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ABSTRACT

Models describing both the "order-disroder" and "displacive" ferroelectric phase transitions are reviewed. By introducing a model pseudospin-phonon Hamiltonian the tunnelling motion of the atoms is also taken into account. On the basis of the self-consistent phonon-field and molecular-field approximations a complete system of self-consistent equations for the two order parameters (average atomic displacement and average population of equilibrium positions) is obtained. The analysis of this system of equations shows that the ferroelectric phase transition (first or second order) can be either the order-disorder, displacive or mixed type, depending on the dimensionless coupling energy of atoms (or their zero-point energy).

АННОТАЦИЯ

Предложены модели для описания сегнетоэлектрических фазовых переходов как типа "порядок-беспорядок", так и типа "смещения". В более общем варианте модели учитываются также эффекты, связанные с туннелированием. Но основе приближений самосогласованного фононного поля и молекулярного поля получена самосогласованная система уравнений для двух параметров порядка /среднего смещения активных атомов и средней заселенности их равновесных положений/. Качественный анализ и также численное решение уравнений показывают, что сегнетоэлектрический фазовый переход /первого или второго рода/ может быть как типа порядок-беспорядок, типа смещения, так и смешанного типа, в зависимости от величины безразмерной энергии связи атомов /или их энергии нулевых колебаний/.

KIVONAT

A ferroelektromos fázisátalakulások tárgyalására modelleket javaslunk, amelyek egyaránt jól leirják a rend-rendezetlen tipusu és a rácstorzulással járó fázisátalakulásokat. A tanulmány második részében az állapotok közötti alagutazással kapcsolatos effektusokat is figyelembe vesszük. A self-consistent fonon-tér és molekuláris tér közelitéseket alkalmazva a két rend-paraméter - az aktiv atomok átlagos elmozdulása és egyensulyi helyzeteik átlagos betöltöttsége - meghatározására egy self-consistent egyenletrendszert nyerünk. Az egyenletrendszer kvalitativ vizsgálatából, éppugy mint a numerikus számitások eredményeiből láthatjuk, hogy az atomok redukált kötési energiájától /illetve a null-ponti rezgések energiájától/ függően lehet /az első-, illetve másodrendü/ ferroelektromos fázisátalakulás rend-rendezetlen tipusu, rácstorzulással járó vagy kevert tipusu.

1. INTRODUCTION

It is generally assumed that there are two basic kinds of phase transitions (PT) in ferroelectrics, one being the order-disorder type and the other being the displacive type (see, for instance, [1], [2]). In the former case the PT results from a statistical disorder of atoms among several (in the simplest case between two) equilibrium positions. In the latter case the PT is caused by lattice instability against a critical vibrational mode (soft mode).

Nevertheless it has been shown in the last years that both types of ferroelectric PT can be described within a single model and there are no essential differences between them (see, for instance, [3]). In the simplest case this model is described by the Hamiltonian which is expressed as a sum of single-site energies, as determined by double-minimum potential wells, and the harmonic couplings between atoms in different cells. The nature of the PT described by such models has been examined by applying both the Curie-Weiss (or molecular-field) and the self-consistent phonon-field approximations. It has been shown [4] by comparing the results of both approximations that for a weak lattice coupling the character of the PT is of the order--disorder type, which is more consistently described by the molecular-field approximation; for a strong lattice coupling the PT has to be related to the displacive type, which can be reasonably described by the self-consistent phonon field

approximation. Such a consistent description can be understood under the circumstances that in the order-disorder transition statistical fluctuations of atoms onto their equivalent equilibrium position play the main role, which is accurately enough described by the pseudo-spin model, while in the displacive transition the dynamical correlations of atomic displacements turn out to be more essential, so the self-consistent phonon-field approximation is more efficient.

However, for a complete description of ferroelectric PT one has to take into account both mechanisms simultaneously in the frame of a universal model. A unified approach of this type has been proposed in [5] and we briefly consider it in Section 2.

However, the single-particle tunnelling motion of atoms has not been taken into account in [5]. The incorporation of the tunnelling motion as an additional degree of freedom leads to collective excitations which may have a soft mode character [2] or cause the appearence of a central peak [6],[7]. Since the tunnelling energies (of the order of the ground state quantum splitting) are usually much smaller than the characteristic phonon energies, the role of such excitations is predominant at low temperatures ($\hbar\Omega \sim k_B T$). On the other hand, in addition to a renormalization of the pseudospin-energy parameters of the De Gennes type [8], the higher phonon excitations can lead to the structural PT of the displacive type (against a certain vibrational mode) at higher temperatures. In [9] ,

[10] the excitations of both types were taken into account self-consistently (within the variational approach of Bogoliubov). This has been achieved by representing the cooperative atomic motion as a slow tunnelling process among several (in the simplest case, among two) equilibrium positions an addition to familiar phonon-like oscillations. This more general type of ferroelectric PT is briefly reviewed in Section 3. Some conclusions are presented in the last Section.

2. UNIFIED MODEL OF FERROELECTRIC PHASE TRANSITIONS

In a model description of the structural PT dynamics it is convenient to use the concept of local normal coordinates [11], [12], [13] involving all active atoms in the given critical vibrational mode. By using this representation a simplified model Hamiltonian can be written in the form:

$$H = \sum_i \{ \frac{\vec{P}_i^2}{2m} + U(\vec{S}_i) \} + \frac{1}{2} \sum_{i \neq j} V(\vec{S}_i, \vec{S}_j) . \qquad (2.1)$$

Here m is the corresponding effective mass of the critical mode, the single-site $U(\vec{S}_i)$ and the pair interaction $V(\vec{S}_i, \vec{S}_j)$ potentials define the critical dynamics of the model. The local normal coordinate $\vec{S}_i$ describes a distortion of the whole unit cell i. $\vec{P}_i$ is the canonical conjugate momentum to $\vec{S}_i$.

It is assumed further, that the single-site potential $U(\vec{S}_i)$ has two minima corresponding to two equilibrium atomic configu-

rations ($\alpha=\pm 1$) in the unit cell. Therefore the local normal coordinate $\vec{S}_i$ can be written as

$$\vec{S}_i = \sum_{\alpha=\pm 1} \vec{S}_i^{\alpha} \sigma_i^{\alpha} \quad . \tag{2.2}$$

Here $\sigma_i^{+} = 1(o)$ and $\sigma_i^{-} = O(1)$ according to whether the atomic configuration corresponds to the state $\alpha = +1(-1)$ respectively. The projection operator σ_i^{α} itself can be expressed by the pseudospin operator

$$\sigma_i^{\alpha} = \frac{1}{2} (1 + \alpha \sigma_i) \; ; \quad (\alpha = \pm 1) \; , \tag{2.3}$$

which is introduced as an independent variable, commuting with the coordinate $\vec{S}_i^{\alpha}$ and the momentum $\vec{P}_i^{\alpha}$ operators.

The coordinate in the state α, $\vec{S}_i^{\alpha}$ can be written as a sum of a static displacement $\vec{b}_i^{\alpha}$ and a thermal fluctuation $\vec{u}_i^{\alpha}$:

$$\vec{S}_i^{\alpha} = \vec{b}_i^{\alpha} + \vec{u}_i^{\alpha} \; ; \quad \vec{b}_i^{\alpha} = < \vec{S}_i^{\alpha} > = \vec{b}_{\alpha} \; , \tag{2.4}$$

where the symbol $< \ldots >$ stands for a statistical average with the Hamiltonian (2.1).

Therefore this representation of distortions as given by Eqs. (2.2), (2.4) enables one to take into account, at first, the atomic random distribution over two equilibrium positions in the cell, using the operator σ_i^{α} and secondly, the thermal fluctuation $\vec{u}_i^{\alpha}$ in the neighbourhood of a given equilibrium position. In describing order-disorder PT the latter variables are usually neglected, whereas in displacive PT it is assumed

that there is only one equilibrium position in the cells (α=+1 or α=-1); thus the operator σ_i^α takes the same value at each lattice site i. In this generalized model we will be able to study both types of PT using the full representation (2.2), (2.4). Such a physical picture is in agreement with recent computer simulation and it is also appealing for the reason of universality [6], [14]. It should be pointed out that the representation (2.2) for atomic coordinates as a sum of pseudospin and phonon variables was proposed by Vaks and Larkin [15] in their discussion of order-disorder type structural PT (see also [1], § 6). We generalize their representation to consider the displacive type PT as well.

Having inserted the definition (2.2) in the Hamiltonian (2.1), it can be written in the form:

$$H = \sum_i \sum_{\alpha=\pm 1} \sigma_i^\alpha \{ \frac{1}{2m} (\vec{P}_i^\alpha)^2 + U(\vec{S}_i^\alpha) \} + \tag{2.5}$$

$$+ \frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta=\pm 1} \sigma_i^\alpha \sigma_j^\beta V(\vec{S}_i^\alpha , \vec{S}_j^\beta) \} \quad .$$

The equilibrium positions of lattice atoms $\vec{b}_\alpha = < \vec{S}_i^\alpha >$ are determined using the equilibrium condition in the form

$$i(\partial/\partial t) < \vec{P}_i^\alpha (t) > = < [\vec{P}_i^\alpha , H] > \tag{2.6}$$

which leads to the equation

$$< \frac{\partial}{\partial \vec{S}_i^\alpha} U(\vec{S}_i^\alpha) > + \sum_{j\beta} < \sigma_j^\beta \frac{\partial}{\partial \vec{S}_i^\alpha} V(\vec{S}_i^\alpha , \vec{S}_j^\beta) > = 0 \quad . \tag{2.7}$$

The phonon spectrum and the average values of the atomic

displacement correlation functions of the model can be considered within the framework of the self-consistent phonon field theory [16] using the thermodynamical Green's functions

$$D_{ij}(t-t') = \langle\langle \vec{u}_i(t) \; ; \; \vec{u}_j(t') \rangle\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, e^{-i\omega(t-t')} \, D_{ij}(\omega) \quad , \tag{2.8}$$

where ordinary notations are used [17].

Dealing with the pseudo-spin subsystem an effective Hamiltonian can be introduced:

$$\tilde{H}_s = \sum_i h_i \sigma_i - \frac{1}{2} \sum_{i \neq j} J_{ij} \sigma_i \sigma_j \quad . \tag{2.9}$$

Here the effective single particle "field" h_i and the effective "exchange energy" J_{ij} can be written on the basis of variational approach [18] in the form:

$$h_i = \sum_{\alpha=\pm 1} \frac{\alpha}{2} \left\langle \frac{1}{2m} (\vec{P}_i^{\alpha})^2 + U(\vec{S}_i^{\alpha}) \right\rangle_o + \sum_{\alpha,\beta=\pm 1} \sum_j \frac{\alpha}{4} \left\langle V(\vec{S}_i^{\alpha}, \vec{S}_j^{\beta}) \right\rangle_o \quad ; \tag{2.10}$$

$$J_{ij} = -\frac{1}{4} \sum_{\alpha,\beta=\pm 1} \frac{\alpha\beta}{4} \left\langle V(\vec{S}_i^{\alpha}, \vec{S}_j^{\beta}) \right\rangle_o \quad ,$$

where the statistical averaging $\langle \ldots \rangle_o$ is performed over phonon variables.

The general model has been considered in [5] for the one particle potential having a double-minimum form

$$U(\vec{S}_i^{\alpha}) = -\frac{A}{2}\ (\vec{S}_i^{\alpha})^2 + \frac{B}{4}\ (\vec{S}_i^{\alpha})^4 \ , \qquad (2.11)$$

and for the pair interaction in the harmonic approximation:

$$V(\vec{S}_i^{\alpha}\ ,\ \vec{S}_j^{\beta}) = \frac{1}{2}\ \varphi''_{ij}\ (\vec{S}_i^{\alpha} - \vec{S}_j^{\beta})^2 \ , \qquad (2.12)$$

where the parameters A and B define, respectively, the height of the potential barrier $U_o = (A^2/4B)$ and the distance between the two minima $2S_o = 2(A/B)^{\frac{1}{2}}$. It has been also assumed that the critical vibrations can be described by a one component local normal coordinata $\vec{S}_i^{\alpha} = (S_i^{\alpha}, 0, 0)$ that corresponds to a one component order parameter $\eta_{\alpha} \sim \langle S_i^{\alpha} \rangle$. The interaction (2.12) acts isotropically between the atoms in the 3-dimensional lattice. Employing the renormalized harmonic approximation [16]

$$\langle\langle (\vec{u}_i^{\alpha})^3\ ;\ \vec{u}_j \rangle\rangle \approx 3 \langle (\vec{u}_i^{\alpha})^2 \rangle\ \langle\langle \vec{u}_i^{\alpha}\ ;\ \vec{u}_j \rangle\rangle \qquad (2.13)$$

for the phonon subsystem and the molecular field approximation for the pseudo-spin subsystem with the effective Hamiltonian (2.9), a closed system of equations has been obtained for the equilibrium displacements η_{α} :

$$\eta_{\alpha}^3 - (1 - 3y_{\alpha})\ \eta_{\alpha} + (\eta_+ + \eta_-)\ f_o\ \sigma_{-\alpha} = 0 \ , \qquad (2.14)$$

for the average thermal fluctuations y_{α} of an atom in state α :

$$y_{\alpha} = \frac{B}{A} \langle (\vec{u}_i^{\alpha})^2 \rangle = \frac{B}{A} \int_0^{\infty} d\omega \coth \frac{\omega}{2k_B T} \left[-\frac{1}{\pi}\ \mathrm{Im} \langle\langle \vec{u}_i^{\alpha} \mid \vec{u}_i \rangle\rangle_{\omega + i\varepsilon} \right] , \qquad (2.15)$$

and for the order parameter $\sigma_{\alpha} = \langle \sigma_i^{\alpha} \rangle$ or $\sigma = \langle \sigma_i \rangle = 2\sigma^{+} - 1$:

$$\sigma = \text{th}\,\frac{(J\sigma - h)}{k_B T} \quad ; \qquad J = \sum_j J_{ij} \quad , \tag{2.16}$$

In (2.14) the dimensionless displacement $\eta_\alpha = (B/A)^{1/2}\, b_\alpha$ and coupling constant $f_o = (1/A) \sum_j \varphi''_{ij}$ were introduced. The effective exchange energy itself is defined by the equilibrium displacements:

$$J_{ij} = (A/4B)\, \varphi''_{ij}\, (\eta_+ + \eta_-)^2 \quad , \tag{2.17}$$

so that above the structural PT, when $\eta_\pm = 0$, J_{ij} becomes zero, leading to the unique solution $\sigma \equiv 0$.

In addition, we quote the expression for the spontaneous polarization, which is dependent in the present model both on the atomic order and on the atomic equilibrium positions, i.e., it is determined by two order parameters $\eta_\pm$ and σ . In dimensionless quantities, the spontaneous polarization is given by

$$\begin{aligned} P_s &= \frac{1}{N} \sum_i \left(\frac{B}{A}\right)^{1/2} \left(\langle \sigma_i^+ S_i^+ \rangle - \langle \sigma_i^- S_i^- \rangle \right) = \\ &= \frac{1}{2} (\eta_+ - \eta_-) + \frac{1}{2}\, \sigma (\eta_+ + \eta_-) \quad . \end{aligned} \tag{2.18}$$

By analysing only the equilibrium conditions (2.14) one finds that in addition to the solutions $\eta_+ = \eta_- = 0$ corresponding to the paraelectric phase (with $J_{ij} \equiv 0$) , nonzero solutions $\eta_\alpha \neq 0$ are also possible. In the case of weak coupling, $f_o \ll 1$ an order-disorder PT can occur since there are two equilibrium displacements η_+ and η_- in the unit cell ($\eta_+ - \eta_- \approx \sigma\, f_o \ll 1$), and there also exists the solution $\sigma = 0$, corresponding to the

complete disorder for an order-disorder PT . While for sufficiently strong coupling, $f_o \geq 0.25$ only one nonzero solution may exist, at all temperatures e.g. $\eta_+ \neq 0$, (for complete atomic order $\sigma=+1$) and therefore only the displacive PT is possible.

The system of self-consistent equations (2.14)-(2.16) obtained for the order parameters $\eta_\pm$ and σ has been solved numerically in the classical limit of high temperatures [5]. The numerical results for $\sigma(\tau)$ and $\eta_\pm(\tau)$ (where $\tau = k_B T/(A^2/B)$ is the reduced temperature) are presented in Figs. 1-3 for certain values of dimensionless coupling parameter f_o . It can be observed that for $f_o \leq 0.1$ an order-disorder PT takes place, for $f_o \geq 0.15$ only a displacive PT is possible, while in a narrow region $f_o \approx 0.12$ the PT is a mixed type one, described by all the three order parameters $\eta_+(\tau)$, $\eta_-(\tau)$ and $\sigma(\tau)$. The temperature dependence of the spontaneous polarization (2.18) for different f_o is shown in Fig. 4. Note that in the region of the order--disorder PT ($f_o < 0.1$), as compared to the ordinary Ising model, the spontaneous polarization is decreased more rapidly as the temperature is increased due to the temperature dependence of the effective exchange energy (2.17).

We note, that these features are also obtained by a more sophisticated calculation [19] based on the coherent potential approximation for the disordered lattice.

We emphasize an important advantage of the present description for ferroelectric PT by two order parameters. It enables one in obtaining the system of self-consistent equations for the order parameters to choose various approximations: the mole-

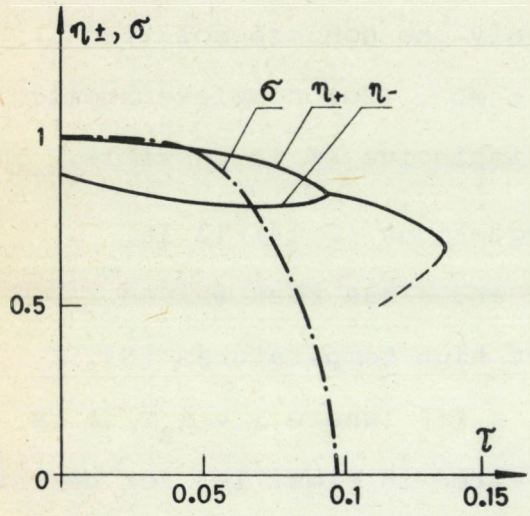

Fig.1. Temperature dependence of the order parameters $\eta_{\pm}$ - average displacement and $\sigma^{\pm}$ - average pseudospin value, for the dimensionless coupling parameter $f_o = 0.10$.

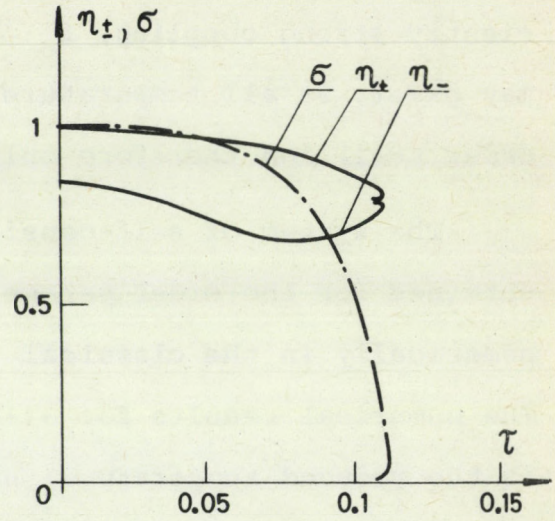

Fig.2. Same as Fig.1., for $f_o = 0.12$.

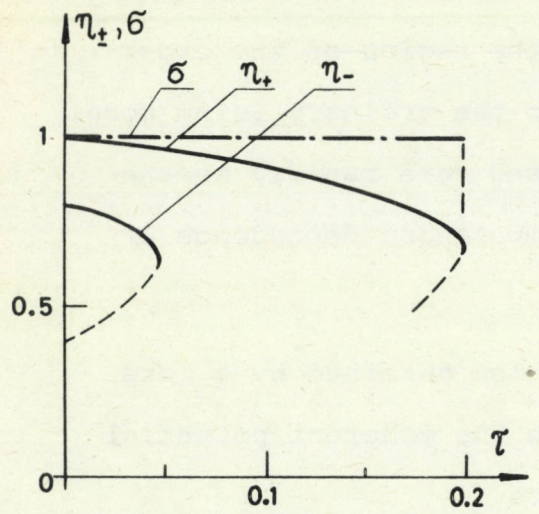

Fig.3. Same as Fig.1., for $f_o = 0.15$.

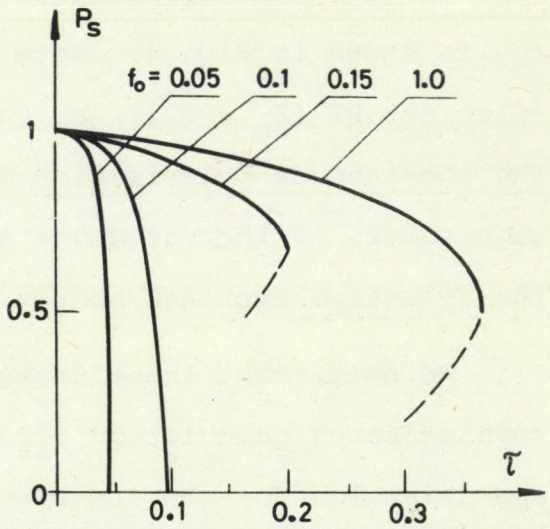

Fig.4. Temperature dependence of the reduced polarization P_s for several values of the coupling parameter f_o.

cular-field approximation for the parameter $\sigma(T)$ in Eq. (2.16) and the self-consistent phonon-field approximation for η_α and y_α in Eq. (2.15), which offers a satisfactory description of the PT, both in the case $f_o \ll 1$ (order-disorder transition of second order) and in the case $f_o \gg 1$ (the displacive PT for the parameter $\eta(T)$, of first order, close to second order), respectively. It is necessary to point out that the true order of the PT (first or second) cannot be predicted in the mean--field approximation (see, for instance, Ref. [1]), so we will not discuss this question here.

3. ORDER-DISORDER, TUNNELLING AND PHONONS IN FERROELECTRIC PHASE TRANSITIONS

In the quantum limit, T=OK, as follows from the Eq. (2.16), a unique solution, $\sigma \equiv 1$ appears (if $J_{ij} > 0$ and $h \geq 0$). The effect of tunnelling between states $\alpha = +1$ and $\alpha = -1$ suggested in [20], makes it possible to generalize the Hamiltonian (2.1) and to introduce in (2.9) the transverse field $\Omega \sum_i \sigma_i^x$, which in turn may lead to the solution $\sigma \to 0$ in the case T=OK. In the quantum limit the displacive PT is determined by the zero--point vibration energy. The limiting values for it has been obtained in both cases of the ordered (σ=1) and disordered (σ=0) lattices [21], assuming that the right choice of the transverse field Ω can ensure the translation from σ=1 to σ=0 in the case of zero temperature (T=OK).

However in the model description in order to take into account the tunnelling motion simultaneously with the statistical order-disorder and the phonon oscillations it is convenient to introduce the time-dependent local normal coordinate S_i participating in the given PT as decomposed into a slow tunnelling-like coordinate r_i with a characteristic frequency Ω and a comparatively fast displacement of the phonon type u_i, with characteristic frequency ω_o.

$$S_i = r_i + u_i \quad ; \qquad < u_i > = 0 \; . \tag{3.1}$$

Such a representation holds under the "adiabatic" condition: $\Omega \ll \omega_o$. Since the tunnelling energies $\hbar\Omega$ are of the order of the ground state quantum splitting, the adiabatic condition means that the latter ones must be much smaller than the characteristic phonon energies $\hbar\omega_o$.

Having inserted the representation (3.1) into the general Hamiltonian (2.1) we obtain a Hamiltonian depending on the variables r_i and u_i. In order to separate these variables the variational approach can be used, assuming that the system can be described by a trial Hamiltonian in the form:

$$H_o = H_{ph}(\{u_i\}) + H_s(\{r_i\}) \; , \tag{3.2}$$

where

$$H_{ph}(\{u_i\}) = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \phi_{ij} \, u_i \, u_j \; , \tag{3.3}$$

$$H_s(\{r_i\}) = \sum_i \{ \frac{p_i^2}{2m} + \tilde{U}(r_i) \} + \frac{1}{2} \sum_{i \neq j} C_{ij} (r_i - r_j)^2 \ . \qquad (3.4)$$

Here ϕ_{ij} , C_{ij} and $\tilde{U}(r_i)$ being the variational parameters, P_i p_i are the canonical conjugate momenta to u_i and r_i , respectively.

For the strongly anharmonic motion described by Eq. (3.4) it is convenient to introduce the pseudospin representation with respect to the ground doublet symmetric (Ψ_s) and antisymmetric (Ψ_a) single-particle states:

$$\{ \frac{p_i^2}{2m} + \tilde{U}(r_i) \} \Psi_{s,a}(r_i) = \varepsilon_{s,a} \Psi_{s,a}(r_i) \ , \qquad (3.5)$$

so that the Hamiltonian (3.4) is cast in the well known form of De Gennes [8]

$$H_s = - \Omega \sum_i \sigma_i^x - \frac{1}{2} \sum_{i \neq j} J_{ij} \sigma_i^z \sigma_j^z + E_o \ , \qquad (3.6)$$

where the energy parameters Ω, J_{ij} and E_o are some functions of ε_α , C_{ij} and the matrix elements $r_{\alpha\beta} = < \alpha \, | r_i | \, \beta >$ and $r_{\alpha\alpha}^2 \ < \alpha \, | r_i^2 | \, \alpha >$ $(\alpha,\beta = s,a)$, calculated with the wave functions in Eq. (3.5) .

The variational parameters ϕ_{ij} , C_{ij} and $\tilde{U}(r_i)$ are determined from the Bogolyubov variational approach, namely from the condition of stationarity of the free energy,

$$F = F_o + < H - H_o >_o = k_B T \, \ell n \, Sp \{ e^{-H_o/k_B T} \} + \\ + Sp \{ e^{(F_o - H_o)/k_B T} (H - H_o) \} \ , \qquad (3.7)$$

with respect to variations over these parameters or, equivalently, over the corresponding correlation functions. By this approach a closed system of self-consistent equations for all parameters entering in Eqs. (3.3), (3.4) and (3.6) can be obtained, which determines the phase transitions of the model and describes the mutual influence of phonon and pseudospin subsystems.

Having chosen the single-site double-well potential $U(S_i)$ in the form (2.11) and the pair-potential $V(S_i, S_i)$ in the harmonic approximation (2.12) the model for the ferroelectric phase transitions was investigated in detail in [9] , [10].

The spontaneous polarization of the system in this model is simply expressed by the "order-disorder" (σ_z) and the displacive (η) order parameters as

$$P_s = \frac{1}{N} \sum_i \left(\frac{B}{A} \right)^{\frac{1}{2}} < r_i > = \left(\frac{B}{A} \right)^{\frac{1}{2}} r_{sa} \sigma_z = \eta \sigma_z \quad , \tag{3.8}$$

where σ_z is the average occupation number. The average "slow" displacement can be written in the form

$$\eta(T) = \left\{ \frac{1-3y}{1-\rho^2} \right\}^{\frac{1}{2}} \quad . \tag{3.9}$$

Here $y = (B/A) < u_i^2 >$ is the reduced average quadratic "fast" displacement, ρ is the overlap of the ground state wave functions of the "left" and "right" unperturbed harmonic oscillators, the linear combination of which was choosed in [22] for the trial wave functions.

The order parameters η and σ_z were obtained on the basis

of the self-consistent phonon-field and molecular field approximation solving the system of self-consistent equations numericaly [22], for certain values of the dimensionless coupling parameter $\tilde{f}_o = (1/\tilde{A}) \sum_j \varphi''_{ij} = [\, 1/(A - 3B < u_i^2 >) \,] \sum_j \varphi''_{ij}$ and the temperature independent reduced quantum parameter $\lambda_o = (A/m)^{1/2}/(A^2/B)$, characterizing the zero-point vibrations. The results of the numerical calculations for $\sigma_z(T)$, $\eta(T)$ and $P_s(T)$ are presented in Figs. 5-8 for $\lambda_o = 0.1$ and $\tilde{f}_o = 0.1$, 0.2 and 0.6 respectively. The corresponding curves in Figs. 5-8 are in agreement with our previous ones: Fig. 1-4. In the weak--coupling limit: $\tilde{f}_o \ll 1$, the tunnelling effects are properly accounted for, consistently to the results by Gillis [3]. The appearance of imaginary solutions in Figs. 5-8 is assigned by open circles. A discontinuity itself in the displacive PT in the case of $\tilde{f}_o \ll 1$ is a very well known characteristic feature of the self-consistent phonon approximation [3]. In the strong--coupling limit the displacive PT does exist and it is properly described as previously in Section 2, since the tunnelling effect can be disregarded. As it can be observed in Fig. 7. the case $\lambda_o = 0.1$ and $\tilde{f}_o = 0.6$ corresponds to a mixed type PT.

In [22] exact self-consistent numerical solution of the Schrödinger equation (3.5) was also performed. The temperature dependence of all relevant parameters for various $\tilde{f}_o$ and λ_o agree fairly well with the results cited above (based on the trial waves functions) for $\rho \leq 0.5$.

Taking into account the tunnelling effects the results for a system with weak coupling in the low temperature limit are

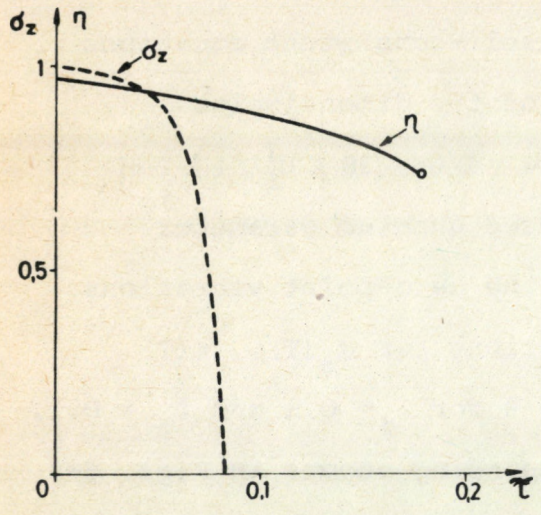

Fig.5. Temperature dependence of the order parameters: η - average displacement and σ_z - average localization, in the case of λ_o=0.1, for the dimensionless coupling parameter $\tilde{f}_o$=0.1 [$\tilde{\tau} = k_B T/(\tilde{A}^2/B)$].

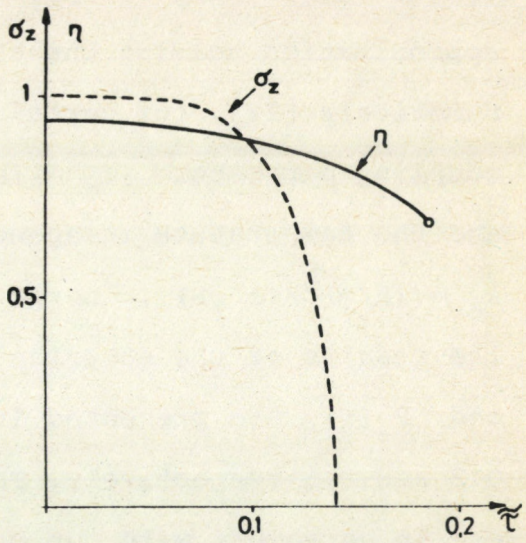

Fig.6. Same as Fig.5., for $\tilde{f}_o$ = 0.2 .

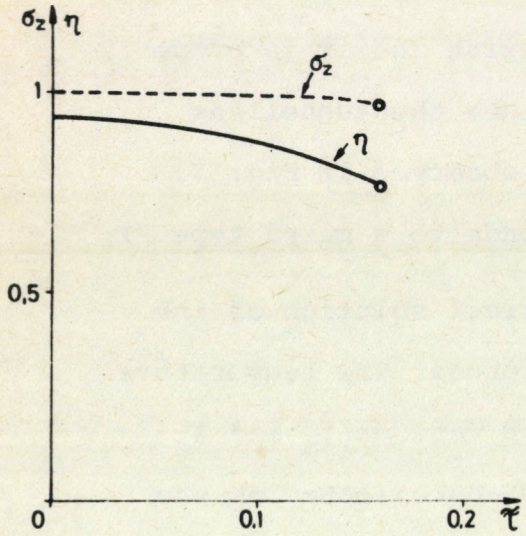

Fig.7. Same as Fig.5., for $\tilde{f}_o$ = 0.6 .

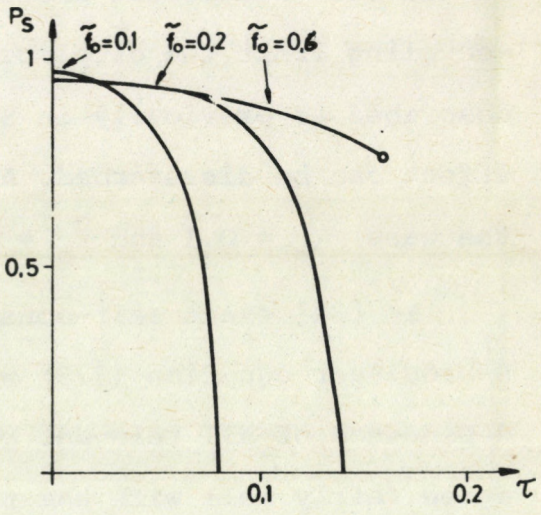

Fig.8. Temperature dependence of the reduced polarization P_s for several values of the coupling parameter f_o [$\tau = k_B T/(A^2/B)$], (λ_o=0.1) .

quite different from the ones, obtained in Section 2. In the quantum limit (T=OK) the order parameter σ_z in the molecular field approximation according Eq. (3.6) reads

$$\sigma_z = \frac{1}{J_o}\sqrt{J_o^2 - \Omega^2} \quad ; \quad \sigma_x = \frac{\Omega}{J_o} \quad , \tag{3.10}$$

where $J_o = r_{sa}^2 \tilde{f}_o$, and consequently it can change between the limits $0 \leq \sigma_z \leq 1$. In such a way the zero-point vibrations can destroy the ground state at T=OK both in the pseudospin and the phonon subsystems. Then according Eq. (3.8), one can expect that the spontaneous polarization P_s vanishes either in σ_z or in η , depending on the mutual competion between $\lambda_{o,s} \approx 1/\ell n(3/4\tilde{f}_o)$ and $\lambda_{o,ph} \approx 2\sqrt{\tilde{f}_o}$, i.e. depending on which is the smaller of the two.

Table 1.

$\tilde{f}_o$	0,05	0,10	0,20	0,30	0,40	0,50
$\lambda_{o,s}$	0.37	0,50	0,76	1,095	1,587	2,50
$\lambda_{o,ph}$	0,44	0,62	0,89	1,099	1,26	1,40

Table 1. shows, that in the quantum limit for $\tilde{f}_o < 0,3$ an order--disorder PT takes place, for $\tilde{f}_o > 0,3$ we can observe a displacive PT and for $\tilde{f}_o \sim 0,3$ the PT has a mixed character.

4. CONCLUDING REMARKS

A novel approximation scheme has been introduced, which takes into account simultaneously all the intriguing features of the

structural PT, i.e. the statistical order-disorder, the tunnelling and phonon oscillation in the frame of only one universal model. Our model description is based on the assumption that the local normal coordinate can be decomposed into a slow "tunnelling (hopping) displacement" and a phonon like one. As a consequence, the energy spectrum of the coupled quartic oscillators is represented as low-lying strong anharmonic excitations (due to the tunnelling - in distinction from Ref. [6], where the pseudospin-flip-type motion is associated with the classical transfer across the barrier) and higher phonon--like excitations, a rather weak anharmonic interaction of which is described in the pseudoharmonic approximation. However, since the energy spectrum of a particle in a local double well potential has quite a complex structure (see e.g. [6]), such a separation has merely an interpolatory character, i.e. it is physically inapplicable for a temperature region $k_B T \sim \hbar\Omega \sim \hbar\omega_o$. In particular, one could expect a more complex renormalization of the pseudospin parameters in order-disorder compounds, especially when the excited atomic states lie in the critical temperature region: $k_B T_c \sim J_o \sim \hbar\omega_o$.

Besides the theoretical and numerical analysis presented, it should be pointed out that our model reveals satisfactorily the essential features both of the order-disorder and displacive type PT at finite and zero temperatures.

Concluding this review it should be pointed out that a further development of this unified approach to the theory of

structural phase transitions is given in [23], where nonlinear effects for the order parameter η are taken into account in the spirit of the central peak dynamics [7], [14] and solitary waves [24] that permits one to go beyond the mean field type approximations discussed in this paper.

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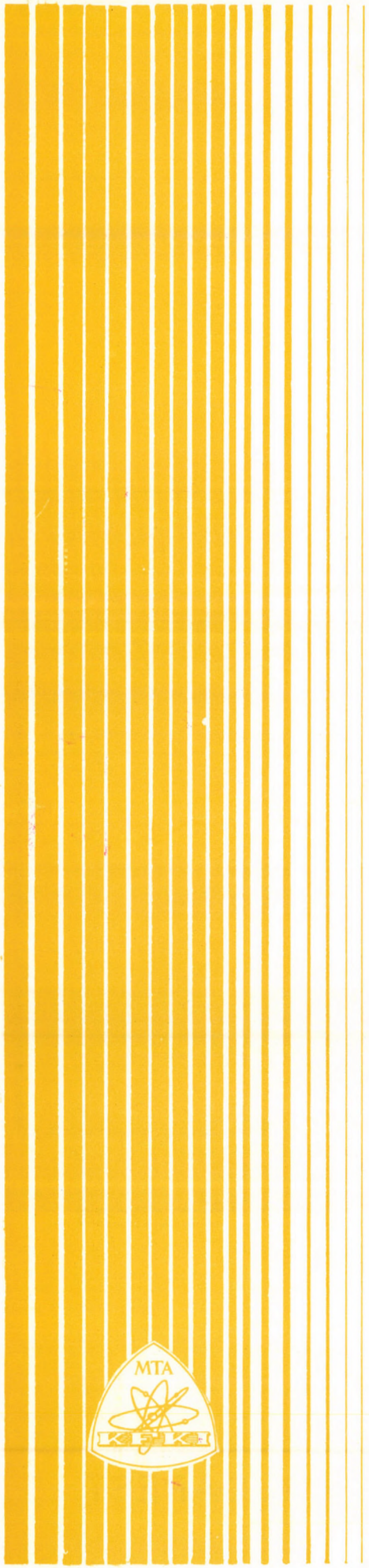

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