

Temperature dependence of velocity of sound in high- T_c superconductors in normal state

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Abstract A microscopic theoretical calculation of temperature dependence of velocity of sound in high temperature superconductors is addressed in this paper. The influence of model parameters of the system in its normal phase is investigated through numerical calculations. The results at the room temperature as well as low temperatures ($\sim 25K$), are discussed. The dimensionless parameters involved in the calculations are the electron-phonon coupling (g), staggered magnetic field (h), hybridization (V), position of the f -level (d), temperature (t) and the conduction band width (\bar{w}). The model Hamiltonian contains the antiferromagnetism in conduction electrons of copper and the electron-phonon interaction through the hybridization between conduction electrons and f -electrons of impurity atoms. The phonon Green's functions are calculated by Zubarev's technique. The velocity of sound is calculated in the long wavelength and finite temperature limit.

Keywords High- T_c compounds, electron-phonon interaction, acoustical properties

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1. Introduction

There has been many experimental and theoretical endeavours to understand the mechanism of superconductivity in hole doped $\text{La}_{1-x}\text{Sr}_x\text{CuO}_4$ (denoted as LSCO) and electron doped $\text{Nd}_{1-x}\text{Ce}_x\text{CuO}_4$ (denoted as NCCO) ceramic compounds. Ultrasonic attenuation peak and minimum in sound velocity is observed in non-superconducting NCCO at $\sim 260K$ and in superconducting sample at $200K$ [1]. Prieur *et al* [2] have measured attenuation and velocity of sound in LSCO for different frequencies and temperatures. At temperature below $200K$, the attenuation increases with decrease in temperature and frequency. For temperatures above $200K$, it increases with frequency and temperature. This may be possible due to tetragonal to orthorhombic phase transition [2]. Longitudinal sound velocities are measured in LSCO in presence of magnetic field and showed presence of superconductivity inhibited by the structural instabilities [3, 4]. Ultrasonic measurements of longitudinal sound waves in LSCO by Zhang *et al*[5] showed a peak at temperature $\sim 27K$ of magnetic origin and another peak

at $37.9K$ due to superconductivity. Rout *et al* [6] have reported a microscopic theoretical model to explain a strong softening in the velocity of sound.

In this paper, we report the microscopic theory of the temperature-dependence of velocity of sound of the above superconducting systems in their normal phase at low temperatures.

2. Formalism

The Hamiltonian in k -space is taken as

$$H_d = \sum_{k,\sigma} \epsilon_0(k) (a_{k,\sigma}^\dagger b_{k,\sigma} + h.c.) \quad (1)$$

with dispersion $\epsilon_0(k) = -2t_0 (\cos k_x + \cos k_y)$

$$H_s = (h/2) \sum_{k,\sigma} \sigma (a_{k,\sigma}^\dagger a_{k,\sigma} - b_{k,\sigma}^\dagger b_{k,\sigma}), \quad (2)$$

$$H_v = V \sum_{k,\sigma} (a_{k,\sigma}^\dagger f_{1,k,\sigma} + b_{k,\sigma}^\dagger f_{1,k,\sigma} + h.c.) \quad (3)$$

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$$H_J = \varepsilon_J \sum_{k,\sigma} f_{1,k,\sigma}^\dagger f_{1,k,\sigma} \quad (4)$$

H_d , H_s , H_v and H_f are conduction electron, staggered field, hybridisation interaction and f -electron Hamiltonian respectively. $a(a^\dagger)$, $b(b^\dagger)$ and $f(f^\dagger)$ are annihilation (creation) operators of conduction electrons and f -electrons respectively. The Fourier transformed electron-phonon interaction Hamiltonian is

$$H_{e-p} = \sum_{k,q,\sigma} f(q) \left[\left(a_{k+q,\sigma}^\dagger f_{1,k,\sigma} + b_{k+q,\sigma}^\dagger f_{1,k,\sigma} \right) + h.c. \right] A_q \quad (5)$$

$$h.c. = \left(f_{1,k+q,\sigma}^\dagger a_{k,\sigma} + f_{1,k+q,\sigma}^\dagger b_{k,\sigma} \right),$$

with $A_q = b_q + b_{-q}^\dagger$ where b_q (b_q^\dagger) are annihilation (creation) operators for phonons with wave vector q and $f(q)$ is the electron-phonon coupling constant. The free phonon Hamiltonian with phonon energy ω_q is written as $H_p = \sum_q \omega_q b_q^\dagger b_q$. The double time phonon Green function of Zubarev type [7] is defined as

$$D_{q,q'}(t-t') = \langle\langle A_q(t); A_{q'}(t') \rangle\rangle = -i\Theta(t-t') \langle [A_q(t), A_{q'}(t')] \rangle \quad (6)$$

Applying Dyson approximation, the phonon Green function can be written as

$$D_{q,q}(\omega) = (\omega_q / \pi) \left[\omega^2 - \omega_q^2 - \Sigma_q(\omega) \right]^{-1} \quad (7)$$

where phonon self energy is given by

$$\Sigma_q(\omega) = 4\pi f^2(-q) \omega_q \chi_{qq}(\omega) \quad (8)$$

$$\chi_{q,q'}(\omega) = \sum_{k,\lambda,\sigma,\sigma'} [\Gamma_3 + \Gamma_4 + \Gamma_5 + \Gamma_6] \quad (9)$$

$\Gamma_i(k, k', q, q', \omega)$'s ($i = 3$ to 6) represent the electron response functions. They are defined by dropping k, k', q, q' and ω as

$$\begin{aligned} \Gamma_3(\omega) &= \langle\langle \alpha^a + \alpha^b; \beta^a \rangle\rangle; \\ \Gamma_4(\omega) &= \langle\langle \alpha^a + \alpha^b; \beta^b \rangle\rangle, \\ \Gamma_5(\omega) &= \langle\langle \alpha^t + \alpha^d; \beta^a \rangle\rangle; \\ \Gamma_6(\omega) &= \langle\langle \alpha^t + \alpha^d; \beta^b \rangle\rangle. \end{aligned} \quad (10)$$

where

$$\alpha^a \equiv a_{k-q,\sigma}^\dagger f_{k,\sigma}; \quad \alpha^b \equiv f_{k-q,\sigma}^\dagger a_{k,\sigma}; \quad \alpha^c \equiv b_{k-q,\sigma}^\dagger f_{k,\sigma};$$

$$\alpha^d \equiv f_{k-q,\sigma}^\dagger b_{k,\sigma}; \quad \alpha^e \equiv a_{k-q,\sigma}^\dagger b_{k,\sigma}; \quad \alpha^f \equiv b_{k-q,\sigma}^\dagger a_{k,\sigma};$$

$$\alpha^g \equiv a_{k-q,\sigma}^\dagger a_{k,\sigma}; \quad \alpha^h \equiv b_{k-q,\sigma}^\dagger b_{k,\sigma}; \quad \alpha^i \equiv f_{k-q,\sigma}^\dagger f_{k,\sigma}; \quad (11)$$

$$\beta^a \equiv a_{k'-q',\sigma'}^\dagger f_{k',\sigma'} + f_{k'-q',\sigma'}^\dagger a_{k',\sigma'},$$

$$\beta^b \equiv b_{k'-q',\sigma'}^\dagger f_{k',\sigma'} + f_{k'-q',\sigma'}^\dagger b_{k',\sigma'}. \quad (12)$$

The renormalized phonon frequency in zero wave vector and low temperature limit is calculated by setting the denominator of the eq. (7) to zero. Then

$$(\omega / \omega_0)^2 = 1 + \left\{ 4\pi f^2(0) \chi_{00}(\omega) / \omega_0 \right\}. \quad (13)$$

The different dimensionless parameters are

$$\begin{aligned} g &= f^2(0) N(0) / \omega_0; \quad d = \varepsilon_f / 2t_0; \quad c = \omega / 2t_0; \\ V &= V / 2t_0; \quad e = v_F k_F / 2t_0; \quad a = \alpha k_F / 2t_0; \\ q &= q / k_F; \quad x_0 = \varepsilon_0(k) / 2t_0; \quad h = h / 2t_0; \\ x &= \varepsilon_k / 2t_0; \quad b = 2t_0 / 2kT; \quad t = 1/b. \end{aligned}$$

3. Results and discussion

The phonon coupling to the hybridisation between f -electron and conduction electrons is considered in the formalism of the model for high temperature superconductors given in [6]. The velocity of sound is evaluated numerically under half filling band situations taking the Fermi level at the middle of the conduction band with $\varepsilon_f = 0$. The dimensionless parameters involved in this calculation are the phonon coupling strength (g), the position of the f -level (d) lying below and above the Fermi level, the hybridisation (V), the antiferromagnetic field strength (h) and the reduced temperature (t). The results of velocity of sound at low temperatures is discussed below.

Figure 1 shows the variation of reduced velocity with temperature for various values of phonon coupling (g) and hybridisation. The reduced velocity (\tilde{v}) softens (decreases) with increase of electron-phonon coupling (g). There occurs dip in \tilde{v} at $t \approx 0.15$ corresponding to a value of $g = 0.018$. The \tilde{v} hardens (increases) with increase of temperature.

Figure 2 shows variation of reduced velocity \tilde{v} of sound for shifting of the f -level. As f -level moves from the top towards the Fermi level, the velocity of sound softens and the hybridisation gap becomes prominent at $t = 0.1$ corresponding to $d = 0.06$, corresponds to a hopping integral $2t_0 (= 2500\text{K})$, the corresponding to a fluctuation temperature of $T^* = 250\text{K}$. As f -level moves towards Fermi level the hybridisation strength

increases and hence the fluctuation temperature shifts from higher to the lower temperatures.

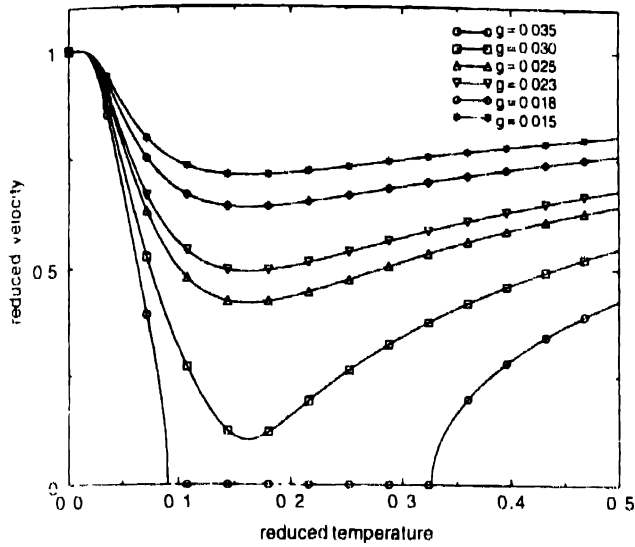


Figure 1. The plot of reduced velocity vs reduced temperature for fixed values of $d = 0.1$, $v = 0.015$, $h = 0.4$ and for different values of $g = 0.035, 0.030, 0.025, 0.023, 0.018, 0.015$

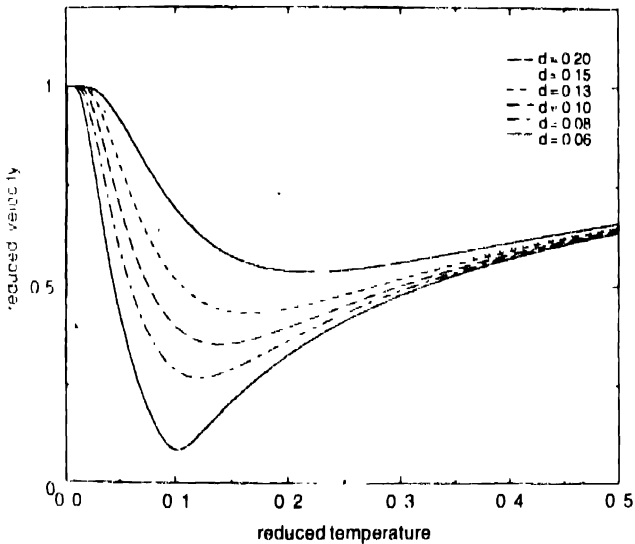


Figure 2. The plot of reduced velocity vs reduced temperature for fixed values of $g = 0.025$, $v = 0.001$, $h = 0.195$ and for different values of $d = 0.2, 0.15, 0.13, 0.10, 0.08, 0.06$

Figure 3 shows the variation of velocity of sound with temperature as f -level moves from the top towards the Fermi

level and further moves below it. Here, velocity of sound softens drastically for a very small change in Fermi level.

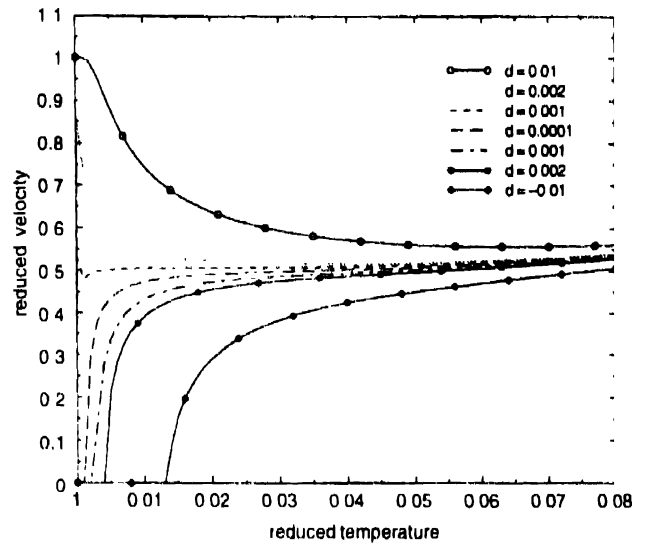


Figure 3. The plot of reduced velocity vs reduced temperature for fixed values of $g = 0.0155$, $v = 0.015$, $h = 0.4$ and for different values of $d = +0.01, +0.002, +0.001, +0.0001, -0.001, -0.002, -0.01$ in the low temperature range

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