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Some Non-Linear Physics in Crystallographic Structures

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I. INTRODUCTION

During the past ten years, the development of neutron scattering techniques and the improvement of the other experimental methods allowed considerable progress in the knowledge of crystallographic structures. Although most crystals can be understood on the basis of an harmonic model with small perturbation terms, many crystals which undergo a change of structure at some temperature, exhibit unexpected features, and sometimes in a rather large region around the transition temperature.

The central peak phenomenon first discovered in 1971 in the strontium titanate¹ is one of the most intriguing. The structural phase transition of this crystal at 105 K, was believed to be of the displacive type, which means that the elastic forces between the atoms are temperature dependent and some of them vanish at the transition temperature, then allowing the change of structure of the crystal. The softening of the elastic atomic constants is experimentally observable by looking (for example, by neutron scattering) at the variation of the phonon peak frequencies of the dynamical response function. In strontium titanate, the softening of one phonon peak was indeed observed but turned out to be incomplete. Close to the transition temperature, instead of vanishing, the soft phonon frequency ceases to decrease and then a zero frequency peak (the central peak) grows with a divergent intensity at the transition. Further experiments did not succeed in determining the width of this central peak. It might be zero as this has been recently shown in KDP², an other compound which exhibits a central peak. However, there are probably several kinds of central peak³ which may have a zero width or not and which require several interpretations. Some theories⁴

interpret the central peak phenomena by a strong anharmonicity of the atomic forces, the others assume the existence of defects or impurities.⁵ These theories might be complementary but until now, none of them has been convincingly shown to explain any given experiment.

Incommensurate structures in crystals are also surprising phenomena. For example, in potassium selenate⁶ which exhibits a structural phase transition at 93 K, the structure of this crystal above the transition temperature (between 93 K and 129.5 K) is modulated by a static periodic distortion. Its period varies with the temperature and so is generally incommensurate with the lattice period.

Other various unexpected features have been observed in compounds which generally undergo structural phase transitions, and also in magnetic structures. They are actually intensively studied and their list grows month after month. For brevity's sake, we will not continue their description but this brief survey demonstrates the ignorance we have of strongly non-linear systems in which the standard approximations may fail drastically.

The aim of this talk is not to present a review of the different theories which have been developed to interpret these phenomena but to present a summary of some of these studies on simple but strongly non-linear models which make use of some methods in stochasticity. I hope this will show the potential applications which might exist in solid state physics for any progress in this field.

Two one-dimensional models will be described. One has been studied to understand some aspects of the non-linear dynamics in crystals when close to the transition temperature. The second one is for commensurability and incommensurability problems.

II. PERIODIC ORBITS AND THE DYNAMICS OF A ONE-DIMENSIONAL COUPLED DOUBLE-WELL CHAIN

The model that we consider is a chain of atoms i , the energy of which is

$$\phi \left[\{ u_i, p_i \} \right] = \sum_i \left[\frac{1}{2} p_i^2 + \frac{1}{2} C (u_{i+1} - u_i)^2 + (u_i^2 - 1)^2 \right] \quad (1)$$

where p_i is the momentum of the atom i with mass unity.

u_i is its displacement with respect its mean position.

C is the elastic coupling constant between two consecutive atoms.

$(u_i^2 - 1)^2$ is a double-well potential (assumed to be created by a rigid sublattice of different atoms).

It is an oversimplified model⁴ to understand the dynamics of structural phase transitions, which contains some of the essential characteristics of the real crystals which undergo a structural phase transition. Its transition temperature is zero; then all the atoms are either in $u_i = +1$ or in $u_i = -1$.

Numerical calculations have been performed⁷ to obtain the space time Fourier transform of the atomic correlation function.

$$\mathcal{S}(q, \omega) = \int e^{i\omega t} \left[\sum_n e^{iqn} \langle u_i(t) u_{i+n}(0) \rangle \right] dt \quad (2)$$

which is an experimentally measurable quantity. Of course, $\mathcal{S}(q, \omega)$ depends on the temperature of the chain (numerically on its initial energy).

Quasi harmonic theories predict, in this model with one atom per unit cell, that $\mathcal{S}(q, \omega)$ must contain (for $\omega \geq 0$) only one phonon peak

at a finite frequency $\omega_{ph}(q)$ with some broadening. In fact, numerical calculation shows that there are (mainly) three peaks, the relative intensity of which varies with the temperature. In addition, one of them is at zero frequency (central peak). We call the two others quasi-phonon peaks. This central peak and one quasi-phonon peak only exist at low temperature. When increasing the temperature, the other quasi-phonon peak appears and develops at the expense of the two first ones which disappear at high temperature. There is a finite region in temperature, where these three peaks coexist.

The central peak is very narrow close to the order-disorder limit $C \ll 1$ while there is almost no softening of the two quasi-phonon frequencies (they are almost independent of the temperature) the spectrum evolves continuously until the displacive limit ($C \gg 1$), where the central peak is then rather broad and where there is an appreciable softening of the two non-zero frequency peak in the quasi-critical region.

This striking behavior can be understood by looking to particular periodic solutions of the non-linear motion equations.

$$\ddot{u}_i + 4 u_i (u_i^2 - 1) + C(2u_i - u_{i-1} - u_{i+1}) = 0 \quad (3)$$

When $C \gg 1$ (displacive limit) a continuous field can be introduced because u_i varies very slowly versus its index i . Considering it as a continuous variable x gives the motion equation

$$\frac{\partial^2 u}{\partial t^2} - C \frac{\partial^2 u}{\partial x^2} + 4u(u^2 - 1) = 0 \quad (4)$$

Propagating solutions with the form $u(qx - \omega t)$ satisfy the equation

$$-(Cq^2 - \omega^2)u'' + 4u(u^2 - 1) = 0 \quad (5)$$

It can be easily integrated, using the three kinds of Jacobi elliptic functions:⁸ dn and cn when $Cq^2 < \omega^2$, sn when $Cq^2 > \omega^2$. These three kinds of solutions are periodic orbits of the whole system.

Considering their energy and their amplitude versus their period in space and time a semi-quantitative interpretation^{4b,7} of the variation of the dynamical correlation function $\mathcal{L}(q, \omega)$ versus the temperature can be given close to the displacive limit.

The family of solutions dn corresponds to small amplitude motions of the atoms in one side of their double-well, and the family cn corresponds to large amplitude symmetric motions from one side to the other side. They interpret the two quasi-phonon peaks with a non-zero frequency.

The third peak, at zero frequency (central peak) is interpreted by the family of solution sn . Some of these solutions are stationary (time-independent) They represent equidistant walls which can be moving uniformly or not. (A single wall separates the chain in two regions with different ordering e.g. $u_i > 0$ for $i > i_0$ and $u_i < 0$ for $i < i_0$. When there are several walls, it is an intuitive concept if they are distinguishable.)

When the wave vector of a solution of this family goes to zero, one obtains a moving single wall (a moving kink). Due to the Lorentz invariance on x and t of the continuous motion equations (4), its energy

is a function of its velocity v by the standard relation:

$$E(v) = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} E(0) \quad (6)$$

with $c = \sqrt{C}$ the limiting velocity of these kinks (physically, it is a sound velocity). Although these kinks are not true solitons (they are not kept when they interact) this particle-like behavior allows us to suppose that they behave independently if they are widely separated.⁴ Then it can be assumed that they are well described by a perfect gas (which at high enough temperature might be relativistic) these assumption allows a quantitative calculation of the shape of the central peak of $\mathcal{S}(q, \omega)$ and of its width.

III. LATTICE LOCKING AND STOCHASTICITY

The above interpretation holds only at the displacive limit ($C \gg 1$). However, it now becomes clear that the central peak of this model is related to the existence of a family of solutions of the motion equations, which contains stationary solutions. These last solutions can be studied in the discrete model far from the displacive limit by considering a non-linear planar mapping. Eq. (3) with $\ddot{u}_i = 0$ yields:

$$C(u_{i+1} + u_{i-1} - 2u_i) - 4u_i(u_i^2 - 1) = 0 \quad (7)$$

The point $\mathcal{P}_{i+1}$ of coordinates (u_{i+1}, u_i) is then a function $T(\mathcal{P}_i)$ of the point $\alpha \mathcal{P}_i = (u_i, u_{i+1})$. This planar transformation T

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = T \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 2x + \frac{4}{c}x(x^2 - 1) - y \\ y \end{pmatrix} \quad (8)$$

is area preserving and has similar properties to those which have been already studied.⁹ Giving an arbitrary initial point $p_1 = (u_1, u_0)$ the iterated sequence $T^n(p_1)$ for $-\infty < n < +\infty$ determine a solution of (7).

The essential feature of the T-mapping, which has physical consequences, is that the sequence of points which do not go to infinity map either analytical curves, or appear to be erratic (in that case, it is a Cantor set which is mapped).

In an exceptional case, it can also map a set of n , n^{th} order fixed points $F_1, F_2 = T(F_1) \dots F_n = T^n(F_1) = F_1$, of the transformation T^n . However, the properties of these fixed points, determine also many properties of the T-mapping. Their iterated sequences represent commensurate configurations in model (1). (We mean that their period is commensurate with the lattice spacing.) The simplest fixed points of our transformation (8) are first order. They are $H_1 = (1,1)$ $H_2 = (-1,-1)$ and $F_0 = (0,0)$. H_1 and H_2 are hyperbolic. In other words, the eigenvalues of the linearized form of T , in H_1 or H_2 are real and their product is unity. The corresponding eigendirections are also real, one is attractive, the other is repulsive. Consequently, these fixed points are unstable with respect to the transformation T but their iterated sequences represent the two classical ground-states of model (1). Fixed point F_0 can be

either elliptic when $C > 1$ (the eigenvalues of the linearized form of T in $\mathbb{F}_0$ are complex with modulus unity and the transformation T is locally equivalent to a rotation on an ellipse) or hyperbolic when $C < 1$. When it is elliptic, it is stable with respect to the transformation T but its iterated sequences represent the dynamically unstable state $u_i \equiv 0$ of model (1).

(K.A.M.theorem)¹⁰

The Kolmogorov-Arnold-Moser theorem predicts that (generally) there exist invariant analytical curves with respect to the non-linear transformation T , around its n^{th} order elliptic fixed points. On these curves, the transformation T^n is topologically equivalent to a rotation incommensurate with 2π . For example, when $\mathbb{F}_0$ is elliptic, there exist connected closed analytical curves around it. A consequence is that the atomic position of the configurations of the model (1) generated by the points of one of these curves can be written as:

$$u_i = f(i + \alpha) \quad (9)$$

α is an arbitrary phase, and f is an analytical periodic function. It is clear that (9) represents an incommensurate periodic configuration of model (1). The perturbation spectrum of this configuration is obtained by linearizing (3) in ϵ_i after setting

$$u_i(t) = f(i + \alpha) + \epsilon_i \exp(i\omega t) \quad (10)$$

where ω is the frequency of the perturbation mode. It yields

$$-\omega^2 \varepsilon_i + C(2\varepsilon_i - \varepsilon_{i+1} - \varepsilon_{i-1}) + \varepsilon_i(3f^2(i + \alpha) - 1) = 0$$

(11)

Differentiating (7)

with respect to i and comparing with (11) show that $\omega = 0$ is an eigenfrequency and that $\varepsilon_i = f'(i + \alpha)$ is the eigenvector. It is the translation mode. Consequently, this configuration is not locked.

The generation of the erratic sequences of the transformation T can be understood by looking first at the wall configuration of model (1) in the discrete case. A stationary configuration with a single wall (with for example $u_{-\infty} = -1$ and $u_{\infty} = +1$) is represented in the T -mapping by a sequence of points $T^n(p_0)$ which go from $H_2 = (-1, -1)$ for $n = -\infty$ to $H_1 = (1, 1)$ for $n = +\infty$. These points belong to the set of points, the successive transformations of which, by T go to H_1 (this set is a line which is called the contracting sheet of H_1) and to the set of points, the successive transformations of which by T^{-1} go to H_2 (it is the dilating sheet of H_2).

For a linear transformation, the contracting and dilating sheets of its unique fixed point exist only in the hyperbolic case and are straight lines parallel at the fixed point to the real eigendirections. In the non-linear cases, these sheets only exist for hyperbolic fixed points but may have extremely complex shapes (see Ref. 11). In addition, contracting and dilating sheets may intersect. The intersection points are called homoclinic if the two involved fixed points are the same, and heteroclinic if they are not. Then, the single wall configurations

are represented by heteroclinic points associated with the couple of hyperbolic fixed points H_1 and H_2 . They do exist as this can be checked numerically.¹¹

A theorem^{10b}, Chapter III theorem 3-7 states that if one homoclinic point exists, there also exists an infinite number of such points. Their closure is a Cantor set Λ which is stable by T and in which this transformation is a Bemoilli shift. As a result, T is ergodic and mixing in Λ . Physically, that means that an infinitely small change of the atomic positions of a configuration generated by such a point is impossible by keeping it stationary. This implies that the perturbation cannot possess any zero frequency mode.

The same property is true for the heteroclinic points which represent the single walls. They are (generally) locked for any value of the coupling constant C . Random distribution of such locked walls (provided that they are not too close to each other) are the physical representation of the erratic trajectories of the transformation T . At high concentration, the walls cannot be considered as independent because they overlap one another; the resulting interaction competes with the lattice locking and an unlocked configuration may result. This is exactly what is proven above by the K. A. M. theorem.

It turns out from these remarks that we can make the physical equivalence in model (1) configuration: representative curve in the T -mapping

unlocked $\leftrightarrow$ analytic (non-stochastic)

locked $\leftrightarrow$ non-analytic or stochastic

We refer the reader to (11) for many more details which also concern the other kind of excitations.

When C is large most of the trajectories of T are analytical

curves. This is consistent with the displacive limit where the continuous model (4) applies and where the stationary configurations are described by elliptic functions which are periodic and analytic. Close to this limit, the lattice locking effects become very weak, the wall dynamics are fast and the central peak broad. When C decreases, these stationary configurations one after the other become locked, the wall dynamics slower and the central peak narrower. At $C=0$ the walls are perfectly locked because the chain is composed of independent particles and the central peak has a zero width.

These results are consistent with the numerical results⁷ and demonstrate the important role of the lattice effects on the dynamics associated with the central peak of this model.

IV. COMMENSURABILITY AND INCOMMENSURABILITY IN CRYSTALLOGRAPHIC STRUCTURES¹²

In the above model (1), the classical ground-state is trivial. However, this is not the case in many models describing the structure of new compounds, as for example K_2SeO_4 mentioned in the introduction. One of the more simple models where such a situation does occur describes a one-dimensional epitaxial monolayer of a gas adsorbed on a crystal surface. Its potential energy is

$$\phi \left(\{u_i\} \right) = \sum_i \left[V(u_i) + W(u_{i+1} - u_i) \right] \quad (12)$$

where u_i is the position of the i^{th} atom of the monolayer, $V(u_i)$ is a periodic potential with period $2a$ which represents the crystal surface, and $W(u_{i+1} - u_i)$ is the interacting potential between neighboring atoms of the chain. Its minimum is obtained for $u_{i+1} - u_i = b$ which is

generally not commensurate with $2a$. The potentials are assumed to be smooth enough (say analytical) function (see ref. 12).

Finding the classical group-state needs to minimize the energy (12). If ϕ in (12) is not considered as an energy but as the action of a single particle with coordinates u_i , with a discrete time i , the equations of extremalization of (12) describe a formal canonical system (see Ref. 10, appendices 32,33). This remark is generalizable to all classical model with short-range interactions for crystallographic or magnetic structures. When V vanishes in (12), this canonical system has a motion invariant

$$u_{i+1} - u_i = \ell = \text{constant} \quad (13)$$

This system is integrable. Considering $V(u_i)$ as a small perturbation, the K.A.M. theorem (Ref.10a, theorem 21.11 and b, theorem 2.11) is applicable. (for details, see Ref. 12) and yields the following conclusion.

For most ℓ incommensurate with the period $2a$ of the potential V (except a zero measure set) and for V small enough, there exist solutions of the extremalization equation of (12) which can be written as

$$u_i = (i + \alpha)\ell + f((i + \alpha)\ell) \quad (14)$$

where f is an analytic function with period $2a$, which goes to zero when V goes to zero, and with zero mean value. α is an arbitrary phase.

Now, if we consider an infinite epitaxial monolayer with fixed ends such that for N going to infinity

$$u_N - u_0 = N\ell \quad (15)$$

with $\frac{\ell}{2a}$ irrational. The analytical solution (14) is the classical ground-state. Since it is represented by an analytical function of i , it is not locked by the substrate potential (see the previous section). It possesses a zero frequency translation mode.

For large enough potential $V(u)$, we can prove (using some assumption (18) on V and W mentioned in the following) that the ground-state can no longer be represented by (14). Mathematically, the invariant torus with period ℓ of the K. A. M. theorem which describes a ground-state disappears. This is a transition from a non-stochastic regime to a stochastic regime. Physically, the monolayer becomes locked by the subtract potential V , for some critical value of its amplitude. This transition can be interpreted by saying that when the potential V becomes strong enough, and the particles are obliged to stay in bounded intervals close to the minima. Then, the $u_i \pmod{2a}$ cannot be dense on the interval $[0, 2a]$ which means that u_i cannot be represented by formula (14) with f periodic analytic.

The Peierls system¹³ in which Fröhlich mode (zero frequency translation mode) is generally assumed to exist, is very similar to this epitaxial model and might exhibit in some cases, the same kind of locking transition simultaneously with the appearance of an insulating phase. This question is to be examined in further studies.

When condition (15)(fixed volume) is relaxed, the model is with free ends. It is convenient in studying it to introduce an additive parameter by changing $W(u_{i+1} - u_i)$ in (12) into

$$\tilde{W}(u_{i+1} - u_i) = W(u_{i+1} - u_i) - p(u_{i+1} - u_i) \quad (16)$$

We get then in the energy an additional term

$$-p(u_N - u_0) = - \sum_{i=0}^{N-1} p(u_{i+1} - u_i) \quad (17)$$

showing that p is the conjugate parameter of the volume $(u_N - u_0)$ of the chain and is then a pressure.

To get more results, we now need to make some assumption about V and W . We assume that

W is a convex function

V is symmetric in addition to being periodic. (18)

This hypothesis is not unreasonable for many physical applications. The ground-state for any boundary conditions can then be proven¹² to have the form

$$u_i = (i + \alpha)\ell + \varepsilon_i \quad (19)$$

where ε_i has a zero mean value. Its modulus is bounded by $2a$, but it is not necessarily an analytic function of i . The equality (19) defines ℓ as the mean distance between neighboring atoms and α as a phase. A consequence is that the coexistence of two phases, in the ground-state with different atomic mean distance is impossible with or without any

boundary conditions. Therefore, no first-order transition can exist in this model by varying the parameters. This sharply contradicts the results which have been obtained by standard variational methods¹⁴ on a particular model (12) which satisfies (18)

The energy of the ground-state with fixed ends (15) versus ℓ is

$$\psi(\ell) = \psi_0(\ell) - p\ell \quad (20)$$

where $\psi_0(\ell)$ is the energy without pressure of the model with fixed ends (15). This function is shown to be convex¹² and the ground-state at constant pressure is given by solving

$$\psi'_0(\ell) - p = 0 \quad (21)$$

which defines ℓ versus p .

We show in Ref. (12) that when ℓ is commensurate with $(2a)$ the left and right derivatives of ψ are generally different and that

$$\psi'_-(\ell) < \psi'_+(\ell) \quad (22)$$

This function $\psi'(\ell)$ makes a jump at any rational value of $\ell/2a$. This jump is shown to be related to the smallest energy of the stationary phase excitations in this commensurate ground-state with period ℓ .¹² Then solving (21) to get $\ell(p)$ the atomic mean distance of the ground-state for a given pressure, shows that this function is constant each time that $\ell/2a$ is a rational number and for p satisfying

$$\psi'_{-}(\ell) < p < \psi'_{+}(\ell) \quad (23)$$

This monotonous increasing function $\ell(p)$ has infinitely many steps and is called a devil's stair. We can go further in choosing particular potentials for V and W in (12)

$$W(u_{i+1} - u_i) = \frac{1}{2} C(u_{i+1} - u_i)^2 \quad (24a)$$

C is a coupling constant.

$$V(u_i) = \frac{1}{2} \omega_0^2 (u_i - 2m_i a)^2 \quad (24b)$$

ω_0^2 is a positive constant and

$$m_i = \text{Int} \left(\frac{u_i}{2a} + \frac{1}{2} \right) \quad (24c)$$

make $V(u)$ periodic with period $2a$. However, this potential (24b) is not well-behaved since it is not differentiable for $u_i/2a$ an integer. All the configurations of this model are readily shown to be locked because this model is locally harmonic. This is consistent with the hypothesis of the version of Moser (Ref. 10, theorem 2.11) of the K. A. M. theorem which requires, when applied to our problem, that V must be at least more than three times differentiable.¹²

Model (12) - (24) is exactly soluble. The atomic mean distance of

the ground-state of this model at constant pressure is proven to be always commensurate with the period $2a$ of the subtract potential V (except perhaps for a zero set of pressure).

Then the function $\ell(p)$ defined by (20) is entirely composed of infinitely many constant steps (the width of them is calculable at any order). When varying the parameters of this model or the pressure, the atomic mean distance of the ground-state varies with infinitely many jumps but without first-order transition.

If such a transition exists in physical compounds as we believe, most of these jumps cannot be observed experimentally except perhaps the largest ones which correspond to simple order of commensurability of ℓ with $2a$ and which might appear as first-order transition but are not. The important feature of these transitions is that for V large enough, the locking forces are practically the same for commensurate (or incommensurate) configurations at any order. Then these sequences of transitions are expected to have a global hysteresis which can be simply described by assuming a solid friction between the monolayer and the substrate. When V is smaller, this friction disappears first for incommensurate configurations. Such phenomena are very similar to the unexplained hysteresis of the apparently continuous variation of the wave vector distortion of some crystal versus the temperature (for example, see Ref. 15).

V. CONCLUDING REMARKS

These exact results obtained on very simple models show that the real behavior of simple non-linear systems might be very different from what is obtained by standard approximations. This occurs because non-

linear systems can exhibit qualitatively different behavior from linear systems. These results of course cannot be obtained, as done usually, by approximating the non-linear system by a linear one. (Solitons, kinks, and stochasticity are examples.) In more complicated models, we may expect that the results are more varied. For example, it might be possible that the ground-state is apparently random although its Hamiltonian is not. Indeed, it turns out that the assumption (18) that we did on potential V and W are essential to get the devil's s stair transition that we just described. If they are relaxed, we ignore what can be the real structure of the ground-state of this model, even if it is periodic or not.

Another problem is to find the effect of the temperature and of the quantum fluctuations. They are well studied by renormalization group techniques.¹⁸ These methods make use of a recursive transformation which transforms a Hamiltonian into a renormalized Hamiltonian. This transformation has usually several kinds of fixed points. The fixed points which are attractive represent the phases of the system. Unstable fixed points with attractive and repulsive directions represent the critical points. The critical surface is simply their contracting sheet (see Sec. III). The behavior of the mapping of the renormalization group transformation has always been found to exhibit such a simple behavior but never stochasticity or only limit cycles. We believe that the explanation of this fact is simply that there are only a few possible structures in the considered models and therefore of possible transitions and fixed points. In systems as simple as the epitaxial model (12) considered in a several dimension version, and in many other models which might be involved in crystal structure, infinitely many

phases are possible and therefore infinitely many fixed points in the recursive renormalization transformation.

In addition, it is now known that new possible features, which are not believed to be exceptional, like a strange (or fractal^{16,17}) attractor may exist in recursive transformations. For example, if a strange attractor exists for the recursive renormalization transformation of some model, it has a finite basin (the set of points which converge to the strange attractor by the recursive transformation) which in some sense plays the same role as the critical surface in usual cases. The corresponding transition should be not at a critical temperature, but extended on a finite interval of temperature $T_1 < T < T_2$. We think that in this range of temperature the crystal structure should be composed of static macrodomains providing then an alternative explanation⁵ for a zero width central peak phenomenon. In other cases, we may have limit cycles for the recursive renormalization transformation which may describe transition with modulated structures like those of K_2SeO_4 .⁶ We believe that models with conflicting interactions between the atoms like the one we considered here in (12) might provide examples of such unexpected behavior of the renormalization group.

These remarks remain still speculative and need detailed studies on particular models. But for this reason, we believe that mathematical progress in non-linear problems should be very useful to help in the understanding of these complex situations and therefore to get explanations of some recent experiments on unusual crystallographic and magnetic structures and perhaps also on amorphous structures.

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