Meissner effect of Dirac electron in superconducting state

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Abstract. We investigate the Meissner effect (ME) of Dirac electrons in a superconducting state on the basis of Kubo formula, and clarify that Meissner kernel becomes finite by use of the inter-band contribution. This mechanism of the ME for Dirac electron is completely different from that for the electron in the usual metals. We also derive the result of the electron gas by taking the non-relativistic limit of Dirac Hamiltonian, and clarify that the diamagnetic term of the Meissner kernel can be regarded as the inter-band contribution between electrons and positrons in terms of the Dirac model.

1. Introduction

Recently, Dirac electron systems have been attracting a great interest. Dirac electron is characterized by the linear dispersion relation, and its low-energy physics is described by relativistic Dirac equation. It has been found that Dirac electron appears in such materials as graphene [1], Bi [2], α-(BEDT-TTF)$_2$I$_3$ [3], and so on. Up to now, many works have been carried out to investigate the properties in normal state of Dirac electron systems, such as the Hall conductivity [4], magnetoresistance [5], orbital magnetism, [6] and spin Hall conductivity [7]. In these studies, it has been pointed out that the inter-band effect plays important roles, since the conduction and valence bands are close to each other.

However, the properties of Dirac electrons in a superconducting state have not been understood completely. One of the most fundamental properties in a superconducting state is the Meissner effect (ME) in which the system becomes perfectly diamagnetic. In the case of parabolic-dispersion system, the ME arises from the diamagnetic term of the current operator. Note that the diamagnetic current term appears when the Hamiltonian has a kinetic energy proportional to $k^2$ with $k$ being the wave vector. [8]. On the other hand, in the Dirac electron system, the diamagnetic term of the current operator is absent since the Hamiltonian contains only up to $k$-linear terms [9]. Therefore, it is not trivial whether the Dirac electron in the superconducting state shows the ME.

In this paper, we discuss the ME of the 4 × 4 massive Dirac electron system in the three-dimensional space. We calculate the Meissner kernel by use of Kubo formula. We clarify that the ME occurs not due to the diamagnetic term of the current operator but due to the inter-band effect. We further study the large band-gap limit, which corresponds to the non-relativistic limit. We clarify that we can reproduce the Meissner kernel of the non-relativistic theory from the Dirac model, and that the paramagnetic and the diamagnetic terms of the kernel correspond to the intra-band and the inter-band terms in Dirac theory.
2. Formulation

Hamiltonian.- We consider the $4 \times 4$ massive Dirac Hamiltonian in the three-dimensional space:

$$H_0(k) = c_k^\dagger \begin{pmatrix} M \hat{I} & ivk \cdot \sigma \\ -ivk \cdot \sigma & -M \hat{I} \end{pmatrix} c_k,$$

where $\hat{I}$ is the $2 \times 2$ unit matrix and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are Pauli matrices. Here, $M$ is the band gap, and $v$ is the Fermi velocity. We use the basis $c_k = (c_{k,1,\uparrow}, c_{k,1,\downarrow}, c_{k,2,\uparrow}, c_{k,2,\downarrow})^T$ where 1, 2 denote the orbital, and $\uparrow$, $\downarrow$ denote the real spin.

Diagonalized form of this Hamiltonian is

$$H_0(k) = a_k^\dagger \begin{pmatrix} \varepsilon(k) \hat{I} & 0 \\ 0 & -\varepsilon(k) \hat{I} \end{pmatrix} a_k,$$

where $\varepsilon(k) = \sqrt{M^2 + (vk)^2}$, and $a_k$ represents the band-basis which is expressed as $a_k = (a_{k,+,\uparrow}, a_{k,+,\downarrow}, a_{k,-,\uparrow}, a_{k,-,\downarrow})^T$. Here, the indices $+$ and $-$ denote the upper and the lower bands respectively, and $\uparrow$ and $\downarrow$ denote pseudo-spins corresponding to the two-fold degeneracy of each band [See Fig. 1(a)] . Two bases, $c_k$ and $a_k$ are related by the unitary transformation as $a_k = U(k)c_k$.

Superconductivity.- We introduce superconductivity in this system. Here we do not discuss the microscopic origin of attractive interaction. Instead, we simply assume the intra-band s-wave interaction as

$$H_{\text{int}} = -V \sum_{|k|,|k'|<k_c} \sum_{\eta,\eta'} a_{k,\eta,\eta'}^\dagger a_{-k',\eta',\eta}^\dagger a_{-k,-\eta',\eta'}^\dagger a_{k',\eta',\eta},$$

where $k_c$ is the cutoff momentum corresponding to the range of energy in which the attractive interaction works. We assume $vk_c \gg M$. Due to this assumption, we obtain the superconducting phase even if the chemical potential is located in the band gap (i.e., there is no density of states...
at the Fermi level) for sufficiently large \( V \), since electrons with \( k < k_c \) can still contribute to the Cooper pairing. Then, we define the superconducting order parameter in the s-wave symmetry,

\[
\Delta_{\pm} = V \sum_{|k'| < k_c} \langle a_{-k',\pm}\hat{a}_{k',\pm} \rangle. \tag{4}
\]

By applying the mean field approximation to the Hamiltonian, \( H = H_0 + H_{\text{int}} \), we obtain the BCS Hamiltonian,

\[
H_{\text{BCS}} = \sum_{|k| < k_c} \sum_{\eta = \pm} \left\{ \xi_{\pm}(k) a_{k,\eta}^\dagger a_{k,\eta} - \Delta a_{-k,\eta}^\dagger a_{k,\eta} - \frac{\Delta}{\sqrt{\sum_{\eta = \pm} \xi_{\pm}(k)}} \right\}
\]

where \( \Delta = \Delta_+ + \Delta_- \) is the sum of the band-dependent order parameters and \( \xi_{\pm}(k) = \pm \varepsilon(k) - \mu \).

Diagonalizing \( H_{\text{BCS}} \), we obtain the excitation energy \( E_{\pm}(k) = \sqrt{\xi_{\pm}(k)^2 + \Delta^2} \) [see Fig. 1(b)]. Then, thermal Green’s function and the anomalous Green’s functions in the band basis are obtained in the form of \( 4 \times 4 \) matrices as follows.

\[
G(k, i\omega_n) = \begin{pmatrix} G_+(k, i\omega_n) & 0 \\ 0 & G_-(k, i\omega_n) \end{pmatrix}, \tag{6}
\]

and

\[
F(k, i\omega_n) = -F_-(k, i\omega_n) = \begin{pmatrix} i\sigma_y F_+(k, i\omega_n) & 0 \\ 0 & i\sigma_y F_-(k, i\omega_n) \end{pmatrix}, \tag{7}
\]

where \( G_\pm(k, i\omega_n) = \frac{\omega^2(k)}{i\omega_n - E_\pm(k)} + \frac{\omega^2(k)}{i\omega_n + E_\pm(k)} \), and \( F_\pm(k, i\omega_n) = -u_\pm(k) v_\pm(k) (\frac{1}{i\omega_n - E_\pm(k)} - \frac{1}{i\omega_n + E_\pm(k)}) \), with \( u^2_\pm(k) = \frac{1}{2} [1 + \frac{\xi_\pm(k)}{E_\pm(k)}] \), \( v^2_\pm(k) = \frac{1}{2} [1 - \frac{\xi_\pm(k)}{E_\pm(k)}] \), and \( u_\pm(k) v_\pm(k) = \frac{\Delta}{2E_\pm(k)} \).

It should be noted that the upper and lower parts of these Green’s functions are decoupled with each other.

**Current operator.** To derive the Meissner kernel, we have to define the current operator in the absence and presence of the vector potential. In the absence of vector potential, \( A \), the current operator in the momentum space is given by

\[
\hat{j}(q) = -e \sum_k \hat{c}_{k-q}^\dagger \partial_q H_0(k) \hat{c}_k^\dagger = -e \sum_k \hat{c}_{k-q}^\dagger \begin{pmatrix} 0 & iv\sigma \\ -iv\sigma & 0 \end{pmatrix} \hat{c}_k \equiv \sum_k \hat{c}_{k-q}^\dagger \hat{J} \hat{c}_k, \tag{8}
\]

where \( e > 0 \) is the absolute value of the charge of an electron. The vector potential \( A \) is introduced in the Hamiltonian by replacing \( k \) by \( k + eA \). However, we can readily see that the current operator in Eq. (8) does not change even in the presence of \( A \), since \( H_0(k) \) contains only linear terms with respect to \( k \).

This property of the current operator is essentially different from that in jellium model in which the current operator is given by \( \hat{j} = \sum_{k,\sigma} c_{k,\sigma}^\dagger \phi_m(k + eA) c_{k,\sigma} \) where the last term is called as the diamagnetic term. Apparently, the current operator of the Dirac electron systems does not have diamagnetic current. As we will show shortly, the absence of the diamagnetic term is crucial for discussing the mechanism of the ME in Dirac electron in superconducting state.

**3. Meissner effect in Dirac electron systems**

**Small band gap case:** Dirac electrons in solids. Using the formulations derived in the previous section, we calculate Meissner kernel, \( K^{(S)}_{xx} \), through Kubo formula. Since we do not have the diamagnetic term of the current operator, \( K^{(S)}_{xx}(q, i\omega) \) is given only by the current-current correlation function.
\[ K^{(S)}_{xx}(q, \omega_n) = \sum_{k, \omega_n} \text{Tr}[\mathcal{G}(k - q, \omega_n - \omega_n) \tilde{j}_x(k, q) \tilde{G}(k, \omega_n) \tilde{j}_x(k - q, -q)] - \mathcal{F}^I(k - q, \omega_n - \omega_n) \tilde{j}_x(k, q) \mathcal{F}(k, \omega_n) \tilde{j}_x^I(-k, -q). \]  

(9)

where \( \tilde{j}_x(k, q) \) is given by \( \tilde{j}_x(k, q) \equiv [U(k - q)j_xU^I(k)] \), and \( \omega_n = \frac{(2n+1)\pi}{\beta} \) \((n = 0, \pm 1, \pm 2, \ldots)\) denotes a fermionic Matsubara frequency. It should be noted that the limit \( \omega \to 0 \) has to be taken before the limit \( q \to 0 \).

By taking the trace in Eq. (9), we obtain the Meissner kernel which consists of two parts as \( K^{(S)}_{xx}(q, 0) = K^{\text{intra},(S)}_{xx}(q, 0) + K^{\text{inter},(S)}_{xx}(q, 0) \); \( K^{\text{intra},(S)}_{xx}(q, 0) \) comes from the term in which the two Green’s functions in Eq. (9), \( \mathcal{G} \) or \( \mathcal{F}^I \) have the same band index \(+, +\) or \(-, -\), and \( K^{\text{inter},(S)}_{xx}(q, 0) \) from the Green’s functions with the opposite band index, i.e., \(+, -\) or \(-, +\).

The explicit forms of these are obtained as

\[ K^{\text{intra},(S)}_{xx}(q, 0) = -\frac{e^2 v^2}{2} \sum_{k} \sum_{\eta = \pm} g^{\text{intra}}(k, q) \left[ (1 + \frac{\xi_{\eta}(k - q) \xi_{\eta}(k) + \Delta^2}{E_{\eta}(k - q) E_{\eta}(k)} f(E_{\eta}(k)) - f(E_{\eta}(k - q)) \right] \] 

\[ -\left(1 - \frac{\xi_{\eta}(k - q) \xi_{\eta}(k) + \Delta^2}{E_{\eta}(k - q) E_{\eta}(k)} f(E_{\eta}(k)) + f(E_{\eta}(k - q)) \right) - \frac{1}{E_{\eta}(k - q) + E_{\eta}(k)}, \]  

and

\[ K^{\text{inter},(S)}_{xx}(q, 0) = \frac{e^2 v^2}{2} \sum_{k} \sum_{\eta = \pm} g^{\text{inter}}(k, q) \left[ (1 + \frac{\xi_{\eta}(k - q) \xi_{\eta}(k) - \Delta^2}{E_{\eta}(k - q) E_{\eta}(k)} f(E_{\eta}(k)) - f(E_{\eta}(k - q)) \right] \] 

\[ -\left(1 - \frac{\xi_{\eta}(k - q) \xi_{\eta}(k) - \Delta^2}{E_{\eta}(k - q) E_{\eta}(k)} f(E_{\eta}(k)) + f(E_{\eta}(k - q)) \right) - \frac{1}{E_{\eta}(k - q) + E_{\eta}(k)}, \]  

(10)

Here, \( f(x) \) is the Fermi distribution function, and \( g^{\text{intra}}_{xx}(k, q), g^{\text{inter}}_{xx}(k, q) \) are given by

\[ g^{\text{intra}}_{xx}(k, q) = \frac{v^2 k^2_{x} (k_x - q_x) - k_y (k_y - q_y) - k_z (k_z - q_z)}{\epsilon(k) \epsilon(k - q)} + \frac{\epsilon(k) \epsilon(k - q) - M^2}{\epsilon(k) \epsilon(k - q)}, \]  

(12a)

\[ g^{\text{inter}}_{xx}(k, q) = \frac{v^2 k^2_{x} (k_x - q_x) - k_y (k_y - q_y) - k_z (k_z - q_z)}{\epsilon(k) \epsilon(k - q)} - \frac{\epsilon(k) \epsilon(k - q) + M^2}{\epsilon(k) \epsilon(k - q)}. \]  

(12b)

In the limit of \( q \to 0 \), we obtain \( K^{(S)}_{xx}(0, 0) = K^{\text{intra},(S)}_{xx}(0, 0) + K^{\text{inter},(S)}_{xx}(0, 0) \) with

\[ K^{\text{intra},(S)}_{xx}(0, 0) = 2 e^2 v^4 \sum_{k} \frac{k^2 x}{\epsilon^2(k)} \left[ \frac{\partial f(E_{+}(k))}{\partial E_{+}(k)} + \frac{\partial f(E_{-}(k))}{\partial E_{-}(k)} \right], \]  

(13)

and

\[ K^{\text{inter},(S)}_{xx}(0, 0) = -2 e^2 v^2 \sum_{k} \left(1 - \frac{v^2 k^2 x}{\epsilon^2(k)} \right) \left[ (1 + \frac{\xi_{+}(k) \xi_{-}(k) - \Delta^2}{E_{+}(k) E_{-}(k)} f(E_{-}(k)) - f(E_{+}(k)) \right] \] 

\[ -\left(1 - \frac{\xi_{+}(k) \xi_{-}(k) - \Delta^2}{E_{+}(k) E_{-}(k)} f(E_{-}(k)) + f(E_{+}(k)) \right) - \frac{1}{E_{+}(k) + E_{-}(k)}, \]  

(14)
Figure 2. \(\mu\) dependence of \(K_{xx}^{(S)}(0,0), K_{xx}^{(N)}(0,0),\) and \(K_{xx}(0,0)\) for (a) \(\Delta = 0.1M\) and (b) \(\Delta = 0.7M\). \(\mu\) dependence of \(K_{xx}\) in a large scale is in the inset.

It should be noted that for \(T = 0\), \(K_{xx}^{\text{intra},(S)}(0,0) = 0\) since the spectrum has a finite gap at the chemical potential. Hence, \(K_{xx}^{(S)}\) only consists of the inter-band contribution. This is in sharp contrast to the conventional BCS case, in which the Meissner kernel from the paramagnetic current vanishes at \(T = 0\), but the Meissner kernel from the diamagnetic current remains which leads to the ME. In contrast, in the Dirac case, the diamagnetic current does not exist from the beginning, but instead the inter-band contribution exists, which leads to the ME.

However, there is an interesting problem appearing from the inter-band contribution. Assume that \(\Delta = 0\), i.e., in the normal state. Even in this case, the kernel \(K_{xx}^{(N)}(0,0)\) does not vanish; the explicit form is

\[
K_{xx}^{\text{intra},(N)}(0,0) = 2e^2v^2 \sum_k \frac{v^2k_z^2}{\varepsilon^2(k)} \left[ \frac{\partial f(\xi_+(k))}{\partial \xi_+(k)} + \frac{\partial f(\xi_-(k))}{\partial \xi_-(k)} \right] \\
= - \frac{e^2v^2}{3\pi^2} \frac{(\mu^2 - M^2)^{3/2}\Theta(|\mu| - M)}{|\mu|v^3}, \tag{15}
\]

and

\[
K_{xx}^{\text{inter},(N)}(0,0) = -2e^2v^2 \sum_k \frac{v^2k_z^2}{\varepsilon^2(k)} \left[ \frac{f(\xi_-(k)) - f(\xi_+(k))}{\varepsilon(k)} \right] \\
= - \frac{e^2v^2}{3\pi^2} \left[ \frac{k_c^3}{\varepsilon(k_c)} - \frac{(\mu^2 - M^2)^{3/2}\Theta(|\mu| - M)}{|\mu|v^3} \right], \tag{16}
\]

with \(\Theta(x)\) being the step function.

In the usual situations in solids with finite Brillouin zone, \(K_{xx}^{(N)} = 0\) hold since the paramagnetic term exactly cancels with the diamagnetic contribution. Therefore we expect that in the Dirac case, there must be some counter-contributions from the vicinity of the Brillouin zone boundary which exactly cancel the contributions from the vicinity of the Dirac point. Therefore, in the following, we calculate the Meissner kernel in superconducting state as

\[
K_{xx} = K_{xx}^{(S)} - K_{xx}^{(N)}. \tag{17}
\]

The mathematical justification of this subtraction can be carried out by studying the slightly modified model [10].
By using Eq. (17), we numerically calculate $K_{xx}(0,0)$ at $T = 0$. In the numerical calculation, we set $k_c = 10 M/v$. Figures 2 (a) and 2 (b) show $\mu$ dependence of $K_{xx}^{(S)}$, $K_{xx}^{(N)}$, and $K_{xx}$ for $\Delta = 0.1 M$ and $\Delta = 0.7 M$ respectively. We can see that although $K_{xx}^{(S)}$ and $K_{xx}^{(N)}$ are both negative, $K_{xx}(0,0)$ is always positive and finite, thus we obtain the Meissner state. (For $\Delta = 0.1 M$, $\mu = 0$, $K_{xx} \sim 0.0007 e^2 v^2$.) In particular, when $|\mu| < M$, the Meissner kernel purely comes from the inter-band contribution, since the intra-band contributions vanish both in $K_{xx}^{(N)}$ and $K_{xx}^{(S)}$.

We can also see in Figs. 2 (a) and 2 (b) that $K_{xx}$ strongly depends on $\Delta$. This is also different from the result of the conventional BCS case in which $K_{xx}$ does not depend on $\Delta$ and depends only on the number and the mass of careers.

Large band gap case: non-relativistic electron.- Up to now, we consider the case in which the band gap is very small ($\sim 10$ meV). On the other hand, we can also consider the opposite case, i.e., the large band gap case. In particular, it is fascinating to test whether our theory can reproduce the results for non-relativistic theory. To access to the non-relativistic limit, we replace our parameters as $M$ to $\mu c^2$, and $v$ to $c$, with $m$ being the mass of an electron and $c$ the speed of light. Then, we can regard the upper band as the real electron, and the lower band as the positron [see Fig. 3]. We further assume that the chemical potential is on the upper band, and that $\mu - mc^2$ is much smaller than $mc^2$. Then we obtain the Meissner kernel in the normal state as

$$K_{xx}^{\text{intra},(N)}(0,0) = -\frac{e^2 c^2}{3\pi^2} \frac{\left(\mu^2 - (mc^2)^2\right)^{3/2}}{\mu c^3} \sim -\frac{e^2 n}{m}, \quad (18)$$

and

$$K_{xx}^{\text{inter},(N)}(0,0) = -\frac{e^2 c^2}{3\pi^2} \left[ \frac{k_F^3}{\varepsilon(k_c)} - \frac{\left(\mu^2 - (mc^2)^2\right)^{3/2}}{\mu c^3} \right] \sim \frac{e^2 n}{m} - \frac{e^2 c^2}{3\pi^2} \frac{k_F^3}{\varepsilon(k_c)}. \quad (19)$$

where $k_F = \sqrt{2m(\mu - mc^2)}$ is the Fermi momentum and $n = \frac{k_F^3}{3\pi^2}$ is the electron density. Here we use the approximantion $\mu \sim mc^2$.

Comparing Eqs. (18) and (19) with the results for the electron gas [8], we can see that $K_{xx}^{\text{intra}}$ equals to the paramagnetic term in the electron gas and that $K_{xx}^{\text{inter}}$ equals to the diamagnetic term apart from the divergent part ($\sim \frac{e^2 c^2}{3\pi^2} \frac{k_F^3}{\varepsilon(k_c)}$). Therefore, this result indicates, first, that we can reproduce the result of the electron gas starting from the Dirac model; second, that the diamagnetic term of the kernel in the electron gas theory originates from the inter-band contribution between positrons and electrons.
4. Summary
In summary, we have investigated the ME of three-dimensional massive Dirac electron in superconducting state on the basis of Kubo formula. We have to care about the finite Meissner kernel in the normal state, but this can be eliminated by subtracting the normal component. Although the diamagnetic term of the current operator is absent in Dirac electron system, the Meissner kernel is finite for any value of the chemical potential. This is due to the inter-band contribution. We also have studied the large band-gap limit to discuss the non-relativistic case. We clarify the relation that the paramagnetic term of the kernel originates from the intra-band term and the diamagnetic term from the inter-band term.

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