IMPACT OF NONLINEAR ELECTRON-PHONON COUPLING IN MgB_2 ON HIGH T_C SUPERCONDUCTIVITY

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"True laws of Nature cannot be linear" - Albert Einstein

The processes of nonlinear electron-phonon coupling in superconductors with two-band electronic structure are considered. It is shown that the mechanism of two-phonon exchange between the carriers has a considerable impact on increasing of T_C of superconductivity in MgB_2 compound.

1. Introduction

The recent discovery of superconductivity at 40 K in magnesium diboride MgB_2 [1] has provoked a keen interest in the structural and electronic properties of this binary inter-metallic compound. Particularly the high T_C caused a lot of interest in this compound and its physical properties. For example the authors of paper [2] have carried out inelastic neutron scattering measurements of the phonon density of states and compared these results with detailed first-principle calculations of the lattice dynamics (and electronic) calculations for MgB_2. Thus they conclude that the electron-phonon coupling is nonlinear, providing the essential ingredient to explain the high T_C and boron isotope effect in MgB_2 [3]. Another research group considers in [4] that the E_{2g} modes in MgB_2 have a significant nonlinear coupling with electrons and suggests that it is stronger than the linear coupling, which signify substantial contribution to the Cooper pairing from the two-phonon exchange.

Also the high T_C superconductivity of MgB_2 has stimulated a strong interest on the role of band-filling in phonon-driven superconductivity when the charge carriers stem from low electron or hole density in the conduction band. There is an agreement among theorists that there are two qualitatively different systems of bands in MgB_2: quasi-2D σ-bands, and 3D π-bands, and that the former strongly couple to optical E_{2g} phonon at ≈ 600 cm^{-1} [5]. This phonon mode is calculated to be highly anharmonic, and it also has significant nonlinear contributions to the electron-phonon coupling. Thus the puzzle of superconductivity in MgB_2 is hidden in it two-gap, nonlinear electron-phonon coupling mechanism (two-phonon in particular) on E_{2g}-mode related with in-hexagonal-plane vibrations of boron ions. This mechanism lays off a bridge for the novel joint model of a *nanotubular* multi-phonon multi-gap room-T_C superconductivity (RTSC) on base of gallery of whispering circular zero-point phonon modes (twistons, rotons), in particular E_{2g}-mode, resulting in resonant electron-phonon coupling. Suggested model is in accordance with some recent experimental data confirming the effect of nanotubular superconductivity and indicating possible RTSC in 2D bundles of carbon nanoscale tubes [6].

In this paper the superconducting properties of magnesium diboride considering the mechanism of nonlinear phonon exchange between the carriers have been studied. The two-band structure of this compound in processes of interband two-phonon scattering of electrons is considered. Taking into account the nonlinear mechanism of electron-phonon interaction as

preponderant in the process of formation of superconducting phase the sophisticated temperature dependence of the order parameter is found, comparatively with the one-phonon BCS-like model. The anomalous behavior of the order parameter as a function of temperature is observed due to the fact that the electron-phonon interaction "constant" in case of two-phonon exchange between the carriers increases as a temperature function. One expects that the nonlinear exchange effects can explain the high T_C superconductivity of MgB_2.

2. The effect of nonlinear electron-phonon interaction in multi-band superconductors: case of two-phonon exchange

The experimental and theoretical results indicate that the compound MgB_2 has a two-band electronic structure [7]. Presence of two bands near the Fermi energy in the electron spectrum of cuprates has stimulated the application of various models with interband interactions to explain their superconductivity, for example see [8]. In framework of these results one can consider the simple case of two-band electronic system which interacts with the phonon subsystem through the two-phonon exchange mechanism. In this model the Columbian interaction between electrons is not taken into consideration without losing of physical essence of this process in superconductors. Therefore the interacting electron-phonon system is governed by the following Hamiltonian, dropping spin indexes

$$H = H_{\text{el}} + H_{\text{ph}} + H_{\text{int}} \tag{1}$$

where $H_{el} = \sum_{m}\sum_{\mathbf{k}} \varepsilon_m(\mathbf{k}) a^{+}_{m,\mathbf{k}} a_{m,\mathbf{k}}$; $H_{ph} = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} b^{+}_{\mathbf{q}} b_{\mathbf{q}}$; $H_{\text{int}} = \frac{1}{\sqrt{V}} \sum_{m,n}\sum_{\mathbf{k},\mathbf{q}} \left(g_{mn}(\mathbf{q}) a^{+}_{m,\mathbf{k}+\mathbf{q}} a_{n,\mathbf{k}} b_{\mathbf{q}} + H.c. \right)$

Here V is the volume of the crystal $b^{+}_{\mathbf{q}}(b_{\mathbf{q}})$ is the creation (annihilation) operator of the phonon with $\mathbf{q}$ wave-vector and $a^{+}_{n,\mathbf{k}}(a_{n,\mathbf{k}})$ is the electron creation (annihilation) operator in n-band (n=1,2) with the quasi-wave vector $\mathbf{k}$. The matrix elements of the electron-phonon interaction constant can be approximated by following expressions

$$g_{11}(\mathbf{q}) \approx i\mathbf{q}\varepsilon_F \sqrt{\frac{\hbar}{2\rho\omega_{\mathbf{q}}}}\,,\; g_{21}(\mathbf{q}) \approx i\varepsilon_{21}\sqrt{\frac{m^{*}\varepsilon_{21}}{\hbar\rho\omega_{\mathbf{q}}}} \tag{2}$$

where ρ is the density of the material, ε_F is the energy of the Fermi level, ε_{21} is the energetic distance between bands, m^* is the effective mass of carriers.

Taking into account the proprieties of the local symmetry of Bloch wave functions for the down and upper bands, it is not difficult to demonstrate that in many cases when the second and the first bands arise from the atomic local levels with different symmetries (for example P and S atomic states) the interband matrix element of the electron-phonon interaction g_{12} is larger than the intraband matrix elements g_{11} ($g_{12} >> g_{11}$) and g_{22}=0. Also it is considered the symmetric form of matrix g, i.e. $g_{12}= g_{21}$.

In the framework of detailed model discussed in [9] the two-phonon cooperative processes between the electrons of the lowest band through the virtual states of the second band are considered (see Fig.2 in [9]). The case of overlapped bands [10] is not taken into account in the proposed model. Thus, it is necessary firstly to eliminate the operators of the second band from Hamiltonian (1). If the second band is situated at the energetic distance larger than $\kappa_B T$, we can eliminate the electronic operators of this band from Hamiltonian (1). After elimination of electronic operators belonging to second band of superconductor the effective electron-electron interaction Hamiltonian resulting from two-phonon exchange

mechanism is obtained [9]. Thus one can write the kinetic equation for any operator *A(t)* of electronic subsystem [6].

$$\left\langle \frac{dA(t)}{dt} \right\rangle = \frac{i}{\hbar}\left\langle \left[H'_{el}; A(t) \right] \right\rangle + \frac{i}{\hbar}\left\langle \left[H^{eff}_{e-e}; A(t) \right] \right\rangle \tag{3}$$

Here $H'_{el} = \sum_{\mathbf{k}} \varepsilon'_1(\mathbf{k}) a^+_{\mathbf{k}} a_{\mathbf{k}}$ and

$$H^{eff}_{e-e} = -\frac{1}{V^2}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\mathbf{q}_1,\mathbf{q}_2} \frac{(1+2N_{q_1})\left|g_{21}(\mathbf{q}_1)\right|^2 \left|g_{21}(\mathbf{q}_2)\right|^2 \phi_1(\mathbf{k})\phi_1(\mathbf{k}')(\hbar\omega_{\mathbf{q}_1}+\hbar\omega_{\mathbf{q}_2}) a^+_{\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2} a^+_{\mathbf{k}'} a_{\mathbf{k}'+\mathbf{q}_1+\mathbf{q}_2} a_{\mathbf{k}}}{(\hbar\omega_{\mathbf{q}_1}+\hbar\omega_{\mathbf{q}_2})^2 - \left(\varepsilon_1(\mathbf{k}'+\mathbf{q}_1+\mathbf{q}_2)-\varepsilon_1(\mathbf{k}')\right)^2}$$

$$-\frac{2}{V^2}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\mathbf{q}_1,\mathbf{q}_2} \frac{N_{q_1}\left|g_{21}(\mathbf{q}_1)\right|^2 \left|g_{21}(\mathbf{q}_2)\right|^2 \phi_2(\mathbf{k})\phi_2(\mathbf{k}')(\hbar\omega_{\mathbf{q}_1}-\hbar\omega_{\mathbf{q}_2}) a^+_{\mathbf{k}+\mathbf{q}_1-\mathbf{q}_2} a^+_{\mathbf{k}'} a_{\mathbf{k}'+\mathbf{q}_1-\mathbf{q}_2} a_{\mathbf{k}}}{(\hbar\omega_{\mathbf{q}_1}-\hbar\omega_{\mathbf{q}_2})^2 - \left(\varepsilon_1(\mathbf{k}'+\mathbf{q}_1-\mathbf{q}_2)-\varepsilon_1(\mathbf{k}')\right)^2} \tag{4}$$

where

$$\phi_1(\mathbf{k}) = \frac{\varepsilon_2(\mathbf{k}+\mathbf{q}_1)+\varepsilon_2(\mathbf{k}+\mathbf{q}_2)-\varepsilon_1(\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2)-\varepsilon_1(\mathbf{k})}{\left[\varepsilon_2(\mathbf{k}+\mathbf{q}_1)-\varepsilon_1(\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2)+\hbar\omega_{\mathbf{q}_2}\right]\left[\varepsilon_2(\mathbf{k}+\mathbf{q}_2)-\varepsilon_1(\mathbf{k})-\hbar\omega_{\mathbf{q}_2}\right]}$$

$$\phi_2(\mathbf{k}) = \frac{\varepsilon_2(\mathbf{k}+\mathbf{q}_1)+\varepsilon_2(\mathbf{k}-\mathbf{q}_2)-\varepsilon_1(\mathbf{k}+\mathbf{q}_1-\mathbf{q}_2)-\varepsilon_1(\mathbf{k})}{\left[\varepsilon_2(\mathbf{k}+\mathbf{q}_1)-\varepsilon_1(\mathbf{k}+\mathbf{q}_1-\mathbf{q}_2)-\hbar\omega_{\mathbf{q}_2}\right]\left[\varepsilon_2(\mathbf{k}-\mathbf{q}_2)-\varepsilon_1(\mathbf{k})+\hbar\omega_{\mathbf{q}_2}\right]}$$

In expression (4) $N_q = \left(\exp[\hbar\omega_q/(\kappa_B T)]-1\right)^{-1}$ is the mean number of phonons in the **q** state.

Thus the effective interaction Hamiltonian (4) of the electrons from the first band through the two-phonon exchange is obtained. From Exp.(4) it results that the interaction is attractive when the difference between the energies of electrons is smaller as $2\hbar\omega_D$ (Debay cutoff). The cooperative interaction between the electrons through the biphonon field is reduced not only to the simple processes of simultaneous absorption or emission of two phonons. As a consequence of effective interaction Hamiltonian, here are possible the scattering processes, i.e. the transitions between two states of the first band can take place with the one-phonon absorption with $\mathbf{q}_1$ wave-vector and the emission of the other phonon with $\mathbf{q}_2$ wave-vector. This cooperative exchange between the electrons increases with increasing of the temperature. In other words the effective Hamiltonian is proportional with the temperature through the mean number of phonons, N_q. This is one of the main differences between the one-phonon Bardeen-Cooper-Schrieffer exchange (BCS, [11]) and the effective electron-electron interaction in case of two-phonon exchange mechanism. Also the temperature dependence of superconductive energy gap in presence of this exchange integral can be modified essentially, as consequence the critical temperature will increase. Thus the two-phonon exchange mechanism can explain the increasing of critical temperature in many-band superconductors.

3. Superconducting properties of MgB_2 considering the two-phonon exchange between electrons

The influence of the second virtual band position on the creation of the two-phonon Cooper effect in the first band plays an important role in this model. For example, if the virtual states of second band are situated near the Fermi level of the first band, the two-phonon scattering effects with the absorption of one phonon from the thermostat and the

generation of another phonon can play a more important role as processes with the simultaneous generation or absorption of phonon pairs.

Considering some approximations in the effective interaction Hamiltonian from Exp.(3) the Hamiltonian of system is obtained taking into consideration spin indexes:

$$H = \sum_k \varepsilon_1'(\mathbf{k}) a_k^+ a_k - \frac{G(T)}{V} \sum_{k,k'} a_{k'}^+ a_{-k'}^+ a_{-k} a_k \ , \tag{5}$$

where $k = (\mathbf{k}, \frac{1}{2})$ and $G(T) = \frac{4}{V} \sum_{\mathbf{q}_1} \frac{|g_{21}(\mathbf{q}_1 - \mathbf{q}_2)|^2 |g_{21}(\mathbf{q}_2)|^2}{\varepsilon_{21}^2} \left\{ \frac{1}{\hbar\omega_{\mathbf{q}_1-\mathbf{q}_2}} + 4N_{q_1} \frac{\hbar\omega_{\mathbf{q}_1-\mathbf{q}_2}}{(\hbar\omega_{\mathbf{q}_1-\mathbf{q}_2})^2 - (\hbar\omega_{\mathbf{q}_2})^2} \right\}$.

Defined the superconductive energy gap $\Delta(T) = \frac{G(T)}{2V} \sum_{k'} \left\langle a_{k'}^+ a_{-k'}^+ \right\rangle$, we can approximate the Hamiltonian (5) in the following form:

$$H = \sum_k \varepsilon_1'(\mathbf{k}) a_k^+ a_k - \sum_k \left(\Delta(T) \langle a_{-k} a_k \rangle + H.c. \right) \tag{6}$$

The diagonalization of Exp.(6) using the Bogoliubov transformations [12] gives us the following relation for the order parameter as a temperature function

$$\Delta(T) = \frac{4\pi\kappa_B T}{\sqrt{14\xi(3)}} \left[\ln\frac{T_c}{T} + \frac{1}{\lambda} \left(\frac{\sigma T^2}{1+\sigma T^2} \frac{\sigma T_c^2}{1+\sigma T_c^2} \right) \right]^{1/2} , \tag{7}$$

where $\xi(3)$ is the value of Riemann zeta-function ($\xi(3) \approx 1.2$), λ, σ are the model parameters and T_C is critical temperature that is calculated in the framework of two-phonon exchange approximation used in proposed model [9].

In Fig.1 the comparison of one-phonon BCS-like model and proposed two-phonon superconductivity model (with $\sigma \neq 0$) is represented. The decreasing of Δ(T) as a temperature function in the proposed model is slower than in one-phonon BCS-like model. This follows from numerical results and analytic dependence (7). The slow decreasing of Δ(T) gives us the higher critical temperature than in conventional superconductivity theory with constant exchange integral when *σ=0*.

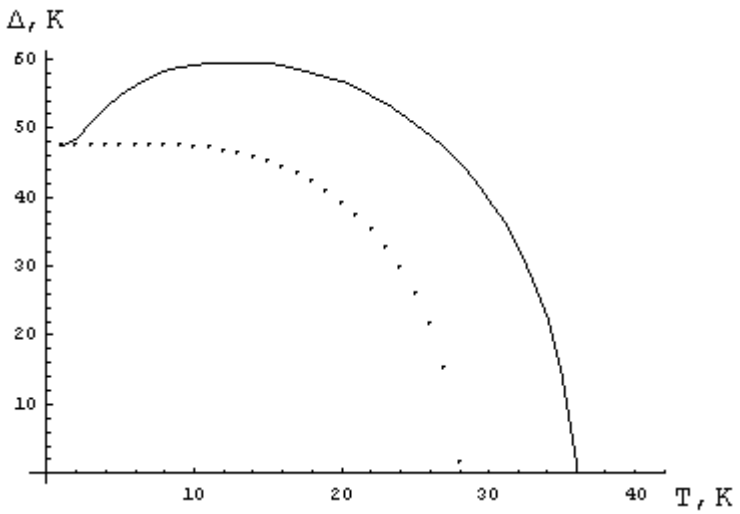

Fig.1 The temperature dependence of the superconductivity order parameter Δ(T). Comparison of one-phonon BCS-like (dotted curve) and two-phonon (solid curve) superconductivity models.

4. Conclusions

In this paper it is shown briefly that the exchange integral between the electrons increases with temperature due to the fact that the two-phonon exchange mechanism stimulates the coherence formation of Cooper-pairs in the two-band superconductors. One of similar superconductor material is MgB_2 and we applied the two-phonon cooperative mechanism of superconductivity [9] for this compound to study its thermodynamic properties. Basing on numerical calculations we plotted the dependence of superconductive energy gap as a temperature function and found the critical temperature of analyzed material. The results of these calculations are in a good agreement with experimental calculations. Thus the two-phonon (nonlinear in general) mechanism of superconductivity opens a new concept on the formation of Cooper-pairs in the processes of multi-phonon exchange between the carriers in multi-band superconductors. The non-traditional temperature dependence of the order parameter (see Fig.1) is described by a complicated two-phonon exchange mechanism between the electrons. Also, from Eq.(7) it results that the temperature of phase transition is higher if the two-phonon interaction is more intensive.

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