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Theoretical investigation of isotope effect of the iron-based superconductors

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ABSTRACT

A two-band BCS-like model in which the mediating interactions arise from both electron–phonon and antiferromagnetically induced interaction as well as ±s-wave gap symmetry has been used to investigate the isotope effect and transition temperature of iron-based superconductors within the Bogoliubov–Valatin approach. Our results show that electron–phonon interaction plays some role in the superconductors and experimentally determined values of the isotope effect exponent as well as transition temperatures of the compounds can be accounted for using the model.

1. Introduction

The discovery of superconductivity in iron-based materials by Kamihara et al. [1] has elicited another round of extensive studies in the field of superconductivity aimed at unraveling the origin of superconductivity in the new high temperature superconductors. The special interest in the iron based superconductors is probably because a material that contains iron is not supposed to be compatible with superconductivity since their magnetic field would not allow the formation of Cooper pairs. It is known that iron based superconductors comprise a broad variety of materials some of which are classified mainly based on the stoichiometric parent compounds, such as, LaFeAsO (the 1111 compounds) [1], $BaFe_2As_2$ (the 122 compounds) [2], FeTe (the 11 compounds) [3] and LiFeAs (the 111 compounds) [4]. All the iron based superconductors appear to have the same phase diagrams [5] and crystallographic motif with the main component being a square lattice of iron atoms sandwiched between two square lattices of pnictogen or chalcogen atoms [6]. In order to understand the gap symmetry and the pairing mechanism in these materials, several studies have been performed and a significant number suggest that the order parameter symmetry has the ±s symmetry in which the order parameter changes sign between different bands in the multiband electronic structure [7–9]. The superconducting gap ratios range from 2 to 3 [10].

The iron pnictides have resemblance to the high-T_c cuprate superconductors since they are layered systems and exhibit antiferromagnetic (AFM) order in the parent phases. However, unlike the cuprates with nine d-electrons, the iron-pnictide parent compounds have six d-electrons. Iron-based compounds are multiband systems which comprise at least two electron bands near the point X, two hole bands at the Γ point and one hole band close to the X point [11,12]. The multiband gap nature of iron based superconductor has been observed in numerous experiments such as: angle resolved photoemission studies [13,14], tunneling spectroscopy [15,16], specific heat measurements [17–20], and infrared reflectivity measurements [21] among others.

Identifying the pairing mechanism in high-T_c superconductors is very difficult task partly due to the complexity of these materials. For iron based superconductors, most researchers believe an electronic or magnetic pairing glue [22] may be involved as the electron–phonon calculation cannot explain the observed high-T_c [23]. The antiferromagnetic fluctuation-mediated attractive interaction mechanism seems favorable [7,24] and has been supported by experimental studies [25].

The isotope effect on T_c has played an important role in identifying the importance of phonon in superconductivity. In the conventional Bardeen–Cooper–Schrieffer's (BCS) theory, the isotope effect exponent β is equal to 0.5 and this has been observed in conventional superconductors [26]. Presently, the available experimental results on isotope effect on T_c of iron based supercon-

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ductors are not conclusive. Liu et al. studied the isotope effect of ^{54}Fe on SmFeAs (O,F) ($T_c \sim 42$ K) and (Ba,K) Fe_2As_2 ($T_c \sim 38$ K) and observed appreciable isotope exponents β's of 0.34 and 0.37 respectively which falls within the BCS limit [27]. On the other hand, Shirage et al. observed a sizable inverse isotope effect exponent $\beta_{Fe} \sim -0.18$ in (Ba,K) Fe_2As_2 [28] and $\beta_{Fe} \sim -0.024$ in SmFeAsO$_{1-y}$ [29]. They interpreted the inverse isotope exponent to originate from the magnetically induced interaction [30].

However, the standard Migdal–Eliashberg theory suggest that the effect of the electron–phonon interaction is non-negligible [31]. Khasanov et al. show that the Fe isotope substitution causes small structural modifications that affect the β. By taking this effect into account, they found that $\beta \sim 0.35$–0.4 for three different families of the Fe-based superconductors [32,33]. Theoretically, it has been proposed that an unconventional s-wave pairing state with a sign reversal of the order parameter between different Fermi surface sheets characterize the pnictide superconductors [6,8,34]. Choi et al. using two-band Eliashberg theory interpreted the inverse isotope effect exponent to arise when the interband electron–phonon interaction is dominant whereas the positive exponent means that the intraband contribution prevails [35]. Recently, Maksimov et al. using two-band BCS model with intra- and inter-band pairing interactions analyzed the optical conductivity and permittivity spectra of Co-doped $BaFe_2As_2$ [36].

In this paper, we shall use a two-band BCS model within the ±s-wave pairing scheme including phonon and non-phonon interactions to account for the superconducting transition temperature and isotope effect in the iron-based superconductors. We present the model in Section 2; Section 3 is devoted to results and discussion while in Section 4 we present the summary.

2. Formalism

Following the original formulation of Suhl et al. [37] on two-band superconductivity, and more recent studies [38,39] on the high-T_c superconductors, the effective Hamiltonian for the two main bands (electron, e band and hole, h band) in the iron-based superconductors is written as

$$H = \sum_{ik\sigma} \epsilon_{ik\sigma} c^{\dagger}_{ik\sigma} c_{ik\sigma} - \sum_{ikk'\sigma} V_{ikk} c^{\dagger}_{ik'\uparrow} c^{\dagger}_{ik'\downarrow} c_{ik\downarrow} c_{ik\uparrow} - \sum_{kk'} V_{ehkk'} \left[c^{\dagger}_{ek\uparrow} c^{\dagger}_{ek\downarrow} c_{hk'\downarrow} c_{hk'\uparrow} + c^{\dagger}_{hk\uparrow} c^{\dagger}_{hk\downarrow} c_{ek'\downarrow} c_{ek'\uparrow} \right] \quad (1)$$

where ϵ_k is the unperturbed kinetic energies of the two ($i = e,h$) bands relative to the Fermi level; $k(k')$ is the Bloch wavevector, σ is spin index, $\uparrow(\downarrow)$; $V_{ikk'}$ are the intraband potential for bands $i = e$, h; and $V_{ehkk'}$ is the net interband interaction. The creation and annihilation operators ($c^{\dagger}_{ik\sigma} c_{ik\sigma}$) with respect to the band from which they arises from using the subscript $i = e$, h.

Assuming the ±s-wave state, we fix the signs of the s-wave gaps as $\Delta_e = |\Delta_e|$ on the electron band and $\Delta_h = -|\Delta_h|$ on the hole band respectively. After applying the standard Bogoliubov–Valatin transformation [40,41] in Eq. (1), the linearized gap equations can be written as

$$\Delta_{ek} = -\sum_{k'} V_{ekk'} \frac{\Delta_{ek'}}{2\epsilon_{ek}} (1 - 2 f(\epsilon_{ek'})) - \sum_{k'} V_{ehkk'} \frac{\Delta_{hk}}{2\,\epsilon_{hk'}} (1 - 2 f(\epsilon_{hk'})) \quad (2)$$

$$\Delta_{hk} = \sum_{k'} V_{hkk'} \frac{\Delta_{hk'}}{2\,\epsilon_{hk}} (1 - 2 f(\epsilon_{hk'})) + \sum_{k'} V_{hekk'} \frac{\Delta_{ek}}{2\,\epsilon_{ek'}} (1 - 2 f(\epsilon_{ek'})) \quad (3)$$

where $\Delta_{ek}(\Delta_{hk})$ is the energy gap for the electron-like (hole-like) band, $f(\epsilon_{ik})$ are the Fermi–Dirac occupation number for quasiparticle states.

For simplicity, we consider a potential pairing model arising from both the attractive electron–phonon (V^{ph}) and the repulsive antiferromagnetic fluctuation-mediated (V^{s}) interaction. Thus,

$$V_{ikk'} = \begin{cases} -V^{ph}_i, & \omega \leqslant \omega_{ph} \\ V^{s}_i, & \omega_{ph} \leqslant \omega \leqslant \omega_s \\ 0, & \omega > \omega_s \end{cases} \quad (4)$$

where the cut-off frequencies ω_{ph} and ω_s are associated with the phonon and spin-fluctuation characteristic Fermi surface energies respectively.

In analogy to the original BCS approach, Eq. (4) is employed in Eqs. (2) and (3) and the momentum summations is replaced by integration over energy, $\epsilon_{ik'}$. Then, following the standard procedure [39,42–44], we consider the phonon and non-phonon contribution on each band. From Eq. (2) for the electron band, the phonon part is

$$\Delta_{eph} = N_e\, V^{ph}_e\, Z_{ph}\, \Delta_{eph} + N_h\, V^{ph}_{eh}\, Z_{ph}\, \Delta_{hph} + \Delta_{es} \quad (5)$$

where $Z_{ph} = \ln(1.14\omega_{ph}/T_c)$, $V^{ph}_e = \langle\langle V^{ph}(k_e, k'_h)\rangle\rangle$ and Δ_{es} is integration constant. N_e (N_h) is the density of states (DOS) of electron (hole) band respectively. The non-phonon (spin) contributions from the electron band is

$$\Delta_{es} = -N_e\, V^{s}_e\, Z_{ph}\, \Delta_{eph} - N_e\, V^{s}_e\, Z_s\, \Delta_{es} - N_h\, V^{s}_{eh}\, Z_{ph}\, \Delta_{hph} - N_h\, V^{s}_{eh}\, Z_s\, \Delta_{hs}. \quad (6)$$

where $Z_s = \ln(\omega_s/\omega_{ph})$.

Similarly, for Δ_{hph} and Δ_{hs} gaps, for the hole-band (Eq. (3)), we get two equations. Combining the resulting four homogeneous equations, we obtain the 4×4 matrix of the form:

$$\begin{bmatrix} -1 & (1 - \alpha N_h V^{ph}_e Z_{ph}) & 0 & -N_h V^{ph}_{eh} Z_a \\ (1 + \alpha N_h V^{s}_e Z_s) & \alpha N_h V^{s}_e Z_{ph} & N_h V^{s}_{eh} Z_s & N_h V^{s}_{eh} Z_{ph} \\ 0 & \alpha N_h V^{ph}_{he} Z_{ph} & -1 & 1 + N_h V^{ph}_h Z_{ph} \\ -\alpha N_h V^{s}_{he} Z_s & -\alpha N_h V^{s}_{he} Z_{ph} & (1 - N_h V^{s}_h Z_s) & -N_h V^{s}_h Z_{ph} \end{bmatrix} \begin{bmatrix} \Delta_{es} \\ \Delta_{eph} \\ \Delta_{hs} \\ \Delta_{hph} \end{bmatrix} = 0 \quad (7)$$

where we have assume the nonsymmetric density of state as $N_e = \alpha N_h$, that is for symmetric density of state $\alpha = 1$ [38].

Solving the secular equation arising from Eq. (7), we obtain after some simplifications, the transition temperature in the form

$$T_c = 1.14\ \omega_{ph} \exp\left(-\frac{1}{\alpha\ N_h\ V_{ph} + \lambda^{*}_s} \right) \quad (8)$$

where

$$V_{ph} = V^{ph}_e - V^{ph}_{he}$$

and

$$\lambda^{*}_s = \frac{\alpha\ N_h (V^{s}_{he} - V^{s}_e)}{1 - \alpha\ N_h (V^{s}_{he} - V^{s}_e)\ Z_s}. \quad (9)$$

The isotope effect exponent β is given by

$$\beta = -\frac{d\ \ln T_c}{d\ \ln M}. \quad (10)$$

Employing the relation $T_c \propto M^{-\beta}$ and assuming that $\omega_{ph} \propto M^{-1/2}$, we get

$$\beta = \frac{1}{2} \left\{ 1 - \left(\frac{\lambda^{*}_s}{\lambda_{ph} + \lambda^{*}_s} \right)^2 \right\} \quad (11)$$

where $\lambda_{ph} = \alpha N_h V_{ph}$.

Eqs. (8) and (11) are the expression for the superconducting transition temperature and the isotope effect exponent in ±s-wave (π-phase shifted s-wave) two-band, two-square-well potentials