Two-Band-Type Superconducting Instability in MgB$_2$

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Using the tight-binding method for the $\pi$-bands in MgB$_2$, the Hubbard on-site Coulomb interaction on two inequivalent boron $p_z$-orbitals is transformed into expressions in terms of $\pi$-band operators. For processes scattering relevant to the problem in which a wave vector $\mathbf{q}$ is parallel to $\hat{z}$, it is found to take a relatively simple form consisting of intra-band Coulomb scattering, interband pair scattering etc. with large constant coupling constants. This allows to get a simple expression for the amplitude of interband pair scattering between two $\pi$-bands, which diverges if the interband polarization function in it becomes large enough. The latter was approximately evaluated and found to be largely enhanced in the band structure in MgB$_2$. These results lead to a divergent interband pair scattering, meaning two-band-type superconducting instability with enhanced $T_c$. Adding a subsidiary BCS attractive interaction in each band into consideration, a semi-quantitative gap equation is given, and $T_c$ and isotope exponent $\alpha$ are derived. The present instability is asserted to be the origin of high $T_c$ in MgB$_2$.

KEYWORDS: MgB$_2$, interband polarization function, superconducting instability, two-band mechanism, interband pair transfer, Coulomb interaction, nesting, isotope effect

The recent finding of 40K superconductivity in MgB$_2$ by the Akimitsu group\cite{1} triggered enthusiastic studies both in experiment and theory to clarify the superconducting properties and mechanism of the new high-$T_c$ superconductor. Given $T_c \approx 40$K amply exceeding the upper bound of $T_c \sim 30$K which was estimated for conventional BCS-type superconductors\cite{2}, it is a very important issue if its superconducting mechanism is conventional or not. Already Bud’ko et al.\cite{3} has reported an isotope effect of $\alpha = 0.26$ with respect of boron, indicating the importance of electron-phonon interaction. Band calculations have suggested that the dimensionless electron-phonon coupling constant $\lambda \sim 0.7$ which would be able to give the $T_c$ value of the order of 40K if the Coulomb pseudo potential term $\mu^*$ is very small. Tunneling results indicate the s-wave nature of superconductivity\cite{4}. All these suggest the BCS-type conventional superconductivity in MgB$_2$.

However, a detailed analysis of the specific heat indicated that the superconducting gap must be anisotropic or two-band-like\cite{1}. Non-conventional features were reported also about the power-law temperature dependence of $H_{c1}\cite{5}$ and the penetration depth\cite{6}. Theoretically, Fukui\cite{7} pointed out that the Fermi surfaces of two $\pi$-bands of MgB$_2$ are close to perfect nesting, which he suggests would give rise to antiferromagnetism; the perfect nesting would be realized if holes did not enter lower $\sigma$-bands, breaking the equality of electron and hole numbers in the $\pi$-bands\cite{8}. In this letter we report that the interband polarization function in the MgB$_2$ band even as it is greatly enlarged for appropriate wave vectors between the two $\pi$-bands and that it can lead to a divergent enhancement of the amplitude of Coulomb-origin interband electron-pair transfer process. The latter means an instability to a two-band-type superconductivity. If this mechanism is the dominant one, the type of superconductivity is s-wave-like in each band with each gap parameter of an sign opposite between the two $\pi$-bands; the gap in the $\sigma$-bands are subsidiary and smaller in a clear contrast to the electron-phonon scenario. This mechanism allows to qualitatively explain the isotope effect when it takes account of the effect of the lattice subsidiary. According to this mechanism $T_c$ can go up further through improvement of the nesting.

Our Hamiltonian is a Hubbard model whose one-particle part is the tight-binding bands giving the two $\pi$-bands on the graphene-structure boron layers. Let us put two boron atoms in the unit cell taken by Wallace\cite{9} at $(\pm a/\sqrt{3}, 0, 0)$, where $a$ is the distance between the equivalent nearest neighbor boron sites in the boron plane. Then the tight-binding bands of the $\pi$-bands are given by

$$\varepsilon_{\pm}(\mathbf{k}) = \pm |h_{21}(\mathbf{k})| + 2t_z \cos(ck_z)$$

$$= \pm t[3 + 2 \cos(ak_y) + 4 \cos(\sqrt{3}ak_x/2) \cos(ak_y/2)]^{1/2} + 2t_z \cos(ck_z),$$

where

$$h_{21}(\mathbf{k}) = t[1 + \exp(-i\mathbf{a}_1 \cdot \mathbf{k}) + \exp(-i\mathbf{a}_2 \cdot \mathbf{k})]$$

with $\mathbf{a}_1 = (\sqrt{3}a/2, a/2, 0)$ and $\mathbf{a}_2 = (0, -a, 0)$; here $t$ and $t_z$ are the absolute value of transfer energy between the nearest neighbor boron $p_z$-orbitals in the plane and along the $z$-direction, respectively; $c$ is the $z$-lattice constant.

The interaction part comes from the on-site Coulomb energy $U_0$ at each boron site. The annihilation operators at two inequivalent sites are Fourier-transformed and here denoted as $a_{\mathbf{k}\sigma}$ and $b_{\mathbf{k}\sigma}$, where $\sigma$ means spin. When the one-electron part is diagonalized into two $\pi$-
bands whose annihilation operators are \( \alpha_{k,\sigma} \) and \( \beta_{k,\sigma} \); the former operators can be linked to the latter through the following unitary transformation:

\[
\begin{align*}
    a_{k,\sigma} &= (1/\sqrt{2}) \exp[-i\phi(k)](\alpha_{k,\sigma} - \beta_{k,\sigma}), \\
b_{k,\sigma} &= (1/\sqrt{2}) \exp[i\phi(k)](\alpha_{k,\sigma} + \beta_{k,\sigma}),
\end{align*}
\]

where \( \phi(k) \) is defined by half of the phase of \( h_{21}(k) \) in Eq. (2). If we restrict \( q \) appearing in the equation below to have only a \( z \)-component, this restricted part \( H' \parallel \) of the interaction Hamiltonian is rewritten in terms of the new operators in a relatively simple form as follows:

\[
H'_{\parallel} = (1/N) \sum_{k_1,k_2,q,\tilde{z},\tilde{g}} \{U[a_{k_1+q}^\dagger \alpha_{k_2} + q_{\parallel} \alpha_{k_2} \alpha_{k_1+q} + (\alpha \leftrightarrow \beta)] \\
+ U'[a_{k_1+q}^\dagger \beta_{k_2+q_{\parallel}} \beta_{k_{1+q}} + (\alpha \leftrightarrow \beta)] \\
+ K[\alpha_{k_1+q}^\dagger \beta_{k_2-q} \alpha_{k_2-q}^\dagger \beta_{k_{1-q}} + (\alpha \leftrightarrow \beta)] \\
+ L[\alpha_{k_1+q}^\dagger \beta_{k_2-q} \alpha_{k_2-q}^\dagger \beta_{k_{1-q}} + (\alpha \leftrightarrow \beta)]\},
\]

where \( U = U' = K = L = U_0/2 \),

The interaction part with \( q \) having non-\( z \)-component is very complicated.

The interband pair-transfer term with \( K \) in Eq. (4) is known to promote superconductivity \[ ] if \( K \) is larger than \( U \), the simple mean-field equation calculates a finite \( T_c \). The amplitude of interband pair-transfer process is known to be enhanced due to the higher order processes illustrated by the ladder-type diagram in Fig. 1. When \( q \) in the diagram is chosen parallel to \( \hat{z} \), the interaction denoted by a dotted line is given by simple coupling constants \( K \) or \( U' \) and summation of the terms represented by this diagram gives the following expression:\[ ]

\[
\Gamma_{12} = K/[1 - (K + U')\Pi_{12}(q)]
\]

when the frequency transfer is set to zero for simplicity. In this diagram with \( q \parallel \hat{z} \) the phase factor disappears.

Next, we first evaluate \( \Pi_{12}(q) \) in the case of the perfect nesting and then discuss on it in the off-set case. The \( xy \)-coordinates of the corner points, \( K \) (and also \( H \)), of the hexagonal Brillouin zone are \((\pm 2\pi/\sqrt{3a}, \pm 2\pi/3a) \) and \((0, \pm 4\pi/3a) \). At these points the intra-plane part of the band \( \pm |h_{21}(k)| \) in Eq. (1) vanishes. So for an appropriate value of Fermi energy \( \varepsilon_F \) in the range between \(-2t_z \) and \( 2t_z \), the Fermi surfaces for the \( \pm \) bands, \( \varepsilon_F \) and electron and hole bands, respectively, cross the corner \( K \)-H-K line at points \( P_{\pm} \) specified by \( k_z = \pm \cos^{-1}(\varepsilon_F/2t_z) \equiv \pm k_{z_0} \), respectively. Then, the Fermi surfaces for the electron and hole bands in the neighborhood of \( P_+ \) are given by the \( \pm \) branch of the following equation:

\[
\pm |h_{21}(k)| = 2t_z \cos(ck_{z_0}) - 2t_z \cos(ck_z) \equiv 2ct_z \sin(ck_{z_0})(k_z - k_{z_0}).
\]

As seen in Fig. (2), at least in the neighborhood of point \( P_+ \), where the second equality in Eqs. (7) is justified, the electron and hole Fermi surfaces form the mirror images with respect of the \( xy \)-parallel plane crossing the corner line at \( P_+ \), as seen in Fig. 2 which is shown for another purpose. There is another set of approximate mirror images around the \( P_- \) point. Therefore, if the electron Fermi surface just below \( P_- \) is translated by \( 2k_{z_0} \) in the \( k_z \)-direction, it nests with the hole Fermi surface just below \( P_+ \). Similarly, the electron Fermi surface part just above \( P_+ \) nests with the hole Fermi surface part just below \( P_- \). The former is translated by \(-2k_{z_0} \). In the neighborhood of the corner line \( K-H-K \) labeled by \((2\pi/\sqrt{3a}, 2\pi/3a) \) in the \( k_x,k_y \)-coordinates, expanding \( h_{21}(k) \) in powers of \( px = k_x - 2\pi/\sqrt{3a} \) and \( py = k_y - 2\pi/3a \), Eq. (7) is approximated as

\[
\pm (\sqrt{3}/2a)t p_{||} \equiv 2ct_z \sin(ck_{z_0})(k_z - k_{z_0}),
\]

where \( p_{||} \equiv \sqrt{p_x^2 + p_y^2} \). This shows the Fermi surfaces around \( P_+ \) are approximated by cones as seen in Fig. 2.

The interband pair-transfer term with \( K \) in Eq. (4) is known to promote superconductivity \[ ]. If \( K \) is larger than \( U \), the simple mean-field calculation gives a finite \( T_c \). The amplitude of interband pair-transfer process is known to be enhanced due to the higher order processes illustrated by the ladder-type diagram in Fig. 1. When \( q \) in the diagram is chosen parallel to \( \hat{z} \), the interaction denoted by a dotted line is given by simple coupling constants \( K \) or \( U' \) and summation of the terms represented by this diagram gives the following expression:\[ ]

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when the frequency transfer is set to zero for simplicity. In this diagram with \( q \parallel \hat{z} \) the phase factor disappears.
and perfectly nest with each other by translation of \( \pi/c \) exactly in the framework of the tight-binding bands in accord with Ref.\[1\]. The interband polarization function between the two \( p \)-bands for zero frequency is defined by

\[
\Pi_{12}(Q) = \frac{1}{N} \sum_{k} \frac{f(\epsilon-(k+Q)) - f(\epsilon+(k))}{\epsilon+(k) - \epsilon-(k+Q)},
\]

where \( N \) is the number of unit cells and \( f(\epsilon) \) is the Fermi-Dirac distribution function. In order to capture gross features, we approximately evaluate this summation in the case of perfect nesting, approximating the right-hand side of Eq. \( (1) \) by terms linear in \( p_{\parallel} \) and in \( k_{z} - k_{z0} \) as \( \epsilon_{\pm}(k) = \pm(\sqrt{3}/2) a t p_{\parallel} + v_{\perp}(k_{z} - k_{z0}) \) with \( v_{\perp} = 2\epsilon_{z}\sin(c k_{z0}) \) and \( k_{z0} = \pi/2c \). Then, the Fermi surfaces are given as in Fig. 2. The hole Fermi surface takes the form of two cones stuck at the bottoms with total height of \( \pi/c \). It centers at \( k_{z} = 0 \). The electron Fermi surface takes the identical form and centers at \( k_{z} = \pi/c \) in the extended zone scheme. Since at each corner integration range is restricted to 120 degrees, we have two 360 degree integrals, counting six corners. The upper bound of \( p_{\parallel} \) is set to \( k_{z0} = 2(\pi/\sqrt{3})^{1/2}/a \) so that the total integration area is equal to the area of the reduced Brillouin zone. For the wave vector \( Q_{0} \equiv (0,0,\pi/c) \) of perfect nesting, we get

\[
\Pi_{12}(Q_{0}) \approx \frac{V_{cell}}{4\pi} \left\{ \frac{3}{4} v_{\perp} \left( \frac{\pi}{2c} \right)^{2} - \frac{1}{2} \ln(1 - \frac{v_{\perp}^{2}}{v_{\parallel}^{2} k_{z0}^{2}}) \right. \\
+ \left. \frac{1}{2} \ln \left( \frac{2v_{\perp}}{v_{\parallel}^{2} k_{z0}^{2}} \right) \right\}^{2} T^{2},
\]

where \( V_{cell} = \sqrt{3a^{2}c/2} \) is the volume of the unit cell, \( v_{\parallel} = \sqrt{3a\delta/2} \), \( \gamma = 1.78107 \) and \( T \) is the temperature. Putting \( a = 3.0844 \) A and \( c = 3.5224 \) A and using \( t \sim 2.5 \) eV and \( t_{z} \sim 1.5 \) eV; \( \Pi_{12}(Q_{0}) \) is estimated as

\[
\Pi_{12}(Q_{0}) \approx 0.053 + 0.139 \ln(30152/T)(\text{eV})^{-1},
\]

where \( T \) is in units of K. Putting \( T = 40 \) K, we get \( \Pi_{12}(Q_{0}) \approx 0.97 \) (eV)\(^{-1} \). This value is much larger than the intra-band polarization function \( \Pi_{1}(0) = V_{cell} v_{\perp}^{2}/4c^{2} \approx 0.139 \) (eV)\(^{-1} \) of band \( i = 1 \) or \( 2 \) for wave vector equal to zero. For wave vector \( Q \) slightly deviating from \( Q_{0} \), \( \Pi_{12}(Q) \) decreases in the way that \( T^{2} \) of \( \ln \) in Eq. \( (10) \) is replaced by \( T^{2} + c_{\perp}^{2}(Q_{z}^{2} + Q_{\perp}^{2}) + c_{\parallel}^{2}(Q_{z} - Q_{z0})^{2} \), where \( c_{\perp} \) and \( c_{\parallel} \) are constants.

In the case of \( k_{z0} \neq \pi/2c \) where the sizes of the cones become different, only a single cone of two electron Fermi cone nests with one of two hole cones for \( \pm Q_{1} \equiv (0,0,\pm 2c) \) which is the nesting vector in this case; the other combination of cones are not nesting at the same time. This situation decreases \( \Pi_{12}(Q_{1}) \) in Eq. \( (10) \) mainly in the way that the term containing \( \ln \) is divided into two terms each with half of the present coefficient; one half is not largely changed, keeping the lnT singularity, and the other diminishes substantially since \( T^{2} \) in the argument of \( \ln \) is replaced by \( T^{2} + c_{\perp}(2\pi/c - Q_{z} - Q_{z1})^{2} \).

The magnitude of \( \Pi_{12}(Q) \) evaluated above and its remarkable growth around \( Q_{z} \approx 2k_{z0} \) are in a fair agreement with Hase’s estimation of \( \Pi_{12}(Q) \) based on FLAPW band calculations.\[19\] However, the prominent peaking with decreasing temperature is moderated to a finite peak height of 0.265(eV)\(^{-1} \). This discrepancy from the above obtained divergent behavior is due to the employed approximation linearizing \( \epsilon_{\pm}(k) \) in \( p_{\parallel} \) and \( k_{z} - k_{z0} \). When \( k_{z0} = \pi/2c \), the second order in \( k_{z} - k_{z0} \) vanishes in \( \epsilon_{\pm}(k) \) and so the linear approximation is not so bad and Eq. \( (10) \) is valid. However, when \( k_{z0} \neq \pi/2c \), the \( (k_{z} - k_{z0})^{2} \) term in \( \epsilon_{\pm}(k) \) suppresses the lnT divergence, leaving a non-divergent peak around \( Q_{z} \approx 2k_{z0} \). In Hase’s result there is another peak at \( Q_{z} = \pi/c \) presumably due to closeness to perfect nesting. Its height is 0.27(eV)\(^{-1} \), slightly higher than the off-set peak. In order to decide which is the highest it is necessary to carry out numerical work taking account of the dependences on parameters such as temperature, band filling and band parameters. Anyway, \( \Pi_{12}(Q) \) is remarkably enhanced around \( Q_{1} \) due to partial nesting and around \( Q_{0} \) due to the closeness to perfect nesting.

As seen above, \( \Pi_{12}(Q) \) is very much enhanced around \( Q_{1} \) and \( Q_{0} \), Eq. \( (10) \) is probable to diverge or to be greatly enhanced with decreasing temperature, if \( U_{0} \) takes a realistic value of \( (2 \sim 4) \) eV since \( K + U' = U_{0} \), from Eq. \( (10) \). This means a great enhancement of the amplitude of the interband pair transfer process. This leads to a superconducting instability due to the two-band mechanism. The above divergence is the first to appear, among other possible divergences, with increasing \( U_{0} \) or with decreasing temperature.

\( T_{c} \) is determined as the temperature where the pair electron scattering diverges in both bands with taking account of other interaction processes, as in Ref.\[18\]. Semi-quantitatively, however, taking account of the effective interband pair scattering coupling constant averaging \( \Gamma_{12} \) in Eq. \( (1) \), by representing it by an effective coupling constant \( K \), and also of the intraband Coulomb coupling constant \( U' \), we obtain the mean-field-like superconducting gap equation with two gap parameters \( \Delta_{1} \) and \( \Delta_{2} \) for the two bands as in Ref.\[19\] as follows:

\[
\Delta_{i} = \frac{1}{N} \sum_{k} \left| W_{i}(\omega_{D} - |\epsilon_{i,k}|) - U_{i} \right| \frac{\Delta_{i}}{2E_{i,k}} \tanh \frac{E_{i,k}}{2k_{B}T} - \frac{1}{N} \sum_{k} \frac{K_{i} \Delta_{i}}{2E_{i,k}} \tanh \frac{E_{i,k}}{2k_{B}T}, \quad (i = 1 \text{ or } 2)
\]

where \( i = 3 - i \) and \( E_{i,k} = \sqrt{\xi_{i,k}^{2} + \Delta_{i}^{2}} \); here we added an intraband phonon-mediated attractive coupling constant \( W_{i} \) in band \( i \) as a subsidiary ingredient to consider about the isotope effect; \( \xi_{i,k} \) is the energy of band \( i \) with reference to the chemical potential, and \( \omega_{D} \) is the Debye energy. In a simple case where the geometrical means of the band half widths of two bands are equal, say \( D \), and the coupling characteristics are identical, the gap equation is easily solved to give

\[
T_{c} = 1.13 \omega_{D} \exp[-1/(\lambda - \mu^{*})],
\]

\[
\lambda = N_{1}(0)W_{1},
\]

\[
\mu^{*} = \frac{N_{1}(0)(U - K)}{1 + N_{1}(0)(U - K) \ln(\frac{D}{\omega_{D}})}.
\]
where $N_1(0)$ is the state density per spin of band 1. In the present case $K$ is enlarged due to the band nesting and the ladder process in Fig. 1, $\mu^*$ becomes small and can be even negative and so $T_c$ can be very much elevated. It should be noted that the effect of $W_i$ is subsidiary; even if $W_i = \lambda = 0$, $T_c = 1.13 \omega_D \exp(-1/N_1(0)(K/U))$ is finite if $K > U$. One feature of this model is that $\Delta_1$ and $\Delta_2$ take the opposite signs although the gap is $s$-wave-like, being constant, in each band.

The isotope exponent $\alpha$ is given by $\alpha = \{1 - [\mu^*/(\lambda - \mu^*)]^2\}/2$. Applying this and Eq. (13) MgB$_2$ with $\alpha = 0.26$ and $\omega_D = 700K$ we get $\mu^* = -0.23$ and $\lambda = 0.103$. The latter value looks much smaller than the experimentally obtained value of $\lambda \sim 0.6$. However, the experimental $\lambda$ value extracted from the specific heat is an upper bound since the mass enhancement due to electron correlation is not taken into account. Further, it should be noted that our $\lambda$ is for a single $\pi$-band while the experimental $\lambda$ is the sum for all bands. So the above-mentioned value of $\lambda$ is not absurd. There is another point to note on the isotope effect, i.e., the increase of $T_c$ by 1K in MgB$_2$ may have been brought about partly through band changes and increase of $\Pi_{12}(Q)$ due to expansion of lattice constant $a$ and slight decrease of $c$.

In the above consideration only the intraband phonon-mediated BCS attraction is taken into account with the interband BCS term neglected. The latter is in conflict with the $K$ term. This neglect is justified since the electron scattering process from one $\pi$-band to the other by the in-plane stretching mode phonons was found to vanish due to symmetry of Bloch wave functions in the close neighborhood of the Brillouin zone boundary where important carriers exist.

Any other combination in MgB$_2$, e.g., between a $\pi$- and a $\sigma$-band, or between two $\sigma$-bands, there is no good nesting enhancing $\Pi_{12}$. Further the interband pair transfer coupling $K$ in these combinations is found to be one order of magnitude smaller than $U_0$. The largest contribution to $K$ among the $\sigma$-bands was found to vanish due to symmetry in another tight-binding approximation. So in the present framework, the role of the $\sigma$-bands are subsidiary with smaller gap parameters. However, there can be an opposite situation, unfortunately to us, where the $\sigma$-bands are primary due to phonon-mediated attraction and the present mechanism of the $\pi$-bands are not important because the above derived superconducting instability happens to be too weak but it does not look natural in view of the jump-wise increase of $T_c$ of MgB$_2$ among diborides and the large value of $\Pi_{12}(Q)$. Recently Imada also presented a two-band consideration on MgB$_2$. He takes no account of nesting and the two bands in consideration are different from ours.

In summary, coupling constant $K$ for the interband pair transfer process, coupling constant $U'$ for interband Coulomb repulsion etc. in two $\pi$-bands of MgB$_2$ were found to be given by half of the on-site Coulomb energy on the boron $p_z$-orbital, specifically in scattering processes relevant to the two-band mechanism. In terms of them the diagrammatic amplitude for the interband pair scattering expressed by ladder diagrams is given by $K/[1 - (K + U')\Pi_{12}(Q)]$, where $\Pi_{12}(Q)$ is the inter-band polarization function between two $\pi$-bands when wave vector $Q$ is parallel to $\hat{z}$. Using the tight-binding bands for $\pi$-bands, $\Pi_{12}(Q)$ was estimated and found to be quite large for $Q$ equal to $Q_1$ and $Q_2$ which are parallel to $\hat{z}$ and allow approximate nesting. Therefore, $K/[1 - (K + U')\Pi_{12}(Q)]$ is very probable to be divergently enlarged in MgB$_2$. This necessarily brings about the two-band-type superconductivity whose $T_c$ can be very high.

A semi-quantitative gap equation was given which takes also account of the BCS interaction in each band as a subsidiary ingredient and $T_c$ and the isotope exponent were derived. Some characteristic features of the gap parameters for various bands were briefly noted. This mechanism was claimed to be a very probable candidate for the superconducting mechanism of MgB$_2$. The isotope exponent $\alpha = 0.26$ and the electron-phonon value $\lambda \sim 0.6$, taken by many researchers as supporting the electron-phonon scenario, were pointed out not to be decisive. The present mechanism gives a guiding principle to further enhance $T_c$ that the nesting between two $\pi$-bands should be improved.

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