Robustness of s-wave superconductivity against Coulomb interactions in Na_xCoO_2

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Abstract

We study the depairing effect due to Coulomb interactions in Na_xCoO_2. We consider the electron-phonon coupling and the Coulomb interactions, and determine T_c for s-wave superconductivity by solving the linearized Eliashberg equation. When we consider shear phonons as well as breathing phonons, T_c is enhanced by Suhl-Kondo (SK) mechanism. Since SK mechanism is strong against Coulomb interactions, T_c remains finite even if strong Coulomb interactions cancel out the attractive force due to breathing phonons. The orbital degree of freedom is important to understand the mechanism of superconductivity in Na_xCoO_2.

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In Na_xCoO_2, although several LDA calculations suggest that there are hole pockets composed of e'_g orbitals. However, the top of the e'_g bands locate below (but very close to) the Fermi level in ARPES measurements. Theoretically, we have shown that a weak pseudogap behavior observed in susceptibility or density of states (DOS) can be explained only when e'_g hole pockets are absent[1]. The closeness of the top of e'_g bands to the Fermi level suggests that the orbital degree of freedom may play a important role in the superconductivity of Na_xCoO_2. We have shown that relatively high s-wave T_c is realized in Na_xCoO_2 in case we consider E_{1g} phonons (shear phonons) as well as A_{1g} phonons (breathing phonons) since the interband transition of Cooper pairs are induced by shear phonons[2]. This enhancement of T_c due to shear phonons is understood as Suhl-Kondo (SK) mechanism where superconductivity is realized by the interband hopping of the cooper pairs. Even if the e'_g bands are valence bands, this mechanism is valid if the top of the e'_g bands locates near Fermi level. We call this mechanism of

superconductivity the valence-band SK mechanism. Thus, we inferred that Na_xCoO_2 is an s-wave superconductor thanks to the orbital degree of freedom. However, it is not clear whether s-wave superconductivity can be realized in Na_xCoO_2 since the strong Coulomb interactions would reduce T_c.

In this paper, we study the depairing effect due to Coulomb interactions in a multi-orbital system which describes the effective bands of Na_xCoO_2. In this model, we consider the direct Coulomb repulsion U and the pair hopping J. The depairing effect on the effective attractive force between electrons in the same orbital is given by U, and that for the interband transition of Cooper pairs due to shear phonons is caused by J. We calculate the reduction of T_c, and find that the SK effect due to the shear phonon is strong against Coulomb interactions.

The electron-phonon coupling between t_{2g} ($a_{1g} + e'_g$) electrons and relevant optical phonon (breathing and shear phonons) are represented by four coupling constant a_1, a_2, b_1, b_2 which is shown elsewhere[2]. We calculate T_c by solving the linearized Eliashberg
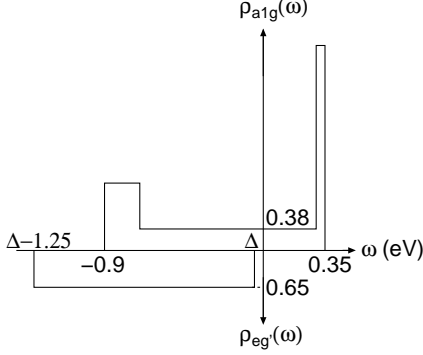
Fig. 1. DOS of Na_xCoO_2. The unit of energy is eV.

Fig. 2. U-dependence of T_c for $J = U/10$.

equation as follows.

$$\lambda\hat{\phi}(i\varepsilon_n) = T\sum_{i\varepsilon_n}\int_{-\infty}^{\infty}d\omega\frac{\hat{z}(\omega)\hat{\rho}(\omega)}{\varepsilon_{n'}^2 + \omega^2}\hat{V}(i\varepsilon_n - i\varepsilon_{n'})\hat{\phi}(i\varepsilon_{n'}),$$
(1)

$$\hat{V}(i\omega_n) = \begin{pmatrix} a_1^2 & 2b_1^2 \\ b_1^2 & a_2^2 + 2b_2^2 \end{pmatrix}D(i\omega_n) - \begin{pmatrix} U & 2J \\ J & U+J \end{pmatrix},$$
(2)

where $\hat{\phi}(i\varepsilon_n) = (\phi_{a1g}(i\varepsilon_n), \phi_{eg'}(i\varepsilon_n))$ is a column vector of gap functions. $D(i\omega_n) = 2\omega_D/(\omega_D^2 + \omega_n^2)$ is the phonon's Green function, where ω_D is the Debye frequency of phonon. We put $\omega_D = 550$ (cm^{-1}) for breathing and shear phonons. $\varepsilon_n = (2n-1)\pi T$ and $\omega_n = 2n\pi T$ are Matsubara frequencies. We show the expression of the renormalization factor $z(\omega)$ for $|\omega| < \omega_D$ elsewhere[3]. We put $z(\omega) = 1$ for $|\omega| > \omega_D$ for simplicity since the energy range where the band structure is renormalized is $|\omega| < \omega_D$. The DOS which we use in this calculation is shown in Fig. 1. This reproduces the bandwidth and the DOS near the Fermi level which is obtained by lattice model[1]. For a_{1g} band, we add the excess DOS in the band edge to reproduce the total number of d-electron and overall shape roughly. Note that the integration of DOS does not reach 1 because the ratio of the number of the d-electron in three t_{2g} bands near Fermi level is about 0.8 in the d-p model. T_c is determined when λ in left-hand side of Eq. 1 is equal to 1.

Fig. 2 shows the U-dependence of T_c for $J = U/10$, $\Delta = -0.02$ (eV) and $a_1 = a_2 = b_1 = 2b_2 = 0.23$ (eV). When we take account of only breathing phonons, T_c reduces rapidly and it vanishes at $U = U_c = 2.8$ (eV). On the other hand, if we consider the shear phonons as well as breathing phonons, $T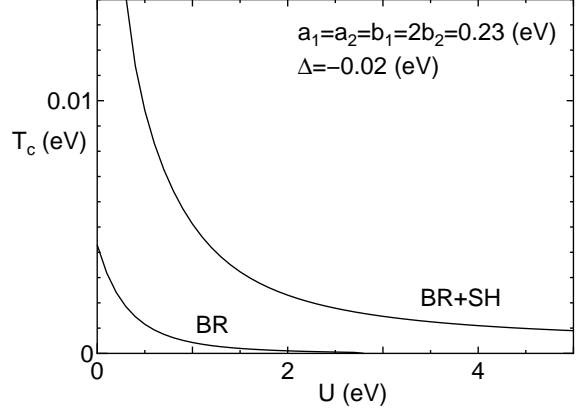_c$ remains finite even if U exceed U_c. This is because there is the effective attractive force due to inter-band hopping induced by shear phonons. This interaction is seldom weakened by Coulomb interactions since $J \ll U$. Thus, the s-wave superconductivity with $T_c \sim 5K$ can be realized by this mechanism even if we consider the strong Coulomb interactions. In this calculation, the renormalization of U and J due to retardation is included automatically because the attractive force due to electron-phonon coupling depend on Matsubara frequency while repulsive force due to Coulomb interactions does not. We derive the renormalized U^* and J^* elsewhere[3]; it is shown that the renormalization for J is larger than that for U. Therefore, interband transition due to shear phonon is not prohibited by the Coulomb interactions.

In conclusion, we studied the depairing effect due to Coulomb interactions in Na_xCoO_2, and found that T_c remains finite even in the presence of the strong Coulomb interactions when we consider both breathing and shear phonons, while T_c vanishes rapidly when we consider breathing phonons only. Even if the direct Coulomb repulsion cancels out the attractive force induced by breathing phonons, the s-wave superconductivity due to SK mechanism would be realized. Thus, the superconductivity due to SK mechanism is realized even if the e_g' bands are valence bands.

References

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