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Analysis of the superconductivity in perovskite oxides using three-square-well BCS formalism

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Abstract. Superconductivity in perovskite, BaKBiO, is studied in the Bardeen–Cooper–Schrieffer (BCS) model, with three-square-well potentials. Components of the new coupling are: the attractive acoustic phonon–electron, optical phonon–electron and repulsive Coulomb interactions. With these in the BCS pairing Hamiltonian, expressions for the superconducting transition temperature and isotope effect exponent are obtained. Results of our analysis are consistent with experiments. Contributions of interactions to system properties are exhibited and analysed. Acoustic phonon–electron and optical phonon–electron interactions have near-identical elevation of transition temperature, holding out possible explanations for high-T_c. Contrastingly, optical phonon–electron and Coulomb couplings cause debilitation of isotope exponent, a possible explanation for low isotope exponent in the cuprates and other high-T_c systems. It is found that BCS electron–phonon coupling appears synonymous with acoustic phonon–electron coupling.

Keywords. Perovskite superconductor; three-square-well potentials; electron–phonon interaction; Bardeen–Cooper–Schrieffer model.

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1. Introduction

Potassium-doped barium bismuth oxide, $Ba_{1-x}K_xBiO_3$ (BKBO), is a non-copper containing oxide superconductor with the transition temperature ($T_c \approx 30$ K, for $x = 0.4$ [1–4]). The important differences between these oxides and cuprates are: (i) absence of metal–oxygen layers (planes), (ii) absence of magnetic degrees of freedom, (iii) overriding presence of electron–phonon coupling (∼Bardeen–Cooper–Shrieffer (BCS) isotope exponent value [5–7]) and (iv) isotropic properties of BKBO [8], as compared with the cuprates.

The most influential difference between BKBO and the cuprates is the electron–phonon coupling which is strongly operative in BKBO but weak or non-existent in the high-T_c cuprates. A direct evidence of the importance of electron–phonon interaction in BKBO has been given by tunnelling measurements [9–11]. The measured values of the coupling constant, $\lambda \approx 0.7$–1.2 are sufficient to explain its high critical temperature within the standard BCS mechanism. Theoretically, Shirai *et al* [12] used tight-binding method and obtained $\lambda \approx 1.09$. Crude rigid-muffin-tin approximation gave $\lambda \approx 3.0$, indicating a strong coupling regime [13]. Early tunnelling data gave the ratio $(2\Delta)/(k_B T_c) \approx 3.5$–$3.9$, which suggested an intermediate coupling $\lambda \approx 1$ [14,15]. Zhao [16] observed large reduced energy gap with $(2\Delta(0))/(k_B T_c) = 4.4$ and a retarded electron–phonon coupling constant $\lambda = 1.4$, suggesting quasi-intermediate interaction. Some tunnelling experiments gave this gap-to-T_c ratio as ∼4.2 [17,18], as found in Nb_3Sn ($\lambda \sim 1.8$), suggesting strong coupling. However, the electronic specific heat coefficient, $\gamma = 1.5$ [17], in conjunction with band-structure density of states, yielded electron–phonon coupling constant, $\lambda \sim 0.35$, consistent with a weak-coupled superconductor.

Electron–phonon coupling in the weak-coupling regime was predominantly given as $\lambda = 0.3$ [19], 0.5 [20] and 0.34 [21], for BKBO, in more recent times. Many other experiments show λ as low as 0.2 [18,22], together with the existence of high-energy excitation [18], suggesting that the dominant coupling mechanism may not be the standard electron–phonon coupling. Although refs [18–23] believed that BKBO is an isotropic s-wave superconductor, they agreed that it was not being driven by the conventional electron–phonon interaction. Meregalli *et al* [21] successfully established a large coupling of the electrons to the bond-stretching oxygen and found, in their Raman scattering results, some high-frequency (energy) optical phonons, as the answer. The large reduced energy gap observed by Zhao [16], is believed by him to have ruled out the possibility of pairing mechanism based on coupling to high-energy electronic excitations.

Raman spectrum of BKBO shows a strong peak close to 348 cm^{-1} due to high-energy optical phonon coupling to electronic states [24]. Inelastic neutron scattering experiment shows that the phonon spectrum comprises two bands near 30 and 60 meV, due to oxygen vibrations [25]. Braden *et al* [26] found that the highest longitudinal optic (LO) branch at ∼17 THz is associated with Bi–O bond-stretching vibrations. These show that in BKBO the carriers may be coupled to high-energy oxygen vibrations. Tunnelling spectroscopy experiments can provide a direct measure of the interactions for superconductivity, although high-quality tunnel junctions on high-T_c materials are difficult to obtain. High-resolution tunnelling measurement on polycrystalline BKBO revealed well-resolved phonon structures corresponding to optical modes of the oxygen in the range 40–65 meV [15]. Huang *et al* [9] have demonstrated that high-energy optical phonons are involved in the carrier pairing with a coupling constant, $\lambda \sim 1$. Other tunnelling measurements on thin films [27] and single crystals [11] of BKBO favour the participation of oxygen optical phonons (∼20–70 meV) in the pairing mechanism.

Among the nonconventional mechanisms that have been proposed for explaining the superconducting properties of BKBO crystals is the concept of negative U centres [28,29], which was originally proposed by Anderson [30] for semiconductor glasses. It associates the tendency of Bi atoms to avoid the Bi^{4+} state while preparing the Bi^{3+} and Bi^{5+} charge states, thereby resulting in an attractive local negative U pairing centre. Hase and Yanagisawa

[31] hold the view that in valence-skip-fluctuation elements, such as BKBO, the effective electron–electron interaction is attractive, contrary to the well-known on-site Coulomb repulsive interaction. However, still a subject of debate, first-principle studies [32–34] have so far ruled out the possibility of the negative U mechanism in BKBO superconductor. Other mechanisms as small polarons [35] and bipolaronic states [36] in the superconductivity of BKBO crystals have been suggested.

At the root of electron–phonon interaction, we recall that acoustic phonons exist in all solids and are defined by the Debye temperature. In some solids, due to the presence of light atoms, there exist optical phonons, in addition, defined by the Einstein temperature. Indeed, in an ionic crystal, such as BKBO, optical phonons are very important. These two interactions constitute the attractive portion of the electron–phonon interaction [6] while the electron–electron (Coulomb) interaction forms the repulsive portion. If we play down on the view of Hase and Yanagisawa, for the moment, these interaction components give rise to the three-square-well potentials [6].

The original phonon-mediated theory of superconductivity by Bardeen, Cooper and Schrieffer assumed attractive interaction energies in the form of a square-well [5]. The theory has also been extended to two-square-well taking into account the Coulombic interaction among others in understanding the properties of high-T_c superconductors [37–41]. The three-square-well potential within one-band BCS model has been employed to study the effect of plasmons on the yttrium- and lanthanum-based superconductors [42]. The effect of spin fluctuations in the superconducting properties of phonon-mediated superconductors have been studied using three-square-well in weak coupling as well as strong coupling regimes [43,44]. Moreover, these potential models have been used to study the properties of two-band high-T_c superconductors [45–49]. Nevertheless, there exist some other non-phonon mechanisms of high-T_c superconductivity [50,51]. In this paper, we shall employ three-square-well potential model to elucidiate the superconducting properties of BKBO.

The longitudinal vibration branch of phonon contribution to pairing can often be guaged from the shift in T_c due to substitution of constituent elements by their isotopes. Batlogg *et al* measured the oxygen isotope effect β in $Ba_{0.6}K_{0.4}BiO_3$ and found $\beta = 0.2$–0.25 [23]. Kondoh *et al* found an isotope exponent of $\beta = 0.35 \pm 0.05$ [52]. Hinks *et al* from DC resistivity and AC susceptibility measurements, found $\beta = 0.41 \pm 0.03$ [53]. Loong *et al*, from inelastic neutron scattering experiment and molecular dynamics simulation, got $\beta = 0.42 \pm 0.05$ [7]. Zhao and Morris reported $\beta = 0.2$–0.3 for BKBO ($x = 0.45$, 0.375 and 0.36) and found that with the decrease of potassium content, the oxygen isotope exponent β increases [54]. However, Hellman interpreted the anomalously small isotope effect as the existence of the exponent depedence on the isotropic substitution fraction [55]. Varshney and Tosi had $\beta = 0.33$ by a theoretical consideration of the mechanism of plasmon–optical phonon pairing [56]. Later, Varshney *et al*, by employing the three-square-well potentials and Nambu–Eliashberg theory, got $\beta = 0.47$ [6].

The Bardeen–Cooper–Schrieffer (BCS) theory is certainly based on the electron–phonon coupling, often alternatively assessed by the isotope effect exponent. From the results outlined so far, both low and high values of λ and β exist abundantly in literature, while the electron–phonon coupling concept appears very much unresolved. Therefore, the concepts of electron–phonon interaction and the associated isotope effect may need reinterpretation. BCS did ignore Coulomb interaction on account of the screening effect.

They worked with simple, attractive, and constant potential. The idea of optical phonons was considered only later. Do we assume, *ab initio*, that the electron–phonon interaction meant by BCS definitely excludes optical phonons? With the present three-square-well potentials as the components of the new 'electron–phonon coupling', the original concepts of electron–phonon coupling and the accompanying isotope effect exponent need enlargement. In the framework of the standard theory, we shall embody these new potentials, and arrive at some physical parameters of the system, BKBO, based on this theory. These will either validate or invalidate the enlarged coupling concept. This will be done with the understanding that perhaps, the problem with BCS model is in their concept of electron–phonon interaction and its effect.

Furthermore, our calculations are motivated by the recent inelastic X-ray scattering measurement of the acoustic and optical modes of BKBO system along the (1 0 0) direction in reciprocal space [57,58]. Khosroabadi *et al* [57,58] observed that there is a large and anomalous softening of the highest energy phonon modes when the system transfers from insulator to the superconducting system. Kang *et al* [59] observed a softening of phonons and a structural phase transition in a superconducting BKBO single crystal using elastic and inelastic neutron scattering measurements. These studies concluded that electron–phonon interaction exists in superconducting BKBO.

In this paper, we shall present the BCS one-band model of superconductivity for $Ba_{1-x}K_xBiO_3$, $x = 0.4$, in §2. In §3 we present our results and discussion and in §4, we give the summary and conclusion.

2. The model

In the weak-coupling BCS model of superconductivity, we start the theory for the cubic perovskite, BKBO, with the reduced Hamiltonian [5]:

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kk'} V_{kk'} c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow} c_{-k\downarrow} c_{k\uparrow}, \tag{1}$$

where ϵ_k is the unperturbed kinetic energy of an electron relative to the Fermi energy, E_F; $c^\dagger_{k\sigma}$ ($c_{k\sigma}$) is the creation (annihilation) operator for the electrons, $V_{kk'}$ is the net attractive pairing interaction, k (k') is the Bloch wave vector and σ is the spin ($\uparrow$ or $\downarrow$) index. After applying the variational analysis, the nonlinear integral equation for the gap, first obtained by BCS [5] is:

$$\Delta_k = -\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2\varepsilon_{k'}} (1 - 2f_{k'}), \tag{2}$$

where $\varepsilon_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$ and f_k is the Fermi–Dirac occupation number of quasiparticle states.

The choice of pairing interaction, $V_{kk'}$, is a major problem in the theory of superconductivity. Even in the face of the observed visual evidence of the existence of space inhomogeneous superconductor–insulator states in high-T_c BKBO by magneto-optical visualization technique [60], we shall take the system as isotropic. The BCS theory assumed a very simple value of an isotropic, constant, net attractive interaction. This was the electron-phonon coupling potential. In our case, we shall assume this interaction to

be made up of three components: attractive acoustic phonon–electron (V_a) and optical phonon–electron (V_p) interactions in addition to electron–electron (V_c) interaction, which is repulsive, all being isotropic. These constitute the three-square-well potentials [6,48]:

$$V_{kk'} = \begin{cases} -V_a - V_p + V_c, & |\omega| < \omega_a \\ -V_p + V_c, & \omega_a < |\omega| < \omega_p \\ +V_c, & \omega_p < |\omega| < \omega_c \\ +0, & |\omega| > \omega_c \end{cases} \tag{3}$$

where ω_a and ω_p are the cut-off frequencies for the attractive acoustic phonon–electron and optical phonon–electron interactions, while ω_c is that for on-site repulsive electron–electron interaction, with $\omega_c > \omega_p > \omega_a$. We note that the phonons are of longitudinal origin and possible contributions to pairing through low-energy collective charge excitation cannot be entirely ruled out. However, the results of the model clearly demonstrate the contribution of various coupling strength constants and their corresponding cut-off energies on the superconducting properties of BKBO.

We substitute eq. (3) in eq. (2) and introduce the constant density of states at the Fermi energy, $N(0)$, after changing the summation to integration, under weak-coupling approximation (with $k_B = h = 1$):

$$\Delta_j = N(0) \int \mathrm{d}\epsilon_{k'}(-V_a - V_p + V_c) \times \frac{\Delta_j(\epsilon_{k'})}{2\,\epsilon_{k'}}(1 - 2\,f(\epsilon_{k'})), \tag{4}$$

where $j = a,\ p,\ c$. Following Su *et al* [61] and considering the acoustic phonon, optical phonon and Coulomb interactions separately, one obtains three homogeneous equations:

$$\begin{aligned} &(1 - \lambda\, Z_a)\Delta_a - \Delta_p = 0, \\ &(1 - \kappa Z_p)\Delta_p - \kappa Z_a \Delta_a - \Delta_c = 0, \\ &(1 + \mu Z_c)\Delta_c + \mu Z_p \Delta_p + \mu Z_a \Delta_a = 0, \end{aligned} \tag{5}$$

where

$$\begin{aligned} &\lambda = N(0)V_a, \qquad \kappa = N(0)V_p, \qquad \mu = N(0)V_c \\ &Z_a = \ln\left(\frac{1.13\omega_a}{T_c}\right), \qquad Z_p = \ln\left(\frac{\omega_p}{\omega_a}\right), \qquad Z_c = \ln\left(\frac{\omega_c}{\omega_p}\right). \end{aligned} \tag{6}$$

λ, κ and μ are acoustic phonon–electron, optical phonon–electron and repulsive Coulomb coupling parameters, respectively.

The equations (eq. (5)) can be rearranged in matrix form and solved simultaneously. The determinant of the resulting square matrix must vanish for non-trivial solutions of the equations. Using the solutions of the determinant and after simplification yield

$$\frac{1}{Z_a} = \left(\lambda - \frac{1}{Z_p - [1/(\kappa - \mu^*)]}\right), \tag{7}$$

where a new Coulomb pseudopotential coupling is defined as $\mu^* = \mu\,(1 + \mu Z_c)^{-1}$. These solutions yield the critical temperature as

$$T_c = 1.13\omega_a\, \exp\left\{-\frac{1}{\lambda_{\mathrm{eff}}}\right\}, \tag{8}$$

where the effective coupling constant λ_{eff} is

$$\lambda_{\text{eff}} = \lambda - \frac{1}{Z_p - [1/(\kappa - \mu^*)]}. \tag{9}$$

This is the expression for transition temperature in terms of the acoustic phonon–electron (λ), optical phonon–electron (κ), Coulomb pseudopotential (μ^*) coupling potentials and logarithmic ratio of optical to acoustic phonon–electron attraction cut-off frequencies. This coincides with the result by Varshney *et al* [6] for this compound using the Nambu–Eliashberg approach in the three-square-well potential formalism.

If the optical phonon–electron coupling contribution to the transition temperature is ignored, the expression for T_c is recovered within the two-square-well, attractive–repulsive potential model as [62]

$$T_c = 1.13\omega_a \exp\left\{-\frac{1}{\lambda - \mu^*}\right\}. \tag{10}$$

The BCS expression for the transition temperature is recovered when both optical phonon–electron and Coulomb couplings are neglected.

The isotope exponent β is derived from the expression for T_c, (eq. (8)), using the relation $-\beta = \mathrm{d}\ln T_c/\mathrm{d}\ln M$, where M is the ionic mass. Employing the relation $T_c \propto M^{-\beta}$ and recalling that $\omega_a \propto M^{-1/2}$, the isotope effect exponent β, after differentiation and simplification, gives

$$\beta = \frac{1}{2}\left\{1 - \left\{\frac{1}{\lambda_{\text{eff}}\,(Z_p - [1/(\kappa - \mu^*)])}\right\}^2\right\}. \tag{11}$$

Equation (11) is the isotope exponent derived in the BCS one-band and three-square-well potential model. It is different from the isotope exponent shift deduced by Varshney *et al* [6]. If $Z_p = \kappa = 0$ is imposed on the system, the expression for the isotope exponent reduces to

$$\beta = \frac{1}{2}\left\{1 - \left\{\frac{\mu^*}{\lambda - \mu^*}\right\}^2\right\}. \tag{12}$$

We observe that λ , κ , μ^* and Z_p influence the values of T_c and β in the present model. However, in two-square-well potential approximation, only λ and μ^* are operative. In pure acoustic phonon–electron interaction regime ($\kappa = \mu^* = 0$), β reduces to 0.5. This happens to be consistent with the BCS 'universality law' of isotope exponent in conventional superconductors. Therefore, the three-square-well approach has revealed that the standard model regarded only acoustic phonon–electron interaction as being synonymous with electron–phonon coupling, while ignoring optical phonon–electron and Coulomb coupling. Here we have shown the contributions by these components in one-band BCS model. These are only intraband effects. In two-band (or multiband) metals, interband interactions do affect superconducting properties [48,63].

3. Results and discussion

With acoustic phonon–electron, optical phonon–electron and Coulomb coupling components operative in perovskite ($Ba_{1-x}K_xBiO_3$, $x = 0.4$) superconductor, the critical temperature

is calculated as $T_c = 29.30$ K, in agreement with experiment [1–4]. The physical parameters used are those commonly employed in literature: $\omega_a = 320$ K [64], $\omega_p = 680$ K [64], $\omega_c = 3$ eV [12], $\lambda = 0.3$ [19], $\kappa = 0.2$ [6], $\mu^* = 0.11$ [65,66] and eq. (8).

In figure 1, the variation of T_c with λ, for three well-separated μ^* values, is shown. It is clear that, although T_c increases with λ in all the three curves, for the same value of λ, it decreases with increase in μ^*. The rate of decrease is not readily discernible in this plot. However, the effect of optical phonon–electron coupling on T_c is depicted by the superposition of T_c of two-square-well, eq. (10), against λ in the plot. The absence of κ in eq. (10) assists greatly the $\mu^* = 0.10$ curve drop by about 20 K, on an average, from the usual highest to the lowest level.

Similarly, T_c increases as κ grows higher. Our analysis shows that the presence of this optical component of electron–phonon coupling elevates T_c as if acoustic phonon–electron coupling strength is about doubled, in its absence. This coupling may be involved as: (i) electrons coupled to bond-stretching oxygen vibrations (phonons) [21], (ii) high-frequency optical phonons coupled to electrons [9,11,23,27]; (iii) the ∼60 meV band in the inelastic neutron scattering due to oxygen phonons [25] and (iv) the LO branch at ∼17 THz [26].

To visualize the overall effect of the Coulomb pseudopotential on transition temperature, we plot, in figure 2, T_c against μ^* and compare this with that for two-square-well ($\kappa = 0$), superimposed. In the present theory, the exact effect of μ^* is to decrease T_c in a near-linear form from the maximum (∼60 K), for very low μ^*, to about 10 K, at about $\mu^* = 0.2$. The presence of μ^* in eqs (8) and (10) greatly reduces T_c on account of their exponential dependence on it. Additionally, in the absence of optical phonon–electron coupling, the reduction leads to all-time low T_c (∼10 K at zero μ^*) to zero at $\mu^* < 0.2$.

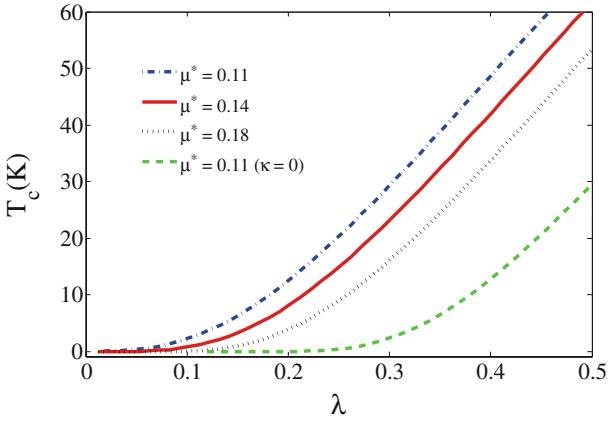

Figure 1. The transition temperature (T_c) as a function of acoustic phonon–electron coupling (λ) for different μ^*. Here, for the present theory, the Coulomb interaction, $\mu^* = 0.11$ (blue, dot–dashed line), 0.14 (red, solid line), 0.18 (black, dotted line) for the parameters $\kappa = 0.2$, $\omega_a = 320$ K, $\omega_p = 680$ K and $\omega_c = 3$ eV. The two-square-well potential approximation ($\kappa = 0.0$ and $\mu^* = 0.11$) (green, dashed line) is superimposed.

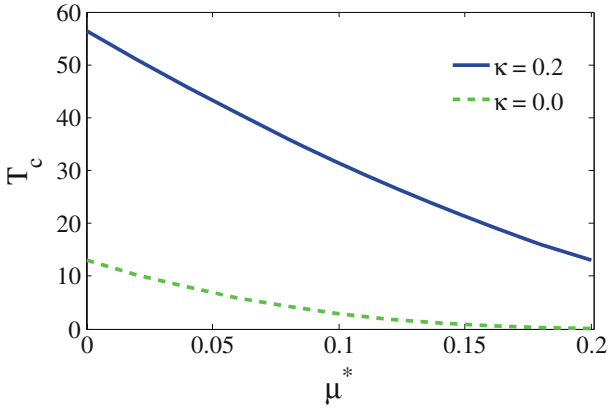

Figure 2. The transition temperature (T_c) against Coulomb interaction coupling (μ^*) for the present theoretical system's optical phonon–electron interaction, $\kappa = 0.2$ (blue, solid line) and for $\kappa = 0.0$ (green, dashed line) for the parameters $\lambda = 0.3$, $\omega_a = 320$ K, $\omega_p = 680$ K, $\omega_c = 3$ eV.

The second physical parameter of BKBO to be calculated from the present theory is the isotope exponent which is given by eq. (11). Using the quoted system parameters ($\lambda = 0.3$, $\kappa = 0.2$, $\mu^* = 0.11$, $\omega_a = 320$ K, $\omega_p = 680$ K and $\omega_c = 3$ eV), the isotope exponent is computed as $\beta = 0.46$. This is consistent with the results [6,7,24,53]. This value of the exponent is reduced from the BCS value for conventional superconductors. The enhanced value of the exponent relative to that of the other high-T_c superconductors, derives from the equally 'enlarged electron–phonon coupling'. Although the Coulomb and optical phonon–electron interactions are not additive, their net effect on the isotope exponent is debilitation. In the absence of optical phonon–electron and Coulomb interactions, what is left is the acoustic phonon–electron coupling. Then the BCS value which is recovered as the isotope exponent, is higher than the value we obtained in the present work. This, again, informs us of the effect of acoustic phonon–electron interaction being the same as BCS electron–phonon coupling.

In figure 3, β against λ is plotted for well-separated μ^*'s. For the present theory, β increases rapidly as λ increases. As λ gets larger, all the curves converge at $\beta = 0.5$ as the saturation point. The saturation point shown here is the same as the BCS universal isotope exponent limit for conventional superconductors. Although the trends are the same, at lower values of λ, the present theory has higher β values than those for two-square-well potential model ($\kappa = 0$) which rapidly take lower β values with reversed μ^*-curve levels. The absence of κ in the two-square-well expression of β may explain the reversed order of the curves. Further analysis shows that β decreases as κ increases for different μ^*. Higher values of β correspond to higher values of μ^*. In all, the dominance of optical phonon–electron interaction reduces isotope exponent, a reverse effect to its role on T_c.

An interesting exposition is that of the plot of β against μ^*, which is presented in figure 4. Here, at $\mu^* = 0$, near-BCS value of isotope effect exponent is obtained for a small κ ($= 0.1$) value. Thereafter, the isotope exponent rises to saturation value (BCS value) as μ^* increases. The small value of κ shows the near-absence of optical

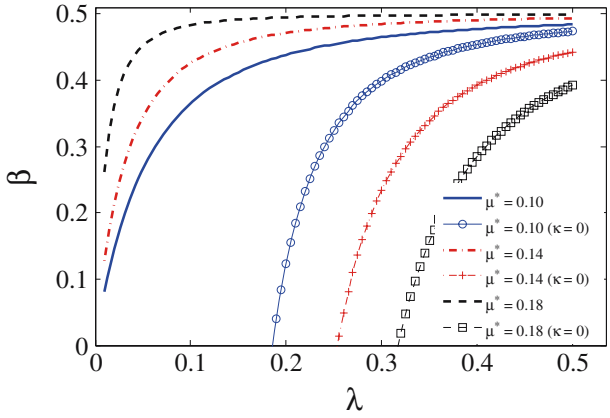

Figure 3. Plot of isotope exponent (β) against acoustic phonon–electron coupling (λ) for various Coulomb interactions ($\mu^* = 0.10$, 014, 0.18) using the parameters $\kappa = 0.2$ (present theory), 0.0 (two-square-well approx.), $\omega_a = 320$ K, $\omega_p = 680$ K and $\omega_c = 3$ eV.

phonon–electron interaction. This point appears confirmed by the superposition of β vs. μ^* from two-well-square approximation ($\kappa = 0$). Here, at $\mu^* = 0$, β takes the BCS value and then falls parabolically to zero at higher values. This is earlier than when the β from the present theory attains saturation. With this action of μ^* on β, we suggest that the graphs of β against μ^*, for $\kappa = 0.2$, 0.3 and 0.4, will all converge at the saturation value, beginning with the lowest $\kappa = 0.4$ curve, up to that for highest 0.1 curve.

Finally, combining (8) and (11), we estimated the transition temperature $T_c \simeq 29.30$ K and the isotope-effect exponent $\beta \simeq 0.46$ in $Ba_{0.6}K_{0.4}BiO_3$ superconductor. These results are close to the experimentally measured value of Hinks *et al* [53] and Loong *et al* [7].

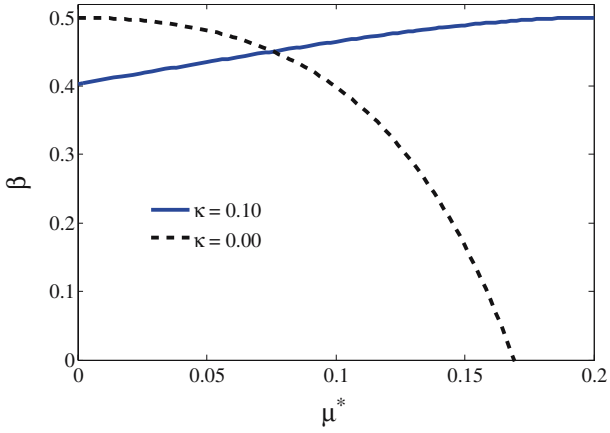

Figure 4. Variation of isotope exponent (β) with pseudopotential coupling (μ^*) for different optical phonon–electron couping, for parameters $\lambda = 0.3$, $\omega_a = 320$ K and $\omega_c = 3$ eV.

4. Summary and conclusion

Superconductivity in cubic perovskite bismuthates ($Ba_{1-x}K_xBiO_3$, $x = 0.4$), has been studied using the well-known BCS model, where the electron–phonon coupling concept is expanded. This is done by including the attractive acoustic phonon–electron, optical phonon–electron and repulsive electron–electron interactions as the components of the new electron–phonon coupling, known as the three-square-well potentials. This is different from the BCS idea which, in effect, excludes the two components from the acoustic phonon–electron interaction, the latter found to be synonymous with BCS electron–phonon interaction. The contributions of these components in the superconducting properties, the transition temperature and the isotope exponent, are analysed afresh. The acoustic phonon–electron interaction causes elevation of both the transition temperature and the isotope exponent, bringing the system, BKBO, to saturation ($\beta \approx 0.5$) as it dominates the others, in obvious compliance to the BCS model. Although the optical phonon–electron interaction also elevates T_c as λ, it causes monotonous decrease in β, down to zero, as it becomes dominant. Gradually, the Coulomb pseudopotential interaction causes a near-linear decrease in T_c while effecting a gradual elevation of the isotope exponent to saturation, as it dominates. These are the findings of the present theory. The absence of optical phonon–electron interaction in the two-square-well approximation leaves T_c and β with similar trends, respectively, but with values lower than in the present. The presence of Coulomb interaction makes T_c drop very low, to a vanishing point, as μ^* grows large. On the isotope exponent, Coulomb pseudopotential interaction makes it to drop from saturation value parabolically to zero, at high μ^*. The realization of the saturation of β-value when $\mu^* = \kappa = 0$ and when acoustic phonon–electron interaction is very dominant, points to the latter being synonymous with BCS electron–phonon interaction.

In conclusion, the involvement of optical phonon–electron interaction in the elevation of the transition temperature, with almost the same strength as acoustic phonon–electron potential, may have explained high-T_c phenomenon in $Ba_{1-x}K_xBiO_3$, $x = 0.4$. In the same way, the combination of optical phonon–electron and Coulomb pseudopotential interactions, that suppresses the isotope effect exponent, has yielded reduced value of isotope exponent below the BCS value. This may, therefore, account for the excessively reduced values of the isotope exponent in the cuprates and high-T_c materials, in general, where electron–phonon interaction is minimal. Indeed, high-T_c occurrence along with almost non-existent isotope exponent, may be a consequence of excessively suppressed acoustic phonon–electron interactions, but with high Coulomb and optical phonon–electron coupling, in those high-T_c systems.

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References

[1] J R Cava *et al*, *Nature* **332**, 814 (1988)
[2] D G Hinks *et al*, *Nature* **333**, 836 (1988)

[3] M Kato *et al*, *J. Phys: Conf. Ser.* **150**, 052100 (2009)
[4] S Larsson, *Physica C* **468**, 113 (2008)
[5] J Bardeen, L N Cooper and J R Schrieffer, *Phys. Rev.* **108**, 1175 (1957)
[6] D Varshney, R P Kumhar and R K Singh, *J. Supercond.* **14**, 623 (2001)
[7] C K Loong *et al*, *Phys. Rev. Lett.* **66**, 3217 (1991)
[8] G E Tsydynzhapov *et al*, *JETP Lette.* **83**, 405 (2006)
[9] Q Huang *et al*, *Nature* **347**, 369 (1990)
[10] N Tralshwala *et al*, *Phys. Rev. B* **51**, 3812 (1995)
[11] P Samuley *et al*, *Phys. Rev. B* **48**, 13904 (1993)
[12] M Shirai, N Suzuki and K Motizuki, *J. Phys.: Condens. Matter* **2**, 3553 (1990)
[13] N Hamada, *Phys. Rev. B* **40**, 4442 (1989)
[14] H Sato *et al*, *Phys. Rev. B* **48**, 6617 (1993)
[15] J F Zasadzinski *et al*, *Physica C* **158**, 519 (1989)
[16] G Zhao, *Phys. Rev. B* **76**, 020501 (2007)
[17] J E Graebner, L F Schneemeyer and J K Thomas, *Phys. Rev. B* **39**, 9682(R) (1989)
[18] H J Kaufmann, O V Dolgov and E K H Salje, *Phys. Rev. B* **58**, 9449 (1998)
[19] A I Liechstenstein *et al*, *Phys. Rev. B* **44**, 5388(R) (1991)
[20] K Kunc and R Zeyher, *Phys. Rev. B* **49**, 12216 (1994)
[21] M Meregalli and S Y Savrasov, *Phys. Rev. B* **57**, 14453 (1998)
[22] K Marsiglio *et al*, *Phys. Rev. B* **53**, 9433 (1996)
[23] B Batlogg *et al*, *Phys. Rev. Lett.* **61**, 1670 (1988)
[24] K F McCarty *et al*, *Phys. Rev. B* **40**, 2662(R) (1989)
[25] C K Loong *et al*, *Phys. Rev. Lett.* **62**, 2628 (1989)
[26] M Braden *et al*, *Europhys. Lett.* **34**, 531 (1996)
[27] H Sato, H Takagi and S Uchida, *Physica C* **169**, 391 (1990)
[28] A Taraphder *et al*, *Phys. Rev. B* **52**, 1368 (1995)
[29] C M Varma, *Phys. Rev. Lett.* **61**, 2713 (1988)
[30] P W Anderson, *Phys. Rev. Lett.* **34**, 953 (1975)
[31] I Hase and T Yanagisawa, *Physica C* **468**, 1129 (2008)
[32] G Vielsack and W Weber, *Phys. Rev. B* **54**, 6614 (1996)
[33] W A Harrison, *Phys. Rev. B* **74**, 245128 (2006)
[34] Z P Yin, A Kutepov and G Kotliar, *Phys. Rev. X* **3**, 021011 (2013)
[35] J Ahmad and H Uwe, *Phys. Rev. B* **72**, 125103 (2005)
[36] M Merz *et al*, *Europhys. Lett.* **72**, 275 (2005)
[37] P Udomsamuthirun, *Pramana – J. Phys.* **66**, 589 (2006)
[38] V L Ginzburg and D A Kirzhnits (eds), *High-temperature superconductivity* (Plenum Publishing Corporation, New York, 1982)
[39] L L Daemen and A W Overhauser, *Phys. Rev. B* **41**, 7182 (1990)
[40] P G deGennes, *Superconductivity of metals and alloys* (Westview Press, USA, 1999)
[41] J B Ketterson and S N Song, *Superconductivity* (Cambridge University Press, Cambridge, 1999)
[42] S P Tewari and P K Gumber, *Physica C* **171**, 147 (1990)
[43] H Shimahara, *J. Phys. Soc. Jpn* **72**, 1851 (2003)
[44] O V Dolgov *et al*, *Phys. Rev. Lett.* **95**, 257003 (2005)
[45] T Örd and N Kristoffel, *Physica C* **370**, 17 (2002)
[46] P Konsin and B Sorkin, *J. Supercond. Nov. Magn.* **18**, 101 (2005)
[47] P Udomsamuthirun *et al*, *Paper presented at 31st Congress on Science and Technology of Thailand* (Suranaree University of Technology, 18–20 Oct., 2005)
[48] O C Abah, G C Asomba and C M I Okoye, *Solid State Commun.* **149**, 1510 (2009)
[49] O A Ogbuu *et al*, *Physica C* **471**, 444 (2011)
[50] R Chaudhury and S S Jha, *Pramana – J. Phys.* **22**, 431 (1984)

[51] V Z Kresin, S A Wolf and H Morawitz, *Mechanism of conventional and high-temperature superconductivity* (Oxford University Press, New York, 1993)
[52] S Kondoh *et al*, *Physica C* **157**, 469 (1989)
[53] D G Hinks *et al*, *Nature* **335**, 419 (1988)
[54] G Zhao and D E Morris, *Phys. Rev. B* **51**, 848 (1995)
[55] E S Hellman *et al*, *Phys. Rev. B* **44**, 9719 (1991)
[56] D Varshney and M P Tosi, *J. Phys. Chem. Solids* **61**, 683 (2000)
[57] H Khosroabadi *et al*, *J. Supercond. Nov. Magn.* **23**, 1385 (2010)
[58] H Khosroabadi *et al*, *Phys. Rev. B* **83**, 224525 (2011)
[59] H J Kang *et al*, *Physica C* **471**, 303 (2011)
[60] A I Golovashkin *et al*, *J. Phys. Ser.* **150**, 042043 (2009)
[61] X-Y Su, J Shen and L-Y Zhang, *Phys. Lett. A* **143**, 489 (1990)
[62] M Tinkham, *Introduction to superconductivity* (Dover Publications, 2004)
[63] O C Abah, G C Asomba and C M I Okoye, *Supercond. Sci. Technol.* **23**, 045031 (2010)
[64] A V Beluschin *et al*, *Physica C* **199**, 103 (1992)
[65] I M Khalatnikov and A Abriksov, *Adv. Phys.* **8**, 45 (1959)
[66] P B Allen and R C Dynes, *Phys. Rev. B* **12**, 905 (1975)