Condensed Matter Physics, 1999, Vol. 2, No. 3(19), pp. 435–446

Local anharmonic effects in high-T_c superconductors. Pseudospin-electron model

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Received September 13, 1999

Some aspects of physical phenomena in high-T_c crystals caused by anharmonicity of the crystal lattice are discussed. Appropriate theoretical models are considered. A review is given of the results obtained while investigating the pseudospin-electron model (PEM) when applied to the description of structural and dielectric instabilities, phase separations and bistability phenomena. The theoretical problems are analyzed arising in PEM when the strong short-range correlations and electron transfer are taken into account simultaneously.

Key words: *phase transitions, local anharmonicity, high-T_c superconductors*

PACS: *71.10 Fd, 71.38.ti, 74.25.Kc, 63.20 Ry*

1. Introduction

The crystals with the high-temperature superconductivity (HTSC) investigated intensively during the last ten years possess a wide spectrum of physical properties. The variety of effects which are realized only separately in the case of other types of crystals is characteristic of these systems. The strong electron correlation, related to the interaction of the Hubbard type in the conductance bands formed mainly by the superconducting Cu_2-O_2 plains, can be pointed out as one of the reasons of this unique situation. Another significant feature connected with the dynamics of HTSC crystals is the presence of strongly anharmonic elements of the structure. As it is known, it can be a source of instabilities of various type. Even in the first publications devoted to the search of mechanisms of the HTSC phenomenon, the amplification of the effective pairing-type coupling between electrons due to the interaction via anharmonic phonons was mentioned to be one of the possible ways leading to this effect [1–3].

Among the most frequently investigated HTSC crystals are the crystals of the $YBa_2Cu_3O_{7-\delta}$ group. The unit cell of these compounds contains, besides two superconducting planes, the chain (at the $\delta \ll 1$ composition) elements Cu_1-O_1, connected by Cu_1-O_4-Cu_2 bridges with plains through the apical oxygen ions O_4. The vibrations of these ions along the c-axis (perpendicularly to the plains) exhibit a strong anharmonicity. Much evidence exists in support of this concept. One can mention the results of experimental investigations (EXAFS data [4,5], Raman scattering [6–9], dielectric measurements [10,11]) where the two equilibrium positions of O_4 ion (two different values of the $R_{O_4-Cu_2}$ distance) have been observed that can point out to the presence of the local double-minimum potential well. Similar conclusions were made based on considerating the local polaron phenomena [12,13], electron transfer processes through O_4 ions [14,15] or bistabilities in the normal phase temperature region [16]. On the other side, the existence of a splitted O_4-ion position was not confirmed by the neutron scattering investigations (see [17]); the first principle LAPW calculations give a one-minimum, though anharmonic, potential [18]. All of it points out to a certain ambiguity in the data available. In spite of that the local double-well picture is considered on the whole to be appropriate [1]. In particular, the recently established fact of the oxygen O_1 vacancy effect on the positions of apical ions [20] testifies in favour of the presence of different possible equilibrium positions of the O_4 ions.

Besides, a connection between positions of O_4 ions and electron states in Cu_2-O_2 plains plays an important role in $YBa_2Cu_3O_{7-\delta}$ crystals. The data given in [21] point to the existence of a significant correlation between the occupancy of electron states of the Cu_2 ion and the $R_{O_4-Cu_2}$ distance as well as to the decrease of this distance at the transition from the metallic orthorombic phase to the semiconducting phase (that takes place at $\delta > \delta^* = 0.55$). These and other similar facts suggest the presence of a large electron-vibrational coupling.

By now, the description of the locally anharmonic subsystem in HTSC crystals develops with the use of two different approaches. The first one, which is chronologically older, is based on the phonon anharmonic model φ^4 [3], or, more recently, on the model $\varphi^3 + \varphi^3$ [16]. The interaction with strongly correlated electrons is treated in the spirit of the Holstein model ($H_{\text{int}} \sim \text{const} \cdot \sum_i x_i n_i$, where x_i is the local normal coordinate, $n_i = \sum_\sigma n_{i\sigma}$ is the occupancy of the electron state on a site) [22]. This approach was used while considerating the polaron effect [23] and also while investigating the effect of anharmonicity on the superconducting transition temperature and on the possibility of the CDW phase creation [24].

In the second approach, which is more appropriate at the strong electron-vibrational coupling and in the cases when two equilibrium positions of anharmonic ions really exist, the pseudospin formalism is used; the pseudospin variable $S_i^z = \pm 1/2$

[1]In this connection, one can mention the work [19] where, on the basis of neutron scattering experiments, the conclusion is made that two equilibrium positions possess Cu_2 ions rather than O_4 ions; this data can be considered as an evidence of the existence of a local anharmonic mode connected with the stretching Cu_2–O_4 vibrations.

defines these two positions. This scheme being applied to the $YBa_2Cu_3O_{7-\delta}$ type systems started from works [25] and [26]. Allowing for the interactions of the $g\sum_i S_i^z n_i$ or $\sum_{ij} g_{ij} S_i^z n_j$ type it was used in investigating the electron pairing correlations [27] and while considering some other aspects of physics of these materials.

In succeeding years, investigations of the second model which was called as pseudo-electron model (PEM) include the structure of its electron spectrum (allowing for the short-range electron correlations) [28], as well as a number of many-particle effects (charge and pseudospin correlations, dielectric susceptibility [29,30]). The various aspects of thermodynamics of this model, in particular equilibrium and metastable states and transitions between them, have been considered as well. This report is devoted to a brief review of the results obtained and their connection with some problems of physics of the mentioned HTSC objects.

It should be mentioned in this connection that the problem of the genesis of structural inhomogeneities (which is manifest, for example, in the Raman scattering spectra [8,9] or mesoscopic structural data [31]) in single crystals of the $YBa_2Cu_3O_{7-\delta}$ type has become urgent in the last years. This situation opens up new possibilities for the application of locally anharmonic models of HTSC systems. Due to the presence of nearly labile elements of the structure (anharmonic ion subsystem) the lattice is potentially unstable. It is favourable to the development of metastabilities or for separation into different phases. The description of these processes can include such models or similar ones.

2. Pseudospin-electron model

Hamiltonian of the pseudospin-electron model has the following form:

$$\begin{aligned} H &= H_0 + \sum_{ij\sigma} t_{ij} a_{i\sigma}^{+} a_{j\sigma} \,, \\ H_0 &= \sum_i H_i = \sum_i \left[U n_{i\uparrow} n_{i\downarrow} - \mu \sum_\sigma n_{i\sigma} + g \sum_\sigma n_{i\sigma} S_i^z - h S_i^z - \Omega S_i^x \right] . \end{aligned} \tag{1}$$

Besides the energy of Hubbard repulsion (U-term), the single-site part of the Hamiltonian includes the interaction with pseudospins (g-term), the energy of double potential well asymmetry (the field h) and the energy of tunnelling splitting (the tunnelling frequency Ω); μ is the chemical potential. The second term in the Hamiltonian describes the electron hopping from site to site (the electron transfer parameter t_{ij}).

When the model is applied to the description of the anharmonic subsystem of apical oxygen ions in the HTSC crystals, the following values of parameters entering expression (1) are adopted: $g = 10\ldots20$, $\Omega = 0\ldots5$, $W = 0\ldots2$ [26]; $g = 1\ldots10$, $\Omega = 1\ldots10$, $W = 1$ [27]; $g = 0.3\ldots0.5$, $\Omega = 0.1$, $W = 1$ [32]; usually $U = 10\ldots20W$ (here $W = \sum_j t_{ij}$ is the parameter defining the width $2W$ of the "bare" electron band appearing due to the electron transfer; for strongly correlated systems in the case of d-electrons $W = 0.2\ldots 0.6$ eV). The asymmetry parameter h can be changed within a rather broad interval of values: $-2 \leqslant h/g \leqslant 2$.

As it follows from the data presented, it is necessary to take into account, in the zero approximation, the short-range interactions which are included into the Hamiltonian H_i. The expansions in powers of the transfer parameter t_{ij} can be used in this situation while applying the perturbation theory. The single-site states form, in this case, the natural basic set $|i,R\rangle = |n_{i\uparrow}, n_{i\downarrow}, S_i^z\rangle$ [28,29]:

$$\begin{array}{ll} |1\rangle = |0,0,1/2\rangle & |\tilde{1}\rangle = |0,0,-1/2\rangle, \\ |2\rangle = |1,1,1/2\rangle & |\tilde{2}\rangle = |1,1,-1/2\rangle, \\ |3\rangle = |0,1,1/2\rangle & |\tilde{3}\rangle = |0,1,-1/2\rangle, \\ |4\rangle = |1,0,1/2\rangle & |\tilde{4}\rangle = |1,0,-1/2\rangle. \end{array} \tag{2}$$

In the presence of tunnelling the H_i matrix is nondiagonal in this representation; by means of the $|i,R\rangle = \sum_r U_{Rr}|i,r\rangle$ transformation it is reduced to a diagonal form:

$$H_i = \sum_{p=1\ldots 4} \lambda_p X_i^{pp} + \sum_{\tilde{p}=\tilde{1}\ldots\tilde{4}} \lambda_{\tilde{p}} X_i^{\tilde{p}\tilde{p}}, \tag{3}$$

$$\lambda_{p,\tilde{p}} = -n_p\mu + U(\delta_{p,2} + \delta_{\tilde{p},2}) \pm \frac{1}{2}[(n_p g - h)^2 + \Omega^2]^{1/2}, \tag{4}$$

where $X_i^{mn} = |i,m\rangle\langle i,n|$ – Hubbard operators acting on the $|i,r\rangle$ basis; $n_p = n_{\tilde{p}}$ ($n_1 = 0$, $n_2 = 2$, $n_3 = n_4 = 1$).

Energies λ_p, $\lambda_{\tilde{p}}$ have a meaning of energies of the single-site states splitted due to the effect of the electron correlation and the interaction with pseudospins. In this case the six sublevels exist instead of the three Hubbard levels with energies 0, $-\mu$ and $U - 2\mu$.

The transitions $\tilde{r} \to r$ are connected with the pseudospin reorientation. The reorientation energy

$$\hbar\omega_r = \lambda_r - \lambda_{\tilde{r}} = [(n_r g - h)^2 + \Omega^2]^{1/2} \tag{5}$$

depends on the filling of electron states on the lattice site (the vibrational mode is splitted into three components, the intensities of which change depending on the electron concentration [33]).

The transitions $(1,\tilde{1}) \to (3,4,\tilde{3},\tilde{4}$ and $3,4,\tilde{3},\tilde{4}) \to (2,\tilde{2})$, at which the change of the electron number on a site takes place, determine the single-electron spectrum. Energy subbands $\varepsilon_{mn}(\vec{q})$ are formed from these transitions in the presence of electron transfer.

The description of the electron spectrum and the electron statistics of the PEM was given in [28] in the framework of the temperature two-time Green function method in the Hubbard-I approximation. In the limit of noninteracting subbands ($W \ll U$, $W \ll g$)

$$\varepsilon_{mn}(q) = \lambda_{mn} + t_q (A_{mn}^{\sigma})^2 \langle X^{mm} + X^{nn}\rangle; \tag{6}$$

here $\lambda_{mn} = \lambda_m - \lambda_n$; t_q is the Fourier transform of the transfer constant; $\langle X^{mm} \rangle$ is the mean occupancy of the m level; A^{σ}_{mn} is the coefficient in the $a^{+}_{i\sigma} = \sum_{mn} A^{\sigma}_{mn} X^{mn}_i$ expansion. The form of spectrum (6) (in particular, the widths and occupancies of subbands) depends on the electron concentration and the asymmetry parameter value [28]. A conclusion was made regarding the effective narrowing of the conduction subbands and the breaking of electron-hole symmetry at $n = 1$ due to the corresponding asymmetry of the model. A renormalization (leading to a decrease) of the Hubbard correlation parameter U takes place due to the interaction with pseudospins. In certain conditions, this can be a reason of negative values ($U_{\mathrm{eff}} < 0$) of this parameter.

3. Thermodynamics of simple PEM

The special features of thermodynamics of a pseudospin-electron model can be considered in a simplest way on the example of the model extended by the inclusion of a direct interaction between pseudospins in the limit case of the zero electron transfer. The results obtained in so doing will be relevant to a great extent to the full model, because the pseudospin-electron interaction forms in its turn the effective pseudospin-pseudospin interaction (having a retarded character).

An investigation, performed in [29,30] in the framework of generalized random phase approximation (GRPA) [34], was devoted to the analysis of the role of such an interaction in the dielectric susceptibility of PEM (GRPA scheme is connected with the summation of diagrams having a structure of sequences of the simple electron loops at the basic allowance for the short-range interactions; the diagrammatic technique for Hubbard operators [35] is used).

In this case the so-called transverse susceptibility

$$\chi^1(\omega_n, q) = \int_0^{\beta} \mathrm{d}(\tau - \tau') \sum_{i-j} \mathrm{e}^{-\mathrm{i}q(R_i - R_j)} \mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')} \langle T P_i(\tau) P_j(\tau') \rangle, \tag{7}$$

that characterizes the response of the unit cell dipole momentum

$$P_i = d_s S^z_i + d_e n_i \tag{8}$$

on the action of the field h_j, was calculated. There exists a divergence of the $\chi^1(0,0)$ function at a certain temperature and h field values in the vicinity of the $h = 0$ and $h = g$ points (within the intervals of the order of W) in the case of $U = \infty$ [29]. This fact as well as the possibility of the similar divergence of the $\chi^1(0, \vec{q}^{*})$ function, where $\vec{q}^{*} = (\pi/a, \pi/a)$ for a two-dimensional structure, were interpreted as a manifestation of the dielectric type instability or the instability with respect to the emerging of modulated charge-ordered states [30,36].

A more complete analysis of this issue requires an investigation of the behaviour of thermodynamic functions. A satisfactory, though simplified, illustration is given just by a model with direct interaction. Its Hamiltonian is written as

$$H = \sum_i H_i - \frac{1}{2}\sum_{ij} J_{ij} S_i^z S_j^z, \tag{9}$$

where the expression for H_i is given by formula (1). The full investigation of the thermodynamics of the model (9) in the case of long-range interaction which allows for the application of the mean field approximation has been performed in [37] and [38] for the ferroelectric and antiferroelectric type interactions, respectively. In particular, in the first of these cases the grand canonical potential of the system is given by the expression

$$\Omega/N = -\Theta \ln \sum_r \mathrm{e}^{-\beta\lambda_r} + \frac{1}{2}J\eta^2, \tag{10}$$

where $\eta = \langle S_i^z \rangle$ is the self-consistency parameter; the single-site energies λ_r are given by the expression (4) with the replacement $h \to h + J\eta$; $J = \sum_j J_{ij}$.

While formulating the thermodynamic equilibrium conditions we consider two different regimes in which the system can exist:

a) the regime $\mu = \mathrm{const}$; it is supposed that the electron states connected with structure elements, which are not included explicitly into the PEM, play a role of a thermostat, that ensures a constant value of the chemical potential μ (despite the possible changes of temperature, field h and other characteristics of the model); the minimum of the potential Ω is a condition of thermodynamical equilibrium;

b) the regime $n = \mathrm{const}$; this situation is more customary at the consideration of electron systems and it means that the chemical potential is now the function of T, h etc. and depends on the electron concentration; the minimum of the free energy $F/N = \Omega/N + \mu n$ is the equilibrium condition in this case.

As it was shown, in the first of these regimes the phase transition of the first order with the jump of the parameter η (and of the electron concentration, correspondingly) takes place in the system at temperatures below the critical temperature T_c. The phase equilibrium line has an inclination with respect to Θ axis, along which the equilibrium curve is directed in the Ising model case ($g = 0$). Because of that, the first order phase transition is possible at the change of temperature (when the values of the field h are in a certain narrow interval, the position of which depends on μ).

When, on cooling below the phase transition temperature, the system remains on a branch of the potential Ω, corresponding to the high-temperature phase, the point of instability of this phase can be achieved. The susceptibility $\chi = \partial\eta/\partial h$ diverges in this point. This corresponds to the above mentioned dielectric instability obtained in the GRPA for the system with electron transfer and may serve as its interpretation.

The behaviour of the system in the regime n =const is more complicated. The existence of a jump of the electron concentration between the n_1 and n_2 values at the crossing of phase equilibrium line gives an evidence that at the transition the phases with these concentrations are in equilibrium. At the fixed value of n the separation on particularly such phases takes place (this situation is similar to the liquid-gas transition at the fixed total volume of the system). The negative sign of derivative $(\partial n/\partial\mu)_{T,h} < 0$ corresponds to instability with respect to the phase separation.

The region of the electron concentration values at which this condition is fulfilled at the given field h and temperature T was established numerically in [37]. At the increase of temperature this area gets narrow, transforming at $T = T_{\mathrm{c}}$ into the line of critical points and disappearing at $T > T_{\mathrm{c}}$. The phases which emerge as the result of separation are also characterised by different values of the parameter of pseudospin ordering η. Thereby, the crystal in a separated state is nonuniform; there exist regions with different electron concentrations as well as the pseudospin orientations corresponding to them (that is, different occupancies of particle positions in the anharmonic potential wells).

4. Two-sublattice PEM with direct interaction

Pseudospin-electron model with direct interaction between pseudospins was generalized in [39] into a two-sublattice case with the aim to take into account the features of real structure of superconducting systems of the $YBa_2Cu_3O_{t-\delta}$ type (the presence of two superconducting planes and two nonequivalent apical oxygen ions in the unit cell). The unit cell Hamiltonian

$$\tilde{H}_i = \sum_{\alpha=1,2} H_{i\alpha} - JS^z_{i1}S^z_{i2} \tag{11}$$

(where α is the sublattice number) includes the interaction between pseudospins from different sublattices besides the sum of terms of type (1) for each sublattice. Asymmetry fields h_α acting on pseudospins are connected by the condition $h_1 = -h_2 \equiv h$. It reflects the centre of symmetry property of the model and corresponds to the structural data for the above mentioned crystal. The total Hamiltonian also contains the term

$$H' = -\frac{1}{2}\sum_{ij}\sum_{\alpha\beta} J^{\alpha\beta}_{ij} S^z_{i\alpha}S^z_{j\beta} \tag{12}$$

describing the long-range direct interaction between pseudospins.

Pseudospin part of the operator

$$H = \sum_i \tilde{H}_i + H' \tag{13}$$

corresponds to the Hamiltonian of the Mitsui model known in the ferroelectrics theory, where such a model was used to describe the sequence of phase transitions in the Rochelle salt crystal (the ferroelectric phase exists only in the intermediate region of temperatures between $T_{\mathrm{c}1}$ and $T_{\mathrm{c}2}$ in this crystal). In this connection, the attempt was made to apply the Mitsui model to the $YBa_2Cu_3O_{7-\delta}$ crystal with the aim to analyze the conditions of emerging of the ferroelectric type phase with the dipole ordering in the subsystem of oxygen apical ions [40] [2]. It was established that this phase can exist as an intermediate one similar to the Rochelle salt case.

An essential addition to this picture can be obtained when the interaction of pseudospins with electrons is taken into account. It was shown [39] that the ground state of the system (which can correspond to the parallel or antiparallel configuration of pseudospins in the unit cell) depends not only on the h and J values but also on the position of the chemical potential μ level. Ferroelectric phase is possible in the narrow range of the μ and h values (the width of the interval of the h values is of the order of J).

This is confirmed by the calculations of phase diagrams of the model. It has been performed in the mean field approximation with the exact allowance for the interaction in the cluster created by pseudospins from the same unit cell. The ferroelectric phase can exist at the intermediate values of the field h ($\frac{h}{J_{11}+J_{12}} \sim 0.5$); the corresponding area in the (T, h) diagram narrows at the strengthening of the intersublattice interaction and completely vanishes at the sufficiently large values of the $a = -\frac{J_{11}-J_{12}}{J_{11}+J_{12}}$ parameter ($a < -1$) or at the increase of the intracluster interaction constant J [39]. As a result, there appears a line of the first order phase transitions that separates two nonpolar phases. These phases differ in the pseudospin orientation in each sublattice; pseudospins are mutually compensated (the abrupt change of the parameter $\xi = \langle S_1^z \rangle - \langle S_2^z \rangle$ takes place; the parameter $\eta = \langle S_1^z \rangle + \langle S_2^z \rangle$ is equal to zero).

The above described feature of phase diagrams remains generally unchanged when we go beyond the mean field approximation taking into account the Gaussian fluctuations of the selfconsistency parameters [43]. At the given values of theory parameters, a certain narrowing of the region of the ferroelectric phase existence takes place.

5. Pseudospin model with random vacancy field

When the PEM is applied to the description of thermodynamics of the anharmonic apical oxygen ions subsystem in the $YBa_2Cu_3O_{7-\delta}$ compounds, it is important to take into account the nonstoichiometry of composition that is manifested in the presence of oxygen vacancies in the chain elements of structure Cu_1...O_1...Cu_1... The data of recent structural investigations show [20] that the emerging of the O_1 ion vacancy leads to the additional shifts of the nearest apical O_4 ions. This fact can be interpreted as the effect of the additional internal field which causes the increase or decrease of the asymmetry of their potential wells. This effect can be described in the framework of the two-sublattice pseudospin model of the Mitsui model type (see section 4). The replacement $h \to h_i$ can be used, where

$$h_i = h_{\mathrm{vac}} + (h - h_{\mathrm{vac}})c_i; \tag{14}$$

[2] Let us mention, that during the experimental investigation of these crystals the manifestations of physical effects, that can be realized in the noncentrosymmetric structures only, were fixed repeatedly, being interpreted as an instabilities of the ferroelectric type (see [41,42])

here h_{vac} – the asymmetry field in the presence of vacancy; $c_i = 0, 1$ is the configurational variable having a meaning of the ion occupation number in the O_1 position [44]. After this extension, the model can be considered as pseudospin-fermionic being conceptually a simplified version of the PEM.

While describing the vacancy statistics, two cases have been considered: a) nonequilibrium distribution (the state of the frozen disorder); the calculations of thermodynamic quantities are performed based on the configurational averaging; b) thermodynamically equilibrium distribution; the vacancy form an equilibrium subsystem and together with the rest of the crystals are described by Gibbs distribution.

In the first of these cases the bimodal distribution function was used [44]

$$P(h_i) = c\delta(h_i - h) + (1-c)\delta(h_i - h_{\mathrm{vac}}), \tag{15}$$

where $1-c = 1-\langle c_i \rangle$ is the vacancy concentration. In the second case the equilibrium consideration of vacancies was based on the extension of the pseudospin basis of states of the (i_1, i_2) cluster by the inclusion of the occupancy number c_i: $|S^z_{i1}, S^z_{i2}\rangle \to |c_i, S^z_{i1}, S^z_{i2}\rangle$ [45]; the interaction with the electron subsystem was not taken into account.

The calculation of thermodynamic function and derivation of equations for ξ and η parameters were performed in the nonequilibrium case in the framework of the mean field approach in the approximation proposed by Holakovsky [46]. The investigation of thermodynamically stable states enables us to build the phase diagrams of the system: in the (T, h) plane at the given vacancy concentration and in the (T, c) plane at a certain value of the host asymmetry field h. The results agree in general with the obtained ones for the PEM. The essential role in the shape of phase diagrams belongs to the relation between the h and h_{vac} fields. The decisive effect is also attributed to the vacancy concentration level. The change of c can lead (as it was shown in [44]) to the emerging and subsequent vanishing of the ferroelectric phase (its existence region is limited to the narrow concentration interval). At the increase in magnitude of the intracluster interaction parameter $j = \frac{J}{J_{11}+J_{12}}$ ($j \leqslant -0.04$) the ferroelectric phase disappears, and only the transition between the described above nonpolar phases remains. Now, it can also take place at the change of the vacancy concentration; the value of the corresponding concentration c^* depends on h and h_{vac} fields. There exists a possibility of the similar transition at the change of temperature. The region of existence of metastable states is rather wide. Because of that, the appreciable hysteresis phenomena can take place in the region of phase transition points which can manifest in the bistability behaviour of various physical characteristics.

An investigation of the system with equilibrium vacancies was performed in the regime of the fixed concentration in the mean field approximation based on cluster states [45]. The calculations of the concentrational dependence of the free energy reveal, similarly to the case of PEM, the possibility of the phase separation on the regions with different concentrations and, respectively, with different pseudospin orderings (nonpolar phases with $\xi^{(\mathrm{I})} \neq \xi^{(\mathrm{II})}$). Taking into account the possibility of the vacancy ordering and the emerging of phases with the different lattice symmetry in the $YBa_2Cu_3O_{7-\delta}$ crystals one can conclude that the above considered separation will mean the coexistence of particularly such phases.

6. Conclusions

The study of thermodynamics of the PEM provides reason enough to conclude that based on this model one can describe a set of the observed structural anomalies, phase transitions and connected with them instabilities in the HTSC of the $YBa_2Cu_3O_{7-\delta}$ type. Among them we should list the bistability effects (at the change of temperature or the vacancy concentration), ferroelectric type instabilities, separation into phases with different electron concentrations, pseudospin orientations (that corresponds to different localization of particles in the anharmonic potential wells) as well as vacancy concentrations which in its turn can correspond to phases with the different crystallographic symmetry. In general, it is in agreement with the picture observed experimentally (some publications in this field were quoted above). At the same time, incompleteness and ambiguity of the experimental material, the complicated influence of factors which had not been taken into account in the model, the absence of confirmed information about the numerical values of the theory parameters do not make it possible to assert that a sufficiently complete qualitative description of the observed phenomena has been achieved.

From the point of view of theoretical aspects, the investigation of the model is far from being ended. The interesting and difficult problem is connected with thermodynamics of the PEM with electron transfer, where the phase diagram should be no less complicated than the similar one in the case of Falicov-Kimball model (at $U = 0$, both models are conceptually close to each other; the distinction between them consists in different regimes of thermodynamical equilibrium [47]). The detailed consideration of the model dynamics, connected with pseudospin reorientation, electron transitions and polaron effect, also deserve attention. A thorough investigation is necessary regarding the applicability conditions of the GRPA and the ways of its improvement while calculating the correlation functions and thermodynamical characteristics. The extension of ideas and approaches which are based on the dynamical mean field method seems to be quite promising.

Some results in this direction were obtained recently. In particular, the thermodynamics and electron spectrum of PEM in $d = \infty$ limit in the case $U = 0$ and $\Omega = 0$ have been investigated [47] within the dynamical mean field approach (in this case the model is exactly solvable). The same simplified version of PEM was considered in [48]; the method of the selfconsistent calculation of thermodynamical and correlation functions was proposed (this approach is based on the GRPA scheme and can be considered as its generalization due to allowance for the mean field type contributions coming from effective pseudospin interactions via conducting electrons). The obtained phase diagrams agree quite sufficiently between themselves and confirm the above described results for models with a direct interaction in the μ =const and n =const regimes. The essential feature which manifests itself in the $d = \infty$ approach only, is a reconstruction of electron spectrum that is similar to the metal-insulator transition, at a certain critical value of the pseudospin-electron coupling constant.

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Локально ангармонічні ефекти у високотемпературних надпровідниках. Псевдоспін-електронна модель

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Отримано 13 вересня 1999 р.

В роботі обговорюються деякі аспекти фізичних явищ у кристалах з високотемпературною надпровідністю, зумовлені локальною ангармонічністю їх кристалічної гратки. Розглядаються відповідні теоретичні моделі. Дається огляд результатів, отриманих при дослідженні псевдоспін-електронної моделі при її застосуванні до опису структурних і діелектричних нестійкостей, фазових розшарувань та явищ бістабільності. Аналізуються теоретичні проблеми, що виникають у ПЕМ при одночасному врахуванні сильних короткосяжних кореляцій та електронного переносу.

Ключові слова: *фазові переходи, локальний ангармонізм, високотемпературні надпровідники*

PACS: *71.10 Fd, 71.38.ti, 74.25.Kc, 63.20.Ry*