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Sound velocity in $La_{0.5}Ca_{0.5}MnO_3$

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ABSTRACT

In this Letter the microscopic theory of the relative change in velocity of sound with temperature of $La_{0.5}Ca_{0.5}MnO_3$ is reported. The phonon Green function is calculated using the Green function technique of Zubarev in the limit of zero wave vector and low temperature. The lattice model electronic Hamiltonian in the presence of the phonon interaction with hybridization between the conduction electrons and the *l*-electrons is used. The relative change in velocity of sound at various temperatures is studied for different model parameters namely the position of the *l*-level, the effective phonon coupling strength and hybridization strength. The phonon anomalies observed experimentally at different temperatures are explained theoretically. An abrupt change in velocity at *Neel* temperature (T_N) is observed clearly. It is observed that different parameters influence the velocity of sound.

1. Introduction

Intense research on experimental and theoretical fronts have been focused on charge-ordered manganites due to the coexistence of charge, orbital, and spin orderings at various temperatures. Charge-ordered manganites in general show different types of ground states depending on the dominance of antiferromagnetic (*AFM*) and/or ferromagnetic (*FM*) interactions, and Jahn–Teller distortions. The half-doped Perovskite manganites $R_{0.5}A_{0.5}MnO_3$ (R = trivalent rare earth ion and A = divalent ion Ca, Sr, Ba) exhibit a wide variety of magnetic structures and magnetotransport behaviors and have been extensively investigated [1–4]. However, the complex physics behind these have not been fully comprehended and, therefore, call for further studies. Qualitative explanation is given by the double exchange (*DE*) mechanism [5]. At higher doping ($x > 0.5$), the ground state becomes again an *AFM* insulator [6,7]. A phase boundary between the *FM* metallic and the *AFM* insulating ground states exists in a narrow range around $x = 0.5$ [8]. In addition, another intriguing phase, the charge ordered (*CO*) state has been found to exist in insulating $La_{1/2}Ca_{1/2}MnO_3$ [9]. A direct evidence of the *CO* state is provided by the electron diffraction for $La_{1/2}Ca_{1/2}MnO_3$ [10].

The *CO* state is characterized by the real space ordering of Mn^{3+}/Mn^{4+} in mixed valent $R_{1/2}A_{1/2}MnO_3$. The *CO* state is expected to become stable when the repulsive Coulomb interacts between carriers dominates over the kinetic energy of carriers [11]. In this respect, the electron lattice of the *CO* state may be viewed as the generalized Wigner crystal. Furthermore, the carriers formed the *CO* state are believed to be manifested in some types of polarons, which arise from the strong electron–phonon interaction, possibly, the *Jahn–Teller* effect [12]. In fact, ordering of such polarons is occasionally observed in 3d transition metal oxides. Ramirez et al. [8] have observed in $La_{1-x}Ca_xMnO_3$ ($0.63 < x < 0.67$) that the *CO* transition is accompanied by a dramatic increase ($> 10\%$) in the sound velocity, implying a strong electron–phonon coupling. Another interesting aspect of the *CO* state is its relevance to the observed magnetic phases. In the half-doped LaCa manganites [9,10], the *CO* state has been realized with *FM–AFM* transition. The common feature is that the *AFM* structure of the specific *CE*-type [6] is observed in the *CO* state of manganites, suggesting a nontrivial effect of the *CO* state on the magnetic phase. The other noteworthy observation is the transport phenomena of the *CO* phase in the presence of the magnetic field. The high magnetic field induces the melting of the electron lattice of the *CO* phase to give rise to a huge negative magnetoresistance (*MR*) [13].

In this work, we report the microscopic theory of the velocity in $La_{1/2}Ca_{1/2}MnO_3$. For this purpose we describe the electronic Hamiltonian of Kondo lattice model and introduce an electron–phonon interaction in Section 2 and calculate phonon Green function in Section 3. The results and discussion are showed in Section 4.

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2. Model

We start from the picture the characteristics of the systems with *Jahn–Teller* (*JT*) ions with an inter-play between electrons localized due to lattice distortions and those in the band states. This situation is typical of manganites and could be described in terms of the Kondo-lattice model in the double exchange limit with account taken for the *Jahn–Teller* distortions and the super-exchange interaction between the localized electrons [14]. The intra-atomic exchange coupling is assumed to be large enough to align the spins of e_g electrons in a Mn ion parallel to spin S of core (t_{2g}) electrons. The *Jahn–Teller* effect leads to the splitting of the double-degenerate e_g level. Then, following [15], we can divide e_g electrons into two groups: "localized" ($l, t^{(l)} \to 0$) producing the maximum splitting of the e_g level and itinerant "band" (b) electrons with nonzero hopping integrals t, leading to smaller distortions of MnO_6 octahedra. The corresponding effective Hamiltonian has the form [14]

$$H_{\text{eff}} = -t \sum_{\langle nm \rangle} c_n^+ c_m - \varepsilon_{JT} \sum_n n_{\text{ln}} + J \sum_{\langle nm \rangle} \cos\theta_{nm} + U \sum_n n_{\text{ln}} n_{bn}. \tag{1}$$

Eq. (1) describes the intra-atomic Hubbard interaction between the l-electrons and l–b-electrons, where $n_{li} = l_i^+ l_i$ and $n_{bi} = c_i^+ c_i$. We linearize the on-site l-electron interaction terms $l_i^+ l_i$ and $c_i^+ c_i$ in the Hamiltonian in the *Hartree–Fock* approximation as $n_{li} n_{bi} \to \langle n_{li} \rangle n_{bi} + n_{li} \langle n_{bi} \rangle$, where $\langle n_{li} \rangle = \langle l_i^+ l_i \rangle$, $\langle n_{bi} \rangle = \langle c_i^+ c_i \rangle$ are the expectation values of n_{li}, n_{bi} and we take $\langle n_{li} \rangle = n_l$, $\langle n_{bi} \rangle = n_b$ for all i. The number of localized, n_{li}, and band, n_{bi}, electrons of per lattice site obeys an obvious relation $n_b + n_l = 1 - x$ (x is doping concentration, value is 0.5).

Then Hamiltonian H_{eff} therefore reduces to

$$H_{\text{eff}} = -t \sum_{\langle ij \rangle} c_i^+ c_j - \varepsilon_{JT} \sum_i n_{li} + J \sum_{\langle ij \rangle} \cos\theta_{ij} + U \left(\sum_i n_{li} c_i^+ c_i + \sum_i l_i^+ l_i n_{bi} \right), \tag{2}$$

$n_{bi} = c_i^+ c_i$; $n_{li} = l_i^+ l_i$, $\varepsilon_{JT} = -g^2/2K$ (where K is the elastic energy and g is the electron-lattice coupling constant).

The Fourier-transformed Hamiltonian of Eq. (2) is written as

$$H_{\text{eff}} = -\sum_k E_k c_k^+ c_k - E_0 \sum_k n_{lk} + J \sum_{\langle ij \rangle} \cos\theta_{ij}, \tag{3}$$

where $E_0 = \varepsilon_{JT} + U n_b$; $E_k = \varepsilon_k + U n_l$; $\varepsilon_k = -2t(\cos k_x a + \cos k_y a + \cos k_z a)$.

In the event of a large *Jahn–Teller* distortion resulting in the band splitting (~ 1 eV) there is the possibility that the lower e_g orbital hybridizes with the localized t_{2g} orbitals which will modify the magnetic ordering of the t_{2g} electrons. Thus the hybridization of the localized electrons with the conduction electrons of band one only is considered, and the Hamiltonian H_v which represents this hybridization effect is given by

$$H_v = V \sum_k \left(c_k^+ l_k + l_k^+ c_k \right). \tag{4}$$

The electron–phonon interaction term in the site representation can be written as

$$H_{e-p} = \sum_{k,q} f(q) \left[c_{k+q}^+ l_k + l_{k+q}^+ c_k \right] \left(b_{-q}^+ + b_q \right). \tag{5}$$

Where b_q (b_q^+) 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

$$H_p = \sum_q \omega_q b_q^+ b_q. \tag{6}$$

The total Hamiltonian of the system then becomes

$$H = H_{\text{eff}} + H_v + H_{e-p} + H_p. \tag{7}$$

3. Calculation of phonon Green function

The phonon self-energy is evaluated by the double-time Green function technique of Zubarev [16] using the equation of motion method. The phonon Green function is defined as:

$$D_{qq'}(t - t') = \left\langle\!\left\langle A_q(t); A_{q'}(t') \right\rangle\!\right\rangle = -i\Theta(t - t') \left\langle \left[A_q(t), A_{q'}(t') \right] \right\rangle, \tag{8}$$

where

$$A_q = b_q + b_{-q}^+ \tag{9}$$

is the qth Fourier component of the displacement. To derive the phonon Green function $D_{q,q'}(t - t')$. We use the equation of motions for phonon operators [17]. The equation of motion for the Fourier transformed phonon Green function $D_{q,q'}(\omega)$ is evaluated for the system using the total Hamiltonian H as given in Eq. (7). The Green function is expressed as

$$D_{q,q'} = \delta_{q,q'} D_q^0(\omega) + 4 f^2(-q) D_q^0(\omega) \chi_{q,q'}(\omega) D_q^0(\omega). \tag{10}$$

Where

$$D_q^0(\omega) = 2\omega_q \left[\omega^2 - \omega_q^2 \right]^{-1} \tag{11}$$