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Impact of superconducting gap on the phonon mode mixing itinerant and localized electron states

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ABSTRACT

The influence of superconducting ordering on the optical lattice vibration modified through the mixing of localized states with Hubbard correlation and itinerant band states is analyzed. We consider the situation where the broad electron band is located between lower and upper Hubbard levels. The hardening or softening of phonon dynamics caused by the opening of superconducting gap in the band of itinerant carriers appears in dependence on the disposition of the electron spectrum and chemical potential. The effect varies substantially if the chemical potential approaches the edges of the band of itinerant carriers or the van Hove singularity.

1. Introduction

The interrelations between superconductivity and phonon dynamics or lattice instabilities have been an object of research for many years, see review [1] for earlier publications in this field. Intensive experimental and theoretical investigations have been conducted to establish the peculiar properties related to the phonon dynamics, structural transformations and symmetry breaking in high-temperature superconductors [2,3]. In particular, the various aspects of phonon self-energy effects caused by superconductivity were analyzed in Refs. [4–7]. A special attention has been paid to the interplay of ferroelectricity and superconductivity in copper-oxide high-T_c systems [8–10]. The involvement of the mixing of vibrational and electronic degrees of freedom for the understanding of relevant physics in cuprate superconductors became particularly essential due to the presence of unconventional isotope effects and phonon as well as lattice anomalies in these systems, see Refs. [11–13] for the theoretical developments.

One of the channels for mutual influence between dynamical lattice destabilization and electronic orderings is served by the vibronic hybridization of electron states which has been accepted as a quite general mechanism for structural phase transitions. This microscopic model considers interband electron-phonon interaction as a dominating cause for structural displacive instabilities and allows one to explain ferroelectricity and related phenomena in several materials [14–17]. Here the virtual transitions of electrons between two bands one of which is filled and the other one is at least partially empty induces the softening of actual optical vibration. In Ref. [18], the behavior of narrow-gap ferroelectric with superconductivity in partially filled conduction band has been examined in the framework of the vibronic theory of ferroelectricity.

Further we use a model where the softening of lattice vibration appears due to the linear electron-phonon interaction mixing localized and itinerant electron subsystems. The ground state of band electrons is supposed to be superconducting. In the absence of superconductivity, the model was examined in Ref. [19] and the special case of such a scheme was suggested as a possible reason for the tetragonal-orthorhombic transition in $La_{2-x}M_xCuO_4$ [20,21]. The main purpose of the present paper is to establish the changes in optical phonon frequency, renormalized by the vibronic hybridization of itinerant and strongly correlated localized electron states, caused by the superconducting pairing gap in the energy spectrum of itinerant carriers.

2. Model

We consider a model where localized and itinerant electron states participate in the electron-phonon interaction leading to the softening of actual phonon mode. The Hamiltonian of the model

$$H = H_0 + H_{\mathrm{el-ph}} \tag{1}$$

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involves the contributions from electron and phonon subsystems

$$H_0 = H_{\rm el} + H_{\rm ph} \tag{2}$$

together with the term of linear electron-phonon interaction $H_{\text{el-ph}}$. The electron subsystem with the Hamiltonian

$$H_{\rm el} = H_{\rm l} + H_{\rm i} \tag{3}$$

contains localized strongly correlated and itinerant carriers. The system of localized electrons is described by the Hamiltonian

$$H_{\rm l} = \sum_j \sum_s \left(\tilde{\varepsilon}_d d_{js}^+ d_{js} + \frac{1}{2} U d_{js}^+ d_{js} d_{j-s}^+ d_{j-s} \right), \tag{4}$$

where d_{js} (d_{js}^+) is the operator of electron annihilation (creation) at the lattice site j with the spin $s = \uparrow, \downarrow$; $\tilde{\varepsilon}_d = \varepsilon_d - \mu$; ε_d is the energy of a localized electron if the electron-electron interaction is absent; μ is the chemical potential; and $U/2 > 0$ is the energy of repulsion between two electrons per one spin direction. For the itinerant electrons which may be in the superconducting state we have the Hamiltonian

$$H_{\rm i} = \sum_{\mathbf{k}} \sum_s \tilde{\varepsilon}(\mathbf{k}) a_{\mathbf{k}s}^+ a_{\mathbf{k}s} + \Delta_{\rm sc} \sum_{\mathbf{k}} a_{\mathbf{k}\uparrow}^+ a_{-\mathbf{k}\downarrow}^+ + \Delta_{\rm sc}^* \sum_{\mathbf{k}} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} . \tag{5}$$

Here $\tilde{\varepsilon}(\mathbf{k}) = \varepsilon(\mathbf{k}) - \mu$; $\varepsilon(\mathbf{k})$ is the energy of an electron with wave vector $\mathbf{k}$; $a_{\mathbf{k}s}$ ($a_{\mathbf{k}s}^+$) is the operator of electron annihilation (creation); and $\Delta_{\rm sc}$ is the superconducting gap. The chemical potential is proposed to be located in the band of itinerant electrons. The term which does not contain operators has been omitted in Eq. (5).

The Hamiltonian of the phonon subsystem is

$$H_{\rm ph} = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left(b_{\mathbf{q}}^+ b_{\mathbf{q}} + \frac{1}{2} \right), \tag{6}$$

where $\hbar\omega_{\mathbf{q}}$ is the energy of an optical phonon with wave vector $\mathbf{q}$ and $b_{\mathbf{q}}$ ($b_{\mathbf{q}}^+$) is the operator of phonon annihilation (creation).

By introducing the Hubbard X-operators [22] representing

$$\begin{aligned} d_{js}^+ &= X_j^{s0} + \eta(s) X_j^{2-s} \\ d_{js} &= X_j^{0s} + \eta(s) X_j^{-s2} \end{aligned} \tag{7}$$

with $\eta(\uparrow, \downarrow) = \pm 1$, the operator (4) takes the form

$$H_{\rm l} = \sum_j \left(\varepsilon_1 \sum_s X_j^{ss} + \varepsilon_2 X_j^{22} \right). \tag{8}$$

Here

$$\varepsilon_1 = \tilde{\varepsilon_d} \tag{9}$$

and

$$\varepsilon_2 = 2\tilde{\varepsilon_d} + U \tag{10}$$

is the energy of one-fold and two-fold occupied states of localized electrons correspondingly with respect to chemical potential. The electron-phonon interaction which mixes itinerant and localized states is determined by the operator

$$H_{\text{el-ph}} = N_0^{-1} \sum_{\mathbf{k}} \sum_j \sum_s \sum_{\mathbf{q}} g(\mathbf{q}) e^{i(\mathbf{k}-\mathbf{q})\mathbf{r}_j} \times a_{\mathbf{k}s}^+ \left[X_j^{0s} + \eta(s) X_j^{-s2} \right] \left(b_{-\mathbf{q}}^+ + b_{\mathbf{q}} \right) + \text{h.c.} , \tag{11}$$

where N_0 is the number of elementary cells; $g(\mathbf{q})$ is the interaction constant; and $\mathbf{r}_j$ is the position vector of the lattice site j.

One can diagonalize the Hamiltonian (5) by means of Bogolyubov–Valatin transformation $a_{\mathbf{k}s} = u_{\mathbf{k}} A_{\mathbf{k}s} + v_{\mathbf{k}}^* A_{-\mathbf{k}-s}^+$, where $u_{-\mathbf{k}} = u_{\mathbf{k}}$, $v_{-\mathbf{k}} = -v_{\mathbf{k}}$ and $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$. As a result we have (omitting ground state energy term)

$$H_{\rm i} = \sum_{\mathbf{k}} \sum_s E(\mathbf{k}) A_{\mathbf{k}s}^+ A_{\mathbf{k}s} , \tag{12}$$

$$E(\mathbf{k}) = \sqrt{\tilde{\varepsilon}^2(\mathbf{k}) + |\Delta_{\rm sc}|^2} \tag{13}$$

together with

$$|u_{\mathbf{k}}|^2 = \frac{1}{2}\left[1 + \frac{\tilde{\varepsilon}(\mathbf{k})}{E(\mathbf{k})} \right], \quad |v_{\mathbf{k}}|^2 = \frac{1}{2}\left[1 - \frac{\tilde{\varepsilon}(\mathbf{k})}{E(\mathbf{k})} \right],$$

$$u_{\mathbf{k}} v_{\mathbf{k}}^* = -\frac{\Delta_{\rm sc}}{2E(\mathbf{k})} . \tag{14}$$

Now the operator of electron-phonon interaction (11) can be presented as

$$H_{\text{el-ph}} = N_0^{-1} \sum_{\mathbf{k}} \sum_j \sum_s \sum_{\mathbf{q}} g(\mathbf{q}) e^{i(\mathbf{k}-\mathbf{q})\mathbf{r}_j} \times \left[u_{\mathbf{k}}^* A_{\mathbf{k}s}^+ + v_{\mathbf{k}} A_{-\mathbf{k}-s} \right] \left[X_j^{0s} + \eta(s) X_j^{-s2} \right] \times \left(b_{-\mathbf{q}}^+ + b_{\mathbf{q}} \right) + \text{h.c.} . \tag{15}$$

3. Squared phonon frequency

One can find the renormalized squared phonon frequency by applying the Shrieffer–Wolff transformation [23], generalized for the case of phonon-mediated dynamic hybridization between itinerant and localized electron states, to the Hamiltonian (1). We exclude from the Hamiltonian (1) the linear contributions of electron-phonon interaction by means of unitary transformation

$$\tilde{H} = U^+ H U, \quad U = e^{iS} \approx 1 + iS - \frac{1}{2} S^2 , \tag{16}$$

$$\begin{aligned} S = N_0^{-1} \sum_{\mathbf{k}} \sum_j \sum_s \sum_{\mathbf{q}} g(\mathbf{q}) e^{i(\mathbf{k}-\mathbf{q})\mathbf{r}_j} \\ \times \Big\{ u_{\mathbf{k}}^* A_{\mathbf{k}s}^+ \left[X_j^{0s} \left(\lambda_1 b_{-\mathbf{q}}^+ + \lambda_2 b_{\mathbf{q}} \right) \right. \\ \left. + \eta(s) X_j^{-s2} \left(\lambda_3 b_{-\mathbf{q}}^+ + \lambda_4 b_{\mathbf{q}} \right) \right] \\ + v_{\mathbf{k}} A_{-\mathbf{k}-s} \left[X_j^{0s} \left(\lambda_5 b_{-\mathbf{q}}^+ + \lambda_6 b_{\mathbf{q}} \right) \right. \\ \left. + \eta(s) X_j^{-s2} \left(\lambda_7 b_{-\mathbf{q}}^+ + \lambda_8 b_{\mathbf{q}} \right) \right] \Big\} + \text{h.c.}, \end{aligned} \tag{17}$$

with the condition

$$H_{\text{el-ph}} + i[H_0, S] = 0 . \tag{18}$$

The equality (18) is satisfied if

$$\begin{aligned} \lambda_{1,2}(\mathbf{k}, \mathbf{q}) &= \frac{i}{-\varepsilon_1 + E(\mathbf{k}) \pm \hbar\omega_{\mathbf{q}}} , \\ \lambda_{3,4}(\mathbf{k}, \mathbf{q}) &= \frac{i}{\varepsilon_1 - \varepsilon_2 + E(\mathbf{k}) \pm \hbar\omega_{\mathbf{q}}} , \\ \lambda_{5,6}(\mathbf{k}, \mathbf{q}) &= \frac{i}{-\varepsilon_1 - E(\mathbf{k}) \pm \hbar\omega_{\mathbf{q}}} , \\ \lambda_{7,8}(\mathbf{k}, \mathbf{q}) &= \frac{i}{\varepsilon_1 - \varepsilon_2 - E(\mathbf{k}) \pm \hbar\omega_{\mathbf{q}}} . \end{aligned} \tag{19}$$

The coefficients $\lambda_{1,2,5,6}$ correspond to the virtual transitions between itinerant and one-fold occupied Hubbard states and the coefficients $\lambda_{3,4,7,8}$ between itinerant and two-fold occupied Hubbard states. It follows from Eqs. (16) and (18) that in the second-order approximation

$$\tilde{H} = H_0 + \frac{i}{2}[H_{\text{el-ph}}, S] . \tag{20}$$

In the random phase approximation one can distinguish in the Hamiltonian (20) the squared phonon frequency $\Omega_{\mathbf{q}}^2$ renormalized