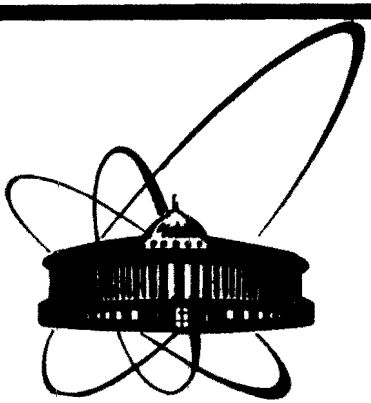

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ANHARMONIC MODEL FOR HIGH-T_c SUPERCONDUCTORS

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In recent experiments new records for superconducting transition temperatures T_c in oxide superconductors have been obtained: $T_c = 30 \div 40$ K in the La—Ba—Cu—O [1-3] and La—Sr—Cu—O [4] systems and $T_c = 93$ K in the Y—Ba—Cu—O [5,6] system. (For additional references see these papers). As has been shown in the subsequent papers [7-9], a two-dimensional character of electron spectrum, that brings about a Peierls instability in a pure La_2CuO_4, and strong-deformation potentials can offer the possibility of enhancement of T_c in these materials. The anharmonic soft modes, structural instability and interfacial effects arising from mixed phases [5] also play an essential role, as generally accepted, in reaching a record value of T_c.

To explain considerable enhancement of T_c in structurally unstable systems an anharmonic model for high T_c superconductors has been proposed in [10]. In this model highly anharmonic quasi-local vibrations in a double-well potential with large amplitudes $d \gg \sqrt{\langle u^2 \rangle}$ were admitted (here $\langle u^2 \rangle$ is a mean-square displacement of ions in the harmonic approximation). Since the effective electron-electron coupling λ is proportional to square of ion displacements, the anharmonic coupling constant λ_s is much larger than λ_{ph} in the harmonic approximation: $\lambda_s / \lambda_{ph} \sim d^2 / \langle u^2 \rangle \gg 1$ (see (8) below). This model was employed in [11] to estimate the enhancement of T_c in metal glasses and to explain the inverse isotope effect in the Zr, Hf—(H,D) systems [12]. The paper [13] should also be pointed out where $T_c \approx 100$ K was obtained in this model for a sufficiently high concentration of two-level anharmonic excitations.

In the present paper the high-temperature superconductivity in oxide materials is considered on the basis of the anharmonic model [10]. According to the results of electronic-structure calculations [8,9] the strong coupling of the oxygen bond-stretching modes with electrons is maintained. In the tetragonal phase a planar breathing type displacement of oxygen atoms coupled with tilting of CuO_6 octahedra (the latter being frozen in the orthorhombic phase [7]) as well as a planar B_{1g} mode of oxygen atoms due to the Jahn-Teller effect for Cu^{2+}, are highly anharmonic. The ferroelectric mode of Cu^{2+} or Cu^{3+} can also be very anharmonic as in other perovskites of $BaTiO_3$ type. Consedering for simplicity only one local anharmonic normal mode (e.g., breathing type) we write down the Hamiltonian of the model in the pseudo-spin notation [10]:

$$H_s = -\Omega \sum_{\ell} S_\ell^x - \frac{1}{2} \sum_{\ell \neq m} C_{\ell m} S_\ell^x S_m^x , \qquad (1)$$

where $\Omega = E_a - E_s > 0$ is the energy difference of the lowest two levels in the anharmonic double-well potential: the anti-symmteric (Ψ_a) and symmetric (Ψ_s) ones; $C_{\ell m}$ is an effective coupling for the excitations in different lattice cells ℓ, m, S^{α}_{ℓ} is the pseudospin operator for $S = 1/2$ acting in the (Ψ_s, Ψ_a) space. The interaction of electron with anharmonic ion vibrations is also written in the pseudospin representation:

$$H_{e-s} = \sum_{\vec{p}\vec{p}'\vec{q},\sigma} V^{\alpha}_{\vec{q}}(\vec{p}, \vec{p}')\, 2x^{\alpha}_{sa} S^{x}_{\vec{q}} a^{+}_{\vec{p}\sigma} a_{\vec{p}'\sigma}, \qquad (2)$$

where the deformation potential is given by

$$V^{\alpha}_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_{\ell} e^{i\vec{q}\vec{\ell}} \langle \vec{p} \,|\, V^{\alpha}_{r}\, U(\vec{\ell} + \vec{r}) \,|\, \vec{p}' \rangle,$$

and $x^{\alpha}_{sa} = \langle \Psi_s | x^{\alpha}_{\ell} | \Psi_a \rangle$ is the matrix element for the local normal mode displacement x^{α}_{ℓ} between the states Ψ_s and Ψ_a. The interaction of electrons with acoustic phonons and other harmonic phonon modes as well as electron-electron Coulomb interaction can be allowed for in the framework of the well-known electron-phonon theory of superconductivity [14].

By applying the double-time Green function method [15] the Eliashberg-type equation can easily be obtained (see [10, 11]) for the anharmonic model (1), (2) and the coupling constant can be calculated:

$$\lambda_s = \frac{1}{N(0)} \int_{S_F} \frac{d^2\vec{p}}{v_{\vec{p}}} \int_{S_F} \frac{d^2\vec{p}'}{v_{\vec{p}'}} |V_{\vec{q}}(\vec{p}, \vec{p}')|^2 \chi_s(\vec{q}) \approx N(0) \overline{J_s^2} \chi_s \equiv \eta_s \chi_s, \qquad (3)$$

where $\overline{J_s^2}$ is the deformation potential averaged over the Fermi surface S_F. The averaged static susceptibility for the anharmonic mode is given by

$$\chi_s = \overline{\chi_s(\vec{q})} \approx (2d)^2 \Omega S^z / \overline{E^2_{\vec{q}}}. \qquad (4)$$

Here $2d = 2|x_{sa}|$ is the characteristic distance between two minima of the anharmonic double-well potential, $S^z = \langle S^z_{\ell} \rangle = (\Omega/2h)\tanh(h/2kT)$, $h^2 = \Omega^2 + (C(0)\langle S^x_{\ell} \rangle)^2$ and the excitation spectrum in the lattice

$$E^2_{\vec{q}} = \Omega[\Omega + C(\vec{q}) S^z] + (C(0)\langle S^x_{\ell} \rangle)^2, \qquad (5)$$

where $C(\vec{q})$ is the Fourier transform of $C_{\ell m}$ in (1). For $T > T_0$ (T_0 is the temperature of structural phase transition to the distorted state with $\langle S^x_{\ell} \rangle \neq 0$) one has $\overline{E^2_{\vec{q}}} \approx \overline{E^2_{\vec{q}}} = \Omega^2$ and for the static susceptibility one gets:

$$\chi_s \approx \frac{2d^2}{\Omega} \tanh \frac{\Omega}{2kT}. \qquad (4a)$$

To compare λ_s (3) with λ_{ph} in the harmonic approximation, we write the latter in the same form as (3) and (4)

$$\lambda_{ph} = N(0) \overline{J^2_{ph}}\, \chi_{ph} \equiv \eta_{ph}\, \chi_{ph}, \qquad (6)$$

where the static susceptibility for the harmonic phonons

$$\chi_{ph} = \frac{1}{M\overline{\omega}^2} \equiv \frac{2\langle u^2 \rangle}{h\overline{\omega}} \tanh \frac{h\overline{\omega}}{2kT}. \qquad (7)$$

Here we introduce the mean-square displacement of ions $\langle u^2 \rangle = (\hbar/2M\overline{\omega}) \times \coth(\hbar\overline{\omega}/2kT)$ in the harmonic approximation with averaged frequency $\overline{\omega} = \sqrt{\overline{\omega^2}}$. By assuming $\overline{J^2_{ph}} \approx \overline{J^2_s}$ and $\Omega \approx \hbar\overline{\omega}$ one gets the estimation

$$\lambda_s / \lambda_{ph} \approx \chi_s / \chi_{ph} \approx d^2 / \langle u^2 \rangle \gtrsim 10, \qquad (8)$$

where values $\langle u^2 \rangle \approx 10^{-3}$ Å^2 and $d \gtrsim 0.1$ Å can be taken from Debye-Waller factors in harmonic crystal and from atomic displacements at structural phase transition, respectively.

It is interesting to point out that structural transformation suppresses this enhancement of λ_s and hence T_c. Since for $T < T_0 < S^x_{\ell} > \neq 0$ in (5) the spectrum of excitation becomes more hard, the susceptibility χ_s(4) decreases thus suppressing λ_s (3) (for details see [10]).

Now we can estimate λ_s for the La(Y)—Ba—Cu—O systems on the basis of the obtained formulae. To calculate T_c we use the formula in the intermediate coupling limit proposed in [16]

$$kT_c \approx 0.05\,\Omega(\lambda_s - 0.25). \qquad (9)$$

For further estimations the Coulomb contribution μ^* as well as contributions from acoustic phonon modes λ_{ph} will be neglected since usually $\lambda_{ph} - \mu^* \ll 1$.

To calculate λ_s one should know three parameters η_s, d and Ω in (3), (4a). According to the results of electronic-structure calculations for La—Ba—Cu—O system [8] one can adopt for density of states N(0) at E_F: N(0) = = 1.3 states/eV. cell and for the deformation potential for breathing mode $J_s \approx 1.6$—3.9 eV/Å near the BZ boundary. But it is very difficult at present to propose some reliable value for the averaged value of $\eta_s = N(0)\overline{J^2_s}$ for the considered anharmonic mode. Therefore we take for crude estimations $\eta_s \approx \approx 2$ eV/Å^2 that seems reasonable (compare, e.g., with $\eta_s \approx 2.4$ eV/Å^2 for

superconducting Pb). For the energy of anharmonic vibrations Ω one can take some average values of optic mode frequencies in perovskites, $\Omega \approx 25$ meV. Then, if one chooses $d \approx 0.14$ Å in (4a), one gets $\lambda_s \approx 3$ and $T_c \approx 40$ K for the anharmonic model of La—Ba—Cu—O system. The adopted value of d seems to be reasonable in comparision with oxygen atoms displacements in the orthorhombic phase of La—Ba—Cu—O: $d \approx 0.2$ Å, due to 5° tilting of the CuO_6 octahedra[7]. For the same values of $\eta_s = 2\ eV/Å^2$, $\Omega = 25$ meV but with $d \approx 0.3$ Å one gets $\lambda_s = 7$ and $T_c \approx 100$ K that can be compared with $T_c \approx 93$ K in the Y—Ba—Cu—O system[5,6]. In the latter system some additional highly anharmonic local vibrations due to structural instability and interfacial effects arising from mixed phases[5] may also be of great importance as in the glass state[11]. The upper limit for T_c in the present model one can get by choosing the higher value for $\eta_s = 7\ eV/Å^2$ (as in the transition metals). Then for $\Omega \approx 25$ meV and $d \approx 0.3$ Å one gets $\lambda_s \approx 27$ and $T_c \approx 270$ K by using the formulae[17]: $kT_c \approx 0.18\ \Omega\sqrt{\lambda_s}$ in the strong coupling limit ($\lambda > 10$).

In conclusion, experiments[1-6] show that high temperature superconductivity of oxyde perovskites can be understood in essential in the framework of the electron-phonon mechanism though at larger electron-phonon coupling constant. The proposed model gives principal explanation of this enhancement of λ due to strongly anharmonic vibration of ions.

The estimations given above for λ_s on the basis of the presently known parameters allow us to obtain the experimentally observed results for T_c for the La—Ba—Cu—O system as well as for the Y-Ba—Cu—O system. To get more reliable numerical results for these new materials in the framework of the proposed model some additional experimental information is needed concerning phonon spectrum, anharmonic parameters of lattice vibration, etc., that can be obtained from X-ray or neutron scattering investigation on a single crystal.

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Ангармоническая модель сверхпроводников с высокой T_c

Заметное повышение температуры сверхпроводящего перехода T_c в перовскитовых оксидных соединениях объясняется на основе ангармонической модели сверхпроводника с структурнонеустойчивой решеткой. Показано, что наличие ангармонических локальных возбуждений, амплитуда флуктуаций которых значительно превышает амплитуду гармонических колебаний, приводит к увеличению константы связи λ. Полученные оценки для T_c согласуются с данными для соединений La(Y)BaCuO.

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Anharmonic Model for High-T_c Superconductors.

A considerable enhancement of the superconducting transition temperature T_c in perovskite oxide compounds is explained in the framework of the anharmonic model for superconductors with structurally unstable lattices. It is shown that anharmonic local excitations with fluctuation amplitudes much greater than harmonic vibrations amplitudes lead to a considerable enhancement of the coupling constant λ. The obtained estimations for T_c are in agreement with experimental data for La(Y)BaCuO systems.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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