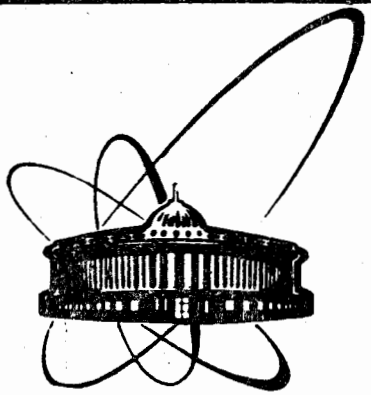

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INELASTIC NEUTRON SCATTERING IN THE ANHARMONIC MODEL OF HIGH-T_c SUPERCONDUCTORS

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Неупругое рассеяние нейтронов
в ангармонической модели высокотемпературных
сверхпроводников

Неупругое рассеяние нейтронов на сильно ангармонических колебаниях ионов кислорода в высокотемпературных сверхпроводниках исследовано с помощью псевдоспинового формализма. Получены выражения для когерентного и некогерентного сечения рассеяния и найдена аномальная зависимость интенсивности рассеяния от температуры.

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Inelastic Neutron Scattering
in the Anharmonic Model of High-T_c
Superconductors

The inelastic neutron scattering on highly anharmonic vibrations of oxygen ions in high-T_c superconductors is studied in the framework of a pseudo-spin model. By evaluating the coherent and incoherent cross-sections it turned out that the scattering intensity exhibits an anomalous temperature dependence.

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

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I. INTRODUCTION

The pairing mechanism of high-T_c superconductivity is still to be elucidated. A number of magnetic pairing models has been proposed as well as excitonic ones. But some experimental findings indicate that the electron-phonon pairing mechanism can not be ruled out. All the cupric oxide superconductors exhibit oxygen isotope effects (see e.g. [1]). The discovery of high-T_c superconductivity [2], a large oxygen isotope effect [3] and tunneling spectroscopy measurements [4] in BaKBiO seem to confirm the importance of phonons for high-T_c superconductivity because BaKBiO is a bridging compound between the conventional "phonon" superconductor BaPbBiO and the new high-T_c superconductors.

Recent neutron diffraction (ND) investigations [5] conclude that the part of the structure between the Cu-O planes in all cupric-oxides is ill defined and indicate that there are always multiple potential wells for the atoms there (see also [6]). In [7] the best ND fit for YBaCuO was obtained by assuming two equivalent sites for the O(1) ion in the Cu(1)-O(1) chain. A similar situation is observed for the O(3) ion in the Tl-O layer in the Tl-based system [8]. Interestingly all these oxygen ions exhibit anomalously large thermal factors.

Although so far the existence of such unstable modes is controversal, first principles calculations predict double-well potentials for the so-called tilting mode in LaSrCuO [9]. Molecular dynamic simulations for YBaCuO [10] show that a linear ordering of the Cu(1)-O(1) chain is not favourable.

Because the proposed anharmonic modes are related to vibrations of atoms, all exclusively situated in the part of the structure supposed to act as the charge carrier "reservoir" their study is

important irrespective of what mechanism underlies the pairing.

The inelastic neutron scattering (INS) is the most appropriate tool for the investigation of the lattice dynamics. Therefore it is important to understand the peculiarities of INS on anharmonic vibrations.

In the present paper we study the INS on an anharmonic potential by the pseudo-spin formalism.

II.Model

The Hamiltonian describing the oxygen ion displacements X_n in the n-th unit cell can be written as:

$$H = \sum_n \frac{m}{2}\dot{x}_n^2 + \frac{1}{2}\sum_{n,k}\phi_{nk}x_n x_k + \frac{B}{4}\sum_n x_n^4 , \qquad (1)$$

with m being the oxygen ion mass and ϕ_{nk}- the harmonic force constant accounting for the interaction of oxygen ion displacements in neighbouring cells. B is the anharmonic model parameter.

We make use of the represantation of the local normal coordinate (LNC) as introduced by Pytte and Feder [11] to describe a soft rotational mode which involves the tilting mode in LaSrCuO or the rotational vibration of O(1)-Cu(1)-O(1) molecules leading to the observed zig-zag ordering of the Cu(1)-O(1) chain in YBaCuO. Then the oxygen-ion displacements x_n in the n-th unit cell (n=1,2,..N) along the x-axis can be written in the form

$$x_n = \frac{b}{2\sqrt{2}mb^2}(R_n - R_{n+b}), \qquad (2)$$

where R_n is a rotational displacement in the n-th unit cell and b the lattice constant along the y-axis. Here we note that if the double-well potential is not related to a rotational mode, which seems to be the case for the oxygen ion in Tl(Bi)-O layer in the Tl(Bi)-based cupric oxides there is no need to introduce LNC.

According implications for the INS will be discussed underneath.

In the LNC representation our Hamiltonian (1) becomes

$$H = \frac{1}{4}\sum_n \dot{R}_n^2 - \frac{\omega_0^2}{2}\sum_n R_n^2 + \frac{\Gamma}{4}\sum_n R_n^4 + \frac{1}{2}\sum_{n\neq k} U_{nk}R_nR_k ; \qquad (3)$$

here

$$\omega_0^2 = \frac{A}{m} = -U_{nn} = \frac{1}{4m}(\phi_{n+a,n} - \phi_{n,n}) > 0 \qquad (4)$$

is the frequency of unstable rotational vibrations in the harmonic approximation and

$$\Gamma = B/4m^2,\ U_{n,k} = (1/8m)[2\phi_{nk} - \phi_{n-a,k} - \phi_{n,k-a}], \qquad (5)$$

are respectively the effective rotational anharmonic and displacement coupling constants. Now, it is convenient to go over to the pseudo-spin representation with spin 1/2. Introducing

$$R_n \to 2\,\xi_{01}S_n^x , \qquad (6)$$

where S_n^x is the Pauli x-matrix and $\xi_{01} = \langle\psi_0|\xi|\psi_1\rangle$- the matrix element between the two lowest eigenstates,the Hamiltonian (3) is cast in the form

$$H = -\Omega\sum_n S_n^z - \sum_{n\neq k} J_{nk}S_n^x S_k^x , \qquad (7)$$

where $\Omega=\varepsilon_1-\varepsilon_0$ is the excitation energy and $J_{nk}=-4(\xi_{01})^2U_{n,k}$- the effective pseudo-spin interaction. Due to the layered structure of the cupric oxides the z-component of the latter can be omitted, i.e.

$$J_{nk} = J_x + J_y . \qquad (8)$$

In the nearest-neighbour approximation the Hamiltonian (7) leads to the two-dimensional dispersion law for the anharmonic pseudo-spin mode ω_q:

$$\omega_q^2 = \tilde{\Omega}^2 - \tilde{\Omega}\tanh(\Omega/2T)(J_x\cos q_x a + J_y\cos q_y b), \qquad (9)$$

where a is the lattice spacing along the x-axis and.

$$\tilde{\Omega}^2 = \Omega^2 + (2J\langle S^z\rangle)^2; \qquad (10)$$

For $T>T_s$ (T_s is the temperature of the structural phase transition i.e. at which the soft mode freezes at BZ boundary)

$$\langle S^z \rangle = \frac{1}{2} \tanh(\Omega/2T) \qquad (11)$$

and $\langle S^x \rangle = 0$, because each site is occupied with equal probability. On the contrary, for $T<T_s$, $\langle S^x \rangle \neq 0$ and $\langle S^z \rangle$ is no longer temperature dependent being equal $\Omega/2J$.

III. INS differential cross section

We start from the general expression of the neutron double-differential cross section per unit solid angle O and unit interval of outgoing energy in the very well known form

$$\frac{1}{N}\frac{d^2\sigma}{dOdE} = \frac{p}{p_0} S(\kappa,\omega), \qquad (12)$$

where $\hbar\vec{\kappa} = \vec{p}_0 - \vec{p}$ and $\hbar\omega = E_0 - E$ are momentum and energy transfers, p_0, $E_0 = p_0^2/2m$ and p, $E = p^2/2m$ being neutron initial and final momenta and energies, respectively. The corresponding Van Hove function for neutron scattering by oxygen ion vibrations of rotational type is given by [12]

$$S(\vec{\kappa},\omega) = \frac{1}{N}\sum_{n,k} a_n a_k e^{i\vec{\kappa}(\vec{n}-\vec{k})} e^{-2W(\vec{\kappa})} \cdot \frac{[1+N(\omega)]}{\pi} \cdot \mathrm{Im}[\chi_{nk}(\vec{\kappa},\omega)], \qquad (13)$$

where a_n is the scattering length for the n-th nucleus, $\exp[-2W(\vec{\kappa})]$ is the anharmonic Debye-Waller factor and $[1+N(\omega)]$ - the Bose factor. For the one-quantum scattering process the above introduced displacement correlation function

$$\chi_{n,k}(\vec{\kappa},\omega) = \langle\langle \vec{\kappa}\vec{x}_n | \vec{\kappa}\vec{x}_k \rangle\rangle =$$

$$= \kappa_x^2 \frac{1}{2m_0}\cdot\frac{1}{4}\langle\langle (\vec{R}_n - \vec{R}_{n+a}) | (\vec{R}_k - \vec{R}_{k+a}) \rangle\rangle_\omega \qquad (14)$$

in the pseudo-spin representation (6) reads

$$\chi_{n,k}(\vec{\kappa},\omega) = \frac{\kappa_x^2}{2m}(2\xi_{01})^2 \cdot \frac{1}{N}\sum_q e^{i\vec{q}(\vec{n}-\vec{k})} \sin^2(\frac{\vec{q}\vec{a}}{2}) \chi_q^{xx}(\omega), \qquad (15)$$

where

$$\chi_q^{xx}(\omega) = -\langle\langle S_q^x | S_{-q}^x \rangle\rangle_\omega \qquad (16)$$

is the resonant (xx-component) Green function.

We note that the contribution of the relaxational (zz-component) Green function $\chi_q^{zz}(\omega)$, being of entirely quasi-elastic nature, is omitted in Eq.(15) as it is predominantly responsible for the central peak dynamics (i.e. the zero-frequency range) in addition being weighted by the small pseudo-spin form-factor $4|(\xi_{00})^2 - (\xi_{11})^2| \ll 1$.

For the coherent scattering from Eqs. (13)-(16) one obtains

$$S_{coh}(\vec{\kappa},\omega) = a_{coh}^2 \Delta(\vec{\kappa}-\vec{q}) e^{-2W(\kappa)} \cdot \frac{\kappa_x^2}{2m}(2\xi_{01})^2 \sin^2(\frac{\vec{\kappa}\vec{a}}{2}) \cdot$$

$$\cdot \frac{[1+N(\omega)]}{\pi} \mathrm{Im}[\chi_q^{xx}(w+i\delta)]. \qquad (17)$$

The corresponding incoherent scattering function is given by the expression

$$S_{inc}(\vec{\kappa},\omega) = \frac{\sigma_{inc}}{4\pi} e^{-2W(\kappa)} \cdot \frac{\kappa_x^2}{2m}(2\xi_{01})^2 \cdot \frac{[1+N(\omega)]}{2\omega} G(\omega), \qquad (18)$$

where the weighted spectral density of vibrational states (DOS) $G(\omega)$ is defined as follows

$$G(\omega) = \frac{1}{N}\sum_q \sin^2(\frac{\vec{q}\vec{a}}{2}) \, 2\omega \frac{1}{\pi} \mathrm{Im}[\chi_q^{xx}(\omega+i\delta)] =$$

$$= \frac{1}{N}\sum_q \sin^2(\frac{\vec{q}\vec{a}}{2}) \Omega \langle S^z \rangle \delta(\omega - \omega_q). \qquad (19)$$

For polycrystalline samples the incoherent approximation for the coherent part (17) can be applied. Therefore the total inelastic scattering function becomes

$$S(\vec{\kappa},\omega) = (a_{coh}^2 + \frac{\sigma_{inc}}{4\pi}) e^{-2W(\kappa)} \cdot \frac{\bar{\kappa}_x^2}{2m}(\frac{2\xi_{01}}{2\omega})^2 [1+N(\omega)] G(\omega). \qquad (20)$$

The above obtained formula (20) for the INS on anharmonic vibrations bears the temperature dependent factor $\langle S^z \rangle$. The

consequency of this factor is an anomalous temperature dependence of the INS intensity above the structural phase transition temperature T_s. For $T>T_s$ the intensity increases with decreasing temperature and below T_s it becomes temperature independent hence one may expect increased intensity at very low temperatures in the lower frequency part of the phonon spectrum as observed in [13]. Another feature of the obtained INS intensity is the appearence of the phase-like factor $\sin^2(qb/2)$ in Eq.(15). It is due to the off-phase rotations in neighbouring cells and predicts decrease in the INS intensity with raising neutron transfer momentum κ. Thus, one has to expect strong scattering intensity in vicinity of the wave vector $q=q_{BZ}=\pi/b$. That can be predominantly revealed in the coherent scattering when

$$\kappa = 2\pi\tau+q \text{ and } \sin^2(qb/2) \to \langle\sin^2(\kappa b)\rangle_\theta = (1/2)[1+(\sin\kappa b/\kappa b)]$$

(τ is the reciprocal lattice vector and the symbol $\langle\ldots\rangle_\theta$ stands for the orientational averaging over κ). As mentioned if the double-well potential is not related to soft rotational modes there is no need to introduce the LNC and consequently the κ-dependence will be dropped. Therefore, it appears that the κ-dependence of the INS intensity is a result of the scattering on vibrations of rotational type. But the anomalous temperature dependence is a peculiarity of the anharmonicity.

IV. Summary

We have investigated the INS on an anharmonic potential and found an anomalous temperature dependence of the scattering intensity. Further the scattering on soft rotational-type modes brings about an anomalous dependence on the transferred neutron momentum κ. In the light of new experimental findings providing some evidence for electron-phonon pairing in the new high-T_c cupric-oxide superconductors the above obtained results may be important for the lattice dynamical study of this compounds.

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