Berry Connection from Many-Body Wave Functions and Superconductivity: Calculations by the Particle Number Conserving Bogoliubov-De Gennes Equations

Hiroyasu Koizumi1 · Alto Ishikawa2

Received: 11 May 2021 / Accepted: 28 July 2021 / Published online: 14 September 2021 © The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2021

Abstract

A fundamentally revised version of superconductivity theory has been put forward since the standard theory of superconductivity based on the BCS theory cannot explain superconductivity in cuprates discovered in 1986, and reexaminations on several experimental results on the conventional superconductors indicate the necessity for a fundamental revision. The revision is made on the origin of the superconducting phase variable, which is attributed to a Berry connection arising from many-body wave functions. With this revision, the theory can be cast into a particle number conserving formalism. We have developed a method to calculate superconducting states with the Berry connection using the particle number conserving version of the Bogoliubov-de Gennes equations.

Keywords Berry connection · The particle number conserving Bogoliubov-de Gennes equations · Berry phase

1 Introduction

In order to orient the fundamental revision of the standard theory of superconductivity presented in this work, we begin with the basis of the current standard theory of superconductivity, the BCS theory [1]. Let \( c_{k\sigma}^{\dagger} \) be the creation operator for the electron in a metal with wave vector \( k \) and spin \( \sigma \). The BCS theory uses the ground state composed of different particle number states

\[
|BCS(\theta)\rangle = \prod_k \left( u_k + v_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} e^{i\theta} \right) |\text{vac}\rangle
\]

where \( u_k \) and \( v_k \) are real parameters that satisfy \( u_k^2 + v_k^2 = 1 \), and \( |\text{vac}\rangle \) is the vacuum that satisfies

\[
c_{k\sigma} |\text{vac}\rangle = 0
\]

The ground state \( |BCS(\theta)\rangle \) is a linear combination of different particle number states, thus, breaks the conservation of the particle number. It has a degeneracy with respect to the choice of \( \theta \), resulting in the breakdown of the global \( U(1) \) gauge invariance; the invariance of the physical state by the change \( c_{k\sigma} \rightarrow e^{-i\theta} c_{k\sigma} \), \( c_{k\sigma}^{\dagger} \rightarrow e^{i\theta} c_{k\sigma}^{\dagger} \), where \( \theta \) is a constant, is violated.

Using the particle number non-conserving formalism, the BCS theory provides a way to calculate the superconducting transition temperature as the energy gap formation temperature by the electron-pairing.

A salient feature of the BCS theory is the presence of the Bogoliubov excitation with an energy gap formed by the electron-pairing [2]. This excitation is most clearly seen if we use the Bogoliubov operators given by

\[
\gamma_{k\uparrow} = u_k e^{-i\theta} c_{k\uparrow} - v_k e^{i\theta} c_{-k\downarrow}^{\dagger}
\]

\[
\gamma_{-k\downarrow} = u_k e^{-i\theta} c_{-k\downarrow} + v_k e^{i\theta} c_{k\uparrow}^{\dagger}
\]

where they satisfy

\[
\gamma_{k\uparrow} |BCS(\theta)\rangle = 0, \quad \gamma_{-k\downarrow} |BCS(\theta)\rangle = 0
\]

This indicates that the superconducting state is the “vacuum of the Bogoliubov quasiparticles”, which replaces Eq. (2).

Using the Bogoliubov operators, the BCS Hamiltonian can be cast into the following,

\[
H_{BCS} = \sum_{k,\sigma} E_k \gamma_{k\sigma}^{\dagger} \gamma_{k\sigma} + E_{\text{const}}
\]
where \( E_{\text{const}} \) is the ground state energy, \( E_k \) is the excitation energy given by

\[
E_k = \sqrt{(E(k))^2 + \Delta_k^2}
\]

with \( E(k) \) being the energy of Bloch electrons measured from the Fermi energy; \( \Delta_k \) is the energy gap given by

\[
\Delta_k = 2E_ku_kv_k, \quad v_k^2 = \frac{1}{2}\left(1 - \frac{E(k)}{E_k}\right), \quad w_k^2 = \frac{1}{2}\left(1 + \frac{E(k)}{E_k}\right)
\]

\( E_k \) explains the energy spectrum with a gap observed in superconductors.

In the BCS theory, the induced current by a magnetic field is calculated as a linear response to \( A^{\text{em}} \). The obtained current is not gauge invariant, and the gauge invariance of the induced current became a big issue. After seminal works by Anderson [3, 4], a final resolution was provided by Nambu [5], culminating to the idea “spontaneous gauge symmetry breaking”. Nambu showed that the Nambu-Goldstone mode appears due to the degeneracy of the ground state with respect to the choice of \( \theta \), and the inclusion of this mode retrieves the gauge invariance.

Before the discovery of high temperature superconductivity in 1986 [6], the BCS theory and its extensions have been very successful, thus, it was believed that superconductivity was a well-understood and solved problem. However, the cuprate superconductivity is markedly different from the BCS superconductivity in a number of ways; for example, the magnetism coexists with superconductivity in the cuprate [7]; the superconducting transition temperature is not the stabilizing temperature for loop currents of \( \xi_{\text{GL}} \) size in optimally doped sample of the cuprates [8], where \( \xi_{\text{GL}} \) is the superconducting coherence length of the Ginzburg-Landau theory [9, 10]; the charge carriers in the room temperature become small polarons at low temperatures [11].

Since the cuprate superconductivity is so different from the BCS superconductivity, a theory significantly departs from the standard one is expected to be needed to explain it. The superconducting state transition temperature indicates the importance of \( \xi_{\text{GL}} \)-sized loop currents [8]. Thus, one of the present author has put forward a theory where \( \xi_{\text{GL}} \)-sized spin-vortices and loop currents appear around the small polarons in the bulk [12–17]. A notable point of this theory is that spin-vortices around small polarons are expected to exit in the cuprates [11, 18], and explain the magnetic excitation spectrum observed by inelastic neutron scattering [19, 20]. The loop current creation is due to the appearance of a Berry connection from the spin-vortex formation.

Efforts toward the elucidation of the cuprate superconductivity have led some researchers to reexamine superconductivity from very fundamental levels. Those efforts revealed the existence of some fundamental experimental facts that disagree with the standard theory even in conventional superconductors [21]. We would like to point out five of them below:

1) Supercurrent in the standard theory contradicts the reversible superconducting-normal phase transition in a magnetic field observed in type I superconductors [22–24].

2) Experiments indicate that the mass in the London moment is the free electron mass, however, the standard theory predicts it to be an effective mass [25, 26].

3) In the standard theory, the breakdown of the global \( U(1) \) gauge invariance or the non-conservation of the particle number is essential. However, it is sensible to consider that the particle number is conserved in an isolated superconductor [27–30].

4) The derivation of the ac Josephson effect takes into account only the half of the contributions [12, 31, 32].

5) The absence of a dissipative quantum phase transition in Josephson junctions [33–35].

In order to remedy above problems, we have developed the particle number conserving Bogoliubov formalism. In this formalism, the \( U(1) \) phase variable that arises from the global \( U(1) \) gauge symmetry braking in the standard theory is replaced by the Berry phase arising from many-body wave functions [36].

Let us explain the essence of the new theory below. In the new formalism, the departure from the current standard theory begins with replacing \( e^{\pm i\theta} \) in Eq. (3) by the number changing operators \( e^{\pm \frac{i}{2} \chi} \) [26, 31, 36]. They are defined using the Berry phase from many-body wave functions [36]; \( e^{\frac{i}{2} \chi} \) increases the number of particles participating in the collective mode arising from the Berry phase by one, and \( e^{-\frac{i}{2} \chi} \) decreases by one.

Then, the Bogoliubov transformation in Eq. (3) becomes

\[
\gamma_{\mathbf{k} \uparrow} = u_k e^{\frac{i}{2} \chi} c_{\mathbf{k} \uparrow} - v_k e^{-\frac{i}{2} \chi} c_{-\mathbf{k} \downarrow}
\]

\[
\gamma_{-\mathbf{k} \downarrow} = u_k e^{\frac{i}{2} \chi} c_{-\mathbf{k} \downarrow} + v_k e^{-\frac{i}{2} \chi} c_{\mathbf{k} \uparrow}
\]

The above Bogoliubov operators conserve particle numbers; terms like \( e^{\frac{i}{2} \chi} c_{\mathbf{k} \sigma} \) can be interpreted that the electron in the \( (\mathbf{k}, \sigma) \) single-particle mode is removed and added to the collective mode described by \( \chi \); those like \( e^{-\frac{i}{2} \chi} c_{\mathbf{k} \sigma}^\dagger \) create an electron in the \( (\mathbf{k}, \sigma) \) and subtract one from the collective mode of \( \chi \). Thus, the Bogoliubov operators cause the fluctuation of the number of electrons participating in the collective mode. The ground state is a total particle number fixed state and replaces the total...
number fluctuating state given by Eq. (1) in the standard theory [36].

In order to use the coordinate dependent functions as the basis single-particle wave functions other than plane waves, we use the label $n$ in stead of the wave number vector $k$. Then, the field operators are given by

$$\hat{\Psi}_\uparrow (r) = \sum_n e^{-\frac{i}{\hbar} \hat{A}(r)} \left( \gamma_{n\uparrow} u_n (r) - \gamma_{n\downarrow}^\dagger v^*_n (r) \right)$$

$$\hat{\Psi}_\downarrow (r) = \sum_n e^{-\frac{i}{\hbar} \hat{A}(r)} \left( \gamma_{n\downarrow} u_n (r) + \gamma_{n\uparrow}^\dagger v^*_n (r) \right)$$

(9)

The particle number conserving Bogoliubov operator $\gamma_{n\sigma}$ satisfies

$$\gamma_{n\sigma} |\text{Gnd}(N)\rangle = 0$$

(10)

where $|\text{Gnd}(N)\rangle$ is the ground state with the total number of particles $N$.

The ground state also satisfies

$$e^{\pm \frac{i}{\hbar} \hat{A}(r)} |\text{Gnd}(N)\rangle = e^{\pm \frac{i}{\hbar} \chi(r)} |\text{Gnd}(N \pm 1)\rangle$$

(11)

The phase factors $e^{\pm \frac{i}{\hbar} \chi(r)}$ give

$$\langle \text{Gnd}(N) | e^{\frac{i}{\hbar} \hat{A}(r_f)} e^{-\frac{i}{\hbar} \hat{A}(r_i)} |\text{Gnd}(N)\rangle = e^{\frac{i}{\hbar} \int_{r_i}^{r_f} \nabla \chi \cdot d\mathbf{r}}$$

(12)

indicating that the phase $\frac{i}{\hbar} \int_{r_i}^{r_f} \nabla \chi \cdot d\mathbf{r}$ is acquired when the particle travels from $\mathbf{r}_i$ to $\mathbf{r}_f$. This takes into account the effects from the vector potential of the Berry connection $A_{\text{fic}}$ given by

$$A_{\text{fic}} = -\frac{\hbar c}{2e} \nabla \chi$$

(13)

The main purpose of the present work is to demonstrate model calculations for properties of superconducting states, such as diamagnetic response current and persistent current generation by including $A_{\text{fic}}$ in the particle number conserving Bogoliubov-de Gennes formalism.

The organization of the present work is as follows:
In Section 2, we explain a model Hamiltonian used in this work. It is constructed as a model for the cuprate superconductivity, originally. In Section 3, the particle number conserving Bogoliubov-de Gennes equations are derived for the model Hamiltonian. In Section 4, the spin-vortex formation and multi-valued wave functions are explained. In Section 5, the appearance of the Berry connection due to the single-valued requirement of the wave function as a function of electron coordinates is explained. We also explain the way to calculate the Berry connection in this section. In Section 6, the results for the diamagnetic current produced by an application of a magnetic field are shown. In Section 7, the results for zero voltage current production by an external current feeding are shown. Lastly, in Section 8, we conclude the present work.

### 2 Model Hamiltonian

In this section, we explain a model that will be used in this work. This model is originally built to study the cuprate superconductivity. The purpose of the present work is to explain the new theory and how to use it; the validity of the model as a model for the cuprate superconductivity will be dealt elsewhere.

The model is composed of two layers, a surface layer and a bulk layer (see Fig. 1). The superconductivity occurs in the bulk; however, many experimental results show contributions from the surface region, thus, the surface layer effects must be included to interpret experiments. The experimental results seem to indicate that the small polaron formation and coexisting magnetic moment effects are strong in the bulk, however, they are weak in the surface region. Thus, we developed a model containing two layers to reproduce experimental results. It is also notable that although the electron-pairing does not occur in the bulk layer, supercurrent flows there in this model. This demonstrates that the primary importance for superconductivity is the appearance of the non-trivial Berry connection.

#### 2.1 Bulk Layer

The model for the bulk layer is constructed based on the fact that the parent compound is a Mott insulator [37], which is

![Fig. 1 Simply connected lattice constructed by removing some bonds for a two-layer model system. We consider the model with two $7 \times 7$ square lattices stacked in the $z$ direction. There are four small polarons in the bulk layer indicated by “M” and “A”. Each “M” indicates a center of a spin-vortex with winding number +1, and “A” a center of a spin-vortex with winding number −1](image-url)
well-described by the two-dimensional Hubbard model with large on-site repulsion

\[ U \gg t_1 \]  

(14)

where \( U \) is the on-site repulsion parameter and \( t_1 \) is the nearest neighbor hopping parameter. The bulk CuO\(_2\) plane of the cuprate is taken as a two-dimensional square lattice, where a copper atom resides at each site. Oxygenes that exist between copper atoms are not explicitly taken into account in the present model.

When holes are doped, they form small polarons in the bulk [11, 18]. At low temperatures, the mobility of the small polaron becomes very small.

The inelastic neutron scattering experiments indicate spin-wave excitations with spin lying in CuO\(_2\) plane [7]. Thus, the magnetic moment coexists with superconductivity in the bulk. The magnetic excitation spectrum has a hourglass-shaped dispersion, suggesting the existence of spin-stripes or spin-vortices [19, 20].

By taking into account the above observation, the following bulk Hamiltonian is constructed,

\[
H_{\text{behfs}} = -t_1 \sum_{\langle i,j \rangle,\sigma} [c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}] + U \sum_j c_{j\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{j\downarrow} + J_h \sum_j S_j \\
+ \lambda \sum_b \left[ (e_{h+y} c_{h-y} - c_{h+y}^\dagger e_{h-y}) + (e_{h-x} c_{h-x} - c_{h+x}^\dagger e_{h-x} ) + (e_{h+y} c_{h-x} + e_{h-x}^\dagger c_{h+y} ) + (e_{h+y}^\dagger c_{h-y} + e_{h-y} c_{h+y}^\dagger ) \right] \\
+ h.c. - \mu_{\text{bulk}} \sum_{j,\sigma} c_{j\sigma}^\dagger c_{j\sigma} 
\]

(15)

where \( c_{j\sigma}^\dagger \) and \( c_{j\sigma} \) are creation and annihilation operators for the electron at \( j \)th site with spin \( \sigma \), respectively.

In this Hamiltonian, the doped holes are assumed to form small polarons and immobile, thus, the effectively half-filled situation (EHFS) is realized, where the number of electrons and the number of accessible sites for the electrons are equal. We take the hole-occupied sites as inaccessible sites for electrons, thus, not included in the sums.

The first term describes the electron hopping with transfer integral \( t_1 \); \( \langle i, j \rangle \) indicates that the sum is taken over 1st nearest neighbor hoppings.

The second term describes the on-site Coulomb repulsion; \( U \) is significantly larger that \( t_1 \) (we adopt \( U = 8t_1 \) in the present work).

The third term describes the antiferromagnetic exchange interaction between electron spins around each doped hole; \( \langle i, j \rangle \) indicates that the sum is taken over pairs around holes, i.e., each hole (denoted by \( h \)) accompanies four sites around it (denoted by \( h-x, h+x, h-y \) and \( h+y \); they are the nearest neighbor sites of \( h \) in \(-x, +x, -y, \) and \(+y\) directions, respectively), and there are six site-pairs that contribute to \( \langle i, j \rangle \) for each doped hole. The parameter \( J_h \) is taken to be 0.5\( J_{\text{AF}} \) where \( J_{\text{AF}} = \frac{4t_1^2}{U} \) is the antiferromagnetic exchange parameter for the parent compound [38].

The fourth term is the Rashba interaction term [39], which we only include around the holes [40]; \( \lambda \) is the coupling parameter. The fifth term is the chemical potential term with \( \mu_{\text{bulk}} \) being the chemical potential for the bulk; the value of \( \mu_{\text{bulk}} \) controls the number of small polarons in the EHFS.

Components of the spin operator \( S_j = (S_j^x, S_j^y, S_j^z) \) are given by

\[
S_j^x = \frac{1}{2}(c_{j\uparrow}^\dagger c_{j\downarrow} + c_{j\downarrow}^\dagger c_{j\uparrow}) \\
S_j^y = \frac{i}{2}(-c_{j\uparrow}^\dagger c_{j\downarrow} + c_{j\downarrow}^\dagger c_{j\uparrow}) \\
S_j^z = \frac{1}{2}(c_{j\uparrow}^\dagger c_{j\uparrow} - c_{j\downarrow}^\dagger c_{j\downarrow}) 
\]

(16)

Since \( H_{\text{EHFS}} \) is too difficult to handle as it is, we use a mean field version of it

\[
H_{\text{EHFS}}^{\text{MF}} = -t_1 \sum_{\langle i,j \rangle,\sigma} [c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}] + U \sum_j c_{j\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{j\downarrow} + J_h \sum_j S_j \\
+ \lambda \sum_b \left[ (e_{h+y} c_{h-y} - c_{h+y}^\dagger e_{h-y}) + (e_{h+x} c_{h-x} - c_{h+x}^\dagger e_{h-x} ) + (e_{h+y} c_{h-x} + e_{h-x}^\dagger c_{h+y} ) + (e_{h+y}^\dagger c_{h-y} + e_{h-y} c_{h+y}^\dagger ) \right] \\
+ h.c. - \mu_{\text{bulk}} \sum_{j,\sigma} c_{j\sigma}^\dagger c_{j\sigma} 
\]

(17)

where \( \langle \hat{O} \rangle \) denotes the expectation value of the operator \( \hat{O} \). This Hamiltonian yields states with spin-vortices around small polarons (see Fig. 2). These spin-vortices induce loop currents called the “spin-vortex-induced loop currents”, due to the appearance of a non-trivial Berry connection.

### 2.2 Surface Layer

The Hamiltonian for the surface layer is following

\[
H_{\text{surf}} = -t_2 \sum_{\langle i,j \rangle,\sigma} [c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}] - t_2 \sum_{\langle i,j \rangle,\sigma} [c_{i\sigma}^\dagger c_{j\sigma}] \\
+ \text{H.c.} + U \sum_j c_{j\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{j\downarrow} - H_{\text{surf}} \sum_{j,\sigma} c_{j\sigma}^\dagger c_{j\sigma} 
\]

(18)

This is the Hubbard model including the second nearest neighbor hopping. The second nearest neighbor hopping
with the parameter $t_2$ is included to have a curved Fermi surface in the angle-resolved photoemission spectrum. We use $t_2 = -0.12t_1$ in this work.

The most important difference from the bulk Hamiltonian is the absence of the small polaron effect. The spin-orbit interaction term is also absent. The chemical potential $\mu_{\text{surf}}$ is so chosen that the bulk and surface hole densities are equal.

Since $H_{\text{surf}}$ is too difficult to handle as it is, we construct a mean-field version via the $t - J$ model [41] for the Hubbard model,

$$H_{\text{surf}}^{\text{MF}} = -t_1 \sum_{\langle i,j \rangle_{1,\sigma}} [(1 - \langle n_{i,-\sigma} \rangle)c_{i\sigma}^+c_{j\sigma}(1 - \langle n_{j,-\sigma} \rangle) + \text{H.c.}]$$

$$- \tau_2 \sum_{\langle i,j \rangle_{2,\sigma}} [(1 - \langle n_{i,-\sigma} \rangle)c_{i\sigma}^+c_{j\sigma}(1 - \langle n_{j,-\sigma} \rangle) + \text{H.c.}]$$

$$+ \sum_{\langle i,j \rangle_{1}} (\Delta_{ij}e^{-\frac{i}{2}\hat{\chi}_i}e^{-\frac{i}{2}\hat{\chi}_j}c_{i\uparrow}^+c_{j\downarrow} + \text{H.c.}) - \mu_{\text{surf}} \sum_{j,\sigma} c_{j\sigma}^+c_{j\sigma}$$

where the pairing amplitude or pair potential $\Delta_{ij}$ is defined as

$$\Delta_{ij} = - \frac{4t_2^2}{U} (e^{\frac{i}{2}\hat{\chi}_i}e^{\frac{i}{2}\hat{\chi}_j}(c_{j\downarrow}c_{i\uparrow} - c_{j\uparrow}c_{i\downarrow})) = \Delta_{ji}$$

(20)

Due to the presence of the number changing operators, $e^{\frac{i}{2}\hat{\chi}_i}$ and $e^{\frac{i}{2}\hat{\chi}_j}$, $\Delta_{ij}$ is obtained in the particle number conserving formalism. The appearance of the number changing operator is due to the spin-vortex formation in the bulk. To have the superconducting state, stable loop currents that can generate a macroscopic persistent current should be realized.

The pair potential $\Delta_{ij}$ gives rise to $d$-wave pairing gap, and explains the Fermi arc [42]. We would like to emphasize that the appearance of the $d$-wave pairing gap is secondary effect enabled by the appearance of the non-trivial Berry connection in the bulk. The Berry connection generates the collective mode for supercurrent, and particle number changing operators $e^{\pm \frac{i}{2}\hat{\chi}_i}$. The existence of the operators $e^{\pm \frac{i}{2}\hat{\chi}_i}$ make it possible to gain energy by the $d$-wave pairing gap formation.

### 2.3 Interlayer Hopping

The bulk and surface layers are connected by the interlayer hopping. The following is the inter-layer hopping Hamiltonian,

$$H_{\text{inter-layer}} = -t_3 \sum_{\langle i,j \rangle_{1,\sigma}} [(1 - \langle n_{i,-\sigma} \rangle)c_{i\sigma}^+c_{j\sigma}(1 - \langle n_{j,-\sigma} \rangle) + \text{H.c.}]$$

$$+ \frac{4t_2^3}{U} \sum_{\langle i,j \rangle_{2}} (S_{i\sigma} \cdot S_{j\sigma} - \frac{1}{4}n_{i\sigma}n_{j\sigma})$$

(21)
where an antiferromagnetic exchange interaction between spins in the bulk-layer and those in the surface-layer is included using a $t$-$J$ model approximation.

Since $H_{\text{inter-layer}}$ is still too difficult to handle, we use the following mean field version,

$$
H^\text{MF}_{\text{inter-layer}} = -t_5 \sum_{\langle i,j \rangle, \sigma} [(1 - \langle n_{i,\sigma} - \sigma \rangle) a_{i,\sigma}^\dagger a_{j,\sigma} (1 - \langle n_{j,\sigma} - \sigma \rangle) + \text{H.c.}]
$$

$$
= \frac{2t_5^2}{U} \sum_{\langle i,j \rangle} \left[ \sum_j \left( \langle S^z_j \rangle - i \langle S^+ \rangle c_{i,j}^\dagger c_{j,i} + \langle S^- \rangle c_{i,j}^\dagger c_{j,i} \right) + \frac{1}{2} \sum_{\langle i,j \rangle} \left( \langle S^z_j \rangle - \frac{1}{2} \langle n_{j,\sigma} \rangle c_{i,j}^\dagger c_{j,i} \right) \right]
$$

$$
= \frac{4t^2}{U} \sum_{\langle i,j \rangle} \left( (S^z_i - \langle S^z \rangle) \cdot (S^z_j - \langle S^z \rangle) + \frac{1}{2} \langle n_{j,\sigma} \rangle c_{i,j}^\dagger c_{j,i} \right) - \frac{4t^2}{U} \sum_{\langle i,j \rangle} \left( (S^z_i - \langle S^z \rangle) \cdot (S^z_j - \langle S^z \rangle) + \frac{1}{2} \langle n_{j,\sigma} \rangle c_{i,j}^\dagger c_{j,i} \right)
$$

$$
- \frac{4t^2}{U} \sum_{\langle i,j \rangle} \left( (S^z_i - \langle S^z \rangle) \cdot (S^z_j - \langle S^z \rangle) + \frac{1}{2} \langle n_{j,\sigma} \rangle c_{i,j}^\dagger c_{j,i} \right)
$$

$$
(22)
$$

We adopt $t_5 = 0.01t_1$ in the following calculations. Through this Hamiltonian, the non-trivial Berry connection generated in the bulk propagates in the surface.

### 2.4 The Total Hamiltonian for the Two-Layer Model

Over all, our model Hamiltonian is given by

$$
H_{\text{eff}} = H^\text{HF}_{\text{EHFS}} + H^\text{HF}_{\text{surf}} + H^\text{HF}_{\text{inter-layer}}
$$

$$
= \sum_{i,j,\sigma} h_{i,j,\sigma} c_i^\dagger c_j + \sum_{i,j} \left[ \Delta_{ij} e^{-\frac{j}{k_B T}} e^{-\frac{j}{k_B T}} c_i^\dagger c_j + \right.
$$

$$
\left. \Delta_{ij} e^{\frac{j}{k_B T}} e^{\frac{j}{k_B T}} c_i c_j \right] + E_{\text{const}}
$$

$$
(23)
$$

### 3 Particle Number Conserving Bogoliubov-de Gennes Equations

In order to obtain the particle number conserving Bogoliubov-de Gennes equations from $H_{\text{eff}}$ in Eq. (23), we perform the following Bogoliubov transformation

$$
c_{i} = \sum_n \left( u_{i}^n \right)^* \gamma_n + (u_{i}^n)^* \gamma_n^* e^{-\frac{j}{k_B T}}
$$

$$
c_{i} = \sum_n \left( u_{i}^n \right)^* \gamma_n + (u_{i}^n)^* \gamma_n^* e^{-\frac{j}{k_B T}}
$$

$$
(24)
$$

Using the Bogoliubov operators $\gamma_n$ and $\gamma_n^*$, $H_{\text{eff}}$ is expressed as

$$
H_{\text{eff}} = \sum_n E_n \gamma_n^* \gamma_n + E_{\text{const}}
$$

$$
(25)
$$

where $E_{\text{const}}$ is a constant and “$\sum_n$” denotes that the sum is taken over $E_n > 0$, and the ground state (Gnd) satisfies

$$
\gamma_n |\text{Gnd}\rangle = 0, \quad E_n > 0
$$

$$
(26)
$$

The Bogoliubov operators are fermion operators that satisfy

$$
\{\gamma_n, \gamma_m^\dagger\} = \delta_{nm}, \quad \{\gamma_n^\dagger, \gamma_m^\dagger\} = 0, \quad \{\gamma_n, \gamma_m\} = 0
$$

$$
(27)
$$

thus, the commutation relations

$$
[\gamma_n^\dagger, H_{\text{eff}}] = -E_n \gamma_n^\dagger, \quad [\gamma_n, H_{\text{eff}}] = E_n \gamma_n
$$

$$
(28)
$$

are obtained.

The following commutation relations are obtained between $H_{\text{eff}}$ and $c_{i,\sigma}$, $c_{i,\sigma}^\dagger$,

$$
[c_{i}^\dagger, H_{\text{eff}}] = \sum_j h_{i,j,\sigma} c_{j,\sigma}^\dagger + \sum_j \Delta_{ij} e^{-\frac{j}{k_B T}} e^{-\frac{j}{k_B T}} c_{j} +
$$

$$
[c_{i}^\dagger, H_{\text{eff}}] = -\sum_j h_{i,j,\sigma} c_{j,\sigma} + \sum_j \Delta_{ij} e^{-\frac{j}{k_B T}} e^{-\frac{j}{k_B T}} c_{j}^\dagger
$$

$$
[c_{i}^\dagger, H_{\text{eff}}] = \sum_j h_{i,j,\sigma} c_{j,\sigma} - \sum_j \Delta_{ij} e^{-\frac{j}{k_B T}} e^{-\frac{j}{k_B T}} c_{j} +
$$

$$
[c_{i}^\dagger, H_{\text{eff}}] = -\sum_j h_{i,j,\sigma} c_{j,\sigma} + \sum_j \Delta_{ij} e^{-\frac{j}{k_B T}} e^{-\frac{j}{k_B T}} c_{j}^\dagger
$$

$$
(29)
$$

Using Eqs. (24), (28), and (29), the Bogoliubov-de Gennes equations are obtained,

$$
E_n u_n^\dagger = \sum_j e^{-\frac{j}{k_B T}} h_{i,j,\sigma} e^{-\frac{j}{k_B T}} u_j^\sigma + \sum_j \Delta_{ij} v_j^\sigma
$$

$$
E_n u_n^\dagger = \sum_j e^{-\frac{j}{k_B T}} h_{i,j,\sigma} e^{-\frac{j}{k_B T}} v_j^\sigma + \sum_j \Delta_{ij} v_j^\sigma
$$

$$
E_n v_n^\dagger = -\sum_j e^{-\frac{j}{k_B T}} h_{i,j,\sigma} e^{-\frac{j}{k_B T}} v_j^\sigma + \sum_j e^{-\frac{j}{k_B T}} h_{i,j,\sigma} e^{-\frac{j}{k_B T}} v_j^\sigma
$$

$$
+ \sum_j \Delta_{ij} u_j^\sigma
$$

$$
E_n v_n^\dagger = -\sum_j e^{-\frac{j}{k_B T}} h_{i,j,\sigma} e^{-\frac{j}{k_B T}} v_j^\sigma + \sum_j e^{-\frac{j}{k_B T}} h_{i,j,\sigma} e^{-\frac{j}{k_B T}} v_j^\sigma
$$

$$
+ \sum_j \Delta_{ij} u_j^\sigma
$$

$$
(30)
$$

In order to solve the above system of equations, we replace the operator $\gamma_j^\dagger$ by its associated scalar value $\chi_j$. Then, the Bogoliubov-de Gennes equations is put into the following matrix form,

$$
\sum_j M_{ij} \phi_j^n = E_n \phi_i^n
$$

$$
(31)
$$
where

\[
M_{ij} = \begin{pmatrix}
    h_{i\uparrow,j\uparrow} e^{\frac{i\pi}{2}(x_i-x_j)} & h_{i\uparrow,j\downarrow} e^{\frac{i\pi}{2}(x_i-x_j)} & 0 & \Delta_{ij} \\
    h_{i\downarrow,j\uparrow} e^{\frac{i\pi}{2}(x_i-x_j)} & h_{i\downarrow,j\downarrow} e^{\frac{i\pi}{2}(x_i-x_j)} & \Delta_{ji} & 0 \\
    0 & \Delta_{ij}^* & -h_{i\uparrow,j\uparrow} e^{-\frac{i\pi}{2}(x_i-x_j)} & h_{i\uparrow,j\downarrow} e^{-\frac{i\pi}{2}(x_i-x_j)} \\
    \Delta_{ji}^* & 0 & h_{i\downarrow,j\uparrow} e^{-\frac{i\pi}{2}(x_i-x_j)} & -h_{i\downarrow,j\downarrow} e^{-\frac{i\pi}{2}(x_i-x_j)}
\end{pmatrix}
\]  

(32)

and

\[
\phi_i^n = \begin{pmatrix}
    u_{i\uparrow}^n \\
    u_{i\downarrow}^n \\
    v_{i\uparrow}^n \\
    v_{i\downarrow}^n
\end{pmatrix}
\]  

(33)

Note that solutions for \( E_n \) and \(-E_n \) are connected; the solution for \(-E_n \) is given by

\[
\begin{pmatrix}
    -(v_{i\uparrow}^n)^* \\
    (v_{i\downarrow}^n)^* \\
    -(u_{i\uparrow}^n)^* \\
    (u_{i\downarrow}^n)^*
\end{pmatrix}
\]  

(34)

Therefore, we only need to obtain half of the solutions to Eq. (31).

Self-consistent solutions are obtained by solving the above equations using the self-consistent fields,

\[
\langle n_{i\uparrow} \rangle = \langle c_{i\uparrow}^+ c_{i\uparrow} \rangle = \sum_{n_1} \sum_{n_2} \langle \hat{c}_{i\uparrow}^+ \rangle \gamma_{n_1} \gamma_{n_2} \\
= \langle \gamma_{n_1} \rangle \gamma_{n_2} \\
= \frac{1}{2} \sum_n [v_{i\uparrow}^n (v_{i\downarrow}^n)^* + c.c] \text{f}(-E_n)
\]

(35)

\[
\langle \gamma_{n_1} \rangle = \text{f}(E_n), \quad \langle v_{i\uparrow}^n \rangle = 1 - \text{f}(E_n) = \text{f}(-E_n), \quad \text{for } f(E_n) \text{ being the Fermi function.}
\]

We solve the system of equations in Eq. (31) by the Car-Parrinello method [43], taking \( \phi_i^n \) as “time-dependent” variable \( \phi_i^t \) at the ith site that follows the Newtonian dynamics

\[
m_{\text{CP}} \ddot{\phi}_i^n(t) = -\sum_j M_{ij} \phi_j^n(t) + E_n \phi_i^n(t) - \eta_{\text{CP}} \dot{\phi}_i^n(t)
\]

(39)

where \( m_{\text{CP}} \) and \( \eta_{\text{CP}} \) are mass and friction coefficient for the variable, respectively; here, the wave functions \( \{\phi_i^n\} \) are orthonormalized during the calculation.
4 Spin-Vortices and Multi-valued Wave Functions

The self-consistent wave functions obtained in the previous section, actually, become multi-valued with respect to electron coordinates due to the presence of spin-vortices. The spin-texture obtained for a model system composed of the two-layers shown in Fig. 1 is depicted in Fig. 2.

If \(
u_{\alpha}^n\) and \(\tilde{v}_{\alpha}^n\) are obtained just by minimizing energy, the resulting state is a currentless state that satisfies the so-called “Bloch’s theorem” [44]. This corresponds to the solution with constant \(\chi\).

Let us examine this currentless state, more closely. Replacing the operator \(\chi\) in Eq. (24) by the scalar value of the underlying Berry connection, we obtain

\[
\begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix} = e^{-\frac{i}{2} \chi_i} \sum_n \begin{pmatrix} \nu_{\alpha}^n \nu_{\alpha}^* \\ \nu_{\alpha}^n \tilde{v}_{\alpha}^* \end{pmatrix} \begin{pmatrix} \gamma_n \\ \gamma_{n'} \end{pmatrix}
\]

and the currentless result corresponds to the solution with coordinate independent (or constant) \(\chi_i\). Since the single-valued solution corresponds to coordinate-dependent multi-valued \(\chi_i\), the currentless \(\nu_{\alpha}^n\) and \(\tilde{v}_{\alpha}^n\) are actually multi-valued.

Now, we need to obtain the multi-valued \(\chi\). The angular variable \(\chi\) is obtained from conditions,

\[
w_{C_i}[\xi] + w_{C_i}[\chi] = \text{even number for any loop } C_i
\]

where \(w_{C_i}[\xi]\) and \(w_{C_i}[\chi]\) are winding numbers given by

\[
w_{C_i}[\xi] = \frac{1}{2\pi} \oint_{C_i} \nabla \xi \cdot d\mathbf{r}, \quad w_{C_i}[\chi] = \frac{1}{2\pi} \oint_{C_i} \nabla \chi \cdot d\mathbf{r}
\]

If the above conditions are satisfied, \(e^{-\frac{i}{2} (\chi+\xi)}\) appearing in Eq. (47) become single-valued.

Due to the presence of spin-vortices, \(\xi\) is multi-valued, and contains jump-of-value points (or bonds) of an integral multiple of \(2\pi\). To establish the condition in Eq. (48), \(\xi\) and \(\chi\) must have the same jump-of-value points.

To have the same jump-of-value points for \(\xi\) and \(\chi\), we do the following: first, we rebuild \(\xi\) from differences of their values between bonds; \(\xi_j\)’s are obtained from the self-consistent fields \(\langle S_i^x \rangle\) and \(\langle S_j^y \rangle\). Since the system has the
antiferromagnetic background $\xi_j^0 = \pi (j_x + j_y + j_z)$ in the units with the lattice constant being one $((j_x, j_y, j_z)$ is the $xyz$ coordinates of the $j$th site), we separate $\xi_j^0$ from $\xi$ by introducing angular variable $\eta_j$.

$$\eta_j = \xi_j - \pi (j_x + j_y + j_z)$$

where $\eta_j$ is $\eta$ at the $j$th site. We take the branch of $\eta_j$ that satisfies the following condition,

$$-\pi \leq \eta_j - \eta_k < \pi$$

where $k$ is a nearest neighbor site of $j$.

From $(\eta_j - \eta_k)$'s, we construct $(\xi_j^1 - \xi_j^0)$'s. After $(\xi_j^1 - \xi_j^0)$'s are obtained, we rebuild $\xi$ from them. The process is as follows: first, we pick a value for the initial $\xi_1$. After fixing the value of $\xi_1$, we calculate $\xi_j$ by $\xi_j = \xi_1 + (\xi_2 - \xi_1)$, where the site 2 is connected to the site 1 by a nearest neighbor bond. The step where value $\xi_j$ is derived from the already evaluated value of $\xi_k$ is given by

$$\xi_j = \xi_k + (\xi_j - \xi_k)$$

where the sites $j$ and $k$ are connected by a bond in the path for the rebuilding of $\xi$. This process is continued until values at all accessible sites are evaluated once and only once.

By this rebuilding process, a single path is constructed from the site 1 to other sites $k \neq 1$, which is achieved by making the region singly connected by removing some bonds (see Fig. 1). We denote the path from the site 1 to the site 2 is connected to the site 1 by a nearest neighbor bond. The step where value $\xi_j$ is derived from the already evaluated value of $\xi_k$ is given by

$$\xi_j \approx \xi_1 + \int_{C_{1 \to k}} \nabla \xi \cdot dr$$

Let us summarize the calculation so far.

1. Solve Eq. (31) self-consistently using the Car-Parrinello method in Eq. (39). Thereby, we obtain self-consistent fields in Eqs. (35), (36), and (37).

2. From Eq. (36), $\xi_1$'s are obtained. Next, $\xi_k$'s are rebuilt using Eq. (53). Thereby, we have $\xi_k$'s for which we know the positions of the jump-of-values.

3. From the rebuilt $\xi_k$'s, construct $c_{j \sigma}^{\dagger}, c_{j \sigma}$ in Eq. (42). Using Eqs. (35), (36), and (37) obtained in Step 1, solve Eq. (44). Thereby, $\hat{u}_{\sigma}^n, \hat{v}_{\sigma}^n$ are obtained.

4. From $e^{\pm i \xi_1}, \hat{u}_\sigma^n, \hat{v}_\sigma^n$, we calculate $u_{\sigma}^n$ and $v_{\sigma}^n$ by using the relations $u_{\sigma}^n = e^{-\frac{i}{\hbar} \xi_1 \hat{u}_\sigma^n}, u_{1\downarrow}^n = e^{\frac{i}{\hbar} \xi_1 \hat{u}_{\sigma}^n}$, $v_{\sigma}^n = e^{-\frac{i}{\hbar} \xi_1 \hat{v}_\sigma^n}, v_{1\downarrow}^n = e^{\frac{i}{\hbar} \xi_1 \hat{v}_{\sigma}^n}$.

Next, we obtain $\chi$'s that satisfy Eq. (48).

We take the branch of $\chi_j$ that satisfies the difference of value from the nearest neighbor site $k$ is in the range,

$$-\pi \leq \chi_j - \chi_k < \pi$$

From $(\chi_j - \chi_k)$'s, we rebuild $\chi$. The rebuilding process is as follows: first, we pick a value for the initial $\chi_1$ (say $\chi_1 = 0$). Then, the value $\chi_k$ is evaluated by

$$\chi_k \approx \chi_1 + \int_{C_{1 \to k}} \nabla \chi \cdot dr$$

The requirement in Eq. (48) is given by

$$w_{C_{\ell}}[\chi] = \frac{1}{2\pi} \sum_{i=1}^{N_\ell} \tau_{C_{\ell}(i+1) \to C_{\ell}(i)}$$

where

$$\tau_{k \to j} = \chi_k - \chi_j$$

and $w_{C_{\ell}}[\chi]$ is the number supplied as a boundary condition. $C_{\ell}(i)$ is the $i$th site in the loop $C_{\ell}$, where $C_{N_\ell+1} = C_1$ with $N_\ell$ being the number of sites in $C_{\ell}$.

In order to impose conditions in Eq. (56), $\tau_{j \to i}$ is split into a multi-valued part $\tau^0_{j \to i}$ and single-valued part $f_{j \to i}$ as

$$\tau_{j \to i} = \tau^0_{j \to i} + f_{j \to i}$$

where $\tau^0_{j \to i}$ is given to satisfy

$$w_{C_{\ell}}[\chi] = \frac{1}{2\pi} \sum_{i=1}^{N_\ell} \tau^0_{C_{\ell}(i+1) \to C_{\ell}(i)}$$

and $f_{j \to i}$ is solved to satisfy

$$0 = \frac{1}{2\pi} \sum_{i=1}^{N_\ell} \sum_{i,j,\sigma} \bar{\gamma}^{j \to i, \sigma, \sigma'} \bar{\gamma}^{i \to j, \sigma, \sigma'} [u_{\sigma}^i u_{\sigma'}^j f(\bar{E}(\sigma)] + \gamma^{j \to i, \sigma, \sigma'} \gamma^{i \to j, \sigma, \sigma'} [v_{\sigma}^i v_{\sigma'}^j f(-\bar{E}(\sigma))]$$

They are imposed on independent loops in the system, as shown in Fig. 3.

The conservation of the local charge at the $k$th site is

$$0 = \sum_{\ell \in b_k} J_{k \to \ell}$$

where $b_k$ is a set of sites that are connected to the $k$th site. $J_{k \to \ell}$ is the current through the bond between sites $k$ and $\ell$ in the direction $k \leftarrow \ell$,
Fig. 3  Loops used to impose boundary conditions in Eq. (48). a Loops in the bulk and surface layers. b Loops in the bulk-surface interface region. Some of the loops in the system are removed since they are not independent; as a consequence, all the cells are accessible from outside without breaking any walls framed by loops.

We employ an iterative improvement of the approximate solutions by using the linearized version of Eq. (61) given by

\[ 0 \approx \frac{2e}{\hbar} \sum_i \frac{\partial E(\{\tau_0^{j\leftarrow i}\})}{\partial \tau_j^{\leftarrow i}} + \frac{2e}{\hbar} \sum_i \frac{\partial^2 E(\{\tau_0^{j\leftarrow i}\})}{\partial (\tau_j^{\leftarrow i})^2} f_j^{\leftarrow i} \tag{64} \]

A system of equations for \( f_j^{\leftarrow i} \)'s composed of Eqs. (60) and (64) are solve for given \( \tau_0^{j\leftarrow i} \)'s by updating them iteratively

\[ \tau_0^{j\leftarrow i}_{\text{New}} = \tau_0^{j\leftarrow i}_{\text{Old}} + f_j^{\leftarrow i} \tag{65} \]

where \( \tau_0^{j\leftarrow i}_{\text{Old}} \) is \( \tau_0^{j\leftarrow i} \) value that is used to obtain the current value of \( f_j^{\leftarrow i} \); \( \tau_0^{j\leftarrow i}_{\text{New}} \) will be used to obtain the next \( f_j^{\leftarrow i} \) value.

The numerical convergence is checked by the condition

\[ \left| \frac{2e}{\hbar} \sum_i \frac{\partial E(\{\tau_0^{j\leftarrow i}\})}{\partial \tau_j^{\leftarrow i}} \right| < \epsilon \tag{66} \]

where \( \epsilon \) is a small number.

For the initial \( \tau_0^{j\leftarrow i} \), we adopt the following,

\[ \tau_0^{j\leftarrow i}_{\text{init}} = \sum_h \frac{w_h \tan^{-1} \left( \frac{j_y - h_y}{j_x - h_x} \right)}{j_x - h_x} - \sum_h \frac{w_h \tan^{-1} \left( \frac{i_y - h_y}{i_x - h_x} \right)}{i_x - h_x} \tag{67} \]

where \((j_x, j_y, j_z)\) and \((i_x, i_y, i_z)\) are coordinates of the sites \( j \) and \( i \), respectively, \( h = (h_x, h_y, h_z) \) is the coordinate of the hole occupied site, and \( w_h \) is the winding number of \( \chi \) around the hole at \( h \).

The number of \( \tau_j^{\leftarrow i} \) to be evaluated is equal to the number of the bonds. The number of equations in Eq. (60) is equal to the number of the plaques. The number of equations from Eq. (61) for the conservation of charge is equal to the number of sites \(-1\), due to the fact that the total charge is fixed in the calculation.

The equality of the number of unknowns and the number of equations gives

\[ \# \text{bonds} = \# \text{plaques} + \# \text{sites} - 1 \tag{68} \]

\[ \# \text{edges} = \# \text{faces} + \# \text{vertices} - 1 \tag{69} \]

When the spin-orbit interaction exists the total energy depends on \( \xi_1 \) as shown in Fig. 4. In Fig. 5, obtained current using \( \xi_1 = 0 \) is depicted.

Fig. 4  Dependence of the total energy on the value of \( \xi_1 \). The zero of energy is taken to be the value for \( \lambda = 0 \) calculation. The units of the energy is \( t_1 \)
6 Diamagnetic Current Produced by an Application of a Magnetic Field

One of the hallmarks of superconducting states is the diamagnetic response to an external magnetic field. Let us consider the situation where a magnetic field $B^{em} = \nabla \times A^{em}$ is applied.

This leads to replace $\tau_{j \leftarrow i}$ in $E$ in Eq. (63) by

$$u_{j \leftarrow i} = \tau_{j \leftarrow i} - \frac{2e}{\hbar c} \int_{j \leftarrow i} A^{em} \cdot \mathrm{d}r$$  \hspace{1cm} (70)

where integration is performed along the bond $j \leftarrow i$.

The calculation can be done similarly to the case for no magnetic field, starting from the initial value

$$u_{j \leftarrow i}^{0 \ init} = \tau_{j \leftarrow i}^{0 \ init} - \frac{2e}{\hbar c} \int_{j \leftarrow i} A^{em} \cdot \mathrm{d}r \hspace{1cm} (71)$$

Note that during the evaluation process of $\nabla \chi$, the ambiguity in the gauge of $A^{em}$ is compensated, thus, the effective vector potential

$$A^{eff} = A^{em} - \frac{\hbar c}{2e} \nabla \chi = A^{em} + A^{fic} \hspace{1cm} (72)$$

is invariant with respect to the choice of the gauge in $A^{em}$.

Now we apply a uniform magnetic field perpendicular to the lattice. In the actual numerical calculations we have adopted

$$A^{em} = \begin{pmatrix} -By \\ 0 \\ 0 \end{pmatrix} \hspace{1cm} (73)$$

but we checked that the calculated current distribution is identical even other gauge is employed.

In Fig. 6a, current distributions with applying the magnetic field are depicted. Numerical calculations indicate the following relation holds

$$J_{j \leftarrow i} \approx -\frac{4e^2}{\hbar^2} \frac{\partial^2 E[\{0\}]}{\partial (u_{j \leftarrow i})^2} \int_{j \leftarrow i} A^{eff} \cdot \mathrm{d}r \hspace{1cm} (74)$$

where $\{0\}$ means all $u_{j \leftarrow i}$’s are zero [45].

The result using the above approximation is shown in Fig. 6b, and the difference between the exact result and approximate one is shown in Fig. 6c. The approximate one is almost identical to the exact one, except the current just around the small polarons; it originates directly from the Rashba interaction.

The induced current is diamagnetic as seen in Fig. 7. This will become a screening current of the magnetic field in a large system size.

7 Zero Voltage Current Production by an External Current Feeding

Another hallmark of superconducting states is the zero voltage current flow through the sample. Let us consider the external current feeding. When external currents are fed, the conservation of the local...
Supercurrent under the application of an external magnetic field. $B = 0.01$ in the units of $t_1 = 1$, $\hbar = 1$, $e = 1$, and lattice constant in the plane $= 1$. a The result from the calculation. b The linear approximation given in Eq. (74). c The difference between the calculated result and its linear approximation.

The charge at site $k$ in Eq. (61) is modified as

$$0 = \sum_{\ell \in b_k} J_{k \leftarrow \ell} + J_{k}^{\text{EX}}$$

(75)

where $J_{k}^{\text{EX}}$ is the external current fed at $k$. Supercurrent obtained by feeding external current is depicted in Fig. 8. A plot for the total energy vs $J_{k}^{\text{EX}}$ is shown in Fig. 9. The energy minimum with nonzero $J_{k}^{\text{EX}}$ occurs for $\lambda \neq 0$ cases. This situation is similar to the one envisaged by Bloch for superconducting states [46]. When the system is at the energy minimum with nonzero $J_{k}^{\text{EX}}$, zero voltage current production is realized. In other words, persistent current flows through the sample.

The energy minimum occurs at zero $J_{k}^{\text{EX}}$ for the $\lambda = 0$ case. This indicates the if the Rashba interaction is absent, the zero voltage current production does not occur in the present model.

Supercurrent induced by the application of an external magnetic field. a The induced current in the two layers. The scale for the current arrow is enlarged from Fig. 6. b The induced current in the bulk layer. c: the induced current in the surface layer.
8 Concluding Remarks

We have presented a fundamentally revised theory for superconductivity, and the method to calculate properties of superconducting states based on it.

Since the early work of London, it has been repeatedly argued that theory of superconductivity needs to have a $U(1)$ gauge field different from the electromagnetic one to have the gauge invariant supercurrent [47]. London called it “superpotential”, and the current standard theory calls it “Nambu-Goldston mode”. In the new theory, the Berry connection $A^\text{fic}$ in Eq. (13) provides the necessary gauge field.

We would like to emphasize that the vector potential provided by the Berry connection $A^\text{fic}$ plays a crucial role in realizing reversible superconducting-normal metal phase transition in a magnetic field [26, 31, 48, 49]. This phenomenon cannot be explained by the standard theory [24, 48].

Besides the reversible superconducting-normal metal phase transition in a magnetic field, the new theory solves four problems described in Introduction (the last one is not yet explained). It also provides a calculation framework for the two of the hallmarks of superconducting states, the diamagnetic response current to an external magnetic field, and the zero voltage current produced by an external current feeding, microscopically.

This theory may be able to elucidate the cuprate superconductivity, where nanoscale inhomogeneity of electronic states is important. The present theory seems to account for the superconducting transition temperature at optimal doping as the stabilization temperature for the spin-vortex-induced loop currents [38, 40]. However, further investigations are necessary to explain its doping dependence.

References

1. Bardeen, J., Cooper, L.N., Schrieffer, J.R.: Phys. Rev. 108, 1175 (1957)
2. Bogoliubov, N.N.: Sov. Phys. JETP 34, 41 (1958)
3. Anderson, P.W.: Phys. Rev. 110, 827 (1958)
4. Anderson, P.W.: Phys. Rev. 112, 1900 (1958)
5. Nambu, Y.: Phys. Rev. 117, 648 (1960)
6. Bednorz, J.G., Müller, K.A.: Z. Phys. B 64, 189 (1986)
7. Kastner, M.A., Birgeneau, R.J., Shirane, G., Endoh, Y.: Rev. Mod. Phys. 70, 897 (1998).
8. Emery, V.J., Kivelson, S.A.: Nature 374, 434 (1995)
9. Leggett, A.J.: Quantum Liquids: Bose Condensation And Cooper Pairing in Condensed- matter Systems. Oxford University Press, Oxford (2006)
10. Koizumi, H.: J. Supercond. Nov. Magn. (2021) https://doi.org/10.1007/s10948-021-05905-y
11. Koizumi, H., Tachiki, M., Supercond. J.: Nov. Magn. 28, 61 (2015)
12. Murani, A., Bourlet, N., le Sueur, H., Portier, F., Altimiras, C., Esteve, D., Grabert, H., Stockburger, J., Anderhold, J., Joyez, P.: Phys. Rev. X 10, 021003 (2020). https://doi.org/10.1103/PhysRevX.10.021003
13. Hakonen, P.J., Sonin, E.B.: Phys. Rev. X 11, 018001 (2021). https://doi.org/10.1103/PhysRevX.11.018001
14. Koizumi, H., Tachiki, M., Supercond. J.: Nov. Magn. 28, 61 (2015)
15. Morisaki, T., Wakaura, H., Koizumi, H.: J. Phys. Soc. Jpn. 86(10), 104710 (2017)
16. Zhang, F.C., Rice, T.M.: Phys. Rev. B 37, 3759 (1988). https://doi.org/10.1103/PhysRevB.37.3759
17. Damascelli, A., Hussain, Z., Shen, Z.X.: Rev. Mod. Phys. 75, 473 (2003)
18. Car, R., Parrinello, M.: Phys. Rev. Lett. 55, 2471 (1985). https://doi.org/10.1103/PhysRevLett.55.2471
19. Bohm, D.: Phys. Rev. 75, 502 (1949)
20. Manabe, D., Koizumi, H.: J. Supercond. Nov. Magn. 32, 2303 (2019). https://doi.org/10.1007/s10948-018-4977-0
21. Bloch, F.: Phys. Today 19(5), 27 (1966)
22. London, F.: Superfluids, vol. 1. Wiley, New York (1950)
23. Koizumi, H.: EPL 131(3), 37001 (2020)
24. Koizumi, H., Ishikawa, A.: Int. J. Modern Phys. B 34(31), 2030001 (2020). https://doi.org/10.1142/S0217979220300017

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.