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SOFT MODE IN LOCALLY ANHARMONIC "$\varphi^3 + \varphi^4$" MODEL

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The dynamics of collective vibrations in the locally anharmonic model is studied. The single ion problem is treated by numerical calculation while interaction between ions in different cells is accounted for in the random phase approximation. The density of vibrational states is obtained at various values of the temperature, single ion asymmetry field and wave vector. The existence in the spectrum of the soft mode whose energy comes to zero at the critical point is verified. The redistribution of intensities among various energy branches at the varying of the wave vector is studied.

Key words: structural phase transitions, anharmonic vibrations, vibrational density of states, soft mode, critical point.

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I. INTRODUCTION

Using the concept of the local normal coordinate denoted below q_i (see, for example, [1]), the model Hamiltonian

$$H = \sum_i \left(\frac{p_i^2}{2M} + V(q_i)\right) - \frac{1}{2}\sum_{ij}\varphi_{ij} q_i q_j, \tag{1}$$

which describes a certain mode of the lattice vibrations, active at the phase transition, is applied to the studies of the mechanism of the structural phase transitions in crystals. The issue of choosing the type of the local potential $V(q)$ is raised. In the harmonic approximation ($V(q) = \frac{\alpha}{2}q^2, \alpha = M\omega_0^2$), the crystal lattice may become unstable in case of the negative value of α. As is mentioned in a number of papers, including [1], the simplest stabilizing interaction may be chosen in the form

$$V(q_i) = -\frac{\mid \alpha \mid q_i^2}{2} + \frac{\beta q_i^4}{4}. \tag{2}$$

In this case the system undergoes the structural phase transition which can be displacive or order–disorder in character, depending on the values of parameters in the initial Hamiltonian. Such a model is often applied to the description of the phase transition in ferroelectrics.

A large number of papers was dedicated to studies of thermodynamics and dynamics of the model described by the Hamiltonian (1), (2). Along with the application of the analytical methods of various degrees of approximation, including the method of self–consistent phonons, the method of renormalized group, etc., the attempts to take into account the effects caused by the local anharmonicity of the model by using numerical methods were made. Particularly, in [2] the energy spectrum of single–ion system described by (2) was calculated, while the interaction of the ions in different cells was taken into account in the mean field approximation; the comparison with the results obtained in the self–consistent phonons approximation was made. This approach is justified in the case of long–range interaction φ_{ij}; the obtained results can be improved by including of the higher order corrections when the expansion in the powers of the inverse radius of interaction is used.

In addition to the description of ion motion in ferroelectrics, the model local anharmonic concept is applied to the description of the lattice anharmonicity in the high temperature superconductors. As is pointed out in [3], such an anharmonicity is inherent to the motion of the apex oxygen ions in YBaCuO and other superconductive compounds. To take into consideration such an anharmonicity in the case of local double–well potential, the approach which introduces pseudospin variables describing the vibrational degrees of freedom was used. The pseudospin — electron model derived in this way, describing also the interaction of the conducting electrons with local anharmonic mode, was the subject of intensive study in the recent years [4–6]. The asymmetry of the anharmonic potential which is characteristic for the systems of this kind was taken into account by including into the Hamiltonian the term which described the interaction with some internal field $\tilde{h}_i$, depending on the occupancy of electronic states ($\tilde{h}_i = h + gn_i$). Structural phase transitions in HTSC systems, including Hg–based superconductors have been recently of wide consideration, in the context of reported connection between the lattice softening in these compounds and transition to the superconducting state. Particularly, in [7] it was mentioned that near the transition point an anomalous abrupt mode softening was observed. Peculiarities related to the presence of the lattice anharmonicity were observed in YBaCuO series on the temperature dependencies of the lattice constant c, coefficients of thermal expansion in the direction of anharmonic vibrations of oxygen ions, as well as specific heat, thermoconductivity and velocity of ultrasonic waves in the form of jump–like and hysteresis behaviour (see [8]).

For the description of such situations, the model potential possessing more general non–symmetrical shape due to the presence of the cubic term, was considered in [8,9]:

$$V(q_i) = \frac{\alpha q_i^2}{2} - \frac{\beta q_i^3}{3} + \frac{\gamma q_i^4}{4}, \ \alpha > 0 \qquad (3)$$

(so called "$\varphi^3 + \varphi^4$" model [10]). Basing on (3) and applying the method of self–consistent phonons it was shown that the behaviour of the apex oxygen in $YBa_2Cu_3O_{7-\delta}$ compound is bistable and the dependence of the order parameter on the temperature has a hysteresis character. However, the question of the applicability of the method of self–consistent phonons to the description of the phase transition in the systems described by (3), including critical areas arises (see [1]).

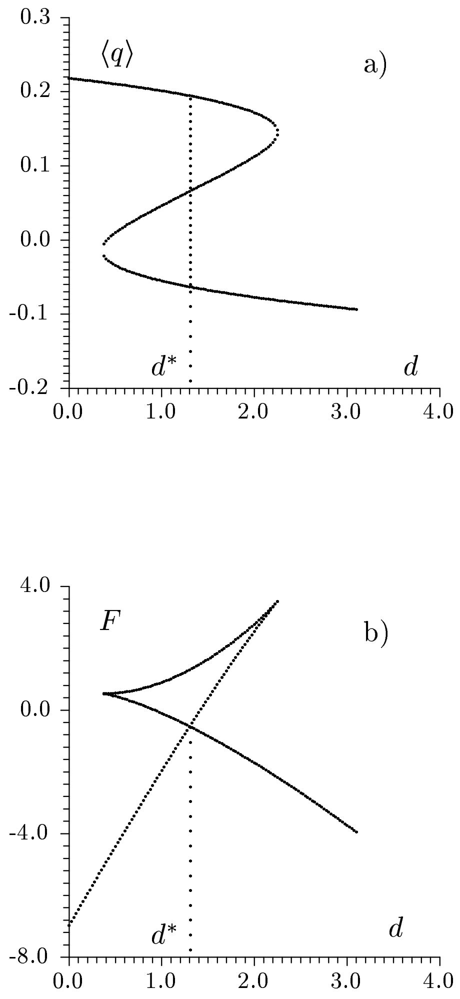

Fig. 1. Dependencies of the order parameter and free energy on the external field, $\frac{kT}{\hbar\omega_0}$=0.17.

Basing on these considerations, we tried to develop further the numerical approaches mentioned above. In [12] we modeled the potential acting on the ion in the form (3) and took into account the anharmonic character of the ion motion by the numerical diagonalization of the Hamiltonian matrix. In [12] we also considered the Gaussian barrier potential in the form $V_G(q_i) = \frac{\alpha q_i^2}{2} + Ce^{-Bq_i^2}$ which was applied to model the double well local potential in [13–15] (see also section III of this paper). The interaction between ions in different cells we took into account in the mean–field approximation, assuming the long–range character of the intercell interaction. Basing on this approach, we derived the dependencies of the order parameter, free energy and dielectric susceptibility on the externally applied field and the order parameter and free energy on the temperature in both models for various model parameters. Analysing these dependencies we investigated the phase transition as the external field varies as well as the temperature, which in the case of potential in form (3) is of the first order; we also considered the behaviour of the dielectric susceptibility near the phase transition point. In addition to that, we constructed the phase diagrams (external field, temperature) and studied the influence of the anharmonicity of potential on the form of the phase diagrams and the location of the critical points. The results obtained in the case of the problem with non–symmetrical potential (3) regarding the character of the phase transitions generally complied with the conclusions of [6], and [16], in which the similar investigations were related to the pseudospin–electron model of HTSC systems. Both in those cases, and in the model (3), the potential asymmetry led to the deviation of the phase coexistence curve from the vertical line on the plane (temperature, field) and to appearance of the first order phase transitions as the temperature varies, in the certain range of the parameters defining mentioned asymmetry; existence of this phase transition corresponded to the bistability of the system with the local potential (3) mentioned in [8,9].

In this paper the dynamical properties of the anharmonic model with potential (3) are studied. We will investigate the behavior of the spectrum of collective vibrations near the phase transition line, particularly addressing the lowest branches in the spectrum and highlighting the so called soft mode. The phonon density of states defined by the imaginary part of the Green function $\langle\langle q_i | q_k \rangle\rangle$ will be calculated. Accounting for the anharmonic motion of the ions will be made, as in [12] by numerical diagonalization of the single–ion matrix. The interaction between vibrations of the ions in different cells will be allowed for in the mean field approximation.

II. NUMERICAL TREATMENT OF SINGLE ION PROBLEM IN THE MEAN FIELD APPROXIMATION

In this section we consider the case of local anharmonic potential in non–symmetric form (3), where

$\alpha = M\omega_0^2 > 0$. Transformation of the last term in (1) in accordance with the mean–field approximation leads to

$$-\frac{1}{2}\sum_{ij}\varphi_{ij}q_iq_j \to \varphi\langle q\rangle q - \frac{1}{2}\varphi\langle q\rangle^2, \qquad (4)$$

$$\varphi = -\sum_i \varphi_{ij}.$$

This results in the following form of H:

$$H_0 = \sum_i H_i,$$

$$H_i = \frac{p_i^2}{2M} + \frac{M\omega_0^2}{2}q_i^2 - \frac{\beta q_i^3}{3} + \frac{\gamma q_i^4}{4} + dq_i + \varphi\langle q\rangle q_i - \frac{1}{2}\varphi\langle q\rangle^2. \qquad (5)$$

Here the asymmetry field described by the parameter d is introduced. On the basis of eigenfunctions of harmonic oscillator operators p and q have the form of the following infinite–dimensional matrices:

$$q_{kj} = \sqrt{\frac{\hbar}{2M\omega_0}}(\delta_{(k+1)j}\sqrt{k} + \delta_{k(j+1)}\sqrt{j}), \qquad (6)$$

$$p_{kj} = i\sqrt{\frac{M\hbar\omega_0}{2}}(\delta_{(k+1)j}\sqrt{k} - \delta_{k(j+1)}\sqrt{j}).$$

After substituting q and p in (6) according to (7), the Hamiltonian matrix has the following form (all terms are divided by $\hbar\omega_0$):

$$\frac{\hat{H}_0}{\hbar\omega_0} = \hat{\alpha} - C_1\hat{\beta} + C_2\hat{\gamma} + C_3\hat{\sigma}(d+\varphi\langle q\rangle) - C_4\langle q\rangle^2, \quad (7)$$

where $C_1 - C_4$ are defined through the initial model parameters, and matrices $\hat{\alpha}-\hat{\sigma}$ are the infinite–dimensional matrices whose elements may be defined using the following relations (see [12] for more detail):

$$\begin{aligned}
\alpha_{ij} &= \delta_{ij}\frac{2i-1}{2},\\
\beta_{ij} &= \delta_{i(j+1)}3j\sqrt{j} + \delta_{j(i+1)}3i\sqrt{i} + \delta_{i(j+3)}\sqrt{j(j+1)(j+2)} + \delta_{j(i+3)}\sqrt{i(i+1)(i+2)},\\
\gamma_{ij} &= \delta_{ij}3(i^2+(i-1)^2) + \delta_{i(j+2)}2(2j+1)\sqrt{j(j+1)} + \delta_{j(i+2)}2(2i+1)\sqrt{i(i+1)}\\
&\quad + \delta_{i(j+4)}\sqrt{j(j+1)(j+2)(j+3)} + \delta_{j(i+4)}\sqrt{i(i+1)(i+2)(i+3)},\\
\sigma_{ij} &= \delta_{(i+1)j}\sqrt{i} + \delta_{i(j+1)}\sqrt{j}.
\end{aligned} \qquad (8)$$

For the purpose of numerical treatment of the Hamiltonian matrix (7) we limit the dimension of this matrix to some finite size. As the calculation of dependencies of thermodynamical functions on model parameters shows, limitation of the size of Hamiltonian matrix (this corresponds to allowing for the finite number of harmonic oscillator levels, starting from the lowest one) to $N = 25$ is sufficient when $\frac{kT}{\hbar\omega_0} \le 5$. All calculations in section II are made within this approximation.

For calculation of the mean value of coordinate q_i which has a meaning of the order parameter we use the expression

$$\langle q\rangle = \frac{Sp(qe^{-\beta H_0})}{Spe^{-\beta H_0}}. \qquad (9)$$

After the unitary transformation is made

$$H_d = V^{-1}H_0V, \qquad (10)$$

which diagonalizes the Hamiltonian matrix (7), we get

$$\langle q\rangle = \frac{Sp(\tilde{q}e^{-\beta H_d})}{Spe^{-\beta H_d}}, \ \tilde{q} = V^{-1}qV. \qquad (11)$$

Note that $\langle q\rangle$ is contained in the Hamiltonian (7). Denoting $f = d + \varphi\langle q\rangle$, we derive the self–consistent system of equations:

$$\begin{cases} \langle q\rangle = \langle q\rangle(f,T), \\ f = d + \varphi\langle q\rangle. \end{cases} \qquad (12)$$

Numerical solution of this system allows to obtain the dependence $\langle q\rangle = \langle q\rangle(d)$ (Fig. 1a) for various values of $\frac{kT}{\hbar\omega_0}$ (in all calculations here, C_1=0.157, C_2=0.025, and $C_3\varphi = -20$; these values of parameters correspond to the ones used in [5]). Substituting this function in the Hamiltonian (7), we can calculate the dependence of the free energy on the external field, according to the expression below:

$$F(d,T) = -T \ln Sp\, e^{-\beta H_d} - \frac{1}{2}\varphi\langle q\rangle^2. \qquad (13)$$

Fig. 1b represents the obtained result for $F = F(d)$. The dependencies shown on Fig. 1 are typical for the first order phase transition. The abscissa of the self–crossing of curve F corresponds to the value d^* at which the phase transition occurs, causing a jump–like change of the order parameter on Fig. 1a. Raising the temperature leads to vanishing of the hysteresis–type of this dependence, i.e., to vanishing of the phase transition.

Temperature increase also results in decrease of d^*. Finding numerically d^* for each value of the temperature and different values of C_1, we construct the phase diagrams (d^*, T) which are shown on Fig. 2.

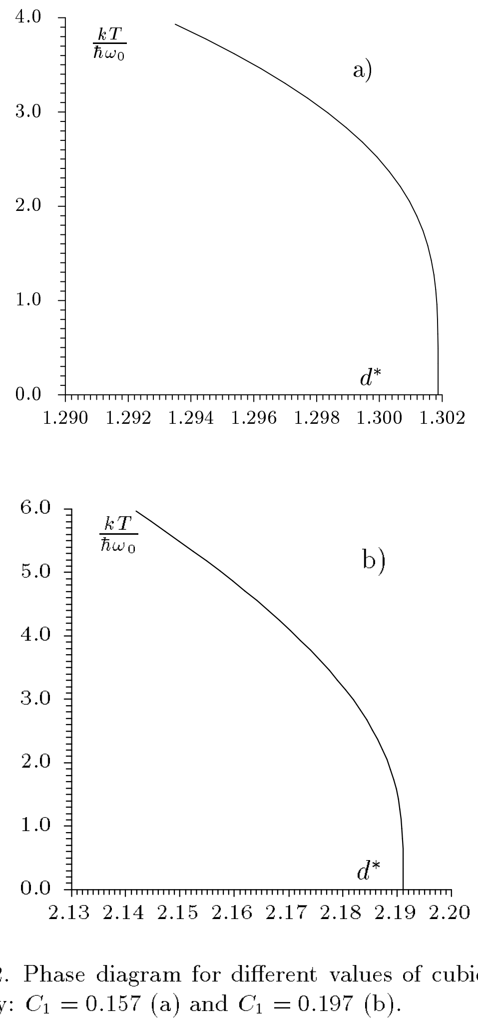

Fig. 2. Phase diagram for different values of cubic anharmonicity: $C_1 = 0.157$ (a) and $C_1 = 0.197$ (b).

The left end of the phase coexistence curve corresponds to values of d^* and $\frac{kT}{\hbar\omega_0}$ at which the phase transition vanishes, having a meaning of the critical point ($\frac{kT}{\hbar\omega_0} \simeq 3.9$, $d_c^* = 1.293$ at $C_1 = 0.157$ and $\frac{kT}{\hbar\omega_0} \simeq 6.0$, $d_c^* = 2.142$ at $C_1 = 0.197$). As was shown in [12], the presence of the anharmonicity of the third order significantly increases the value of the critical temperature.

III. PHONON SPECTRUM IN THE RANDOM PHASE APPROXIMATION

In the case of the investigated one–particle problem

$$\left(\frac{p_i^2}{2M} + V(q_i)\right)\psi_{ia} = W_a\psi_{ia}, \qquad (14)$$

we introduce Hubbard operators $X_i^{ab} = |i,a\rangle\langle i,b|$ on the basis of ψ_{ia} which describe transitions between the states of this basis (see [17]). Operator X_i^{ab} is the matrix which has only one non–zero element equaling 1 located at the intersection of row a and column b. Displacement q_i may be therefore written as

$$q_i = \sum_{ab} d_{ab} X_i^{ab}, \qquad (15)$$

where d_{ab} is the matrix element of displacement q

$$d_{ab} = \int \psi_{ia}^* q_i \psi_{ia} d\tau \qquad (16)$$

After introducing Hubbard operators the Hamiltonian (1) may be rewritten as

$$H = \sum_{ia} W_a X_i^{aa} - \frac{1}{2}\sum_{ij}\varphi_{ij} q_i q_j \qquad (17)$$

Let us consider now ions vibrations relatively to their average displacements q_i. Separating terms which correspond to the mean field approximation, Hamiltonian (17) may be rewritten in the form

$$H = -\frac{1}{2}N\varphi\langle q\rangle^2 + H_0 + H', \qquad (18)$$

where

$$H_0 = \sum_i \left[\sum_a W_a X_i^{aa} + \langle q\rangle\varphi q_i\right], \qquad (19)$$

and

$$H' = -\frac{1}{2}\sum_{ij} V_{ij}(q_i - \langle q\rangle)(q_j - \langle q\rangle) \qquad (20)$$

Diagonalization of Hamiltonian H_0 by means of unitary transformation (10) is accompanied by the following transformation of Hubbard operators:

$$X_i^{ab} = \sum_{\mu\mu'} q_{a\mu}^* q_{b\mu'} \tilde{X}_i^{\mu\mu'} \qquad (21)$$

where $q_{a\mu}$ are eigenfunctions of the one–site Hamiltonian matrix

$$\sum_b (W_a \delta_{ab} - \langle q \rangle J \tilde{d}_{ab}) q_{b\mu} = E_\mu q_{a\mu}, \qquad (22)$$

here

$$\tilde{d}_{\mu\mu'} = \sum_{ab} d_{ab} q_{a\mu}^* q_{b\mu'}, \qquad (23)$$

so that

$$q_i = \sum_{\mu\mu'} \tilde{d}_{\mu\mu'} \tilde{X}_i^{\mu\mu'} \qquad (24)$$

Then H_d is written in the form

$$H_d = \sum_{i\mu} E_\mu \tilde{X_i^{\mu\mu}}, \qquad (25)$$

Having transformed the Hamiltonian (17) this way, we construct the Green function

$$\langle\langle q_i | q_k \rangle\rangle = -i\Theta(t - t') \langle [q_i(t) q_k(t')] \rangle, \qquad (26)$$

where operators are written in Heisenberg representation, and statistical averaging is performed with Hamiltonian H.

After writing equation of motion for operators $\tilde{X}_i^{\mu\mu'}$, performing necessary linearization in the random field approximation, the Fourier image of the Green function can be written in the form:

$$G(q, E) = \frac{1}{2\pi} \frac{1}{Z^{-1}(E) + \varphi(q)}, \qquad (27)$$

where

$$Z(E) = \sum_{\mu\mu'} \tilde{d}_{\mu\mu'} \frac{\langle \tilde{C}^{\mu\mu'} \rangle}{E - E_{\mu\mu'}} \qquad (28)$$

Here

$$\tilde{C}_i^{\mu\mu'} = \sum_\nu (\tilde{d}_{\mu'\nu} \tilde{X}_i^{\mu'\nu} - \tilde{d}_{\nu'\mu} \tilde{X}_i^{\nu'\mu});$$

$$E_{\mu'\mu} = E_{\mu'} - E_\mu \qquad (29)$$

$G(q, E)$ in form (27–29) was derived in [17]. We need to transform $G(q, E)$ to the form convenient for further treatment and investigation. Denoting $A_{\mu\mu'} = \tilde{d}_{\mu\mu'} \langle \tilde{C}^{\mu\mu'} \rangle$, we rewrite (27) in the form

$$G(q, E) = \frac{1}{2\pi} \frac{P(E)}{\prod_{\mu\mu'} (E - E_{\mu\mu'}) + \varphi(q) P(E)}, \qquad (30)$$

where

$$P(E) = \sum_{\mu\mu'} A_{\mu\mu'} \prod_{\nu\nu' \neq \mu\mu'} (E - E_{\nu\nu'}) \qquad (31)$$

Assuming that we are able to solve equation

$$\prod_{\mu\mu'} (E - E_{\mu\mu'}) + \varphi(q) P = 0, \qquad (32)$$

or find roots of the polynomial in the denominator of (30), we write this denominator as

$$Q = \prod_j (E - \tilde{E}_j), \qquad (33)$$

where $\tilde{E}_i$ are the roots of equation (32).

This gives a possibility to expand (30), using a well–known formula, into the sum of simple fractions in a way that each fraction's denominator contains $E - \tilde{E}_i$:

$$G(q, E) = \frac{1}{2\pi} \sum_i \frac{P(\tilde{E}_i)}{Q'(\tilde{E}_i)} \frac{1}{E - \tilde{E}_i}. \qquad (34)$$

From (33) it follows that

$$Q'(\tilde{E}_i) = \prod_{i \neq j} (\tilde{E}_i - \tilde{E}_j). \qquad (35)$$

Form (34) immediately allows to write the phonon density of states $\rho(E) = 2\mathrm{Im}(G(q, E - i\epsilon))$. After making the analytical continuation to the complex plane and applying a well–known formula we derive:

$$2\mathrm{Im}(G(q, E - i\epsilon)) = \sum_i \frac{P(\tilde{E}_i)}{Q'(\tilde{E}_i)} \delta(E - \tilde{E}_i). \qquad (36)$$

Now we can interpret (36) as a set of peaks the heights of which are equal to $\frac{P(\tilde{E}_i)}{Q'(\tilde{E}_i)}$ (see Figs. 5–7).

After making simple transformations, $\langle \tilde{C}^{\mu\mu'} \rangle$ may be written as

$$\langle \tilde{C}^{\mu\mu'} \rangle = \tilde{d}_{\mu\mu'} \frac{e^{-\beta E_\mu} - e^{\beta E_{\mu'}}}{\sum_k e^{-\beta E_k}} \qquad (37)$$

In calculating $G(q)$, the quantities E_μ, $\tilde{d}_{\mu\mu'}$ are derived according to the procedure described in (15)–(25) and using the method outlined in section I. We assume that the double–well potential has the form of that in $\phi^3+\phi^4$ model, and use the model parameters mentioned in Chapter 1. The values of $\tilde{E}_i$, or spectrum of phonon vibrations is obtained by a numerical solution of equation (32). The values of roots $\tilde{E}_i = \tilde{E}_i(q)$ are between values of E_i and E_{i+1} and depend on $\varphi(q)$ (if $\varphi(q)=0$, $\tilde{E}_i = E_i$). The number of roots corresponds to the number of differences $E_{i\,i+1}$ and is equal to $N(N-1)$.

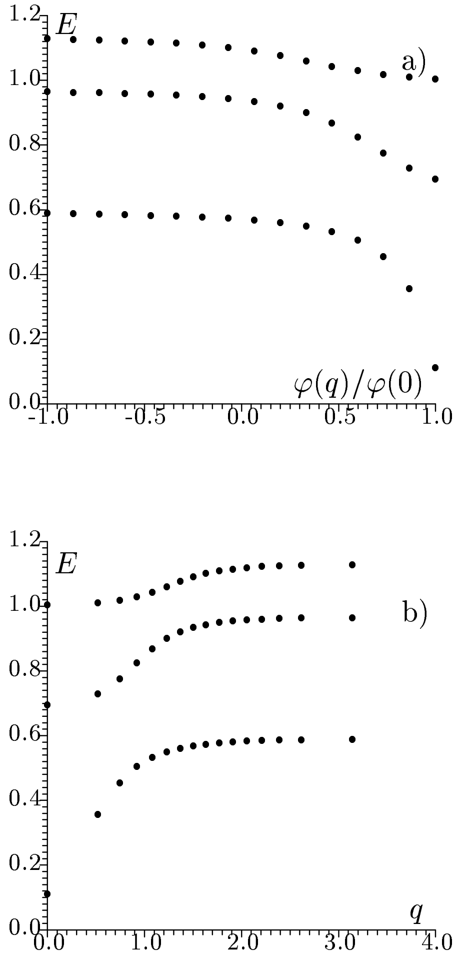

Fig. 3. Dependencies of the three lowest energy levels on $\varphi(q)/\varphi(0)$ (a), and on q (b).

The smallest value of $\tilde{E}_0(q)$ is the peculiar mode referred as the soft mode, as it will be shown below. Its value becomes small near the center of the Brillouen zone and comes to zero at $q=0$, or $\varphi(q)/\varphi(0)=1$ at the critical point. Before discussing the behavior of this mode, we comment on the results related to this matter found previously in [17]. Particularly, it was pointed out that the existence of a barrier and two minima in the local potential leads to the grouping of the lower energy levels into pairs. Two lowest energy levels pair at the beginning, while pairing of other levels is much less significant and quickly disappears with the energy increase. Such an effect was proved in [12] for the model with Gaussian barrier potential by the numerical approach mentioned above, i.e., by the diagonalization of the single–ion Hamiltonian: the existence of two parts of the spectrum of different character was found, with quasidoublet (at the lower values of energy) and quasi equally distanced (at the higher values of energy) structures. The crossover from one part to another is relatively sharp and takes place in the range of energies which are of the height of potential barrier by the order of magnitude. Thus, assuming that only two lowest levels are paired while all others stay equally distanced ("low anharmonicity double well") and applying random phase approximation, behavior of the soft modes was studied in [17]. Three modes were found in the energy spectrum and analysis of their statistical weights showed that there is effectively one soft mode which seemed to consist of three parts. The energy of this mode tends to come to zero near $T=T_c$ at $q=0$.

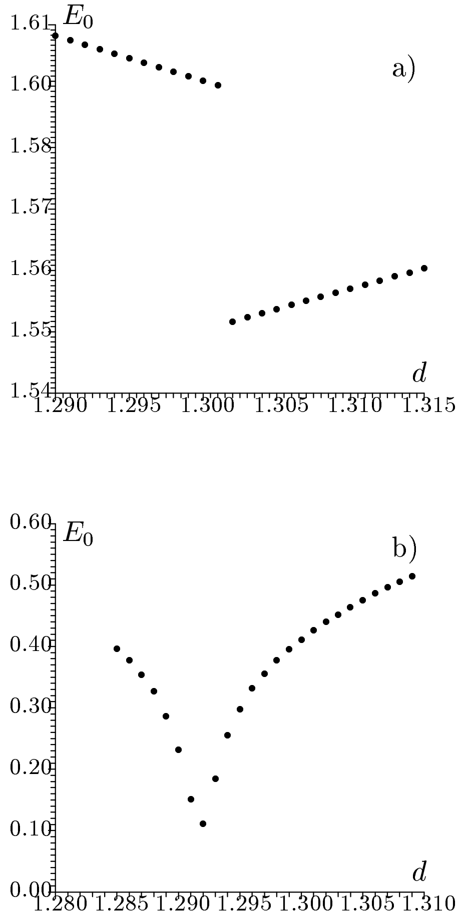

Fig. 4. Dependencies of the three lowest energy levels on d at $\tilde{t}=1.6$ (a), and at the critical point $\tilde{t}=4$ (b).

We plot three lowest energies $\tilde{E}$ found as solutions of (32), as functions of $\varphi(q)/\varphi(0)$ on Fig. 3a (dependence of $\tilde{E}$ on q is shown on Fig. 3b), for the values of d and $\tilde{t}=\frac{kT}{h\omega_0}$ which correspond to the critical point on the phase diagram shown on Fig. 2. As follows from Fig. 3, the lowest energy branch $\tilde{E}_0$ goes to zero when $\varphi(q)/\varphi(0) = 1$ [18]. As calculations show, at other values of $(d, \tilde{t})$ this does not happen; energy $\tilde{E}_0$ decreases as q comes to zero, but stays finite. This suggests that the lowest energy branch is the soft mode which becomes zero at $q = 0$ only at the critical point.

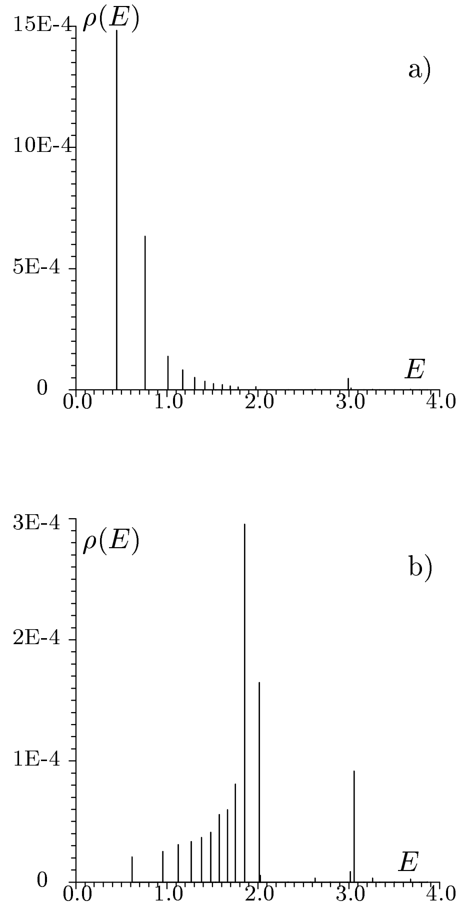

Fig. 5. Dependencies of $\rho(E)$ on E at $\varphi(q)/\varphi(0) = 0.8$ (a) and at $\varphi(q)/\varphi(0) = -0.8$ (b) at the critical point.

In order to study the behavior of the lowest energy branch at $\varphi(q)/\varphi(0) = 1$ near phase transition line, we also plot the dependencies $\tilde{E}_0 = \tilde{E}_0(d)$ for two different values of $\tilde{t}$ on Fig. 4. The jump–like change of the energy $\tilde{E}_0$ at $\tilde{t} = 1.6$ occurs at $d \simeq 1.301$ (Fig. 4a), i.e. at the point which falls on the phase coexistence line on Fig. 2. Such a change is understood since $\tilde{E}_\mu$ depends on E_μ, and in turn, as it follows from (5), E_μ depends on $\langle q \rangle$. At the phase transition point $\langle q \rangle$ changes jump–like, thus causing jump–like change of $\tilde{E}_0$. As calculations show, the height of this jump decreases as one moves to the critical point. At the critical point (Fig. 4b) no jump–like change occurs in $\langle q \rangle$ and therefore $\tilde{E}_0 = \tilde{E}_0(d)$ has no abrupt changes going to zero at the critical point.

Fig. 5 represents dependencies $\rho(E) = 2\mathrm{Im}(G(q, E - i\epsilon))$ in the energy range $0 < E < 4$ for different values $\varphi(q)/\varphi(0) = \pm 0.8, \pm 0.4$ at values $(d, \tilde{t})$ which correspond to the critical point. Comparing intensities which are shown as height peaks on Fig. 5 and Fig. 6 of energy branches for those values one concludes that moving to the lower values of $\varphi(q)/\varphi(0)$, or to the larger values of wave vector q leads to a gradual redistribution of intensities of phonon vibrations energy branches. At $q \sim 0$ the major branch with the maximum intensity is the lowest in the spectrum soft mode (Fig. 5a). As one moves from the center of the Brillouen zone this maximum moves to the upper energies (Fig. 5b, 6b). Such a redistribution of intensities was foreseen in [17], basing on approximation of "low anharmonicity double well".

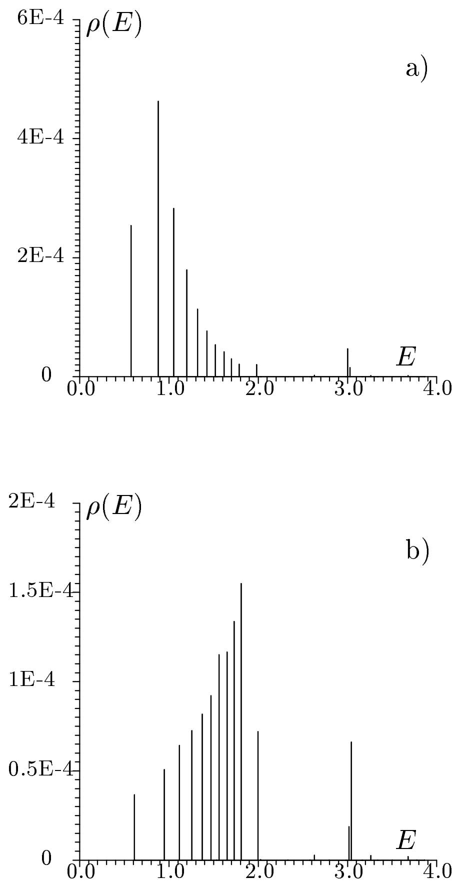

Fig. 6. Dependencies of $\rho(E)$ on E at $\varphi(q)/\varphi(0) = 0.4$ (a) and at $\varphi(q)/\varphi(0) = -0.4$ (b) at the critical point.

We also plot $\rho(E)$ for values $(d, \tilde{t})$ where d corresponds to the critical value of $d = d_{cr}$ but $\tilde{t} = \tilde{t}_{cr}/2$ and $\tilde{t} = \tilde{t}_{cr}/4$ on Fig. 7. This figure illustrates how the soft mode increases as one moves away from the critical point by temperature decrease; no substantial change of the spectrum density is observed. This soft mode increase is consistent with the one observed on Fig. 4b when we decrease parameter d starting from its critical value.

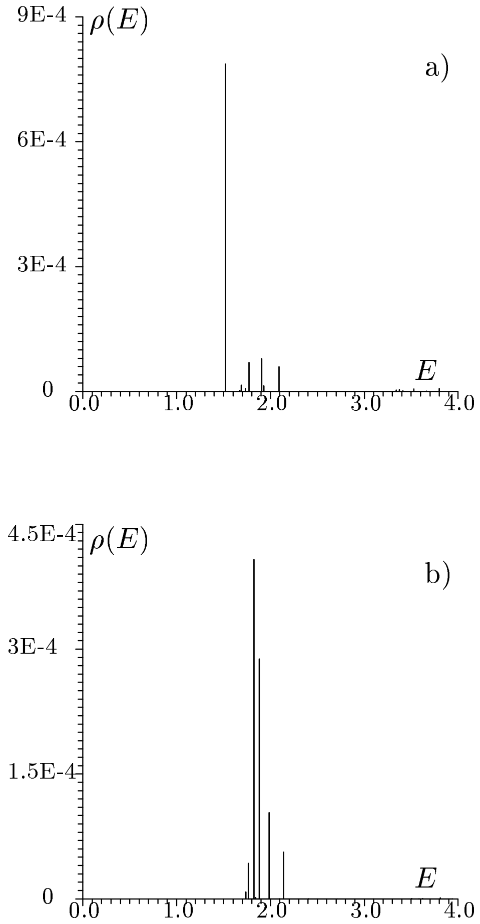

Fig. 7. Dependencies of $\rho(E)$ on E at $(d_{cr}, \tilde{t}_{cr}/2 = 2)$ (a) and at $(d_{cr}, \tilde{t}_{cr}/4 = 1)$ (b) at $\varphi(q)/\varphi(0) = 0.8$.

IV. CONCLUSIONS

In this paper the dynamics of collective vibrations in the locally anharmonic "$\varphi^3 + \varphi^4$" model is studied. The single ion problem is solved by numerical method and the interaction between ions in different cells is accounted for in the random phase approximation while calculating the phonon Green function. The density of vibrational states at various values of temperature $\tilde{t}$, single ion asymmetry field d and wave vector q is derived. The existence in the spectrum of the soft mode whose energy comes to 0 at the critical point is verified. The redistribution of intensities among various energy branches in the spectrum as the wave vector changes is established. It can be interpreted as manifestation of certain effective complex phonon vibration the energy and effective width of which are functions of the wave vector and also vary as the temperature and asymmetry field d are changed. A more detailed study of this effect in the "$\varphi^3 + \varphi^4$" model as well as in the related models and comparing it with the results which may be obtained in the approaches using various approximations (for example, self–consistent phonon approximation) deserve attention and may be the subject of further investigation.

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SOFT MODE IN LOCALLY ANHARMONIC "$\varphi^3 + \varphi^4$" MODEL

М'ЯКІ МОДИ В ЛОКАЛЬНО АНГАРМОНІЧНІЙ МОДЕЛІ "$\varphi^3 + \varphi^4$"

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Проведено дослідження динаміки колективних коливань локально ангармонічної моделі. Однойонну задачу розв'язано числовим методом, міжйонну взаємодію враховано при розрахунку фононних функцій Ґріна в наближенні хаотичних фаз. Отримано густину коливних станів при різних значеннях температури, поля асиметрії однойонного потенціялу та хвильового вектора. Встановлено існування в спектрі м'якої гілки коливань, енергія якої прямує до нуля в критичній точці. Виявлено перерозподіл інтенсивностей між різними гілками в спектрі при зміні значень хвильового вектора.