Field Dependence of Electronic Specific Heat in Two-Band Superconductors

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The vortex structure is studied in light of MgB$_2$ theoretically based on a two-band superconducting model by means of Bogoliubov-de Gennes framework. The field dependence of the electronic specific heat coefficient $\gamma(H)$ is focused. The exponent $\alpha$ in $\gamma(H) \propto H^\alpha$ is shown to become smaller by adjusting the gap ratio of the two gaps on the major and minor bands. The observed extremely small value $\alpha \sim 0.23$ could be reasonable in this two-band model with the gap ratio $\sim 0.3$.

KEYWORDS: MgB$_2$, two-band superconducting model, two gaps, vortex structure, electronic specific heat coefficient $\gamma(H)$, Bogoliubov-de Gennes equations

Much attention has been focused on the recently discovered MgB$_2$ because of its relatively high superconducting transition temperature $T_c \sim 39$K and simple crystalline structure.$^1$ General consensus obtained so far is that the electron-phonon interaction is mainly responsible for the pairing mechanism in this system because the large isotope effect is observed.$^2,3$ There is, however, little consensus as to the microscopic description for the record high $T_c$ due to the electron-phonon interaction.

Apart from the much debated pairing mechanism, it is rather urgent to determine the precise pairing function or gap function realized in MgB$_2$. There are several important, but conflicting experimental data concerning the superconducting energy gap $\Delta$, ranging from the strong electron-phonon coupling $2\Delta/k_B T_c \sim 5$ to extremely weak coupling value $2\Delta/k_B T_c \sim 2$. These come from the earlier experiments, such as position-dependent tunneling or Raman experiments.$^4$ More recent experiments show unequivocally that these two gap values come from a single sample and converge to definite values: the larger $\Delta_L$ and the smaller $\Delta_S$ whose ratio $\Delta_S/\Delta_L$ falls around 0.3$\sim$0.4. These experiments include photoemission ($\Delta_L=5.6$meV, $\Delta_S=1.7$meV, $\Delta_S/\Delta_L=0.30$)$^5$ the $T$-dependent specific heat analysis ($\Delta_S/\Delta_L=0.27$$^6,7$) and tunneling experiment ($\Delta_S/\Delta_L=0.42$)$^8$. Through these analyses, they are able to obtain systematic and smooth $T$ evolutions of each gap value. This implies that the two gap structure is an intrinsic property in MgB$_2$.

According to the band structure calculations,$^9,10$ there are two distinctive Fermi surface sheets; one is a two-dimensional cylindrical Fermi surface arising from $\sigma$-orbitals due to $p_z$ electrons of B atoms and the other is a Fermi surface coming from $\pi$-orbitals due to $p_z$ electrons of B atoms. They are weakly hybridized with electron orbitals of Mg atoms. Since the $\sigma$-orbital is strongly coupled to the in-plane B-atom vibration with $E_{2g}$ symmetry simply because the hopping integral between the $\sigma$-orbitals is modulated by this bond stretching motion. On the other hand, it is shown by the band calculation$^{10}$ that the $\pi$-orbital is weakly coupled with this phonon mode. Thus it is quite conceivable that these two Fermi surfaces with different electron characters have different energy-gap values if this particular in-plane vibrational mode is responsible for the attractive interaction which induces superconductivity in MgB$_2$.

Here we are going to analyze the field dependence of the $T$-linear electronic specific-heat coefficient $\gamma(H)$ in the superconducting mixed state by investigating the vortex lattice structure in two-band superconductors. It is known that $\gamma(H)$ is a sensitive and useful quantity to reflect the gap structure through the zero-energy excitation spectrum inside and outside the vortex core.$^{11-14}$ In particular, the exponent $\alpha$ in $\gamma(H) \propto H^\alpha$ at low fields reflects the nodal structure of the superconducting gap at the Fermi surface, playing a vital role to identify the gap function.$^{15}$ Several recent specific heat experiments on MgB$_2$ show a very small exponent$^{6,16,17}$ $\alpha \sim 0.23$, implying that on increasing $H$ the zero-energy density of states (DOS) in the mixed state quickly recovers its normal state value, compared with those in $d$-wave superconductors$^{11-14}$ with $\alpha \sim 0.5$ or clean limit $s$-wave case$^{12,13}$ with $\alpha \sim 0.7$. Since there are no definitive reports which claim a line or point node in the superconducting gap in MgB$_2$, this small exponent remains mystery and requires a proper explanation by microscopic calculations. This is one of our purposes in this paper based on the microscopic theory of Bogoliubov-de Gennes (BdG) framework.$^{14,18,19}$

We start with a model pairing Hamiltonian for a two-band superconductor described by tight binding form:

$$
\hat{H} = \hat{H}_0 + \hat{H}_{pair},
$$

(1)

$$
\hat{H}_0 = \sum_{i,j,\sigma,\gamma} (\hat{t}_{ij\sigma} - \mu_{ij}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\gamma},
$$

(2)

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\[ \hat{H}_{\text{pair}} = \frac{1}{2} \sum_{i,\sigma,\gamma,\gamma'} \gamma_{\gamma'} (a_{i\sigma\gamma} a_{i-\sigma\gamma'})^\dagger a_{i\sigma\gamma} a_{i-\sigma\gamma'} \]  

with the nearest neighbor (NN) hopping integral

\[ \tilde{t}_{ij\gamma} = t_{ij} \exp[i \frac{\pi}{\phi_0} \int_{\gamma} A(r) \cdot dr], \]

where \( A(r) \) is the vector potential and \( \phi_0 = \hbar c/2e \) is the unit flux. The two-dimensional square lattice whose lattice constant is unity is assumed. The index \( \gamma \) denotes the two bands \( \gamma = L \) and \( S \). Assuming the singlet pairing, we can derive the BdG equations for \( \gamma = L \) and \( S \) in a standard way:

\[ \sum_i \begin{pmatrix} K_{ji\gamma} & \delta_{ij} \Delta_{i\gamma} \\ \delta_{ij} \Delta_{i\gamma} & -K_{ji\gamma}^* \end{pmatrix} \begin{pmatrix} u_{\gamma\epsilon}(r_i) \\ v_{\gamma\epsilon}(r_i) \end{pmatrix} = E_{\gamma\epsilon} \begin{pmatrix} w_{\gamma\epsilon}(r_i) \\ \gamma_{\gamma'}(r_i) \end{pmatrix} \]

(5)

where

\[ K_{ji\gamma} = -\tilde{t}_{ij\gamma} - \mu \delta_{ij}. \]

(6)

The gap equation is given by

\[ \Delta_{i\gamma} = \sum_{\gamma'} g_{\gamma\gamma'} d_{\gamma'}(r_i) \]

(7)

with the order parameter

\[ d_{\gamma}(r_i) = \langle a_{i\gamma\epsilon} a_{i-\epsilon\gamma}^\dagger \rangle = -\sum_\epsilon \delta_{\gamma\epsilon}(r_i) u_{\gamma\epsilon}(r_i) \tanh \frac{E_{\gamma\epsilon}}{2T}. \]

(8)

The local density of states (LDOS) at site \( i \) for the \( \gamma \) band is calculated by

\[ N_{\gamma}(r_i, E) = \sum_\epsilon \{ |u_{\gamma\epsilon}(r_i)|^2 \delta(E - E_{\gamma\epsilon}) + |v_{\gamma\epsilon}(r_i)|^2 \delta(E + E_{\gamma\epsilon}) \}. \]

(9)

We assume an isotropic \( s \)-wave pairing for both bands \( \gamma = L \) and \( S \) characterized by the order parameters (the energy gaps) \( d_L(\Delta_L) \) and \( d_S(\Delta_S) \). The attractive interactions are chosen as \( g_{LL} \neq 0 \), \( g_{LS} = g_{SL} \neq 0 \) and \( g_{SS} = 0 \), namely in eq. (5) the gap \( \Delta_S \) on the \( S \)-band is induced by the Cooper pair tunneling via \( g_{LS} \). As for the normal state band parameters we take \( t_L = t_S = t(= 1) \) and \( \mu_L = -1 \) and \( \mu_S = +1 \), thus the Fermi surface for \( \gamma = L(S) \) is close (open) around the \( \Gamma \)-point. The DOS for both bands is same at the Fermi level. As two vortices are accommodated in a unit cell of \( N_x \times N_y \) atomic sites, the applied magnetic field is given by \( H_{N_x \times N_y} = 2\phi_0/N_x^2 \). By introducing the quasi-momentum of the magnetic Bloch state we obtain the wave function under the periodic boundary condition for a large number of unit cells (See detailed numerical calculations in ref. 19).

First, we study the case \( g_{LL} = 2.0 \) and \( g_{LS} = 0.2 \), which gives \( \Delta_L = 0.322 \) and \( \Delta_S = 0.086 \) at zero field. It is designed to adjust the gap ratio for MgB2 \( \Delta_S/\Delta_L = 0.27 \). If we consider a single band superconductor with the small gap \( \Delta = 0.086 \), the superconductivity vanishes at the following magnetic field discussed below, since

\[ H > H_{c2}. \]

But, in this two band superconductor, the small gap superconductivity survives in the \( S \)-band because of the cooper pair transfer \( g_{LS} \).

The spatial profiles of the order parameters \( d_L(r) \) and \( d_S(r) \) are shown in Fig. 1 where the unit cell of the square vortex lattice is displayed. Vortices are accommodated at the center and four corners. It is seen that the vortex core radius for the \( L \)-band (\( S \)-band) is small (large) and the depression of \( |d(r)| \) is apparent along the

Fig. 1. Spatial profiles of the order parameter \( |d_L(r)| \) for the \( L \)-band and \( |d_S(r)| \) for the \( S \)-band at lower field \( H_{30 \times 30}(a) \) and at higher field \( H_{18 \times 18}(b) \). They are normalized by the zero field values \( |d_L|_{H=0} (= 0.145) \) and \( |d_S|_{H=0} (= 0.055) \), respectively.

Fig. 2. Zero energy local density of states \( N_L(r, E \sim 0)/N(E_F) \) and \( N_S(r, E \sim 0)/N(E_F) \) at lower field \( H_{30 \times 30}(a) \) and at higher field \( H_{18 \times 18}(b) \). They are normalized by \( N(E_F) \), the normal state DOS at the Fermi level.
with
\[ \gamma_{L,S}(H) = \langle N_{L,S}(r,E \sim 0) \rangle_{r:\text{unit cell}}. \] (11)

We have done extensive computations for various \( H_{N_x \times N_y} \) cases. In Fig. 3, it is seen that \( \gamma(H) \) described by a power law: \( \gamma(H) \propto H^{\alpha} \) with small \( \alpha \). If only the low field points are fitted, we obtain \( \alpha = 0.38(\text{thick line}) \). The fitting by \( \gamma(H) \sim \gamma_N(H/H_c2)^\alpha \) under the condition that \( \gamma(H) \) is reduced to the normal state value \( \gamma_N \) gives \( \alpha = 0.33(\text{thin line}) \). The small exponents \( \alpha \), or the sharp rise of \( \gamma(H) \) in small fields, can be attributed to the \( S \)-band contribution \( \gamma_S(H) \propto H^{0.20} \), while \( \gamma_L(H) \propto H^{1.00} \) in the \( L \)-band. That is, the small \( \alpha \) is due to the overlap of the low energy states outside of vortex cores at the \( S \)-band. Physically it is because the energy gap for the \( S \)-band is suppressed by a weak field, while the total superconductivity is maintained by the larger energy gap up to \( H_{c2} \). This intuitively appealing picture is actually confirmed by the present microscopic calculation. This is, however, different from the two independent gaps with different transition temperatures and different \( H_{c2} \). In such a case, we would have double transitions and \( \gamma(H) \) would be a simple addition of two independent curves, which has a kink structure at the lower \( H_{c2} \). This is not the case for MgB2.

To study the dependence of \( \alpha \) on the gap ratio \( \Delta_S/\Delta_L \), we perform the calculation for various pairing parameter sets. In Fig. 4, we show the \( \Delta_S/\Delta_L \)-dependence of \( \gamma(H) \) behavior. There, we show the results using the two kinds of fitting; the fitting for low field data in Fig. 4(a), and overall fitting by \( \gamma(H) \sim \gamma_N(H/H_c2)^\alpha \) in Fig. 4(b), while the numerical data are the same in both figures. In the insets, we show the \( \Delta_S/\Delta_L \)-dependence of \( \alpha \) for each fitting case. 

NN direction, in particular, for the \( S \)-band. By increasing \( H \), \( |d(r)| \) is further suppressed as is seen in Fig. 1 where the core radius is widened. The suppression by \( H \) is eminent in the \( S \)-band.

The corresponding spatial profiles of the LDOS are shown in Fig. 2, where \( N_L(r,E \sim 0) \) and \( N_S(r,E \sim 0) \) have a peak at the vortex center and the ridges connecting the vortex cores are clearly seen. While the high density of states is concentrated at the vortex core in \( N_L(r,E \sim 0) \), it rather spreads out in \( N_S(r,E \sim 0) \). This is because the vortex bound states are highly confined in the \( L \)-band vortex corresponding to the narrow core radius while in the \( S \)-band vortex the core states are loosely bounded. The spatial profiles for \( N_L(r,E \sim 0) \) and \( N_S(r,E \sim 0) \) are resemble to those of the low field case and the high-field case in the single band superconductor (see Fig. 1 and Fig. 2 in ref. 13). In \( N_S(r,E \sim 0) \), the low energy states extending from vortex cores overlap with each other, and the LDOS is suppressed along the line connecting the NN or next NN vortices. With increasing \( H \), the effect of the overlap becomes eminent, and the LDOS is reduced to the flat profile \( N_S(r,E \sim 0)/N(E_F) \sim 0.5 \) in the \( S \)-band \( (N(E_F) \) is the total DOS in the normal state at the Fermi level). The spatial average of \( N_L(r,E \sim 0) \) and \( N_S(r,E \sim 0) \) gives rise to the total DOS under a given field, leading to \( \gamma(H) \) which is defined by

\[ \gamma(H) = \gamma_L(H) + \gamma_S(H) \] (10)

\[ \gamma_{L,S}(H) = \langle N_{L,S}(r,E \sim 0) \rangle_{r:\text{unit cell}}. \] (11)
is reduced to the exponent in the single band case. In Fig. 4(b), it gives \( \alpha \sim 0.7 \) in accord with the previous quasi-classical calculation.\(^{12}\) In both cases, \( \alpha \) monotonically decreases with decreasing \( \Delta_S/\Delta_L \). It should be emphasized that we may identify the gap ratio \( \Delta_S/\Delta_L \) uniquely by measuring the electronic specific heat under varying external field, providing a rather unique spectroscopic method for determining the gap ratio. In Fig. 4, for the gap ratio \( \Delta_S/\Delta_L \sim 0.3 \) observed by the several groups with different methods, we obtain small exponent \( \alpha \), as in the specific heat data on MgB\(_2\).

There are several factors which might alter our conclusion on the relation \( \alpha \) vs. \( \Delta_S/\Delta_L \).

1) We assume that the DOS in the normal state for each Fermi surface sheet is equal. According to the band calculation by Belashchenko et al.\(^{20}\) the ratio of the two DOS is 0.55 (\( \pi \)-band) : 0.45 (\( \sigma \)-band). This small difference causes potentially to alter our conclusion, but not in an essential way.

2) It is assumed that in the minor \( S \)-band there is no direct attractive interaction \( g_{SS} = 0 \). The gap in the \( S \)-band is exclusively induced by the Cooper pair tunneling process via \( g_{LS} \neq 0 \). According to Kortus et al.\(^{9}\) the electron-phonon coupling in the \( S \)-band due to the bond stretching mode is smaller than that in the \( L \)-band, but yet non-vanishing. Thus \( g_{SS} \) might not completely vanish in MgB\(_2\). We might regard it vanish as a first approximation because our conclusion relies exclusively on the gap ratio \( \Delta_S/\Delta_L \). The effect of \( g_{SS} \neq 0 \) will be studied in the future for more details.

3) We comment on the small discrepancy of the exponent \( \alpha \) between our calculation based on BdG theory and that of the experiment. Since our parameters belong to a rather quantum limit case (the coherent length \( \xi \) is an order of the atomic lattice constant), the quasi-classical calculation\(^{12,13}\) is more appropriate for MgB\(_2\). We believe, however, that the overall relation \( \alpha \) vs. \( \Delta_S/\Delta_L \) is not greatly altered in that calculation. We will study this case in a future publication.

Haas and Maki\(^{21}\) analyze an anisotropic s-wave pairing state in connection with MgB\(_2\). Their single band model is designed to describe the anisotropic superconducting properties such as the upper critical field or the penetration depth. According to the recent penetration depth measurement\(^{22}\) for single crystals of MgB\(_2\), the anisotropy of the penetration depths for \( H \parallel c \) and \( H \perp c \) in the hexagonal crystal is almost absent, which is at odd with the prediction by Haas and Maki. Since their single band model is similar to our two band model in the sense that the gap anisotropy is implemented in the reciprocal space in Haas and Maki or implemented in the energy space in ours. In order to fully describe the three dimensional superconducting nature in MgB\(_2\) our model should consider the anisotropic s-wave pairing state for both major and minor bands, which may better explain the above penetration depth experiment.

We speculate that the present multi-gap model may have potentially wide applicability. It is quite usual that a superconductor has a multiple gap because the underlying Fermi surface consists of multiple sheets, on each of which the gap value could be different. It is true even for elemental metals. MgB\(_2\) may belong to an extreme case. To reveal this feature, the measurement of \( \gamma (H) \) is demonstrated to be a useful tool. The analysis for the \( p \)-wave pairing case,\(^{23}\) focusing on Sr\(_2\)RuO\(_4\), is reported in ref. 24.

In conclusion, we have evaluated the exponent \( \alpha \) in the \( T \) linear specific heat coefficient \( \gamma (H) \propto H^\alpha \) for a simple two-band superconductor and succeeded in reproducing the extremely small \( \alpha \cong 0.3 \), as in observed in MgB\(_2\), by taking the two gap ratio \( \Delta_S/\Delta_L \cong 0.3 \), each coming from the different Fermi sheets. Thus we conclude that the gap functions are distinctly different for the different Fermi sheets, the major is the \( \sigma \)-band (\( p_x \) and \( p_y \) characters of B atoms) while the minor is the \( \pi \)-band (\( p_z \) characters of B atoms), yet each gap being isotropic on its own Fermi sheet. Thus we do not need exotic anisotropic gap function for describing superconductivity here. This two-band feature is intrinsic in MgB\(_2\).

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