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ISOTOPE EFFECT ($O^{16} - O^{18}$) IN THE ANHARMONIC MODEL OF HIGH-T_c SUPERCONDUCTORS

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The results of a numerical simulation are presented for the oxygen isotope effect in the high-T_c oxides by solving the Schrödinger equation for a local vibrational mode of oxygen ions in a double well anharmonic potential of the form $-Ax^2/2+Bx^4/4$.

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

Изотопический эффект ($O^{16}-O^{18}$) в ангармонической модели ВТСП

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Представлены результаты моделирования кислородного изотопического эффекта в высокотемпературных сверхпроводниках, полученные численным решением уравнения Шредингера для квазилокальной моды движения атомов O^{16}, O^{18} с потенциалом вида $Ax^2/2 + Bx^4/4$.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

The recent discovery of new cuprate oxide superconductors having transition temperatures T_c up to 114K [1–3] have caused an immense activity in research of the mechanism(s) responsible for the superconductivity, in particular, whether it is mediated by phonons or not; a question which is still open. However, the recent experimental observations of the oxygen isotope effect in the LaSrCuO and YBaCuO systems [4] indicate that phonons play a certain role in the formation of superconductivity. Thus, in the light of the new high-T_c superconductors the isotope effect becomes an important issue with respect to testing any theory intending to explain such high T_c's.

Calculations of the electronic structure [5] demonstrate overlapping of the 3d states of copper with the 2p states of oxygen indicating the importance of the Cu-O chain for such high T_c's. It was shown [6] that interactions of electrons with the high frequency Cu-O

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bond-stretching mode can produce strong electron-phonon coupling leading to T_c around 40K. However, the pure phonon mechanism in the harmonic approximation fails to explain experimentally observed 90K in the YBaCuO system [9]. Structural studies of the high-T_c cuprate oxides have revealed features as evidence of structural instabilities and the existence of soft modes in LaSrCuO system. The investigation of the phonon behaviour of $YBa_2Cu_3O_7$ by neutron inelastic scattering shows larger phonon density states in lower frequency modes rather than in high frequency ones [6] which turned out to be in agreement with theoretical calculations [9] of the phonon spectra for large coupling constant λ_s. As it was demonstrated earlier within the anharmonic model of the high-T_c superconductors [10] large values of λ_s can be obtained as a result of interaction of electrons with the so-called soft bond-bending mode, related to the highly anharmonic vibrations of oxygen ions of the CuO_6 octahedron, due to the high susceptibility of the lattice χ_s. This idea has been backed up by the observation of unusual large Debye-Waller factors in $YBa_2Cu_3O_7$ [13]. In this paper we suggest for the vibration of the oxygen ions a double-well anharmonic model potential

$$U(x) = -Ax^2/2 + Bx^4/4 + A^2/4B, \qquad (1)$$

where A and B are both positive and related through

$$U_0 = A^2/4B \qquad \text{and} \qquad x_0 = (A/B)^{1/2} \qquad (2)$$

to real physical quantities, the central barrier height U_0 and it's average width x_0, respectively, thus $2x_0$ being the distance between the two minima of the potential. Units are used where $h = k_B = 1$. By introducing the dimensionless coordinate and energy

$$\xi = x/x_0 \qquad \text{and} \qquad E_n = E_n'/U_0 \qquad (3)$$

one obtains the Schrödinger equation in the following form

$$-d^2\phi(\xi)/d\xi^2 + 1/\beta^2[(1-\xi^2)^2 - E_n]\phi(\xi) = 0, \qquad (4)$$

which was numerically solved for a broad set of the dimensionless parameter $\beta = \omega_0/4U_0$, where $\omega_0 = \sqrt{\frac{2A}{m}}$ is a characteristic frequency; and m, the reduced mass of the Cu-O-Cu cluster, thus a complete replacement of O^{16} by O^{18} in the cluster is simulated through de-

creasing β by 5%. The cluster approach is motivated by the fact that superconductivity has been observed in crystalline as well as in ceramic states. The eigenvalues E_n and eigenfunctions ϕn of the anharmonic oscillator are calculated as well as the matrix elements of the dipole moment ξ_{01} and the mean square amplitude of vibrations Q^2. The obtained anharmonic eigenfunctions ϕ_n are expanded in terms of the eigenfunctions $u_j(x)$ of the harmonic oscillator

$$\phi_n(x) = \sum_{j=0}^{N_{max}} a_j u_j(x) , \qquad (5)$$

where N_{max} is fixed by the condition that $\sum_{j=0}^{N_{max}} a_j^2$ be unity within the given accuracy.

A study of the convergence accuracy of (5) indicates that it improves from 0.25% to better than 0.0001% when the number of the expansion coefficients is increased from 40 to 100. This demonstrates the strong effect of the anharmonicity on the eigenfunctions. The behaviour of the energy spectrum is illustrated in Fig. 1 in terms of $\Lambda_{1,2}/\epsilon_{01}$.

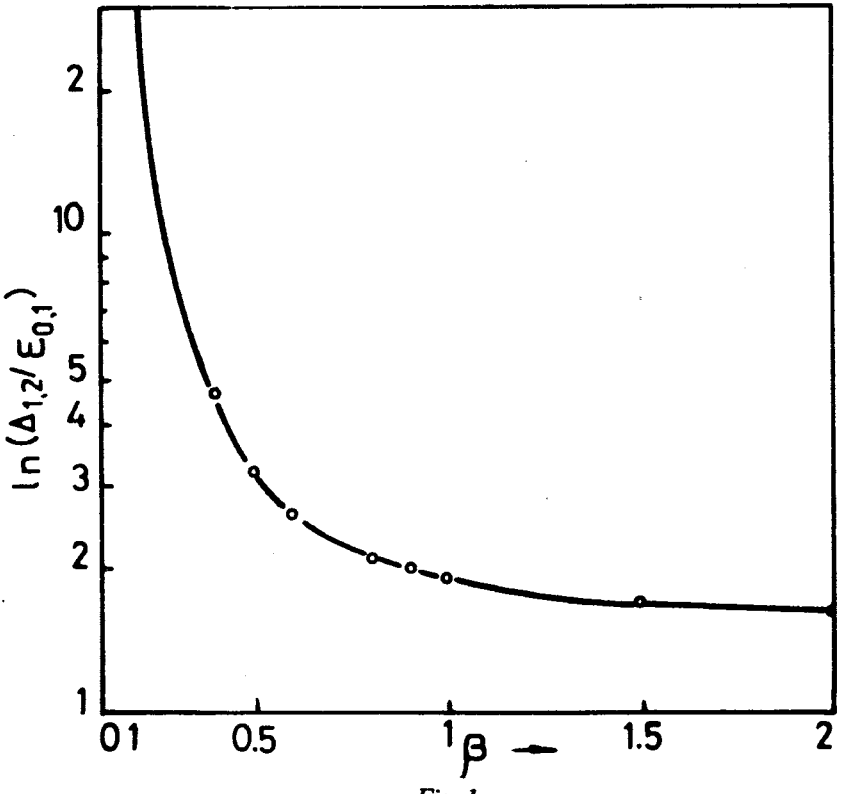

Fig. 1.

Here is

$$\Delta_{1,2} = E_2 - E_1 . \tag{6}$$

There, one can see two features of the above ratio demonstrating for higher levels weak and for lower ones strong anharmonicity. The same effect is observed in the dependence of the mean square amplitude of vibration (Table 1) on the anharmonicity, too, calculated by

$$Q^2 = < n \mid \xi^2 \mid n > . \tag{7}$$

We found that while for larger β it steadily increases with temperature, for lower values of β an oscillating behaviour is observed.

The values of β can be estimated by the relation $\Omega_{01} = (E_1 - E_0) U_0 = \epsilon_{01} U_0$. We reckon the frequency Ω_{01} , in the case of the soft bond bending mode at range 10-30 meV. Then, for values of $\beta \sim 0.2\, U_0$ becomes very large (~1000 meV) which is unphysical. In the region $\beta = 0.4 \div 0.8\ U_0$ takes values between 10-150 meV, thus values of β in this range can be considered as physically meaningful. As one can see from Fig. 1 in this region the application of a two level approximation is allowed. According to /10/ the coupling constant is given by

$$\lambda_s = N(0) < J_s^2 > \chi_s , \tag{8}$$

Table 1

The mean-square amplitude of vibration Q^2 (dimensionless) for different values of β . Underneath the corresponding eigenvalues E_n (dimensionless) are given.

β / n	0	1	2	3	4	5	6	7	8
0.125	0.951	0.932	0.753	0.785	0.452	0.718	0.717	0.815	0.897
E_n	0.242	0.243	0.681	0.689	0.985	1.09	1.30	1.53	1.77
0.42	0.650	0.922	0.801	1.08	1.24	1.38	1.54	1.65	1.79
E_n	0.631	0.842	1.79	2.71	3.84	5.12	6.51	8.00	9.57
0.6	0.594	1.01	1.04	1.31	1.53	1.69	1.89	2.04	2.27
E_n	0.777	1.33	2.82	4.48	6.41	8.58	10.88	13.37	15.99
0.84	0.597	1.13	1.29	1.59	1.68	2.07	2.32	2.51	2.73
E_n	0.982	2.12	4.51	7.26	10.41	13.89	17.64	21.64	25.85

where N(0), J_s and χ_s denote the density of states at Fermi level E_F, the deformation potential and the static susceptibility of the lattice, respectively. The latter is described in a two-level approximation by

$$\chi_s = \frac{2x_0^2 \xi_{01}^2}{\Omega_{01}} \text{th}(\Omega_{01}/2T) , \tag{9}$$

where $x_{01} = x_0 \xi_{01}$ is the matrix element of the dipole moment between the states ϕ_0 and ϕ_1. This expression can be derived from the spectral representation

$$\chi_s = Z^{-1} \sum_{n,m} e^{-\beta E_n} \frac{1 - e^{-\beta(E_m - E_n)}}{(E_m - E_n)/U_0 - \omega/U_0} <m | \xi | n>^2 , \tag{10}$$

where $Z = \sum e^{-\beta E_n}$, in the static limit $\omega = 0$ by considering the two lowest levels, only. We studied the convergence of (10) taking into account up to four levels. As one can see from Table 2 it is convergent, thus the application of the two-level approximation is justified.

Table 2

The static susceptibility χ (dimensionless) calculated by taking into account 2,3 and 4 levels, respectively for three different values of β at T = 92K.

β	χ_s		
	n=2	n=3	n=4
0.2	262.191	262.199	262.208
0.5	3.236	3.249	3.251
1.0	0.711	0.719	0.720

The transition temperature has been calculated by the general relation

$$T_c = \Omega_{01} f(\lambda_s, \mu^*) , \tag{11}$$

where Ω_{01} is the frequency of the phonon mode under consideration, $f(\lambda_s, \mu^*)$ is given for the weak and strong coupling cases by the McMillan [11] and the Allan-Dynes [12] formulas, respectively, μ^* is the

Coulomb pseudopotential. Differentiating (11) with respect to the isotopic mass one obtains the following relation for the relative shift in T_c

$$\delta T_c = dT_c / T_c = -\alpha dm/m , \qquad (12)$$

where

$$\alpha = 0.5 \left(1 + \frac{\beta d\epsilon}{\epsilon d\beta}\right)\left(1 - \frac{\lambda}{f}\frac{df}{d\lambda} - \frac{\mu^{*2} df}{f d\mu^*}\right) . \qquad (13)$$

The isotope effect thus depends on λ_s and μ^* through the second term while the first term gives the effect of the anharmonicity on the value of α. To calculate the coupling constant we estimate x_0, N(0) and J_s^2 in the following ranges: $x_0 = (0.1 \div 0.3)$ Å, N(0) = $= (1 \div 3)$ states/eV and $J_s^2 = (0.5 \div 1)$ $(eV/Å)^2$. As is shown in Fig. 2 in the anharmonic case even an inverse isotope effect is possible for $T_c < 33K$, while in the narrow region 34-35K a nearly zero or heavily suppressed one is observed. At T_c slightly above 36K α lies in the range 0.1-0.2, depending on β; thus, it is in agreement with experimental observation for the LaSrCuO system. However, for higher T_c we found normal isotope effect with a trend of α to increase with temperature and then to saturate at 0.3-0.4, which is in contradiction with the up-to-date observed trend of α to decrease. We conclude from our numerical calculation that in the anharmonic model the phonon mechanism permits one to obtain an agreement with the experimentally observed isotope effect in the LaSrCuO system ($\alpha \sim 0.1$-0.2) whereas it is not the case for the YBaCuO system. This may be an indication that higher energy levels have to be taken into account, otherwise a nonphonon mechanism should be considered.

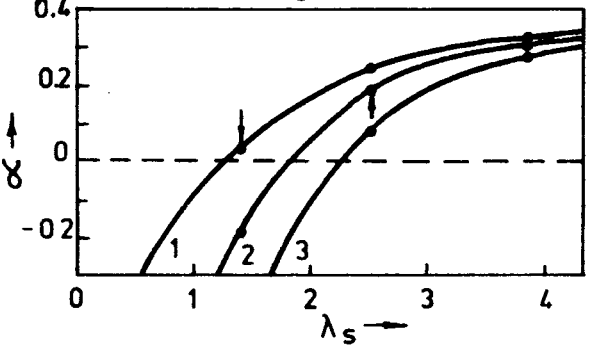

Fig. 2.

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