Superconductivity Driven by the Interband Coulomb Interaction and 
Implications for the Superconducting Mechanism of MgB₂

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Superconducting mechanism mediated by interband exchange Coulomb repulsion is examined
in an extended two-band Hubbard models with a wide band crossing the Fermi level and co-
existing with a narrower band located at moderately lower energy. We apply newly developed
path-integral renormalization group method to reliably calculate pairing correlations. The cor-
relation shows marked enhancement at moderate amplitudes of the exchange Coulomb repulsion
taken smaller than the on-site repulsion for the narrower band. The pairing symmetry is s-wave
while it has unconventional phases with the opposite sign between the order parameters on the
two bands, in agreement with the mean-field prediction. Since the band structure of recently
discovered superconductor MgB₂ shares basic similarities with our model, we propose that the
present results provide a relevant clue for the understanding of the superconducting mechanism
in MgB₂ as well as in this class of multi-band materials with good metallic conduction in the
normal state.

KEYWORDS: MgB₂, pairing mechanism,

Mechanisms of superconductivity have been a long-
sort issue since the discovery in 1911 but are still under active studies with aiming at novel mechanisms and
searching for materials with higher transition temperatures. In particular, mechanisms driven by the electron-
electron interaction in general are widely and intensively studied issue since the discovery in 1911 but are still un-
change mechanism works in realizing the ferromagnetic
relativistic effect. With this background, the double ex-
change Coulomb interaction strongly favors the spin singlet formation and heavily renormalized effective mass of the quasiparticles in lattice. On the other hand, if the
hybridization is vanishing or small between the two or-
bital wave function, the exchange Coulomb interaction becomes relatively important, the Hund’s rule works efficiently and the atomic high-spin state generically appears, if the level difference between the two atomic orbitals, \( \Gamma \) is relatively small. With this background, the double exchange mechanism works in realizing the ferromagnetic
ground state in metals. The high-spin state appears especially when the ratio between the onsite Coulomb interaction for the lower-level orbital, \( U \), and \( \Gamma \), namely \( U/\Gamma \) is large. If the interorbital on-site repulsion \( V \) is taken into account, this rough estimate of the ratio is replaced with \( (U - V)/\Gamma \).

However, if \( (U - V)/\Gamma \) becomes relatively small or compara-
tible, the low-spin state may be stabilized and the
Hund’s rule coupling becomes irrelevant. Near this stab-
ilization point, \( (U - V)/\Gamma \leq 1 \), another term of the exchange Coulomb interaction between the lower and higher orbitals may work for the stabilized low-spin ground state. This term of the exchange transfers the up and down spin electrons on the same orbital (band) to the other one in pair. In contrast to the ferromagnetism driven by the Hund’s rule term, we show that this pair transfer part of the exchange interaction strongly favors the singlet superconducting order in an appropriate range of the parameter space.

In 1963, using the BCS approximation, Kondo\[15\] considered the pairing mechanism assisted by the interband exchange Coulomb interaction between s and d bands for the mechanism of the superconductivity of transition metals. Yamaji\[14, 16\] also considered the similar mechanism in a specific condition of two-band Hubbard models. A similar interband mechanism was also examined in strongly correlated models by the authors\[12, 13\].

Here, we reexamine the mechanism driven by the exchange Coulomb interaction and show by a newly developed numerical technique that this mechanism works for simple metal compounds mixed with elements with
a localized orbital (or relatively narrow band) located moderately below the Fermi level. Its implication for the mechanism of the superconducting transition in MgB$_2$ recently discovered by Akimitsu et al. above temperature 39K is an important subject of discussions in this letter. We discuss that this mechanism may drive or substantially enhance the superconducting transition of MgB$_2$.

Our Hamiltonian

$$H = H_1 + H_2 + H_3 + H_4$$

(1)

consists of the conduction band $H_1$ with the wide and narrow bands or localized level part with the on-site Coulomb repulsion terms $H_2$ and $H_3$ and with their interorbital Coulomb interaction $H_4 = H_{4E} + H_{4P} + H_{4V}$:

$$H_1 = - \sum_{(i,j),\lambda,\sigma} t_{ij}(c_{i\sigma}^\dagger c_{j\lambda} + H.c.) - \mu N_1 - (\mu + \Gamma)N_2$$

(2)

$$H_2 = U_1 \sum_i n_{1i\uparrow} n_{1i\downarrow}$$

(3)

$$H_3 = U_2 \sum_j n_{2j\uparrow} n_{2j\downarrow}$$

(4)

$$H_{4E} = -J \sum_{i,\sigma'} c_{1i\sigma}^\dagger c_{1i\sigma'} c_{2i\sigma'} c_{2i\sigma}$$

(5)

$$H_{4P} = J \sum_{i,\sigma'} (1 - \delta_{\sigma\sigma'})(c_{1i\sigma}^\dagger c_{1i\sigma'} c_{2i\sigma'} c_{2i\sigma} + H.c.)$$

(6)

$$H_{4V} = V \sum_j n_{1j} n_{2j}$$

(7)

$$N \equiv N_1 + N_2,$$

(8)

$$N_1 \equiv \sum_{i,\sigma} n_{1i\sigma},$$

(9)

$$N_2 \equiv \sum_{i,\sigma} n_{2i,\sigma},$$

(10)

In Eq.(1-10), the annihilation (creation) operator of the orbital $l(l=1,2)$ at the site $i$ with the spin $\sigma$ are represented by $c_{i\sigma}$($c_{i\sigma}^\dagger$). In this letter, we assume that $U_1$ is small by considering a wide metallic band 1 while $t_{2ij}$ is smaller than $t_{1ij}$.

For the region characterized roughly by $U_2 - V \leq \Gamma - J$, the atomic ground state of the orbital 2 is fully filled singlet. However, when $J$ becomes not too smaller than $\Gamma$, the singlet pair can transfer to the conduction band 1 through the term (6) and it generates a charge fluctuation with a singlet cloud around a site of the local orbital 2. In this letter we show that the overlap of such singlet clouds formed around the neighboring atomic orbitals 2 may drive the delocalization of the singlet pair and lead to coherent ground state with the superconducting symmetry breaking. Such formation of itinerant singlet pairs survives, as we show later, when the orbitals 2 form a band through their mutual transfer. If we take the region with the low-spin ground state, the terms (5) and (7) do not play relevant roles and we neglect these terms in the following discussion for simplicity.

Here we first neglect the dispersion of the lower-level band, $t_2$ in (2) and the Coulomb repulsion $U_1$ within the conduction band in (3) for simplicity and discuss their effects later. When we take the mean field approximation with the uniform superconducting order parameter

$$\Xi_1 = \frac{J}{N} \sum_i (c_{1i\uparrow}^\dagger c_{1i\downarrow} + \text{H.c.})$$

(11)

$$\Xi_2 = \frac{J}{N} \sum_i (c_{2i\uparrow}^\dagger c_{2i\downarrow} + \text{H.c.})$$

(12)

the selfconsistent equation for the order parameters obtained from the decoupling of the term (6) for $t_{2ij} = 0$ is given by

$$2\Xi_1 = \Xi_2 J/\sqrt{\Xi_2^2 + \Gamma^2}$$

(13)

$$2\Xi_2 = -U_2 \Xi_2/\sqrt{\Xi_2^2 + \Gamma^2} + \Xi_1 J \int_{-W_1/2}^{W_1/2} dc \frac{D_1(c)}{\sqrt{c^2 + \Xi_1^2}}$$

(14)

where the density of states of the conduction band 1 is $D_1(c) = 1/\pi$ with the dispersion $\epsilon(k) = \sum_{i,j} t_{1i,j} \exp(ik(r_i - r_j) - \mu + W_1/2$ is the bandwidth of the band 1 in proportion to $1/t_1$. When the density of states is replaced with the rectangular constant one for the conduction band for simplicity, namely, $D_1(c) = 1/W_1$, the selfconsistent solution at temperature $T = 0$ in the weak coupling BCS limit is given by

$$\Xi_1 \sim W_1 \exp[-2W_1 J/\Xi_1 (U_2 + \Gamma/\mu)].$$

(15)

Here $x$ denotes the number of the orbital 2 in a unit cell and if the orbital 2 forms a band through nonzero $t_{2i,j}$, basically $x$ may be replaced with the integrated density of states of this narrower band with the width $W_2$.

An important point of this pairing mechanism is that the prefactor in Eq.(15) is determined from the bare bandwidth of the wide band 1. In addition, the argument of the exponential function may have order unity when we may assume that $J, U, \Gamma$, and $W_1$ would have comparable values. This may necessarily requires the consideration in a strong coupling region. However, here we took a BCS weak-coupling approach as a starting
point and by assuming that $W_1$ is the largest parameter among the energy scales. The strong coupling correction is left for further studies.

Even more important point of this mechanism is that the pairing order parameters on the bands 1 and 2 have the opposite sign, namely $\sum_{i,j} [c_{i\sigma}^\dagger c_{i\sigma}^\dagger c_{j\sigma} c_{j\sigma}] < 0$ because the pairing is mediated by repulsive interband exchange interaction. This anisotropy may enable us to distinguish the present pairing mechanism from that of the conventional phonon-mediated BCS theory.

This weak coupling mean-field picture is complemented by numerical study of the Hamiltonian (1) in the following. We employ recently developed path-integral renormalization group method to perform a controlled calculation in the ground state. Since our basic picture applies to any type of lattice structure, we first employ a numerically feasible square lattice for simplicity and introduce orbital 2 by replacing a fraction of the lattice points (denoted by B in Fig. 1) regularly and assign orbital 1 to the rest of the lattice sites (denoted by A in Fig. 1). We have introduced the B sites periodically in $x$ and $y$ directions with the period $l_B$. The wide band 1 is formed from the nearest neighbor transfers $t_1$ between the sites A while the narrower band is formed from the nearest neighbor transfer $t_2$ between the sites B. The unit cell of this lattice becomes $l_B \times l_0$ and it causes a folding of the Brillouin zone with multi-band structure instead of the band 1. However it does not alter our basic argument especially near the Fermi level. The transfer between A and B sites is switched off. We also introduce an onsite Coulomb repulsion $U_2$ for the sites B (on the band 2) while the onsite Coulomb interaction for the free-electron like band 1, $U_1$ is taken small. The exchange Coulomb interaction $J$ given by Eq. (6) is introduced between nearest neighbor A and B sites. The atomic level difference like band 1, $J$ is mostly negative values as we expect. The overrealistic situation, $J$ of comparable $/t$ is expected in the region $U_1$, $J$ and $\Gamma$ are retained. The overall feature of the enhancement is in qualitative agreement with that expected from the parameter dependence of the mean-field result Eq.(15).

We next discuss the implication of this result for the mechanism of superconductivity discovered in MgB$_2$. The crystal of MgB$_2$ has so called AlB$_2$-type hexagonal structure with an alternate stacking of Mg and B honeycomb layers. The band structure suggests that degenerate bands with two-dimensional anisotropy are formed from B $2p_\sigma$ band and its bonding part crosses the Fermi level near the top of the band. In the band structure calculations, the center of the B $2p_\sigma$ bonding band is 1-2 eV below the Fermi level and two cylindrical hole Fermi surface appears around the axis through $\Gamma$ to A points due to the bandwidth of the order of 4 eV. A rather separate free-electron like band also crosses the Fermi level, which is formed from the hybridization of Mg sp and B $p_z$ bands and has a bandwidth larger than 10 eV. The Mg sp band is expected to have a rather small electron correlation while B $p_\sigma$ band may have a moderate correlation due to dominant $p$ character confined in the two-dimensional honeycomb layer. Because of their symmetries, these two bands do not seem to be appreciably hybridized and are clearly separated near the Fermi level. This band structure is essentially similar to our model with the band 1 (corresponding to Mg$sp$-B$p_z$) and the band 2 (B-$p_\sigma$). Although the amplitude of the electron correlation is not well known in this compound, the choice of the parameters in our calculations in comparison with plausible values of parameters for MgB$_2$ does not seem to be unrealistic and provides a good starting point in the present stage. Our calculated result shows that the pairing enhancement becomes optimized.
for comparable $U$ and $\Gamma$ while it is suppressed, for example, for too large $\Gamma$. This is consistent with the fact that AlB$_2$ does not show superconductivity because the B $p_\sigma$ level is deep in AlB$_2$. On the other hand, if $\Gamma$ becomes too small, the Hund's rule coupling starts working and the ferromagnetic state becomes more stable. In a series of the binary compounds of boronides, we expect that the ferromagnetic and superconducting phase may appear rather close each other with competitions.

In this compound, phonon modes of Boron oscillation may have relatively high frequencies and may take a strong electron-phonon coupling which support the phonon-mediated conventional pairing [10, 11]. Our proposal gives an alternative possibility or may play a complementary role. In comparison with the phonon mechanism, our mechanism contains a specific prediction where the phases of the order parameter on the B $p_\sigma$ band and B $p_z$ bands hybridized with Mg $sp$ should have the opposite sign. This is a crucial test for the role of the interband Coulomb exchange as a driving force of the superconductivity. This may be tested in a carefully designed junction to pick up the opposite phase. Although the pairing symmetry is $s$-wave as supported also experimentally [12], our theory suggests that it is not a simple BCS isotropic pairing.

In summary, we have analyzed a superconducting mechanism mediated by the interband Coulomb exchange repulsion. The numerical simulation results suggest enhancements of pairing for the combination of wide and narrower bands crossing the Fermi level without mutual hybridization but with a moderate amplitude of the exchange Coulomb interaction. We have proposed that this mechanism may be relevant to the occurrence of superconductivity recently discovered in MgB$_2$.

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