region (with respect to the given interaction, chemical potentials, and temperature). The equilibrium state ρ is a Gibbs state, and has a unique decomposition into extremal (i.e. indecomposable) Gibbs states. This means that there is an integral representation

$$\rho = \int_\Gamma \sigma \ m(d\sigma) \tag{1}$$

where m is a probability measure on extremal Gibbs states. The integral representation (1) may be obtained by diagonalization of the algebra at infinity : the Abelian algebra of observables which can be measured outside of any bounded region (see Lanford and Ruelle [11]). The Euclidean group acts on the space Γ of Gibbs states on which σ is defined, and this permits a precise definition of periodic, quasiperiodic, and turbulent crystals as we shall now indicate.

First we may decompose ρ into ergodic states with respect to the normal subgroup H consisting of translations in the Euclidean group G. This decomposition may be written in the form

$$\rho = \int_{G/H} \tau_g \rho_o \ \mu_o(d\bar{g}) \tag{2}$$

where μ_o is the Haar measure on the compact rotation group G/H ; $\tau_g \rho_o$ is the image under $g \in G$ of a suitable H-ergodic state ρ_o, and $\bar{g}$ is the class of g in G/H (see Ruelle [15] 6.4, and references quoted there). The decomposition (2) is coarser than (1); this means that ρ_o is again a Gibbs state, which may be further decomposable.

Remember now that ρ_o is a probability measure on the space K of infinite configurations such that ρ_o is ergodic under the translation group H. There is thus a natural unitary representation U of H in $L^2(K,\rho_o)$, and there is a projection-valued measure E on the character group $\hat{H}$ of H such that

$$U(a) = \int_{\hat{H}} E(dx) e^{iax}$$

Note that $\hat{H}$ is isomorphic to $\mathbb{R}^3$. Let X be the subset of $\hat{H}$ consisting of the points x such that the corresponding projection does not vanish : $E(\{x\}) \neq 0$. One can show (using the ergodicity of ρ_o) that X is a subgroup of $\hat{H}$, and that $E(\{x\})$ is a one-dimensional projection when $x \in X$. (For this, and the following details, see Ruelle [15] §4 , and the references quoted there). Define

$$P = \sum_{x \in X} E(\{x\})$$

This is a projection on the space of almost periodic vectors in $L^2(K,\rho_o)$. The operators PFP , where F is multiplication by a continuous function on K , generate an Abelian algebra, and the diagonalization of this algebra corresponds to an "almost periodic" decomposition of ρ_o . This representation may be written as

$$\rho_o = \int_M \tau_\lambda \rho_1 \, \mu_1(d\lambda) \tag{3}$$

In this formula, M is the compact Abelian group of characters of X , where X is equipped with the discrete topology. There is a natural homomorphism $H \to M$ with dense image, which permits the extension of the representation τ from H to M on suitable states; μ_1 is Haar measure on M . The state ρ_1 is again a Gibbs state.

Let us suppose that $X \simeq \mathbb{Z}^d$. The case $d = 3$, with $\hat{H}/X$ compact, and ρ_1 an extremal Gibbs state, corresponds to the idea we have of a periodic crystal. If $X^\perp \subset H$ is the group of periods of the crystal, the decomposition (3) coincides then with the decomposition of ρ_o into $X^\perp$-ergodic states. A quasiperiodic crystal would correspond to $d > 3$, and liquid crystals might correspond to $d < 3$. There are other possibilities than $X \simeq \mathbb{Z}^d$. For instance, we can imagine a "Feigenbaum crystal" where X would have a subgroup isomorphic to $\{p2^q : p,q \in \mathbb{Z}\}$. A turbulent crystal would correspond to the situation where ρ_1 is not an extremal Gibbs state, so that the decomposition of ρ_o into extremal Gibbs states is strictly finer than the almost periodic decomposition (3).

To prove the existence of turbulent crystals would presumably not be easier than to prove the existence of periodic ones. Here we shall only indicate one way in which a turbulent crystal structure might arise. Suppose that a quasiperiodic crystal with $X \simeq \mathbb{Z}^5$ is given, corresponding to two rationally unrelated modulations of a periodic lattice $\mathbb{Z}^3$. The compact Abelian group M is here a 5-torus : $M \simeq T^5$. Writing $T^5 = T^2 \times T^3$, and using $H \simeq \mathbb{R}^3$, we may define a group of "return maps" $\varphi_\xi : T^2 \to T^2$, labelled by $\xi \in \mathbb{Z}^3$ (we may think of ξ as defining a translation of the unmodulated crystal lattice). One (at least) of the maps φ_ξ has dense orbits in T^2, and it can be shown (see Ruelle and Takens [17], Newhouse, Ruelle and Takens [13]) that a small perturbation of φ_ξ will lead to "chaotic" behavior (sensitive dependence on initial condition). It appears therefore likely that, in situations where quasiperiodic crystals with two independent modulations are present, turbulent crystals may also appear.

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