What is the phase variable in superconductors?:
theory of superconductivity based on the spin-vortex formation

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Abstract. When Schrödinger solved the Schrödinger equation for the hydrogen atom, he
assumed the single-valuedness of the electronic wave function. Thereafter, this assumption
has been one of the fundamental postulates of quantum mechanics. When wave functions are
multi-component, however, the imposing of the single-valued condition may become nontrivial.
The spin-degree-of-freedom of electron makes electronic wave functions two-component.
When spin-vortices are created by the conduction electrons and they move in the self-consistent
field with the spin-vortices, the twisting of the spin basis occurs; then, the imposing of the single-valued condition becomes nontrivial, and a vector potential is induced. As a consequence, the
effective vector potential becomes the sum of the vector potential from the induced one and
that originates from the electric current. This effective vector potential is gauge invariant
and the persistent current is generated by it.

In the present work, we argue that if interactions that are omitted in the BCS reduced
Hamiltonian are included, spin-vortices may be generated upon the application of a magnetic
field. Then, the vector potential is induced and provides with the phase variable, \( \theta \), of
the electron pair amplitude. The appearance of the spin-vortex provides with a new origin of \( \theta \); it
originates from the induced gauge potential. This origin is compatible with the superselection
rule for charge in contrast to the currently-accepted origin.

1. Introduction
The mechanism of the cuprate superconductivity is still not elucidated although a large
amount of researches have been performed for more than 26 years. Recently, it is argued
that the superconductivity without the Cooper pairs may occur in the cuprate [1, 2]. This
superconductivity is based on the stable spin-vortex formation, thus, called the spin-vortex
superconductivity [1].

If we look back the currently-accepted BCS theory, its superconducting order parameter is
the electron pair amplitude given by

\[
\langle \hat{\psi}_\uparrow \hat{\psi}_\downarrow \rangle = |\langle \hat{\psi}_\uparrow \hat{\psi}_\downarrow \rangle| e^{i\theta},
\]

where \( \hat{\psi}_\sigma \) is the field operator of conduction electrons with spin \( \sigma \), and \( \langle \hat{O} \rangle \) denotes
the thermal average of the operator \( \hat{O} \) [3]. We notice that if the expectation value in Eq. (1)
is calculated with fixed-particle-number states, it is zero. Since it is sensible to consider that
superconductivity occurs in fixed-particle-number systems, the use of the above order parameter is for a mathematical convenience rather than for taking into account of a physical reality.

However, in the currently-accepted theory of superconductivity, \( \theta \) arises from the phase difference between different charged states. This origin of \( \theta \) requires the interference of different charged states, thus, is against the superselection rule for charge (SSRC); the SSRC dictates that such a phase is physically meaningless due to the nonexistence of interactions that connect different charged states [4, 5].

In the present work, we argue that the appearance of \( \theta \) may be attributed to the fundamental postulate of quantum mechanics, the single-valuedness of wave functions, employed by Schrödinger [6]. If the interactions that are omitted in the BCS reduced Hamiltonian are included, spin-vortices will be created by the conduction electrons. Then, their wave functions have twisted spin basis since they are moving in the self-consistent field with the spin-vortices.

The twisting of the spin basis induces the following vector potential as will be explained later;

\[
A^{\text{fic}} = \frac{e\hbar}{2q} \nabla \chi \tag{2}
\]

where the charge unit \( q \) is given by \( q = -e \); \( \chi \) is a harmonic function that is optimized under the condition that the conduction electron wave functions are single-valued in the presence of spin-vortices [1]. Here the superscript ‘fic’ in \( A^{\text{fic}} \) stands for ‘fictitious’ and denotes that the vector potential is not the electromagnetic field origin. Since \( \nabla \times A^{\text{fic}} = 0 \), the effect is an Aharonov-Bohm type. A remarkable point is that \( A^{\text{fic}} \) generates spin-vortex-induced loop currents (SVILCs) [7]. If the spin-vortices are long-lived, the induced loop currents, i.e., SVILCs are also long-lived. The spin-vortex superconductivity is the theory of superconductivity with the SVILC as the current element [1].

The appearance of \( A^{\text{fic}} \) in the spin-vortex superconductivity shows a marked similarity between the ferromagnetic phase and the superconducting phase. With the vector potential from the electromagnetic field \( A^{\text{em}} \), the effective vector potential becomes the sum,

\[
A^{\text{eff}} = A^{\text{em}} + A^{\text{fic}}. \tag{3}
\]

It reminds us of the fact that a molecular field \( B^{\text{mol}} \) exists in addition to the real magnetic field \( B^{\text{em}} \) in ferromagnets, and the effective magnetic field is given as a sum of the two

\[
B^{\text{eff}} = B^{\text{em}} + B^{\text{mol}}. \tag{4}
\]

The occurrence of the ferromagnetic phase is attributed to the appearance of \( B^{\text{mol}} \); the order parameter is the magnetization \( M \), which is calculated at \( T = 0 \) K as

\[
M = -\frac{\delta E[B^{\text{eff}}]}{\delta B^{\text{eff}}} \tag{5}
\]

with taking the external magnetic field zero. Therefore, the appearance of the ferromagnetic phase is attributed to the appearance of \( A^{\text{fic}} \) that yields nonzero \( M \) even without an external magnetic field.

The similarity between Eqs.(3) and (4) suggests that in the phase in which \( A^{\text{fic}} \) is nontrivial, a spontaneous current density \( j \) given by

\[
j = -e\frac{\delta E[A^{\text{eff}}]}{\delta A^{\text{eff}}} \tag{6}
\]

may appear even without an external magnetic field. We may identify such a phase as superconducting phase.
The spin-vortex superconductivity does not require Cooper pairs; on the other hand the BCS superconductivity does. Therefore, it seems they are unrelated. However, we will show that the former may actually incorporate the latter.

Using $\theta$, the persistent current is given by
\[
\mathbf{j} = \Lambda (\mathbf{A}^{\text{em}} - \frac{\hbar c}{q} \nabla \theta),
\]
in the currently-accepted theory if the spatial variation of the magnetic field is much slower than the coherence length, where $\Lambda$ is a function of the coordinate $r$, and $\theta$ is an angular variable with period $2\pi$. The observed flux quantization unit $\frac{\hbar c}{2e}$ in superconductors is obtained by taking the charge unit $q$ as $-2e$ in Eq.(7).

On the other hand the current density in the spin-vortex superconductivity is given by
\[
\mathbf{j} = \Lambda \mathbf{A}^{\text{eff}} = \Lambda (\mathbf{A}^{\text{em}} + \frac{\hbar c}{2q} \nabla \chi),
\]
where $q = -e$. The above current density also yields the observed flux quantization unit $\frac{\hbar c}{2e}$. Whether the charge unit $q$ is $-e$ or $-2e$ is a very important issue. The recent re-derivation of the AC Josephson frequency including the charge flow through the leads connected to the Josephson junction indicates $q = -e$ is the right one [1]; this point will be further discussed in Appendix.

The comparison of Eqs. (7) and (8) suggests the relation
\[
\theta = -\chi.
\]
in the present work, we will argue that this identification is adequate. Then, the phase of the Cooper pair amplitude is attributed to the appearance of $\mathbf{A}^{\text{fc}}$. If we take this origin of $\theta$, the current carrying state of the BCS theory becomes the one compatible with the SSRC.

2. Appearance of $\mathbf{A}^{\text{fc}}$

In this section we explain the appearance of $\mathbf{A}^{\text{fc}}$ using a model for the cuprate.

In the model construction, experimental results that probe the bulk properties were utilized. They indicate the appearance of significant local lattice deformations upon hole doping, and the presence of spin-configurations that generate the hourglass-shaped magnetic excitations. Since the latter is explained by the existence of spin-vortices, we construct a model with the spin-vortices [7, 8].

The minimal model for the parent antiferromagnetic insulator of the cuprate is a half-filled 2D Hubbard model with large on-site Coulomb repulsion. We include hole-lattice interaction in the Hubbard model since a number of experiments indicate that the doped holes become polarons:
\[
H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{j} c_{j\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} c_{j\downarrow} c_{j\uparrow} + H_{\text{hole+lattice}},
\]
the first two terms are those of the Hubbard model, where $t_{ij}$ is $t$ when the sites $i$ and $j$ are nearest neighbors, and zero otherwise. The strong correlation condition, $0 < t \ll U$, is assumed. The third term describes the interaction between holes and underlying lattice, and also lattice vibrations.

To simplify the above Hamiltonian, we utilize the following observations: 1) the Hall coefficient measurement in a strong magnetic field indicates that the charge carriers in the magnetically-produced normal state below the superconducting transition temperature $T_c$ are
electrons, not holes [9]; 2) a molecular orbital cluster calculation indicates that the energy lowering by the deformation of CuO unit is large enough to localize the hole. They indicate that holes becomes small polarons and immobile below $T_c$ [10]. Then, the above Hamiltonian is simplified as

$$H_{\text{EHFS}} = - \sum_{i,j \in \text{acc. sites}, \sigma} t_{ij} c_i^\dagger c_j^\sigma + U \sum_{j \in \text{acc. sites}} c_j^\dagger c_j^\sigma c_j^\dagger c_j^\sigma$$

(11)

where EHFS stands for the ‘effectively-half-filled situation’; the summation is taken only over accessible sites.

Due to the large on-site Coulomb repulsion, an effectively-half-filled situation where the number of accessible sites and that of electrons are equal, is realized; then, the ground state is well-approximated by a Slater determinant of fully-occupied lower band. Usually, the filled band does not contribute to electric current; however, the current flow by SVILCs is possible in the present model as will be explained below.

In order to obtain the wave function for the conduction electron in the self-consistent field with the spin-vortices, the following new particle operators

$$\left( \begin{array}{c} a_j \\ b_j \end{array} \right) = \frac{e^{i x_j}}{\sqrt{2}} \left( \begin{array}{cc} e^{i \xi_j^x} & e^{-i \xi_j^x} \\ -e^{i \xi_j^x} & e^{-i \xi_j^x} \end{array} \right) \left( \begin{array}{c} c_j^\uparrow \\ c_j^\downarrow \end{array} \right),$$

(12)

are employed. The angular variable $\xi_j$ describes the spin direction at site $j$ in the $x$-$y$ plane. In the cuprate, the spins are observed to lie in the CuO$_2$ plane [11], and we take the CuO$_2$ plane as the $x$-$y$ plane.

The angular variable $\chi_j$ with period $2\pi$ is added; it is necessary for the single-valuedness of the above transformation matrix. Since $\xi_j$ is an angular variable with $\xi_j$ and $\xi_j + 2\pi$ physically equivalent, the sign-change occurs in $e^{\pm \frac{i}{2} \xi_j}$ by the phase shift $\xi_j \to \xi_j + 2\pi$; the sign-change brought about by $e^{\pm \frac{i}{2} \xi_j}$ must be compensated by the sign-change of $e^{\frac{i}{2} \chi_j}$. This condition is given using the winding numbers of $\chi$ and $\xi$ as

$$w_\ell[\chi] + w_\ell[\xi] = \text{even number}, \quad \text{for any loop } C_\ell$$

(13)

where the winding number for function $f$ around the loop $C_\ell$ is defined as

$$w_\ell[f] = \frac{1}{2\pi} \oint_{C_\ell} \nabla f \cdot dr.$$ 

(14)

After the basis transformation in Eq. (12), $H_{\text{EHFS}}$ becomes

$$H_{\text{EHFS}}[\nabla \chi] = - \sum_{k,j \in \text{acc. sites}} t_{kj} e^{\frac{i}{2} \int_c^k \nabla \chi \cdot dr} \left[ \cos \frac{\xi_k - \xi_j}{2} (a_k^\dagger a_j + b_k^\dagger b_j) - i \sin \frac{\xi_k - \xi_j}{2} (a_k^\dagger b_j + b_k^\dagger a_j) \right] + U \sum_{j \in \text{acc. sites}} a_j^\dagger a_j b_j^\dagger b_j$$

(15)

A notable point in Eq. (15) is that the transfer integrals acquire phase factor $e^{\frac{i}{2} \int_j^k \nabla \chi \cdot dr}$, thus, the transfer integral is modified as

$$t_{kj} \to t_{kj} e^{\frac{i}{2} \int_j^k \nabla \chi \cdot dr}$$

(16)

This modification of the transfer integral is the one that will appear if the Peierls substitution for a magnetic field with the vector potential $A^\text{fc}$ is performed.
We now consider the situation where $\xi$ is given, and obtain $\chi$ that minimizes the total energy under the constraints given in Eq. (13). The optimization with respect to $\nabla \chi$ is performed under the following constraints;

$$
\frac{1}{2\pi} \oint_{C_\ell} \nabla \chi \cdot d\mathbf{r} = w_\ell, \quad \ell = 1, \ldots, N_{\text{loop}},
$$

(17)

where $w_\ell$ is the winding number of $\chi$ along a loop $C_\ell$, and $N_{\text{loop}}$ is the number of independent loops.

Including the above constraints, the functional to be optimized is given by

$$
F[\nabla \chi, \lambda_1, \ldots, \lambda_{N_{\text{loop}}}] = E[A_{\text{fic}}] + \sum_{\ell=1}^{N_{\text{loop}}} \lambda_\ell \left( \oint_{C_\ell} \nabla \chi \cdot d\mathbf{r} - 2\pi w_\ell \right),
$$

(18)

where $E[\nabla \chi]$ is the energy of the system for a given $\nabla \chi$, and $\lambda_\ell$ are the Lagrange multipliers.

From the stationary condition for $F$, we have

$$
0 = \frac{\delta E[A_{\text{fic}}]}{\delta A_{\text{fic}}} \frac{c}{2q} + \sum_{\ell=1}^{N_{\text{loop}}} \lambda_\ell \frac{\delta}{\delta \nabla \chi} \oint_{C_\ell} \nabla \chi \cdot d\mathbf{r}.
$$

(19)

In reality, the vector potential from the real electromagnetic field $A_{\text{em}}$ must be included. Then, $E[A_{\text{fic}}]$ is replaced by $E[A_{\text{eff}}]$.

We note that the current density is obtained from the functional derivative of energy by the vector potential as

$$
\mathbf{j}(x) = -\frac{c}{2q} \delta E[A_{\text{eff}}] \delta A_{\text{eff}}(x);
$$

(20)

thus, from Eqs. (19) and (20), we have

$$
\mathbf{j}(x) = \frac{2q}{\hbar} \sum_{\ell=1}^{N_{\text{loop}}} \lambda_\ell \frac{\delta}{\delta \nabla \chi(x)} \oint_{C_\ell} \nabla \chi \cdot d\mathbf{r}.
$$

(21)

This shows that a current is generated by the constraints. This is a novel current generation mechanism that occurs even in the filled-band situation. The current element is a loop current induced by the spin-vortex; thus, we call it the spin-vortex-induced loop current (SVILC). Note also that a similar calculation was done by Vergès et al. in Ref. [12]. Since they did not take care of the multi-valuedness arising from the twisting of the spin basis, they did not obtain the electric current.

3. Appearance of $A_{\text{fic}}$ in the BCS current carrying state

Let us start with presenting the state vector employed in the BCS theory;

$$
|\text{BCS}\rangle = \prod_k (u_k + v_k c_{-k}^d c_{k}) |\text{vac}\rangle,
$$

(22)

where $u_k$ and $v_k$ are real variational parameters that satisfy $u_k^2 + v_k^2 = 1$ [13]. The BCS used this variational state vector to facilitate calculations involving the electron pair-correlation. Although it is a linear combination of states with different particle numbers, the obtained wave function can be practically regarded as that for a state with $N$ particles since the particle number distribution has a sharp peak at the mean-value $N$. 

Currently, $u_k$ and $v_k$ are extended to complex numbers from real numbers, and their relative phases are considered physically meaningful. This extension, however, violates the SSRC [4, 5]. We stick to the BCS’s original intention, and show below that what is believed to arise from the phase between $u_k$ and $v_k$ actually may be explained to arise from the modification of the electron pairing. The strong point of this origin is that it is in accordance with the SSRC.

In the BCS ground state the pairing occurs between two states whose annihilation operators are given by

$$c_{\downarrow} = \frac{1}{\sqrt{N}} \sum_j c_j e^{ik \cdot r_j},$$
$$c_{\uparrow} = \frac{1}{\sqrt{N}} \sum_j c_j e^{-i k \cdot r_j},$$

where the coordinate of the system is described as discrete lattice points; the total number of sites is denoted as $N$; $r_j$ denotes the coordinate of the $j$th site.

Now we consider the case where an external magnetic field is applied in the $z$-direction. We anticipate that the state corresponding to $|BCS\rangle$ is replaced by the state with non-trivial $A^{bc}$; i.e., the ground state is shifted from $|BCS\rangle$ to the new one denoted by $|BCS[\chi]\rangle$ which contains the multi-valued harmonic function $\chi$. This shift will be caused by two interactions that are omitted in the BCS reduced Hamiltonian.

The first interaction we include is the Zeeman interaction between the magnetic field and electron spin. This interaction will create a tilting of up-spin components of electrons.

The second interaction we include is the spin-orbit interaction derived by Dirac [14]; the electron spin $s = \frac{\hbar}{2} \sigma$ is shown to interact with electric field $E$ as

$$H_{SO} = \frac{\mu_B}{2c^2} (v \times E) \cdot \sigma,$$

where $\mu_B$ is the Bohr magneton, $v$ is the velocity operator; $\sigma$ is the vector of the Pauli matrices.

At the instant when the magnetic field in the $z$-direction is turned on, eddy currents flow in the $x$-$y$ plane. If the internal electric field $E$ exists along the $z$-direction, the eddy current in the direction $v$ and the electric field $E$ create a circular effective magnetic field that acts on electron spins in the $x$-$y$ plane in the direction $v \times E$. This is a circular effective magnetic field since the eddy current is a circular current. Thus, it will generate a circular change of spin-direction along the eddy current. As a consequence, spin-vortices will be created.

We assume that the wave function for the above situation is constructed by modifying the electron-pairing from $\{c_{\uparrow}, c_{\downarrow}\}$ to $\{a_k, b_{-k}\}$, where $a_k$ and $b_{-k}$ are given by

$$a_k = \sum_j \frac{e^{ij}}{\sqrt{N}} \left( \sqrt{1 - \epsilon_j^2} e^{i \xi_j} \xi_j e^{-i \xi_j} e^{-i \xi_j} c_j \right) e^{i k \cdot r_j},$$
$$b_{-k} = \sum_j \frac{e^{ij}}{\sqrt{N}} \left( \sqrt{1 - \epsilon_j^2} e^{i \xi_j} \xi_j e^{-i \xi_j} e^{-i \xi_j} c_j \right) e^{-i k \cdot r_j},$$

where the phase factor $e^{i \xi}$ is added as in Eq. (12) to satisfy the single-valued condition since as before the angular variable $\xi$ describes the spin-direction in the $x$-$y$ plane, and it may give rise to singularities for the single-valued condition of wave functions.

New creation and annihilation operators satisfy the following anti-commutation relations;

$$a_k a_{k'}^\dagger + a_{k'}^\dagger a_k = b_{kk'} b_{k'}^\dagger + b_{k'}^\dagger b_k = \delta_{kk'}.$$
and

\[ a_k b_{k'} + b_{k'}^d a_k = \frac{1}{N_s} \sum_j \varepsilon_j e^{i(k-k') \cdot r_j}. \]  

(27)

If \( \varepsilon_j \)'s are non-zero in a small region along the eddy current, we may consider that the right-hand side in Eq. (27) is practically zero. If this is the case, we may ignore contributions from the right-hand side in Eq. (27) and treat them as orthogonal although states created by \( a_k^\dagger \) and \( b_{k'}^\dagger \) are actually not orthogonal. If the following, we assume that this is the case.

The BCS-like state vector using the \( \{ a_k, b_{-k}^\dagger \} \) pairing is given by

\[ |BCS[\chi] \rangle = \prod_k (u_k + v_k a_k^\dagger b_{-k}^\dagger) |\text{vac} \rangle. \]  

(28)

The state \( |BCS[\chi] \rangle \) has local moments; the expectation value of electron spin at the \( j \)th site is calculated as

\[ S_x^j = \frac{\hbar N}{2N_s} \varepsilon_j \sqrt{1 - \varepsilon_j^2} \cos \xi_j \approx \frac{\hbar N \varepsilon_j}{2N_s} \cos \xi_j \]

\[ S_y^j = \frac{\hbar N}{2N_s} \varepsilon_j \sqrt{1 - \varepsilon_j^2} \sin \xi_j \approx \frac{\hbar N \varepsilon_j}{2N_s} \sin \xi_j \]

\[ S_z^j = -\frac{\hbar N \varepsilon_j^2}{2N_s} \approx 0. \]  

(29)

The above formulae indicate that \( \xi_j \) describes the angle of the direction of the spin in the \( x-y \) plane at the \( i \)th site. The circular change of \( \xi \) means the existence of spin-vortices.

It is noteworthy that paramagnetic responses have been observed in the BCS superconductors [15, 16]; the pairing shift given above agrees with this fact.

Due to the appearance of the spin-vortices, the eddy currents turn into the SVILCs that persist as long as the spin-vortices persist. The collection of these SVILCs acts as the Meissner current. For a large sample, the exclusion of the applied magnetic field by the Meissner current is always energetically favorable, thus, the appeared Meissner current will persist as long as the external magnetic field is present.

The argument above suggests that if the Cooper pair condensation occurs, the system may acquire the ability to generate \( A_{\text{eff}} \). If this is the case, the Cooper pair condensation temperature corresponds to \( T_c \). It is also suggested that in some materials, the superconducting phase may be realized even without the Cooper pair formation if the long-lived spin-vortex formation occurs.

The effective vector potential in the superconductor becomes \( A_{\text{ed}} \) when \( A_{\text{bc}} \) arises. Then, the vector potential for the magnetic field, \( A_{\text{em}} \), in the Meissner current in the BCS theory should be replaced by \( A_{\text{eff}} \).

If we calculate \( \langle \hat{\psi}_\uparrow \hat{\psi}_\downarrow \rangle \) using \( |BCS[\chi] \rangle \) in Eq. (28), we obtain

\[ \langle \hat{\psi}_\uparrow \hat{\psi}_\downarrow \rangle = \langle BCS[\chi] | \hat{\psi}_\uparrow \hat{\psi}_\downarrow | BCS[\chi] \rangle = \frac{1}{N_s} \sum_k v_k u_k e^{-i\chi(r)}, \]  

(30)

where the limit \( \varepsilon_j \rightarrow 0 \) is taken. Then, we can identify that \( \theta = -\chi \).

4. Concluding remarks

The currently-accepted origin of \( \theta \) assumes that the superconducting state is a coherent superposition of different charged states. Although such a treatment is against the SSRC, the observation of Josephson effects is regarded as a proof for it.
However, it was recently found that the Josephson’s derivation of the AC Josephson frequency may be defective due to the lack of the inclusion of the charge flow through the leads connected to the Josephson junction [1]; the Josephson’s derivation is based on the situation given in Fig. 1(a), however, the real situation is more like that given in Fig. 1(b). This point needs a serious investigation. By examining the AC Josephson problem very carefully, we may come to the conclusion that the currently accepted $q = -2e$ theory must be replaced by the $q = -e$ theory.

By the present origin of $\theta$, the BCS theory can be incorporated into the spin-vortex superconductivity theory by identifying $\theta$ to be $\chi$. Currently, $\theta$ is believe to arise from the modification,

$$\prod_k (u_k + v_k c_{k\uparrow} c_{-k\downarrow}^\dagger) |\text{vac}\rangle \to \prod_k (u_k + e^{i\theta} v_k c_{k\uparrow} c_{-k\downarrow}^\dagger) |\text{vac}\rangle$$

(31)

where the spatial variation of $\theta$ gives rise to the persistent current.

We have shown that the current carrying state is generated from the following modification,

$$\prod_k (u_k + v_k c_{k\uparrow} c_{-k\downarrow}^\dagger) |\text{vac}\rangle \to \prod_k (u_k + v_k a_k b_{-k}^\dagger) |\text{vac}\rangle,$$

(32)

where $a_k$ and $b_{-k}$ are given in Eq. (25).

The important point to remember is that the modification in Eq. (31) cannot be achieved by the known interactions [5]. On the other hand, the modification in Eq. (32) is achieve by the known interactions that are omitted in the BCS reduced Hamiltonian, i.e., the Zeeman interaction and the spin-orbit interaction of conduction electrons. They are energetically very small; however, they will introduce the singularities in $\xi$, thus, induces the vector potential $A^{\text{fic}}$.

**Appendix A. The time-dependence of $\chi$ and the derivation of the AC Josephson frequency**

In this appendix, we derive the AC Josephson frequency $2eV/h$ by including the charge flow through the leads connected to the junction.

Let us consider the situation where $\chi$ and $\rho$ are only active variables for the current generation, where $\chi$ is the angular variable that appears in $A^{\text{fic}}$ and $\rho$ is the electron density. Then, the Hamiltonian is given as a functional of $\chi$ and $\rho$ as $H = H[\chi, \rho]$ [1].

The gauge invariant vector potential $A^{\text{eff}}$ in Eq. (3) implies that the following scalar potential

$$\phi^{\text{eff}} = \phi^{\text{em}} - \frac{h}{2q} \frac{\partial \chi}{\partial t},$$

(A.1)

since it is a time-component partner of $A^{\text{eff}}$, where $\phi^{\text{em}}$ is the scalar potential for electromagnetic field.

Then, the term of the electrostatic interaction in the Lagrangian should be given as

$$-q \int d^3x \rho \left( \phi^{\text{em}} - \frac{h}{2q} \frac{\partial \chi}{\partial t} \right),$$

(A.2)

where $q = -e$ is electron charge.

Let us obtain the canonical momentum for $\chi$, which we denote as $p_\chi$. The Lagrangian $L$ is written using $\chi$ and $p_\chi$ as

$$L = \int d^3x \ p_\chi \dot{\chi} - H.$$  

(A.3)
Figure 1. (a) The SIS junction considered by Josephson. The electric field in the insulator produces the voltage difference $V$. The Cooper-pair tunneling with unit charge $q = -2e$ across the two superconductors gives rise to the AC frequency $2eV/h$ [17]. (b) The SIS junction including the current flow through the leads connected to it. The electric field in the insulator produces the voltage difference $V$. The chemical potential difference $eV$ exists between the two leads. The electron tunneling with unit charge $q = -e$ across the two superconductors is added by the energy gain due to the flow-in and flow-out through the leads. The values of the former and the latter are the same. Overall, the AC frequency is given by $2eV/h$ with the charge unit $q = -e$ [1].

The term in Eq. (A.2) implies that $p_\chi$ is given by

$$p_\chi = \frac{\delta L}{\delta \dot{\chi}} = \frac{\rho \hbar}{2}. \tag{A.4}$$

Thus, $\chi$ and $\frac{\rho \hbar}{2}$ are conjugate variables.

Then, the Hamilton’s equations are given by

$$\dot{\rho} = -\frac{2\delta H}{\hbar \delta \chi},$$

$$\dot{\chi} = \frac{2\delta H}{\hbar \delta \rho}. \tag{A.5}$$

Now we consider the SIS junction depicted in Fig. 1(b). The number of particles in the left superconductor is $N_L$ and the right superconductor is $N_R$; the chemical potential on the left and right superconductors are $\mu_L$ and $\mu_R$, respectively. The phase $\chi$ on the two superconductor are written as

$$\chi(r) + \chi_L \tag{A.6}$$
and
\[ \chi(r) + \chi_R, \]  
respectively, where \( \chi_L \) and \( \chi_R \) do not depend on the position in each superconductor. Actually, for the time-dependent change of the current flow to occur, \( \chi(r) \) will change in time; however, we neglects its contribution by assuming that it is negligibly small; this also corresponds to the situation assumed by Josephson [17].

Let us assume that the link between the two superconductors is so weak that the optimized \( \nabla \chi \) in \( S_L \) and \( S_R \) are not affected by the presence of the link. The conjugate variables for \( \chi_R \) and \( \chi_L \) are calculated using Eq. (A.4) as \( \hbar N_R/2 \) and \( \hbar N_L/2 \), respectively.

Then, the canonical equations for \( N_X \) and \( \chi_X \) are obtained as
\[
\dot{N}_X = -\frac{2}{\hbar} \frac{\partial H}{\partial \chi_X}, \\
\dot{\chi}_X = \frac{2}{\hbar} \frac{\partial H}{\partial N_X},
\]
where \( X \) is either \( L \) or \( R \).

The quantum mechanical version of them are given by
\[
\dot{N}_X = i \frac{\hbar}{\hbar} [\hat{H}, \hat{N}_X], \\
\dot{\chi}_X = i \frac{\hbar}{\hbar} [\hat{H}, \hat{\chi}_X].
\]

Since \( \hbar \hat{N}_X/2 \), and \( \hat{\chi}_X \) are canonical conjugate operators, the commutation relation of them are given by
\[
[\hat{N}_X, \frac{1}{2} \hat{\chi}_X] = -i.
\]

By introducing the following operators,
\[
\hat{C}_X = e^{-\frac{i}{2} \hat{\chi}_X} \hat{N}_X^{1/2}
\]
and
\[
\hat{C}^\dagger_X = \hat{N}_X^{1/2} e^{\frac{i}{2} \hat{\chi}_X},
\]
the commutation relation in Eq. (A.11) becomes,
\[
[\hat{C}_X, \hat{C}^\dagger_X] = 1;
\]
this shows that \( \hat{C}_X \) and \( \hat{C}^\dagger_X \) are the annihilation and creation operators for particles in \( S_X \). Note that the commutation relations are used, although the particles are fermions. This is allowable since we consider not the individual particle levels, but just the number in each superconductor with the condition \( N_X \gg 1 \).

Then, the operator for the transfer of particles between \( S_R \) and \( S_L \) is constructed as
\[
\hat{K}_J = t_{RL} \hat{C}^\dagger_R \hat{C}_L + \text{h.c.}
\]
where the hopping matrix element between \( S_L \) and \( S_R \), \( t_{RL} \), is given by a real parameter \( t_J \).
Let us employ a semiclassical approximation in which $\hat{\chi}_R, \hat{\chi}_L, \hat{N}_R, \hat{N}_L$ are replaced by their mean values $\chi_R, \chi_L, N_R, N_L$, respectively. Then, the semiclassical version of $K_J$ is given by

$$K_J = E_J \cos \left( \frac{1}{2}(\chi_L - \chi_R) \right), \quad (A.16)$$

where

$$E_J = 2t_J(N_RN_L)^{1/2}. \quad (A.17)$$

If a real magnetic field exits, the hopping matrix element becomes

$$t_{RL} = t_J \rightarrow t_{RL} = t_J e^{i \frac{q}{\hbar c} \int_R^L A_{em} \cdot \mathbf{d}r}, \quad (A.18)$$

thus, the kinetic term in Eq. (A.16) becomes

$$K_J = E_J \cos \left( \frac{1}{2}(\chi_L - \chi_R) - \frac{q}{\hbar c} \int_R^L A_{em} \cdot \mathbf{d}r \right). \quad (A.19)$$

Then, the current through the junction is given by

$$J = \frac{qE_J}{\hbar} \sin \phi, \quad (A.20)$$

where $\phi$ is given by

$$\phi = \frac{1}{2}(\chi_L - \chi_R) - \frac{q}{\hbar c} \int_R^L A_{em} \cdot \mathbf{d}r = -\frac{q}{\hbar c} \int_R^L A_{eff} \cdot \mathbf{d}r. \quad (A.21)$$

The time-derivative of $h\phi$ yields,

$$h\dot{\phi} = \frac{\partial \bar{H}}{\partial N_L} - \frac{\partial \bar{H}}{\partial N_R} + q \int_R^L \mathbf{E} \cdot \mathbf{d}r, \quad (A.22)$$

where $\bar{H}$ is a part of the Hamiltonian that excludes the electrostatic potential term

$$\bar{H} = H - q \int d^3 x \rho_{em}. \quad (A.23)$$

The electric field $\mathbf{E}$ inside the insulator region is given by

$$\mathbf{E} = -\nabla \varphi_{em} - \frac{1}{c} \frac{\partial A_{em}}{\partial t}. \quad (A.24)$$

In order to calculate the r.h.s in Eq. (A.22), we may use the following relation

$$\frac{\partial \bar{H}}{\partial N_L} - \frac{\partial \bar{H}}{\partial N_R} = \bar{H}(N_L + 1, N_R - 1) - \bar{H}(N_L, N_R), \quad (A.25)$$

where $\bar{H}(N_L, N_R)$ denotes the energy of the system excluding the electrostatic potential with $N_L$ particles on the left superconductor and $N_R$ particles on the right superconductor.

In the situation where particle flow occurs through the leads as shown in Fig. 1(b), the following two processes contribute to the r.h.s in Eq. (A.22):

$$\mathbf{E} = -\nabla \varphi_{em} - \frac{1}{c} \frac{\partial A_{em}}{\partial t}. \quad (A.24)$$
(i) Particle transfer by tunneling (indicated by the black solid arrow in Fig. 1(b)). It gives rise to
\[ q \int_{L}^{R} \mathbf{E} \cdot d\mathbf{r} = qV. \] (A.26)
This contribution can be interpreted as the energy gain from the acceleration during the tunneling from \( S_L \) to \( S_R \).

(ii) Particle flow through the leads (indicated by the red dotted arrows in Fig. 1(b)). The particle flows from \( L_L \) has the Fermi energy of the left lead which is equal to \( \mu_L \); the particle flows from \( L_R \) has the Fermi energy of the right lead which is equal to \( \mu_R \). Thus, we have
\[ \hat{H}(N_L + 1, N_R - 1) - \hat{H}(N_L, N_R) = \mu_L - \mu_R = qV \] (A.27)
This can be regarded as the energy gain by the particle flow-in from \( L_L \) to \( S_L \) and the flow-out from \( S_R \) to \( L_R \).

The total contribution is the sum of the above two, i.e., \( 2qV \). It corresponds to the total energy gain for the particle flow from \( L_L \) to \( R_L \) via the tunneling between \( S_L \) to \( S_R \).

Therefore, the time derivative of \( \phi \) is given by
\[ \dot{\phi} = \frac{2qV}{\hbar}. \] (A.28)
This yields the observed AC frequency \( \frac{2eV}{\hbar} \) with \( q = -e \).

The same frequency was obtained by taking into account only the first process in Eq. (A.26) with \( q = -2e \) by Josephson and others [17]. Since the current is measured in one of the leads, it is sensible to include the effect of the charge flow through the leads. If the contribution from it is included, the AC frequency for the \( q = -2e \) case becomes \( \frac{4eV}{h} \), which disagrees with the experiment.

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