Theory of Supercurrent generation in BCS Superconductors

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Abstract

We revisit the supercurrent generation mechanism for the type of superconductors whose superconducting transition temperature is explained by the BCS theory (we call them BCS superconductors). This revisit is motivated by the reexamination of the ac Josephson effect [H. Koizumi, M. Tachikii, J. Supercond. Nov. Magn. (2015) 28:61] that indicates the charge on the charge carrier for the ac Josephson effect is $q = -e$, which strongly suggests that the supercurrent generation mechanism is lacking in the BCS theory since the charge carrier in the BCS theory is the Cooper pair with $q = -2e$. We present a new mechanism for the supercurrent generation in BCS superconductors. We first argue that the origin of the supercurrent generation is the formation of Dirac strings with $\pi$ flux inside. Then, the ground state is not the functional of the electron density at sites alone (assumed by the density functional theory), but also the Berry connection between sites that ensures the conservation of charge and the single-valuedness of the wave function. The $\pi$-flux Dirac strings are realized when the Rashba spin-orbit interaction is added to the BCS model. The Rashba spin-orbit interaction modifies the electron pairing from the original BCS one to the pairing of spin-twisting circular itinerant motion states. Then, the energy minimizing wave function becomes multi-valued with respect to electron coordinates due to the sign-change of the wave function around the centers of spin-twisting, and the lines composed of the centers of spin-twisting become the $\pi$-flux Dirac strings. The Berry connection provides a $U(1)$ instanton given by $A^{\text{fic}} = -\frac{\hbar}{2e} \nabla \chi$, $\varphi^{\text{fic}} = \frac{\hbar}{2e} \partial_t \chi$, where $\chi$ is an angular variable of period $2\pi$. The appearance of the flux quantum $\Phi_0 = \hbar/2e$ and the voltage quantum $V_0 = hf/2e$ are explained as topological effects of this $U(1)$ instanton without referring to the electron pair charge $2e$.

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I. INTRODUCTION

In the present work, we revisit the supercurrent generation mechanism for the type of superconductors whose superconducting transition temperature is explained by the BCS theory (we call it the BCS superconductor)\(^1\). In the BCS superconductor, the superconducting transition temperature is determined by an energy gap formation temperature, where the energy gap is created by the electron pairing due to an effective attractive interaction between them caused by the virtual exchange of phonons. Through the success of the BCS theory, it is now widely-believed that the electron pair formation is the origin of superconductivity. The electron pairing energy gap is often called the ‘superconducting gap’; \(2e\) in the flux quantum \(\Phi_0 = h/2e\), where \(e\) is the absolute value of the electron charge and \(h\) is Planck’s constant, and the voltage quantum \(V_0 = hf/2e\) appearing across the Josephson junction in the presence of a radiation field with frequency \(f\), are regarded as due to the pairing electron charge.

Now, superconductivity of a different type is known in cuprates\(^2\). The cuprate superconductors show marked differences from the BCS ones. For example, the superconducting transition temperature is not given by the energy gap formation temperature, but corresponds to the stabilization temperature of coherent-length-sized loop currents for optimally doped samples\(^3\); the normal state from which the superconducting state emerges is not an ordinary metallic state described by the Fermi liquid theory but a doped Mott insulator state; the local magnetic correlation that is a remnant of the parent Mott insulator still exists in the doped compound, giving rise to the hourglass-shaped magnetic excitation spectrum\(^4\); actually, the magnetic excitations persist entire superconducting hole doping range\(^5\), thus, a close relationship between the superconductivity and magnetism is plausible. In spite of all the differences, \(\Phi_0 = h/2e\) and \(V_0 = hf/2e\) are observed; thus, it is widely-believed that the origin of the cuprate superconductivity is still the electron pairing.

However, a challenge has been put forward on the above widely-held view; a new theory of superconductivity has been presented in order to explain the cuprate superconductivity\(^6\). For the appearance of supercurrent, it uses the fact that persistent current generation is possible if the wave function has singularities that exhibit non-trivial topological phases or Berry phases\(^10,11\). In this theory, the key ingredient is the Dirac string with \(\pi\) flux inside (\(\pi\)-flux Dirac string); a Dirac string is a line of singularities of wave functions in
the coordinate space, and the $\pi$-flux inside it causes the sign-change of the wave function when it is transported around it. The $\pi$-flux Dirac string arises due to the spin-twisting itinerant motion of electrons, where the centers of the spin-twisting are singularities of the wave function.

There is an indication that the new theory may supersede the currently accepted one and extends the possibility of realizing superconductivity\textsuperscript{12}. The phenomenon of superconductivity is associated with external current flow through the system without voltage drop; it indicates the existence of an energy minimum under the current feeding boundary condition. Although the BCS theory is an established theory of superconductivity, such an energy minimum has never been obtained by it. However, such a minimum is found in the system exhibiting spin twisting itinerant motion of electrons with the Rashba spin-orbit interaction without referring to the electron pairing\textsuperscript{12}.

It is also notable that a misfit was found between the experimentally observed ac Josephson effect and the Josephson’s prediction\textsuperscript{6,9}. Since this is the major motivation of the present work, we shall explain it succinctly, below. The details are given in Section IV.

First, we note that the true cause of superconductivity is the appearance of an angular variable $\phi$ with period $2\pi$ that makes the followings gauge invariant,

$$A^{em} = \frac{\hbar}{2e} \nabla \phi; \quad \varphi^{em} + \frac{\hbar}{2e} \partial_t \phi$$  \hspace{1cm} (1)

where $(\varphi^{em}, A^{em})$ is the electromagnetic gauge potential, and the gauge invariance means that the above sums are not affected by the choice of the gauge in $\varphi^{em}$ and $A^{em}$ due to compensational changes in $\phi$.\textsuperscript{13,14} This $\phi$ is required to explain the Meissner effect, persistent current generation, and Josephson effect. In the BCS superconductors, the required phase $\phi$ appears when the electron pairing is established, and $\phi$ is associated with charge $-2e$ particles.\textsuperscript{13,14}

The misfit arises from the difference in boundary conditions between the Josephson’s derivation\textsuperscript{15} and the experiment. The Josephson’s derivation assumes a simple appearance of a dc voltage across the Josephson junction; however, a dc voltage does not appear by a simple application of a dc voltage; instead, when a dc voltage is applied, a dc Josephson effect takes over, resulting in a zero voltage across the junction\textsuperscript{16}. In the experimental situation where a finite voltage exists, there also exist a radiation field and a dc current flow. In this situation, an extra contribution to $\dot{\phi}_J$ arises, where $\dot{\phi}_J$ is the difference of $\phi$ across the
Josephson junction. By including the extra contribution, there are two contributions to \( \dot{\phi}_J \); one from the chemical potential difference between the leads connected to the junction, and the other from the electric field in the non-superconducting region between the two superconductors in the junction. Their contributions are equal due to the balance between the voltage and chemical potential difference. In the Josephson’s derivation, only one of them is included. By taking into account the two contributions and also the fact that \( \dot{\phi}_J = \frac{2eV}{h} \) is observed experimentally, we have \( q = -e \) for the carrier charge (if we use \( q = -2e \) as in the Josephson’s prediction, we have \( \dot{\phi}_J = \frac{4eV}{h} \)). This suggests that the electron pairing is not the true cause of the supercurrent generation, although the pairing energy gap formation temperature is the superconducting transition temperature.

In the new theory that attributes the supercurrent generation to the formation of Dirac strings with \( \pi \)-flux, the flux quantum \( \Phi_0 = h/2e \) and the voltage quantum \( V_0 = hf/2e \) can be explained with \( q = -e \). In the present work, we argue that the spin-twisting itinerant motion of electrons occurs in the BCS superconductors and \( \pi \)-flux Dirac strings are created if the Rashba spin-orbit interaction is included.

The organization of the present work is as follows: in Section II, Berry connection for many-body wave functions is introduced to deal with the situation where the energy minimizing wave function becomes multi-valued with respect to electron coordinates. In Section III, the effective gauge potential in materials is explained. In Section IV, the ac Josephson effect is revisited. In Section V, the wave packet motion of electrons in the presence of the Rashba spin-orbit interaction and magnetic field is considered. The gap equation for the new pairing is given in Section VI. The modification of the kinetic energy due to the Rashba interaction is derived and the London equation is obtained in Section VII. In Section VIII, the problem of the choice of the gauge in the BCS theory is revisited. Lastly, we conclude the present work in Section IX.

II. BERRY CONNECTION FOR MANY-BODY WAVE FUNCTIONS AND SINGLE-VALUED REQUIREMENT OF THE GROUND STATE WAVE FUNCTION AS A FUNCTION OF COORDINATES

Let us consider the wave function of a system with \( N_e \) electrons,

\[
\Psi(x_1, \cdots, x_{N_e}, t)
\]
where \( \mathbf{x}_j = (r_j, s_j) \) denotes the coordinate \( r_j \) and spin \( s_j \) of the \( j \)th electron.

We can define a Berry connection associated with this wave function\(^{10}\). Actually, it is a \( U(1) \) gauge field for the electron. We first construct a normalized single-particle wave function from \( \Psi \),

\[
\int d\mathbf{x}_2 \cdots d\mathbf{x}_{N_e} \frac{\Psi(\mathbf{r}, \mathbf{x}_2, \cdots, \mathbf{x}_{N_e}, t)}{|C(\mathbf{r}, t)|^{\frac{1}{2}}}
\]

where

\[
|C(\mathbf{r}, t)| = \int ds d\mathbf{x}_2 \cdots d\mathbf{x}_{N_e} \Psi(\mathbf{r}, \mathbf{x}_2, \cdots, \mathbf{x}_{N_e}, t) \Psi^*(\mathbf{r}, \mathbf{x}_2, \cdots, \mathbf{x}_{N_e}, t)
\]

From it, the Berry Connection for Many-Body Wave Functions is defined:

\[
A_{MB}(\mathbf{r}, t) = -i \int ds d\mathbf{x}_2 \cdots d\mathbf{x}_{N_e} \left[ \nabla_{\mathbf{r}} \frac{\Psi(\mathbf{r}, \mathbf{x}_2, \cdots, \mathbf{x}_{N_e}, t) \Psi^*(\mathbf{r}, \mathbf{x}_2, \cdots, \mathbf{x}_{N_e}, t)}{|C(\mathbf{r}, t)|^{\frac{1}{2}}} \right]_{\mathbf{r} = \mathbf{r}'}
\]

Let us consider the kinetic energy part of the Hamiltonian,

\[
K_0 = \frac{1}{2m} \sum_{j=1}^{N_e} \left( \frac{\hbar}{i} \nabla_j \right)^2
\]

We can construct a currentless wave function \( \Psi_0 \) using \( \Psi \) and \( A_{MB} \),

\[
\Psi_0(\mathbf{x}_1, \cdots, \mathbf{x}_{N_e}, t) = \Psi(\mathbf{x}_1, \cdots, \mathbf{x}_{N_e}, t) \exp \left( -i \sum_{j=1}^{N_e} \int_{r_j}^{\mathbf{r}} A_{MB}(\mathbf{r}', t) \cdot d\mathbf{r}' \right)
\]

We now consider the case where \( A_{MB} \) is not the magnetic field origin and satisfies,

\[
\nabla \times A_{MB} = 0
\]

From Eq. (8), we may write

\[
A_{MB} = -\nabla \theta
\]

As a consequence, \( \Psi(\mathbf{x}_1, \cdots, \mathbf{x}_{N_e}, t) \) is expressed as

\[
\Psi(\mathbf{x}_1, \cdots, \mathbf{x}_{N_e}, t) = \Psi_0(\mathbf{x}_1, \cdots, \mathbf{x}_{N_e}, t) \exp \left( -i \sum_{j=1}^{N_e} \theta(\mathbf{r}_j, t) \right)
\]

Let us consider the case where the electromagnetic vector potential \( A_{em} \) is included. The kinetic energy operator is modified as

\[
K[A_{em}] = \frac{1}{2m} \sum_{j=1}^{N_e} \left( \frac{\hbar}{i} \nabla_j - qA_{em}(\mathbf{r}_j) \right)^2
\]
where $q = -e$ is the charge of electron.

The kinetic energy is calculated as

$$E_{\text{kin}} = \langle \Psi | K [ A^\text{em}] | \Psi \rangle = \langle \Psi_0 | K \left[ A^\text{em} + \frac{\hbar}{q} \nabla \theta \right] | \Psi_0 \rangle$$

(12)

The total energy is given by

$$E_{\text{tot}} = \langle \Psi | H [ A^\text{em}] | \Psi \rangle = \langle \Psi_0 | H \left[ A^\text{em} + \frac{\hbar}{q} \nabla \theta \right] | \Psi_0 \rangle$$

(13)

If we treat $\nabla \theta$ as parameters that are optimized to minimize the total energy $E_{\text{tot}}$, the optimization condition for the $A^\text{em} = 0$ case is given by

$$0 = \frac{\delta E_{\text{tot}}}{\delta \nabla \theta} = \frac{\hbar}{q} \frac{\delta E_{\text{tot}}}{\delta A^\text{em}} \bigg|_{A^\text{em}=0} = -\frac{\hbar}{q} \cdot \frac{\delta E_{\text{tot}}}{\delta A^\text{em}}$$

(14)

where $\mathbf{j}$ is the current density, and the identity

$$\mathbf{j} = -\frac{\delta E_{\text{tot}}}{\delta A^\text{em}}$$

(15)

is used. This shows that the optimized state is that of zero current; thus, it is actually $\Psi_0$ if the ground state is not degenerate. This is in accordance with the Bloch theorem, "the energy minimizing ground state is currentless". However, the energy minimizing wave function $\Psi_0$ may be multi-valued if singularities of wave functions arise, then, it is not allowed. In this situation, the Bloch theorem may be violated.

Actually, if spin-twisting circular itinerant motion of electrons occurs, the centers of the spin-twisting are singularities of it. Such a motion can be realized by the spin-orbit interaction

$$H_{\text{so}}^\text{Dirac} = -\frac{q \hbar}{4m^2c^2} \sigma \cdot [E^\text{em} \times (\mathbf{p} - qA^\text{em})]$$

(16)

as is demonstrated in our previous work.

The singularities from the spin-twisting itinerant motion form lines, $\pi$-flux Dirac strings. A Dirac string is a line of singularities of the wave function considered by Dirac. When $\Psi_0$ is transported around the $\pi$-flux Dirac string, it changes sign, showing that $\Psi_0$ is multi-valued.

Since the legitimate wave function of the Schrödinger equation is a single-valued function of the electron coordinates, the multi-valuedness of $\Psi_0$ must be compensated by
\[ \exp \left( -i \sum_{j=1}^{N_e} \theta(r_j, t) \right) \] in Eq. (10). For later convenience, we introduce angular variable \( \chi \), which is related to \( \theta \) as
\[ \chi = \frac{1}{2} \theta \] (17)

Since \( \Psi_0 \) changes sign after a circular transport along loop \( C \) around the \( \pi \)-flux Dirac string, \( e^{-\frac{i}{2} \chi} \) must change sign also. This means that \( \chi \) is an angular variable with period \( 2\pi \) and the winding number along \( C \) given by
\[ w_C[\chi] = \frac{1}{2\pi} \oint_C \nabla \chi \cdot d\mathbf{r} \] (18)
is an odd integer.

Actually, we can construct \( \chi \) if we know the positions of \( \pi \)-flux Dirac strings, and the winding numbers for \( \chi \) around them. In other words, we can obtain \( \chi \) from the topological properties of the wave function. Let us describe how to obtain \( \chi \). First, we discretize the three-dimensional continuous space by a cubic lattice of length \( a \). Then, the wave function is given as values at the lattice points. The system we consider occupies a region of \( N_s \) sites (lattice points) that are composed of \( N_c \) cubes of volume \( a^3 \); each of them has 6 faces and 12 bonds, some of them are shared by other cubes. To obtain \( \chi \) means to obtain \( \nabla \chi \) along all bonds. We denote the number of bonds in the system by \( N_b \). The value of \( \nabla \chi \) along the bond \( k \leftarrow j \) is denoted as
\[ \tau_{k \leftarrow j} = \chi_k - \chi_j \] (19)

We need to know all \( N_b \) values of \( \tau_{k \leftarrow j} \)'s.

According to Eq. (14), the current through the bond \( k \leftarrow j \) is given by
\[ J_{k \leftarrow j} = \frac{2e}{\hbar} \frac{\partial E_{\text{tot}}}{\partial \tau_{j \leftarrow i}} \] (20)

The conservation of charge at site \( j \) is given by
\[ 0 = \sum_i \frac{2e}{\hbar} \frac{\partial E_{\text{tot}}}{\partial \tau_{j \leftarrow i}} + J_j^{\text{EX}} \] (21)
where \( J_j^{\text{EX}} \) is the current that is fed externally from the \( j \)th site. We have \( (N_s - 1) \) conditions from the conservation of local charge, where the subtraction 1 comes from the fact that the calculation is done with total charge conserved, thus, one condition is redundant. It is worth
noting that \( J_j^{EX} \neq 0 \) energy minimal states can be realized if the spin-orbit interaction is included\(^{12}\).

We restrict the situation when each \( \pi \)-flux Dirac sting enters a unit cube, it enters through one of the faces of the cube and exits from another one. Then, we have the following condition

\[
\nabla \cdot \mathbf{A}^{MB} = 0
\]

for each cube.

The spin-twisting is detected by calculating the winding number of the projection of the spin on the plane containing the face, \( S_\ell \), along the boundary loop of the face, \( C_\ell = \partial S_\ell \). If the surface normal of \( S_\ell \) is in the \( z \) direction, the expectation value of the projection of the spin \( S_j \) at the site \( j \) is \( (S_j^x, S_j^y) \), given by

\[
S_j^x = S_j \cos \xi_j \sin \zeta_j \\
S_j^y = S_j \sin \xi_j \sin \zeta_j
\]

where \( \zeta \) and \( \xi \) are polar angle and azimuthal angle, respectively. Then, the spin-twisting is detected by calculating the winding number of \( \xi \) along \( C_\ell \) given by

\[
w_{C_\ell}[\xi] = \frac{1}{2\pi} \sum_{k \leftarrow j} L_{k \leftarrow j}^\ell (\xi_k - \xi_j)
\]

where the sum is taken over the bonds \( k \leftarrow j \) and \( L_{k \leftarrow j}^\ell \) is defined as

\[
L_{k \leftarrow j}^\ell = \begin{cases} 
-1 & \text{if } j \leftarrow i \text{ exists in } C_\ell \text{ in the clockwise direction} \\
1 & \text{if } j \leftarrow i \text{ exists in } C_\ell \text{ in the counterclockwise direction} \\
0 & \text{if } j \leftarrow i \text{ does not exist in } C_\ell
\end{cases}
\]

If \( w_{C_\ell}[\xi] \neq 0 \), there is a center of spin-twisting in \( S_\ell \). If \( w_{C_\ell} \) is odd, \( S_\ell \) is penetrated by a \( \pi \)-flux Dirac string.

The winding number of \( \chi \) along \( C_\ell \) is given by

\[
w_{C_\ell}[\chi] = \frac{1}{2\pi} \sum_{k \leftarrow j} L_{k \leftarrow j}^\ell \tau_{k \leftarrow j}
\]

The single-valuedness of the wave function is given by

\[
w_{C_\ell}[\xi] + w_{C_\ell}[\chi] = \text{ even number}
\]
since by this condition, the sign-change of \( \Psi_0 \) is compensated by that of \( e^{-\frac{i}{2} \chi} \). The number of conditions from the single-valued requirement is \((N_f - N_c)\), where \( N_f \) and \( N_c \) are the numbers of faces and cubes, respectively. The subtraction \( N_c \) comes from the fact that one of its faces is omitted from each cube due to the condition in Eq. (22).

We need to know \( \tau_{k\leftarrow j} \)'s for \( N_b \) bonds. The equality between the unknowns and the conditions is given by

\[
N_b = (N_s - 1) + N_f - N_c
\]

Actually, the above relation is the Euler’s theorem for a three dimensional object.

The necessity to obtain \( \tau_{k\leftarrow j} \)'s to construct the ground state can be viewed as an extension of the Hohenberg-Kohn theorem “the ground state energy is determined by the electron density alone\(^{19}\).” This theorem does not take into account the presence of Dirac strings; the present work indicates that if they exist, we need to know \( \tau_{k\leftarrow j} \)'s for all bond in addition.

From the knowledge of the electron density at sites \( \rho_j \)'s and the Berry connection for bonds \( \tau_{k\leftarrow j} \)'s, the reduced density matrix of order one, \( \Gamma^{(1)}(r, r', t) \), in the region \(|r - r'| \to 0 \) can be constructed. It is given in the continuous limit by

\[
\Gamma^{(1)}(r, r', t) \approx \frac{\rho^{1/2}(r, t)}{\rho^{1/2}(r', t)} \exp \left( \frac{i}{2} \int_{r}^{r'} \nabla \chi(r'', t) \cdot dr'' \right)
\]

and yields the correct kinetic energy in Eq. (12).

Then the approximate density matrix can be expressed as

\[
\Gamma^{(1)}(r, r', t) \approx \gamma(r, t) \gamma^*(r', t)
\]

where

\[
\gamma(r, t) = \rho^{1/2}(r, t) \exp \left( -\frac{i}{2} \int_{0}^{r} \nabla \chi(r', t) \cdot dr' \right)
\]

The above form of \( \Gamma^{(1)}(r, r', t) \) is actually the form suggested by Penrose and Onsager for Bose-Einstein condensation systems with the condensate wave function \( \gamma(r, t)\(^{20}\). Thus, the present system has the form of density matrix for a long-range off-diagonal order in the Penrose and Onsager’s sense although the region is restricted.

The wave function \( \gamma(r, t) \) is multi-valued with respect to the coordinates, thus, will not be convenient for calculations. We can construct a single-valued one by considering the
electron pair. The resulting wave function is given by

$$\gamma_{\text{pair}}(r, t) = \left( \frac{\rho(r, t)}{2} \right)^{1/2} \exp \left( -i \int_0^r \nabla \chi(r', t) \cdot dr' \right)$$  (32)

This may be identified as the macroscopic wave function in the Ginzburg-Landau formalism\textsuperscript{21}.

The current density is calculated with Eq. (29), using the kinetic operator Eq. (11), neglecting the contribution from the spin-orbit interaction Eq. (16) assuming it is small, as

$$j = -\frac{e^2 \rho(r)}{m} \left( A_{\text{em}} - \frac{\hbar}{2e} \nabla \chi \right)$$  (33)

This is the London equation. If we take a loop $C$ along which $j = 0$, we have

$$\oint_C A_{\text{em}} \cdot dr = \frac{\hbar}{2e} \oint_C \nabla \chi \cdot dr = \frac{\hbar}{2e} \omega_C[\chi]$$  (34)

This shows the flux quantization in $\frac{\hbar}{2e}$.

III. EFFECTIVE GAUGE POTENTIAL IN MATERIALS

Let us derive the equations of motion for $\chi$ and its conjugate variable $\rho$. For that purpose, we use the time-dependent variational principle using the following Lagrangian\textsuperscript{22},

$$L = \langle \Psi | i \hbar \partial_t - H[A_{\text{em}}, \varphi_{\text{em}}] | \Psi \rangle = \int dr \left[ \rho \frac{\hbar}{2} \nabla \chi, A_{\text{em}} + \frac{\hbar}{2q} \nabla \chi, \varphi_{\text{em}} \right]$$  (35)

where $E_{\text{tot}}[A_{\text{em}} + \frac{\hbar}{2q} \nabla \chi, \varphi_{\text{em}}]$ is given in Eq. (13). Here, we assume the situation where only $\chi$ and its conjugate variable are important variables.

From the above Lagrangian, the conjugate momentum of $\chi$ is obtained as

$$p_{\chi} = \frac{\delta L}{\delta \dot{\chi}} = \frac{\hbar}{2} \rho$$  (36)

thus, $\chi$ and $\rho$ are canonical conjugate variables.

We assume that $\langle \Psi_0 | \partial_t | \Psi_0 \rangle = 0$ due to the reality of $\Psi_0$ or time-independence of $\Psi_0$ in the following.

By separating the Coulomb term that is proportional to $\varphi_{\text{em}}$, we define $\tilde{H}$ as

$$\tilde{H} \left[ A_{\text{em}} + \frac{\hbar}{2q} \nabla \chi \right] = H \left[ A_{\text{em}} + \frac{\hbar}{2q} \nabla \chi, \varphi_{\text{em}} \right] - q \int dr \rho \varphi_{\text{em}}$$  (37)
Then, we have

\[
\tilde{E}_{\text{tot}} \left[ A^{\text{em}} + \frac{\hbar}{2q} \nabla \chi, \varphi^{\text{em}} \right] = \tilde{E}_{\text{tot}} \left[ A^{\text{em}} + \frac{\hbar}{2q} \nabla \chi \right] - q \int \text{d} \mathbf{r} \ \rho \varphi^{\text{em}}
\]  

(38)

where \( \tilde{E}_{\text{tot}} \left[ A^{\text{em}} + \frac{\hbar}{2q} \nabla \chi, \varphi^{\text{em}} \right] \) is defined by

\[
\tilde{E}_{\text{tot}} \left[ A^{\text{em}} + \frac{\hbar}{2q} \nabla \chi \right] = \langle \Psi_0 | \hat{H} \left[ A^{\text{em}} + \frac{\hbar}{2q} \nabla \chi \right] | \Psi_0 \rangle \quad \text{(39)}
\]

Using \( \tilde{E}_{\text{tot}} \left[ A^{\text{em}} + \frac{\hbar}{2q} \nabla \chi, \varphi^{\text{em}} \right] \), \( \mathcal{L} \) is written as

\[
\mathcal{L} = -\tilde{E}_{\text{tot}} \left[ A^{\text{em}} + \frac{\hbar}{2q} \nabla \chi \right] - q \int \text{d} \mathbf{r} \ \rho \left( \varphi^{\text{em}} - \frac{\hbar}{2q} \dot{\chi} \right)
\]

(40)

The Lagrangian \( \mathcal{L} \) indicates that \( A^{\text{em}} \) and \( \varphi^{\text{em}} \) always appear in the following combinations,

\[
A^{\text{eff}} = A^{\text{em}} + \frac{\hbar}{2q} \nabla \chi
\]

(41)

and

\[
\varphi^{\text{eff}} = \varphi^{\text{em}} - \frac{\hbar}{2q} \dot{\chi}
\]

(42)

Thus, we may consider \((\varphi^{\text{eff}}, A^{\text{eff}})\) as the basic field. We call it the effective gauge potential in materials.

The Hamilton’s equations for \( \chi \) and \( \rho \) are obtained as

\[
\dot{\chi} = 2 \frac{\delta E_{\text{tot}}}{\hbar \delta \rho} = 2 \left( \frac{\delta E_{\text{tot}}}{\delta \rho} + q \varphi^{\text{em}} \right)
\]

(43)

\[
\dot{\rho} = 2 \frac{\hbar}{\nabla} \cdot \frac{\delta E_{\text{tot}}}{\delta \nabla \chi} = \frac{2}{\hbar} \nabla \cdot \frac{\delta E_{\text{tot}}}{\delta \nabla \chi}
\]

(44)

The equation (44) describes the conservation of the charge

\[
q \dot{\rho} + \nabla \cdot \mathbf{j} = 0
\]

(45)

with the current density given by

\[
\mathbf{j} = -\frac{2q}{\hbar} \frac{\delta E_{\text{tot}}}{\delta \nabla \chi} = -\frac{\delta E_{\text{tot}}}{\delta A^{\text{em}}}
\]

(46)

which is equal to Eq. (15).
The equation (43) is rewritten as

\[ q\varphi_{\text{eff}} = -\frac{\delta \tilde{E}_{\text{tot}}}{\delta \rho} \]  

This indicates that \(-q\varphi_{\text{eff}} = e\varphi_{\text{eff}}\) plays a role of the chemical potential by taking \(\tilde{E}_{\text{tot}}\) as the total energy.

For a stationary and isolated system, we have \(\dot{\chi} = 0\) and \(\dot{\rho} = 0\). From \(\dot{\chi} = 0\), we have

\[ \frac{\delta E_{\text{tot}}}{\delta \rho} = 0 \]  

This agrees with the condition for the ground state electron density in the density functional theory\(^1\).

Let us consider the gauge invariance problem in \((\varphi_{\text{eff}}, A_{\text{eff}})\). In classical theory, the gauge invariance is the invariance for the electric field \(E_{\text{em}}\) and the magnetic field \(B_{\text{em}}\)

\[ E_{\text{em}} = -\partial_t A_{\text{em}} - \nabla \varphi_{\text{em}} ; \quad B_{\text{em}} = \nabla \times A_{\text{em}} \]  

with respect to the following modifications,

\[ A_{\text{em}} \rightarrow A_{\text{em}} - \frac{\hbar}{2q} \nabla \phi ; \quad \varphi_{\text{em}} \rightarrow \varphi_{\text{em}} + \frac{\hbar}{2q} \partial_t \phi \]  

where \(\phi\) is a scalar function. Here, the charge of charged particles \(q\) is included for later convenience.

In quantum mechanics, the gauge transformation requires an additional change in the phase of the wave function for the material interacting with the electromagnetic field

\[ \psi(x, t) \rightarrow e^{-\frac{i}{\hbar} \phi} \psi(x, t) \]  

This means that we need to adjust the \(U(1)\) phase factor of the wave function for the material in response to the change of the gauge.

From the conditions in Eqs. (21) and (26), the gauge invariant \(A_{\text{eff}}\), which absorbs the change of gauge, is obtained. Then, substituting this gauge invariant \(A_{\text{eff}}\) in Eq. (17), the gauge invariant \(\varphi_{\text{eff}}\) is obtained, where the arbitrariness in gauge chosen for \(\varphi_{\text{em}}\) is absorbed in the arbitrariness of \(\partial_t \chi\) in this process. Thus, if we stick to \((\varphi_{\text{eff}}, A_{\text{eff}})\) that satisfies Eqs. (21), (26), and (17), it is gauge invariant.

Note that the phase change in Eq. (51) in the wave function may be explained as a particular case for the above mentioned evaluation of \(\chi\) that satisfies Eqs. (21), (26), and
Let us assume $\Psi_0$ in Eq. (10) is the exact solution for the first chosen $(\varphi^{em}, A^{em})$; the fact that $\Psi_0$ is optimized for the first chosen $(\varphi^{em}, A^{em})$ means that for the gauge transformation in Eq. (50), the solution $\chi$ evaluated by the conditions Eqs. (21), (26), and (47) will yield $\chi = \phi$ within a constant added to it, since the gauge invariant $(\varphi^{eff}, A^{eff})$ is obtained as

$$A^{eff} = A^{em} + \frac{\hbar}{2q} \nabla \chi = A^{em} - \frac{\hbar}{2q} \nabla \phi + \frac{\hbar}{2q} \nabla \chi$$

(52)

$$\varphi^{eff} = \varphi^{em} - \frac{\hbar}{2q} \partial_t \chi = \varphi^{em} + \frac{\hbar}{2q} \partial_t \phi - \frac{\hbar}{2q} \partial_t \chi$$

(53)

$\Psi_0$ is optimized for $(\varphi^{em}, A^{em})$ means that we have $\nabla \phi = \nabla \chi$ and $\partial_t \phi = \partial_t \chi$.

IV. REVISITING AC JOSEPHSON EFFECT

We revisit the ac Josephson effect problem here. This is a modified and extended version of our previous work. In the following the charge on the carrier is $q = -e$, not $q = -2e$ that is adopted in the original Josephson derivation.

Let us consider a Josephson junction and denote two superconductors in the junctions as $S_L$ and $S_R$. The angular variable $\chi$ is assumed continuous along the line connecting $S_L$ and $S_R$, and it is denoted as $\chi_L$ and $\chi_R$ when it is on $S_L$ and $S_R$, respectively. Then, according to Eq. (15) the current-flow through the junction is a function of

$$\int_{L}^{R} A^{eff} \cdot d\mathbf{r} = \int_{L}^{R} A^{em} \cdot d\mathbf{r} + \frac{\hbar}{2q} (\chi_R - \chi_L)$$

(54)

Since the change of $\chi_R \to \chi_R + 4\pi n$ ($n$ is an integer) or $\chi_L \to \chi_L + 4\pi n$ ($n$ is an integer) does not change the wave functions on the superconductors, the current is a function of the angular variable

$$\phi_J = \frac{q}{\hbar} \int_{L}^{R} A^{eff} \cdot d\mathbf{r}$$

(55)

with period $2\pi$. The current through the junction is often approximated as

$$J = J_0 \sin \phi_J$$

(56)

but we do not assume the above form in the following.

The chemical potential $\mu = q\varphi^{eff}$ is also continuous through the junction. From Eq. (42), the difference of the chemical potential on $S_L$ and on $S_R$ is given by

$$\int_{L}^{R} \nabla \mu \cdot d\mathbf{r} = q \int_{L}^{R} \nabla \varphi^{em} \cdot d\mathbf{r} + \frac{\hbar}{2} \int_{L}^{R} \nabla \chi \cdot d\mathbf{r}$$

(57)
Let us consider the situation where a radiation field with frequency \( f \) is applied in the absence of the static electric field in the insulator region; then, \( \nabla \varphi^\text{em} \) arises only from this radiation field. The current is a dc current (dc Josephson effect is operating) with \( \partial_t A^\text{eff} = \frac{\hbar}{2q} \partial_t \nabla \chi = 0 \). Then, from Eq. (57), the average of the chemical potential difference between time interval \( 0 < t < f^{-1} \) is calculated as

\[
eV = \frac{\hbar f}{2} \int_0^{f^{-1}} dt \int_L^R \partial_x \partial_t \chi dx = -\frac{\hbar f}{2} \int_0^{f^{-1}} dt \int_L^R (\partial_x \partial_t - \partial_t \partial_x) \chi dx = \frac{\hbar f}{2} n
\]

where the direction of the junction is taken to be in the \( x \) direction and \( n \) is the winding number of \( \chi \) along boundary of integration given by

\[
n = \frac{1}{2\pi} \int_0^{f^{-1}} dt \int_L^R (\partial_x \partial_t - \partial_t \partial_x) \chi dx = \frac{1}{2\pi} \oint_{\partial([0,f^{-1}] \times [L,R])} d\chi
\]

The contribution from the first term in the r.h.s. of Eq. (57) is averaged out. The chemical potential difference \( \frac{\hbar f}{2} n \) arises from the topological object “instanton” created by the radiation field.

Next we consider the stationary state after the instanton is created. Actually, in this stationary situation, we have \( \dot{\chi} = 0 \), thus, the instanton disappears. The chemical potential difference created by the instanton is now balanced by the electric field generated by charging of the junction as a capacitor. Then, the second term in Eq. (57) becomes zero, and the first term becomes the sum of the contribution from the radiation field and the static electric field generated by the charging.

Let us obtain \( \phi_J \) for this stationary situation. We take the time derivative of \( \phi_J \),

\[
\dot{\phi}_J = \frac{q}{\hbar} \int_L^R \hat{A}^\text{em} \cdot dr - \frac{1}{2} \int_L^R \nabla \chi \cdot dr
\]

\[
= -\frac{q}{\hbar} \int_L^R E^\text{em} \cdot dr - \frac{q}{\hbar} \int_L^R \nabla \phi^\text{eff} \cdot dr
\]

\[
= -\frac{q}{\hbar} \int_L^R E^\text{em} \cdot dr + \frac{e}{\hbar} V
\]

The balance of the chemical potential difference and the electric field in the insulator region of the junction requires

\[
V = -\int_L^R E^\text{em} \cdot dr
\]

Thus, we have

\[
\dot{\phi}_J = \frac{2e}{\hbar} V
\]
Actually, $E^{em}$ contains a contribution from the radiation field with frequency $f$; however, it does not change the average voltage $V$. Thus, this relation is valid in this averaged sense.

A dc current is generated when the condition

$$\frac{2e}{h} V = 2\pi f n$$  \hspace{1cm} (63)

is satisfied, where $n$ is an integer. This relation is equal to the one in Eq. (58), and gives rise to the voltage quantization

$$V = \frac{hf}{2e} n$$  \hspace{1cm} (64)

observed as "Shapiro steps"\textsuperscript{16}.

The applied radiation field actually plays two roles; one is the creation of the instanton that generate the chemical potential difference in Eq. (58), and the other is the maintenance of the dc voltage by the resonance condition in Eq. (63).

V. WAVE-PACKET DYNAMICS OF BLOCH ELECTRONS IN THE PRESENCE OF RASHBA SPIN-ORBIT INTERACTION AND MAGNETIC FIELD

In the following sections, we present a possible mechanism for the appearance of spin-twisting itinerant motion of electrons in the BCS superconductors. When this motion is realized, the energy minimizing wave function becomes multi-valued with respect to electron coordinates. Then, the wave function has the from in Eq. (10) with non-trivial Berry connection.

The normal state of the BCS superconductors is a band metal. It exhibits quantum oscillations when a magnetic field is applied. This oscillation is due to the reorganization of electronic states near the Fermi surface. In this section, we examine this reorganization in the presence of the Rashba spin-orbit coupling.

In order to include the effect of the magnetic field $B^{em} = \nabla \times A^{em}$ that gives rise to the cyclotron motion, we use the wave-packet dynamics formalism\textsuperscript{23}. We consider electrons in a single band and denote its Bloch wave as

$$|\psi_q\rangle = e^{i\mathbf{q} \cdot \mathbf{r}} |u_q\rangle$$  \hspace{1cm} (65)

where $\mathbf{q}$ is the wave vector and $|u_q\rangle$ is the periodic part of the Bloch wave.
\( |u_q| \) satisfies the Schrödinger equation,

\[
H_0[q]|u_q| = \mathcal{E}(q)|u_q|,
\]

(66)

where \( H_0 \) is the zeroth order single-particle Hamiltonian for an electron in a periodic potential.

According to the wave packet dynamics formalism \( H_0[q] \) is modified as

\[
H_0[q] \rightarrow H_0 \left[ q + \frac{e}{\hbar} \mathbf{A}^{em}(r) \right].
\]

(67)

in the presence of the magnetic field \( \mathbf{B}^{em} = \nabla \times \mathbf{A}^{em} \).

Using the Bloch waves, a wave-packet centered at coordinate \( r_c \) and with central wave vector \( q_c \) is expressed as

\[
\langle r|(q_c, r_c)\rangle = \int d^3q a(q, t) e^{\frac{i}{\hbar} \tau(r) \cdot \sigma} e^{-i\frac{\chi(r)}{2}} \begin{pmatrix} \langle r|\psi_q \rangle \\ 0 \end{pmatrix}
\]

(68)

where \( a(q) \) is a distribution function, \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) is the vector of Pauli matrices, and \( \tau(r) \) describes the direction of spin.

Note that

\[
e^{\frac{i}{\hbar} \tau(r) \cdot \sigma} = I \cos \frac{\tau}{2} + i e_{\tau} \cdot \sigma \sin \frac{\tau}{2}
\]

(69)

produces the rotation \( \tau = |\tau| \) around the axis \( e_{\tau} \), where \( e_{\tau} \) is the unit vector in the direction of \( \tau \). When a spin-vortex exists, \( \tau \) shifts by \( 2\pi n \) (\( n \) is an integer) around the center of it; thus, if \( n \) is odd, sign change occurs for \( e^{\frac{i}{\hbar} \tau(r) \cdot \sigma} \), making it multi-valued. \( \chi(r) \) is an angular variable that makes the wave function single-valued as a function of \( r \) by compensating this sign change.

The distribution function \( a(q, t) \) satisfies the normalization

\[
\int d^3q |a(q, t)|^2 = 1
\]

(70)

and the localization condition in \( k \) space,

\[
\int d^3q q |a(q, t)|^2 = q_c
\]

(71)

The distribution of \( |a(q, t)|^2 \) is assumed to be narrow compared with the Brillouin zone size so that \( q_c \) can be regarded as the central wave vector of the wave packet.
The wave packet is also localized in $r$ space around the central position $r_c$:

$$ r_c = \langle (q_c, r_c) | r | (q_c, r_c) \rangle. \quad (72) $$

The crucial ingredient for realizing the spin-twisting itinerant motion is the Rashba spin-orbit interaction. We include the following term in the Hamiltonian

$$ H_{so} = \lambda(r) \cdot \frac{\hbar \sigma}{2} \times (\hat{p} - q A^{em}(r)), \quad (73) $$

where $\lambda(r)$ is the spin-orbit coupling vector (its direction is the internal electric field direction), $r$ is the spatial coordinates, $\hat{p} = -i\hbar \nabla$ is the momentum operator, and $q = -e$ is electron charge.

Let us construct the Lagrangian $L'(r_c, \dot{r}_c, q_c, \dot{q}_c)$ using the time-dependent variational principle,

$$ L' = \langle (q_c, r_c) | i\hbar \frac{\partial}{\partial t} - H | (q_c, r_c) \rangle. \quad (74) $$

For convenience sake, we introduce another Lagrangian $L$ that is related to $L'$ as

$$ L = L' - \hbar \frac{d}{dt} [\gamma(q_c, t) - r_c \cdot q_c], \quad (75) $$

where $\gamma$ is the phase of $a(q, t) = |a(q, t)| e^{-i\gamma(q, t)}$.

By following procedures for calculating expectation values for operators by the wave packet\textsuperscript{23}, $L$ is obtained as

$$ L = -\mathcal{E} \left( q_c + \frac{e}{\hbar} A^{eff}(r_c) \right) + \hbar q_c \cdot \dot{r}_c + i\hbar \left\langle u_q \left| \frac{du_q}{dt} \right\rangle \right. $$

$$ + \hbar \lambda(r_c) \cdot \left[ s(r_c) \times \left( q_c + \frac{e}{\hbar} A^{eff}(r_c) \right) \right], \quad (76) $$

where $s(r_c)$ is the expectation value of spin for the wave packet centered at $r_c$ given by

$$ s(r_c) = \frac{\hbar}{2} \langle (q_c, r_c) | \sigma | (q_c, r_c) \rangle. \quad (77) $$

We introduce the gauge invariant wave vector $k_c$,

$$ k_c = q_c + \frac{e}{\hbar} A^{eff}(r_c) \quad (78) $$

and change the dynamical variables from $q_c, \dot{q}_c$ to $k_c, \dot{k}_c$\textsuperscript{23}. 

17
Then, the Lagrangian with dynamical variables \( r, \dot{r}, k, \dot{k} \) is given by
\[
L(r, \dot{r}, k, \dot{k}) = -\mathcal{E}(k) + \hbar \lambda(r) \cdot [s(r) \times k] \\
+ \hbar \left[ k - \frac{e}{\hbar} \mathbf{A}^{\text{eff}}(r) \right] \cdot \dot{r} + i\hbar \dot{k} \cdot \left( u_q \frac{\partial u_q}{\partial q} \right)_{q=k} 
\]
Using the above Lagrangian \( L \), the following equations of motion are obtained:
\[
\dot{r} = \frac{1}{\hbar} \frac{\partial \mathcal{E}}{\partial k} + \lambda(r) \times s(r) - \dot{k} \times \Omega, 
\]
\[
\dot{k} = \frac{\partial}{\partial r} [\lambda(r) \times s(r) \cdot k] - \frac{e}{\hbar} \dot{r} \times B^{\text{em}},
\]
where \( \Omega \) is the Berry curvature in \( k \) space defined by
\[
\Omega = i\hbar \nabla_q \times \langle u_q | \nabla_q | u_q \rangle.
\]
In the following, we consider the case where \( \Omega = 0 \). Then, Eq. (80) becomes
\[
\dot{r} = \frac{1}{\hbar} \frac{\partial \mathcal{E}(k)}{\partial k} + \lambda(r) \times s(r).
\]
Using Eq. (83), and (81) becomes,
\[
\dot{k} = \frac{\partial}{\partial r} \left[ \left( \dot{r} - \frac{1}{\hbar} \frac{\partial \mathcal{E}(k)}{\partial k} \right) \cdot k \right] - \frac{e}{\hbar} \dot{r} \times B^{\text{em}} \\
= -\frac{e}{\hbar} \dot{r} \times B^{\text{em}}
\]
Eqs. (83) and (84) indicate that the wave packet exhibits cyclotron motion for the electron in the band with energy
\[
\mathcal{E}(k) + \hbar \lambda(r) \times s(r) \cdot k
\]
VI. THE PAIRING ENERGY GAP

In stead of the pairing between single particle states \( (k \uparrow) \) and \( (-k \downarrow) \), we consider the pairing between \( (k, s_0(r)) \) and \( (-k, -s_0(r)) \). We will obtain the pairing energy gap at \( r \) by treating the wave packets with \( k \) in each coarse-gained cell at \( r \) as basis states.

The single-particle energy for the states \( (k, s_0(r)) \) and \( (-k, -s_0(r)) \) are given by
\[
\mathcal{E}_+(k, r) = \mathcal{E}(k) + \hbar \lambda(r) \times k \cdot s_0(r) 
\]
where $\mathcal{E}(\mathbf{k}_c) = \mathcal{E}(-\mathbf{k}_c)$ is assumed.

Another pairing of states $(\mathbf{k}_c, -\mathbf{s}_0(\mathbf{r}_c))$ and $(-\mathbf{k}_c, \mathbf{s}_0(\mathbf{r}_c))$ are possible. Their single-particle energy is

$$
\mathcal{E}_-(\mathbf{k}_c, \mathbf{r}_c) = \mathcal{E}(\mathbf{k}_c) - \hbar \lambda(\mathbf{r}_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(\mathbf{r}_c)
$$

(87)

Let us briefly review the BCS theory. The model Hamiltonian is given by $H_{\text{kin}} + H_{\text{int}}$, where $H_{\text{kin}}$ is the kinetic energy given by

$$
H_{\text{kin}} = \sum_{\mathbf{k}_\sigma} \xi_0(\mathbf{k}) c_{\mathbf{k}_\sigma}^\dagger c_{\mathbf{k}\sigma}
$$

(88)

$\xi(\mathbf{k})$ is the energy measured from the Fermi energy $\mathcal{E}_F$ given by

$$
\xi_0(\mathbf{k}) = \mathcal{E}(\mathbf{k}) - \mathcal{E}_F
$$

(89)

and $H_{\text{int}}$ is the interaction energy given by

$$
H_{\text{int}} = \frac{1}{2} \sum_{\mathbf{k}\ell} V_{\mathbf{k}\ell} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{\ell}\downarrow} c_{\mathbf{\ell}\uparrow}.
$$

(90)

The electron pairing occurs between electrons near the Fermi surface since attractive $V_{\mathbf{k}\ell}$ only exists in that region. In the BCS interaction, $V_{\mathbf{k}\ell}$ is nonzero ($V_{\mathbf{k}\ell} = -g$) only when $|\xi_0(\mathbf{k})|, |\xi_0(\mathbf{\ell})| < \hbar \omega_D$ ($\omega_D$ is the Debye frequency) is satisfied. Then, $\Delta_k$ becomes independent of $\mathbf{k}$, and we express it as $\Delta$.

The superconducting state is given by the following state vector,

$$
|\text{BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|\text{vac}\rangle.
$$

(91)

This state exploits the attractive interaction between electron pairs $(\mathbf{k} \uparrow)$ and $(-\mathbf{k} \downarrow)$ and the following energy gap equation is obtained,

$$
\Delta = g \sum_{|\xi_0(\ell)| < \hbar \omega_D} u_{\ell} v_{\ell}
$$

(92)

and $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are parameters given using $\Delta$ and $\xi(\mathbf{k})_0$ as

$$
u_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left( 1 + \frac{\xi_0(\mathbf{k})}{\sqrt{\xi_0^2(\mathbf{k}) + \Delta_k^2}} \right)^{1/2}
$$

(93)

and

$$
v_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left( 1 - \frac{\xi_0(\mathbf{k})}{\sqrt{\xi_0^2(\mathbf{k}) + \Delta_k^2}} \right)^{1/2},
$$

(94)
respectively.

The total energy by the formation of the energy gap is given by

\[ E_{\text{BCS}}^{\text{n}} = E_{\text{BCS}}^{\text{n}} - \frac{1}{2} N(0) \Delta^2 \] (95)

where \( E_{\text{BCS}}^{\text{n}} \) is the normal state energy, and \( N(0) \) is the density of states at the Fermi energy\(^{\dagger}\).

Now, we come back to the pairing of \((k_c, s_0(r_c))\) and \((-k_c, -s_0(r_c))\), and also \((k_c, -s_0(r_c))\) and \((-k_c, s_0(r_c))\). The parameters for the pairing and energy gap are now functions of \(k_c\) and \(r_c\); \(u_k\) and \(v_k\) are replaced by \(u_\pm(k_c, r_c)\) and \(v_\pm(k_c, r_c)\) given by

\[ u_\pm(k_c, r_c) = \frac{1}{\sqrt{2}} \left( 1 + \frac{\xi_\pm(k_c, r_c)}{\sqrt{\xi^2_\pm(k_c, r_c) + \Delta^2(r_c)}} \right)^{1/2}, \] (96)

\[ v_\pm(k_c, r_c) = \frac{1}{\sqrt{2}} \left( 1 - \frac{\xi_\pm(k_c, r_c)}{\sqrt{\xi^2_\pm(k_c, r_c) + \Delta^2(r_c)}} \right)^{1/2}, \] (97)

where

\[ \xi_\pm(k) = E_\pm(k) - E_F = \xi_0(k_c) \pm \hbar \lambda(r_c) \times k_c \cdot s_0(r_c) \] (98)

and the gap function \( \Delta(r_c) \) is the solution of the gap equation given by

\[
\begin{aligned}
\Delta(r_c) &= \frac{g}{2} \sum_{|\xi_0(\ell)| < \hbar \omega_D} \left\{ u_+ (\ell_c, r_c) v_+ (\ell_c, r_c) + u_- (\ell_c, r_c) v_- (\ell_c, r_c) \right\} \\
&= \frac{g \Delta(r_c)}{4} \sum_{|\xi_0(\ell)| < \hbar \omega_D} \left\{ \frac{1}{\sqrt{\xi^2_\pm(k_c, r_c) + \Delta^2(r_c)}} + \frac{1}{\sqrt{\xi^2_\pm(k_c, r_c) + \Delta^2(r_c)}} \right\} \\
&\approx \frac{g \Delta(r_c)}{4} \sum_{|\xi_0(\ell)| < \hbar \omega_D} \left\{ \frac{2}{\sqrt{\xi^2_0(k_c, r_c) + \Delta^2(r_c)}} - \lambda^2 [\xi^2_0(k_c, r_c) + \Delta^2(r_c)]^{3/2} \right\} \\
&\approx \frac{g \Delta(r_c) N(0; r_c)}{4} \int_{-\hbar \omega_D}^{\hbar \omega_D} de \left\{ \frac{2}{\sqrt{e^2 + \Delta^2(r_c)}} - \frac{\lambda^2}{[e^2 + \Delta^2(r_c)]^{3/2}} \right\} \\
&\approx g \Delta(r_c) N(0; r_c) \left\{ \log \frac{2\hbar \omega_D}{\Delta} - \frac{\lambda^2}{\Delta^2} \right\}
\end{aligned}\] (99)

where \( N(0; r_c) \) is the density of states at the Fermi energy in the coarse grained cell of center \( r_c \).
Then, we have
\[
\Delta(r_c) \approx 2\hbar\omega_D \exp\left(-\frac{1}{g N(0; r_c)} - \frac{\lambda^2}{\Delta_0^2}\right); \quad \Delta_0(r_c) = 2\hbar\omega_D \exp\left(-\frac{1}{g N(0; r_c)}\right) \tag{100}
\]
where we assume that \(\hbar\omega_D \gg \Delta\). If the spin-orbit interaction parameter \(\lambda\) is significantly smaller than \(\Delta_0\), the gap is the same as the original pairing. The gap \(\Delta\) is reduced by the spin-orbit interaction, generally.

VII. THE KINETIC ENERGY WITH RASHBA INTERACTION AND LONDON EQUATION

The kinetic energy density including the Rashba interaction is given by
\[
2 \sum_k \xi_-(k, r)v^2_k(k, r) + 2 \sum_k \xi_+(k, r)v^2_+(k, r) \tag{101}
\]
For simplicity, we approximate it using the Fermi distribution functions \(f(\epsilon) = (1 + e^{\epsilon/k_BT})^{-1}\) \((k_B\) is Boltzmann’s constant) and density of states \(N(\epsilon; r_c)\) as
\[
\int \frac{N(\epsilon; r_c)}{2} \left\{ [\epsilon + \hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)] f(\epsilon + \hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)) + [\epsilon - \hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)] f(\epsilon - \hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)) \right\} d\epsilon
\approx \int \frac{N(\epsilon; r_c)}{2} \left\{ [\epsilon + \hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)] f(\epsilon + \hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)) + f(\epsilon - \hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)) \right\} d\epsilon
- \int \frac{N(\epsilon; r_c)}{2} \left\{ 2\epsilon f(\epsilon) + 2 |\hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)|^2 \frac{\partial f(\epsilon)}{\partial \epsilon} \right\} d\epsilon \tag{102}
\]
At temperature \(T = 0\), \(\frac{\partial f(\epsilon)}{\partial \epsilon} = -\delta(\epsilon)\); thus, the above becomes,
\[
\int d\epsilon N(\epsilon; r_c) f(\epsilon) d\epsilon - N(0; r_c) |\hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)|^2 \tag{103}
\]
The first term may be approximated as
\[
\int d\epsilon N(\epsilon; r_c) f(\epsilon) \approx \sum_{\xi_0(q)<0} \frac{\hbar^2}{2m} \left[ \mathbf{q} + \frac{e}{\hbar} \mathbf{A}^{\text{eff}} \right]^2 \approx \sum_{q < q_f} \frac{\hbar^2}{2m} q^2 + \frac{e^2 \rho(r_c)}{2m} |\mathbf{A}^{\text{eff}}|^2 \tag{104}
\]
assuming that the term linear in \(\mathbf{q}\) cancels out.

The second term may be approximated as
\[
-N(0; r_c) |\hbar\lambda(r_c) \times \mathbf{k}_c \cdot \mathbf{s}_0(r_c)|^2 \approx - \sum_{\xi_0(q)=0} |\hbar\lambda(r_c) \times [\mathbf{q} + \frac{e}{\hbar} \mathbf{A}^{\text{eff}}] \cdot \mathbf{s}_0(r_c)|^2
\approx -\hbar^2 \sum_{\xi_0(q)=0} |\lambda(r_c) \times \mathbf{q} \cdot \mathbf{s}_0(r_c)|^2 - \hbar^2 N(0; r_c) \left| \lambda(r_c) \times \mathbf{s}_0(r_c) \cdot \mathbf{A}^{\text{eff}} \right|^2 \tag{105}
\]
assuming that the term linear in $q$ cancels out.

To minimize the kinetic energy, $s_0$ is so chosen to satisfy

$$\lambda(r) \times s_0(r) \parallel A^{\text{eff}}(r)$$

(106)

Then, the current density is given by

$$j_{\text{tot}}(r) = -e^2 \left[ \frac{\rho(r)}{m} - N(0; r)|\lambda(r) \times s_0(r)|^2 \right] A^{\text{eff}}(r)$$

(107)

where the contribution from the energy gap term is neglected by assuming it is negligible. This is the London equation, and the system should exhibit the Meissner effect.

VIII. CRITICAL LOOK AT THE GAUGE INVARIANCE PROBLEM IN THE BCS THEORY

In the original BCS calculation, the Meissner effect is explained as a linear response to an applied magnetic field by treating $A^{\text{em}} \neq 0$ as a perturbation for the wave function obtained for the gauge $A^{\text{em}} = 0$.

The BCS employed the following gauge,

$$\nabla \cdot A^{\text{em}} = 0; \quad A^{\text{em}} = 0 \quad \text{if the magnetic field is zero.}$$

(108)

The obtained current was not gauge invariant, and the validity of using the gauge $\nabla \cdot A^{\text{em}} = 0$ was intensively studied by a number of researchers, and believed to be solved. However, the misfit of the ac Josephson effect indicates the necessity for the new mechanism for the supercurrent generation. Thus, we reexamine this problem from the viewpoint of the new supercurrent generation mechanism.

First, we consider the gauge choice $\nabla \cdot A^{\text{em}} = 0$. In the present new theory, the vector potential $A^{\text{eff}}$ appears in physical observables instead of $A^{\text{em}}$. It is gauge invariant, thus the choice of the gauge $\nabla \cdot A^{\text{em}} = 0$ does not cause any problems.

Second, we take up the second assumption, ‘$A^{\text{em}} = 0$ if the magnetic field is zero’, in Eq. (108). The condition $\nabla \cdot A^{\text{em}} = 0$ still leaves arbitrariness of the gauge for the zero magnetic field case; for example,

$$A^{\text{em}} = A_0 = \text{const.}$$

(109)
also fulfills the zero magnetic field and $\nabla \cdot \mathbf{A}^\text{em} = 0$; however, if this vector potential is employed, it yields the Meissner current for zero magnetic field.

This problem is a very serious one in the calculation of the wave vector $\mathbf{q} = 0$ Fourier component of $\mathbf{j}$. In the BCS theory, if $\mathbf{q} \to 0$ limit is taken, we have the following $\mathbf{q} = 0$ Fourier component of the current

$$i(0) = \Lambda a^\text{em}(0) \quad (110)$$

where $\Lambda$ is a parameter, and $i(0)$ and $a^\text{em}(0)$ are $\mathbf{q} = 0$ Fourier components of $\mathbf{j}$ and $\mathbf{A}^\text{em}$, respectively. This corresponds to Eq. (5.26) in the BCS paper\textsuperscript{1}. If we use a different gauge, this $a^\text{em}(0)$ can be removed. Thus, this current carrying state becomes a currentless state. Since the currentless state is lower in energy than the current carrying state, and $a^\text{em}(0)$ gives rise to zero magnetic field, the limit just yields the currentless ground state for zero magnetic field. Thus, the explanation of the Meissner effect in the BCS theory actually gives a currentless state.

Actually, if the condition in Eq. (108) is replaced by

$$\nabla \cdot \mathbf{A}^\text{em} = 0; \quad \mathbf{A}^\text{eff} = 0 \quad \text{if the magnetic field is zero.} \quad (111)$$

this problem is lifted. The constant vector potential is removed by taking $\frac{\hbar}{2e} \nabla \chi = -\mathbf{A}^\text{em} = -\mathbf{A}_0$.

Another problem arises if we consider the situation where the magnetic flux quantization is observed. In this case, the vector potential in the magnetic field expelled region is given by

$$\mathbf{A}^\text{em} = -\frac{\hbar}{2e} \nabla g \quad (112)$$

where $g$ is an angular variable with period $2\pi$. In this case, we may set $\chi = -g$ from $\mathbf{A}^\text{eff} = 0$.

The above results suggest that the BCS results obtained from the perturbation theory using $\mathbf{A}^\text{em}$ as small parameters may be valid if $\mathbf{A}^\text{em}$ is replace by $\mathbf{A}^\text{eff}$ and taking them as the results for the case of very small spin-orbit interaction.

**IX. CONCLUDING REMARKS**

When Schrödinger solved the Schrödinger equation for hydrogen atom, he required the wave function to be a single-valued function of the electron coordinate\textsuperscript{32}. The single-valued
requirement of the wave function is a postulate which may be rephrased as the existence of the basis composed of the eigenfunctions $|\mathbf{r}\rangle$ for the coordinate operator $\hat{\mathbf{r}}$. Here, $|\mathbf{r}\rangle$ satisfies

$$\hat{\mathbf{r}}|\mathbf{r}\rangle = r|\mathbf{r}\rangle,$$

(113)

where $r$ is the eigenvalue uniquely determined by $|\mathbf{r}\rangle$. With this basis, the wave function for a state vector $|\varphi\rangle$ is given by $\langle \mathbf{r}|\varphi\rangle$, which must be single-valued with respect to the coordinate since $\mathbf{r}$ is uniquely determined by $|\mathbf{r}\rangle$.33

Before the Schrödinger equation was put forward by Schrödinger, quantum mechanics was formulated as the Matrix mechanics by Heisenberg.34 Schrödinger showed that his version of quantum mechanics can be transformed into the Heisenberg’s Matrix version by expressing the linear operators by matrices using the basis functions; then, the Schrödinger’s differential equation can be transformed into the matrix equation or the integral equation if the indices of the matrix elements are continuous.35

However, von Neumann argued that these two forms are not equivalent; there are situations where differential equations cannot be simply transformed into integral equations, but require Dirac delta functions.36 In this respect, the $\pi$-flux Dirac string is such an object. Actually, Dirac noticed the possibility for the appearance of a phase factor in the displacement operator, and also considered the possibility of the appearance of the singular phase factor in the wave function.18 The Berry phase factor in the present work can be viewed as an example of such a phase factor. The important point is that this phase factor is necessary to satisfy the single-valued requirement of the wave function as a function of coordinates, and the conservation of local charge.

Hohenberg an Kohn argued that the ground state can be obtained from the electron density alone.19 However, their argument tacitly assumes the absence of singularities in the ground state wave function that might arise from many-body effects. When such singularities exist, we need to specify how to handle them; namely, we need to require that the wave function to be a single-valued function and the current calculated by it conserves the local charge. Thus, the ground state cannot be obtained solely by the electron density, but require the Berry connection. The present work indicates that if the Berry connection is included, the phenomenon of superconductivity is a natural consequence.

There is a connection between the Berry phase considered in the present work and the change of the $U(1)$ phase factor on the wave function when the gauge transformation is
performed. This change is conveniently incorporated if we use the effective gauge potential in materials ($\phi_{\text{eff}}, A_{\text{eff}}$) given in Eqs. (41) and (42); it is invariant with respect to the choice of the gauge adopted in the ordinary electromagnetic gauge potential ($\phi_{\text{em}}, A_{\text{em}}$) due to the fact that the arbitrariness in the gauge is absorbed in the Berry connection. It is noteworthy that the introduction of the effective gauge potential in materials solves a long-standing puzzling problem of the ‘flux rule’, the Faraday’s induction formula is consist of one of the Maxwell equations and the Lorentz force calculation$^{38}$, as due to the the duality that a $U(1)$ phase factor added on a wave function describes a whole system motion and also plays the role of a $U(1)$ gauge potential$^{39}$. We expect there will be more cases where ($\phi_{\text{eff}}, A_{\text{eff}}$) is useful.

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