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SOME REFLEXIONS AND QUESTIONS ABOUT APERIODIC CRYSTALS

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I enjoyed tremendously this workshop ! Denis Gratias and I thank cordially all the participants to have made it. I learned a lot; mainly about experimental facts and methods. How clever are experimentalists ! I sympathized very much with the theorists : it is amusing to play with models ! I was fascinated by the works of mathematicians here. Thanks to the excellent logistic of Les Houches "Centre de Physique", I could be very relaxed from the responsabilities I had; so I had a lot of time for thinking and discussing. As a result, many questions arise that I cannot answer so I will share them with you.

As you know, in the XIX century, crystallography was in the forefront of studies on symmetry in Nature : the 32 point groups were determined (Frankenstein, Hessel) before the word groups was introduced by Galois (1830) and the 230 space groups were cataloged independently by a mineralogist Fedorov and a mathematician Schönflies in 1892. (It is true that space groups were not applied for the study of crystals before the twenties). In the last quarter of the XIXth century, symmetry arguments were used more and more by physicists for explaining or predicting physical properties of matter (e.g., Jacques and Pierre Curie prediction of piezoelectricity) and P. Curie paper on the symmetries of physical states [1] is a classic still very much worth reading. In the XXth century, the symmetry of physical laws was a central subject in physics. After special relativity it lead Einstein to formulate its general relativity theory. It also guided Dirac for the discovery of its famous equation; and after three years of extraordinary intellectual struggle, Dirac predicted from it the existence of a new type of symmetry in physics : that of charge conjugation (between matter and antimatter). Fifteen years ago emerged a new step in the unification of physics : QED (quantum electrodynamics) gauge group $U(1)$ could be enlarged to $U(2)$ to unify weak and electromagnetic interaction and to $U(3)$ for chromodynamics and electromagnetism; so now, physicists are at work for discovering the grand unified theory (and even the supersymmetric theory which will also include gravitation). Hence physical laws have a huge and beautiful symmetry which is realized nowhere in the physical states, but which may have been the symmetry of the universe at the big bang. Tremendous efforts are made by physicists for observing predicted effects : proton decay (life time of $10^{32\pm 2}$ years), t'Hooft - Polyakov monopole with mass in the range $10^{-8} \sim 10^{-6}$ grams ! It will take so many years and so much money for these and other experiments to be completed that it is very refreshing to look simply at the intriguing symmetry of a phase of some Al-Mn alloys.

It is a strange paradox that physicists were able to predict from symmetry arguments the existence of antimatter, of the $N^{\pm}$, Z° bosons but not that of the icosahedral quasi-crystal phase. On the contrary it was a much believed dogma that such crystals could not exists ! Thanks to D. Schechtman and his collaborators to have observed them !

It must be said that theoricians are just beginning to explain the existence of crystals from first physical principles (statistical mechanics of the interacting atoms of the crystal) and works of this kind are not very well known (see e.g. /2/, /3/, /4/ and their bibliography). It is true that, similar to the geometrical deduction of the space group classification, there exists a general scheme for predicting the symmetry group of the mesomorphic phases /5/:they are the closed co-compact (i.e. the set of their cosets is compact) subgroups of the Euclidean group $E(3)$. These groups form an infinite (but compact) set; so the predictive value of the scheme is weak (while only 8 space groups are not yet illustrated by actual crystals). However, on such general grounds, one can also classify the topologically stable symmetry defects of those phases /6/ and this has been quite useful for recognizing recently new phases of liquid crystals. The same general scheme (decomposition of Euclidean invariant states into extremal states of the C^*-algebra of local observables) predict also a great variety of equilibrium phases without symmetry group corresponding to the ergodic action of $E(3)$. Their classification has not been done : surely, it must contain the incommensurate and aperiodic crystal phases.

To my knowledge, the first prediction of an aperiodic (in one direction) crystal state was made independently by J. Villain /7/ and Yoshimori /8/ in 1959. That was helimagnetism, which was observed by Herpin et al./9/. It is really aperiodic because the ratio of the helix period to the distance between neighbour reticular planes containing the spins is a continuous function of temperature (in general there is no locking). The next observation of an incommensurate structure by De Wolf et al. /10/ is well known here and both Janner and Janssen had the opportunity to convince us once more that the best way to describe these structures is to use quasi-periodic functions; they are restrictions of 4, 5 or 6 period functions. The latter can be considered as the description of a crystal (a simple and elegant auxiliary thinking tool) in 4, 5,6 dimensions.

The first time I discussed with Denis Gratias about the icosahedral phase it was perfectly clear in his mind that it had also to be described by quasi periodic functions in 3 dimension, restriction of 6-period functions with periods in ratio $1,1,1,\tau,\tau,\tau$, ($\tau = (1+\sqrt{5})/2$) . This is a unique fixed point in 6 dimensional space, while the representative point of a modulated crystal depends on temperature, pressure, external fields, etc... We heard also very convincing argument, e.g. by P. Bak, that this is the good frame for describing this new phase. Of course, as we were explained by several colleagues, Penrose patterns, and their extensions to three dimensional space (A. Mackay; Kramer and Neri) were already avalaible and give us a very concrete model to play with. They will help to explain the structure of the different alloys. There is however a difficulty not yet met by crystallographers : the existing software for crystal analysis does not work. How to describe most economically the position of the atoms ? I believe that it will be by giving the "motive" of the six dimensional crystal, and to check the predictions from this structure with every possible experimental analysis. I do hope that the simplet 1^3 , τ^3 hypercubic structure in 6-dimension will work. If it were not the case, one may go higher in dimension (10 and 15 were already suggested). The trouble is that the choice may be too large. Indeed what is needed is to know the n-dimensional lattices whose holohedry group G contains Y_h , the 120-element symmetry group of the dodecahedron or icosahedron, with the condition that the corresponding n dimensional representation of Y_h by integer matrices must contain, when extended to real matrices, its 3-dimensional vector representation. However a finite group representation by integer matrices might be reducible (i.e. it leaves a subspace invariant) without being indecomposable into a direct sum of irreducible representations. This does not occur in 2 or 3 dimensions but already begins in dimension 4. In ref. /11/ see Bravais lattices XVII/IV and XVII/VI . Their holohedries is isomorphic to O_h ; the integer representations is reducible on R (vector + one dimensional representation) but indecomposable on the integers Z . And for Y_h the member of indecomposable, Z-inequivalent representations on the integers is infinite! This is also true for Y, it is due to the fact that its 2-Sylow group ~ $Z_2 \times Z_2$ is not cyclic([1]) /12/. It does not seem that the non-decomposable representations of Y or Y_h have been yet classified. However there is no reason to worry about this problem as long as the 6-dimensional simple hypercublic lattice works.

There is also the T phase, quasi-crystal in 2 dimensions periodic in one, not to speak of the phases known for several years, crystal in two dimensions and quasi crystal in one. There is therefore a challenge to theorists to give a list of such possible new phases, and to experimentalists: find them if they exist.

It was very interesting to see how Landau theory can accomodate the existence of icosahedral and similar phases. I would like in the written report to refer to some impressive work that I did not quote in the oral talk but which were mentionned by Jean Taylor : those of C. Radin /13/ . His statistical mechanic models yield both crystals and aperiodic crystal. There were also private discussions for the possibility to observe what Ruelle /14/ calls "turbulent" crystals; and I did note less ignorance and more scepticism as usual among the participants

We heard the great news that there are now icosahedral phase crystals with a size of few millimeters (instead of microns !). So we will soon learn a lot more, not only about their structure, but also on their physical properties; there is much work ahead for the theorists to explain them ! How do these crystals grow ? This seems to be a completely new problem, quite different from that of periodic or modulated crystals. A detailed study of their shape will probably gives us some hints.

To conclude, I want to thank you all again to be here, I think we did well what we had to do, as I heard it expressed by Niels Bohr in my youth : "We tried to explain to each other what we do not yet understand".

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([1]) Thanks to Andreas Dress for discussion on this point.

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