Estimation of electron-phonon coupling constant in $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$

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Abstract. The Holstein model was used to determine the value of electron-phonon coupling in BaBiO$_3$-based compounds in the framework of the dynamical mean-field theory calculations for various levels of doping with potassium. The results obtained characterize the electron-phonon interaction as strong. The phase diagram of the model was calculated with reference to experimental data.

1. Introduction
Perovskite materials based on BaBiO$_3$ doped with potassium ($\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ or BKBO) have been the subject of research for more than three decades, since there is still no universally accepted theory of the superconductivity mechanism in these compounds. The reason of this issue is due to the complex crystal structure, which includes different types of BiO$_6$ octahedra complexes. These octahedra have different occupations of the hybridization Bi(6s)–O(2p) orbital, that leads to their inequality in sizes and to the distortion of the formed crystal structure (Fig. 1). It was suggested recently in [1] that bipolaron conductivity could be a good explanation of superconductivity mechanism in $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ because of

Figure 1. Structure of BaBiO$_3$ consists of two different types of BiO$_6$ that tilted to each other by 11’.

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the lack of electron carriers. The local electron structure in BKBO was explained by the existence of a spatially separated Bose-Fermi mixture and the presence of a pair density wave (PDW). The PDW phase is formed due to the distortions of the crystal structure and a local double-well potential caused by them. The parameters of this potential were obtained experimentally in [2] for various degrees of doping of the BKBO compound. The presence of a strong electron-phonon coupling is the crucial part of this phenomenological theory. The aim of this work is to estimate the value of the electron-phonon interaction coupling constant in the framework of a microscopic model of BKBO.

2. Model
The Holstein model is the simplest one that takes into account electron-phonon coupling. The Hamiltonian of the model reads

$$H = \sum_{i,j,\sigma} t_{ij} c_{i,\sigma}^+ c_{j,\sigma} + g \sum_i (b_i^+ + b_i)(n_i - 1) + \omega_0 \sum_i b_i^+ b_i + \mu \sum_i n_i,$$  

(1)

where $c_{i,\sigma}^+ (c_{i,\sigma})$ is the creation (annihilation) operator of an electron with spin $\sigma$ at a lattice site $i$; $n_i$ is the particle number operator; $b_i^+ (b_i)$ is the phonon creation (annihilation) operator; $t_{ij}$ is the amplitude of electron hopping between lattice sites $i$ and $j$; $g$ is the constant of electron-phonon coupling.

The value of $g$ will be used later to construct the phase diagram of the model (1). It should be noted that the physically meaningful value of the strength of the electron-phonon interaction is $\lambda_{\text{eff}}$, which includes renormalization phonon effects [3], and is defined as

$$\lambda_{\text{eff}} = \frac{\partial \Sigma(\omega)}{\partial \omega} \bigg|_{\omega=0},$$

(2)

where $\Sigma(\omega)$ is the self-energy. In practice, the value of $\lambda_{\text{eff}}$ occurs larger than $\lambda_0 = 2g^2 N(\epsilon_F)/\hbar \omega_0$, where $N(\epsilon_F)$ is the density of states on the Fermi level.

3. DMFT method
To solve (1), we have used the method of dynamical mean-field theory (DMFT) [4]. The DMFT approach is based on the theoretical discovery that in the limit of infinite dimensions the electron self-energy does not depend on the momentum $k$ but only on the frequency $i\omega_n$.

The idea of DMFT is to map the lattice model to an effective impurity model (in our case, to the single-impurity Anderson model, or SIAM) and exactly take into account all interactions within it; the correspondence between the systems is achieved by a properly adjusted free electron baths, which are defined self-consistently. The resulting mapping is shown in Fig. 2.

Figure 2. An example of SIAM: interacting site (blue) surrounded by baths (non-interacting sites).
A significant feature of the DMFT approach is the assumption that short-range correlations prevail over long-range ones. In the case of SIAM this implies that the self energy $\Sigma_k$ has no spatial dependence, and

$$\Sigma_k(i\omega_n) \to \Sigma(i\omega_n).$$

(3)

In the limit of infinite dimensions $d \to \infty$ the expression (3) became exact. The mapping between the model (1) and the auxiliary system is fulfilled by the equality of the local self-energy of the model (the lattice self-energy $\Sigma(i\omega_n)$) and the self-energy of the SIAM (the auxiliary self-energy $\Sigma_{aux}(i\omega_n)$); this constitutes one of the the convergence conditions of the DMFT cycle, in which the mapping is realized.

The lattice Green’s function (GF) is defined as

$$G(i\omega_n) = \sum_k (i\omega_n + \mu - \epsilon_k - \Sigma(i\omega_n))^{-1},$$

(4)

where $i\omega_n$ are fermion Matsubara frequencies, $\mu$ is the chemical potential, and $\epsilon_k$ is the kinetic energy of electrons. The corresponding non-interacting lattice GF $G_0(i\omega_n) = G(i\omega_n, \Sigma(i\omega_n) = 0)$ may be calculated from the tight-binding model.

The convergence conditions of the DMFT cycle are

$$G(i\omega_n) = \mathcal{G}(i\omega_n); \quad \Sigma(i\omega_n) = \Sigma_{aux}(i\omega_n),$$

(5)

where $\mathcal{G}^{-1}(i\omega_n)$ is the interacting GF of the auxiliary system, which is calculated by the solution of the SIAM. The auxiliary self-energy $\Sigma_{aux}$ may be obtained from the Dyson equation,

$$\Sigma_{aux}(i\omega_n) = \mathcal{G}^{-1}_0(i\omega_n) - \mathcal{G}^{-1}(i\omega_n),$$

(6)

where $\mathcal{G}^{-1}_0(i\omega_n)$ is the non-interacting GF of the auxiliary system.

The general scheme of the DMFT calculation procedure consists of the following steps:

(i) Set $\Sigma_k(i\omega_n) = 0$ and compute $G$ from (4);
(ii) Calculate the non-interacting auxiliary GF:

$$\mathcal{G}_0(i\omega_n) = (i\omega_n - \epsilon_0 - \Delta(i\omega_n))^{-1},$$

(7)

where the hybridization function $\Delta(i\omega_n) = \sum_b |V_{0b}|^2 / i\omega_n - \epsilon_b$ and $b$ is the number of baths in the auxiliary system; $V_{0b}$ and $\epsilon_b$ are the parameters of the SIAM;
(iii) Solve the SIAM with the use of exact diagonalization technique and compute the interacting GF of the auxiliary system $\mathcal{G}(i\omega_n)$;
(iv) Calculate $\Sigma_{aux}(i\omega_n)$ from (6) and set $\Sigma(i\omega_n) = \Sigma_{aux}(i\omega_n)$;
(v) Check the convergence condition (5). If the DMFT cycle does not converge, calculate new lattice GF $G(i\omega_n)$ (4) and go to (ii).

4. Evaluation of electron-phonon coupling constant

The method described above was applied to the tight-binding model (1); we have used the parameters of the Hamiltonian for BKBO obtained in [5] from \textit{ab initio} calculations (Fig. 3). The dispersion of free electrons in this lattice geometry is

$$\epsilon(k) = 2t_1[\cos(k_x) + \cos(k_y) + \cos(k_z)] + 2t_4[\cos(2k_x) + \cos(2k_y) + \cos(2k_z)] +$$

$$+ 2t_2[\cos(k_x)\cos(k_y) + \cos(k_y)\cos(k_z) + \cos(k_z)\cos(k_x)],$$

(8)
where $k_x, k_y, k_z \in [-\pi, \pi]$. The values of $V_{0b}$ and $\varepsilon_b$, which characterize the hybridization function, should be tuned to satisfy the condition $G_0(i\omega_n) = \mathcal{G}_0(i\omega_n)$; this was achieved by a minimization procedure. Finally, the Hamiltonian of the SIAM has the following form:

$$
\hat{H}_{\text{SIAM}} = \sum_{i,\sigma} V_{0i}(c_{i\sigma}^+ c_{i\sigma} + c_{i\sigma}^+ c_{i\sigma}^-) + \sum_{i,\sigma} \varepsilon_i c_{i\sigma}^+ c_{i\sigma}^- + g \sum_{q,\sigma} (b_q^+ + b_q^-)(c_{0\sigma}^+ c_{0\sigma}^- - \delta) + \omega_0 \sum_q b_q^+ b_q - \mu(n_{0\uparrow} + n_{0\downarrow}),
$$

(9)

where $\delta$ was used to control the correct level of doping in the auxiliary system.

The interacting GF $\mathcal{G}(i\omega_n)$ of the auxiliary system was obtained by solving (9) with the use of the exact diagonalization technique.

Figure 3. The tight-binding model for BKBO from [5]. The hopping amplitudes (in eV) are $t_1 = -0.45$, $t_2 = -0.09$, $t_4 = 0.10$.

After the DMFT-cycle completion, the obtained lattice GF $G(i\omega_n)$ and self-energy $\Sigma(i\omega_n)$ may be used to determine the phase state of the system. Specifically, taking into account the relation between the density of states at the Fermi level and Matsubara GF [6],

$$
N(0) = \frac{\beta}{\pi} \sum_{\mathbf{k}} G(\mathbf{k}, \tau = \beta/2) = \frac{\beta}{2\pi} \sum_{\mathbf{k}} \int \frac{A(\mathbf{k}, \omega)}{\cosh(\beta\omega/2)} d\omega,
$$

(10)

where $A(\mathbf{k}, \omega)$ is the spectral density, it is possible to determine the value of electron-phonon coupling corresponding to the metal–insulator transition. Varying the level of doping in (10) and comparing the phase state of the system with experimental results [7], one obtains proper critical values $g_c$ and the phase diagram of the model (Fig. 4).

These values of $g_c$ were used to solve (1) again to obtain $\lambda_{\text{eff}}$ from (2) for various levels of doping. The results are presented in Table 1; the electron-phonon coupling may be actually classified as strong [8].

5. Conclusions
In this work, we have applied the Holstein model to study the role of electron-phonon interaction in the formation of properties of BaBiO$_3$-based compounds. The values of the effective electron-phonon coupling constant were obtained within DMFT calculations for various levels of doping with potassium. It was found that the electron-phonon interaction in Ba$_{1-x}$K$_x$BiO$_3$ may be characterized as strong at all degrees of doping. The phase diagram of the model in the coordinates doping level – electron-phonon coupling was calculated.
Figure 4. The phase diagram “doping level–electron-phonon coupling” of the model (1).

Table 1. Values of electron-phonon coupling $\lambda_{\text{eff}}$ for various degrees of doping.

|            | BaBiO$_3$ | Ba$_{0.8}$K$_{0.2}$BiO$_3$ | Ba$_{0.7}$K$_{0.3}$BiO$_3$ |
|------------|-----------|-----------------------------|-----------------------------|
|            | 1.52      | 3.54                        | 4.26                        |

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