Note on the Improper Bogoliubov Transformation

An Example in the Many-Quark System

Masaharu IWASAKI

Department of Physics, Kochi University, Kochi 780

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We study the improper Bogoliubov transformation which is an improper rotation in the \( SO(2N) \) group in Fermion systems. The mathematical properties of the Bogoliubov transformation are investigated generally, when the dimension \( N \) is odd. It is shown that the improper transformation appears naturally and some quasi-particles become gapless. This leads to the property that some physical quantities have singularities in momentum space across the Fermi surface. Moreover it is pointed out that such a case may be realized in quark matter.

1. Introduction

It is well-known that several Fermion systems become superconducting at low temperature. Such systems are described using the generalized Hartree-Fock (Hartree-Bogoliubov) theory. This is a kind of mean field approximation, and the Hamiltonian obtained by this method is diagonalized in terms of the unitary transformations which are referred to as the Bogoliubov transformations. Usually these transformations are assumed to be proper, that is, their determinants are unity. Some time ago, however, Fukutome\(^1\) pointed out the usefulness of a new type of Bogoliubov transformation whose determinant is negative in contrast to the usual ones. He named it as an improper Bogoliubov transformation. Later Fukutome, Yamamura, Nishiyama and the present author\(^2\) demonstrated that these transformations are especially suitable to Fermion systems with odd-particle number.

In this note, our aim is to point out that there exists another type of the improper Bogoliubov transformation. To this end we generally consider Fermion systems where the number of the single-particle state is odd. Then it is noted that the improper Bogoliubov transformation appears irrespective of the particle number of the system. Moreover it is shown that such a property may be realized in quark matter and that the resultant quasi-particles have an unusual property.

In 2 we develop a general theory of the Bogoliubov transformation based on the group \( SO(2N) \) with odd \( N \). Thus an example of the improper transformation is given in quark matter if the one-gluon-exchange interaction between quarks is assumed. Finally concluding remarks are given.

2. Improper Bogoliubov transformation

First let us consider a Fermion system with \( N \) single-particle states. Let \( c_a \) and \( c_a^\dagger \), \( a=1,2,\ldots,N \), be the annihilation-creation operators of the Fermion particle with the single particle state \( a \). As is well known, the Hartree-Bogoliubov Hamiltonian which is a generalization of the mean field approximation is written as

\[
H_{\text{RB}} = \sum_{ab} \left[ \varepsilon_{ab} c_a^\dagger c_b + \frac{1}{2} \Delta_{ab} c_a^\dagger c_b c_b^\dagger + \frac{1}{2} \Delta^*_{ab} c_b^\dagger c_a c_a^\dagger \right],
\]

(1)
where the single particle energy and the pairing field are given by the matrices \( \varepsilon \) and \( \Delta \), respectively. These can be regarded as \( N \times N \) matrices with the following symmetry properties:

\[
\varepsilon^* = \varepsilon \quad \text{and} \quad \Delta^T = -\Delta ,
\]

without loss of the generality. The Hamiltonian (1) may be expressed in matrix form as follows:

\[
H_{HB} = \frac{1}{2} \left( c^+ \begin{pmatrix} \varepsilon & \Delta \\ -\Delta^* & -\varepsilon^* \end{pmatrix} c \right) + \text{const.}
\]

In order to diagonalize this Hamiltonian, we introduce the unitary transformation (the Bogoliubov transformation),

\[
\begin{pmatrix} c \\ c^+ \end{pmatrix} = \begin{pmatrix} u & \nu^* \\ \nu & u^* \end{pmatrix} \begin{pmatrix} a \\ a^+ \end{pmatrix} = U \begin{pmatrix} a \\ a^+ \end{pmatrix} .
\]

The quasi-particles \( a_a \) and \( a_a^+ \) introduced on the right-hand side satisfy the anticommutation relations of the Fermion. The unitary conditions \( UU^+ = U^+U = 1 \) lead to the following relations:

\[
\begin{aligned}
uu^* + \nu^*\nu^T &= 1 , \\
\nu\nu^* + \nu^*u^T &= 0 , \\
u^*u + \nu^+\nu &= 1 , \\
u^*\nu^* + \nu^+u^* &= 0 .
\end{aligned}
\]

Using this unitary matrix, we can obtain the eigenvalue equation for the Hamiltonian matrix appearing in Eq. (3),

\[
\begin{pmatrix} \varepsilon & \Delta \\ \Delta^* & -\varepsilon^* \end{pmatrix} \begin{pmatrix} u & \nu^* \\ \nu & u^* \end{pmatrix} = \begin{pmatrix} \nu & u^* \\ u & \nu^* \end{pmatrix} \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix} ,
\]

where \( E \) is the \( N \times N \) diagonal matrix whose diagonal elements are arranged so as to be positive.

Now we will investigate general mathematical properties of the above-mentioned Bogoliubov transformation. It is assumed here that the number of the single-particle state is odd. Note that this assumption is essential in the subsequent discussion. Thus the following properties hold:

(i) \( \det U = \pm 1 \).

Noting that \( \det U^* = \det U \) and \( \det U \det U^* = 1 \), this follows at once.

(ii) \( \det \Delta = 0 \).

Since the \( \Delta \) is an anti-symmetric matrix, one obtains \( \det \Delta = \det \Delta^T = (-1)^N \det \Delta \). When \( N \) is odd, Eq. (8) is obtained.
This relation is derived directly from the last equation (5d);
\[ \det u \det \nu = (-1)^n \det \nu \det u. \] 
\[ \text{(iv)} \quad \det U = \begin{cases} +1, & (\det u \neq 0) \\ -1, & (\det \nu \neq 0) \end{cases} \] 

**Proof** First we must recall the formulae
\[ \det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det A \det (D - CA^{-1}B), \] 
where \( A, B, C \) and \( D \) are any \( N \times N \) matrices, and \( \det A \neq 0 \) is assumed. Applying this identity to our unitary transformation with \( \det u \neq 0 \), we obtain
\[ \det U = \det u \det (u^* - \nu u^{-1} \nu^*) = \det u \det (u^* + \nu \nu^* (u^T)^{-1}). \] 
In the second equation, use is made of Eq. (5b). Moreover, using Eq. (5a), the right-hand side of Eq. (12) is transformed into
\[ \det U = \det u \det (u^* + (1 - u^* u^T) (u^T)^{-1}) \] 
\[ = \det u (\det u^T)^{-1} = 1. \] 
On the other hand, let us consider the case \( \det \nu \neq 0 \). If we interchange the two matrices \( u \) and \( \nu \), we obtain
\[ \det \begin{pmatrix} u & \nu^* \\ \nu & u^* \end{pmatrix} = (-1)^n \det \begin{pmatrix} \nu & u^* \\ u & \nu^* \end{pmatrix}. \] 
The determinant on the right-hand side becomes unity by the procedure described above. Consequently we obtain \( \det U = -1 \).

\[ \text{(v)} \quad \text{If} \ \epsilon^* = \epsilon \ \text{and} \ [\epsilon, \Delta] = [\Delta, \Delta^*] = 0, \ \text{then} \ E = \sqrt{\tilde{\epsilon}^2 + \tilde{\Delta}^2}, \] 
where the \( \tilde{\epsilon} \) and \( \tilde{\Delta} \) are diagonal matrices of \( \epsilon \) and \( \Delta \), respectively.

**Proof** The square of the Hamiltonian matrix is written as
\[ \begin{pmatrix} \epsilon & \Delta \\ \Delta^* & -\epsilon \end{pmatrix}^2 = \begin{pmatrix} \epsilon^2 + \Delta \Delta^* & 0 \\ 0 & \epsilon^2 + \Delta^* \Delta \end{pmatrix}. \] 
Since the hermite matrix \( \epsilon \) and the normal matrix \( \Delta (\Delta^* = \Delta^* \Delta) \) commute, these can be diagonalized by the unitary matrix simultaneously. The diagonal matrices are denoted by \( \tilde{\epsilon} \) and \( \tilde{\Delta} \), respectively. It should be noted that at least one of the diagonal elements of \( \tilde{\Delta} \) vanishes because of \( \det \Delta = \det \tilde{\Delta} = 0 \). Therefore it is proved that some gapless quasi-particles necessarily appear.

3. **Application to the quark matter** Here we give an example of the improper Bogoliubov transformation mentioned above. Recently it has been pointed out that
the ground state of the quark matter may be a superconducting (BCS) state.\textsuperscript{3,4) Although the quark matter has not been observed in nature, its existence is expected to be realized inside high density stars.\textsuperscript{5)} Our aim is not to discuss the possibility of the quark matter but to study the mathematical structure of the Bogoliubov transformation assuming a simple BCS-type model Hamiltonian for the quark matter.

If quarks interact with each other via the one-gluon exchange interaction, there exists an attractive force between two quarks in the color-anti symmetric and spin-parallel state, as shown in Ref. 4). Thus the pairing scheme is expected to be

\begin{equation}
\langle c_{-\mathbf{k},ab}c_{\mathbf{k}0a}\rangle = \begin{pmatrix}
0 & 1 & -1 \\
-1 & 0 & 1 \\
1 & -1 & 0
\end{pmatrix}_{a,b} F_{\mathbf{k}} \equiv \bar{\varepsilon}_{a,b} F_{\mathbf{k}} .
\end{equation}

Here a single particle state is designated by momentum $\mathbf{k}$ ($|\mathbf{k}|$), helicity $s$ along the momentum $\mathbf{k}$ and color $a$. Since we have assumed that the expectation value is independent of the helicity and the direction of the $\mathbf{k}$, our Cooper pair is in the $s$-wave and spin-parallel (spin-triplet) state. From this type of the pairing field, the Hartree-Bogoliubov Hamiltonian is given by\textsuperscript{4)}

\begin{equation}
H_{\text{HB}} = \sum_{\mathbf{k}} (c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + c_{-\mathbf{k}}^\dagger c_{-\mathbf{k}}) \begin{pmatrix}
\varepsilon_{\mathbf{k}} & \Delta_{\mathbf{k}} \\
\Delta_{\mathbf{k}}^* & -\varepsilon_{\mathbf{k}}
\end{pmatrix} + \text{const} ,
\end{equation}

where the $3 \times 3$ matrices $\varepsilon_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$ are given by\textsuperscript{4)}

\begin{equation}
\varepsilon_{\mathbf{k}} = e_{\mathbf{k}} - \mu \text{ and } \Delta_{\mathbf{k}} = id_{\mathbf{k}} \bar{\varepsilon} ,
\end{equation}

with the use of the anti-symmetric matrix $\bar{\varepsilon}$ introduced in Eq. (17). The quantities $e_{\mathbf{k}}$ and $d_{\mathbf{k}}$, which should be determined self-consistently, are real numbers, and $\mu$ and $\lambda$ Lagrange multipliers.\textsuperscript{4)} The suffix of the matrices appearing in 3 refers to the degrees of the color space. The whole Bogoliubov transformation discussed in 2 is composed of these $6 \times 6$ matrices. Each matrix can be diagonalized by a unitary transformation,

\begin{equation}
\begin{pmatrix}
c_{\mathbf{k}}^\dagger \\
c_{-\mathbf{k}}^\dagger
\end{pmatrix} =
\begin{pmatrix}
u_{\mathbf{k}} & \nu_{\mathbf{k}}^* \\
u_{\mathbf{k}} & \nu_{\mathbf{k}}^*
\end{pmatrix}
\begin{pmatrix}
a_{\mathbf{k}}^\dagger \\
a_{-\mathbf{k}}^\dagger
\end{pmatrix} = U_{\mathbf{k}} \begin{pmatrix}
a_{\mathbf{k}}^\dagger \\
a_{-\mathbf{k}}^\dagger
\end{pmatrix} .
\end{equation}

This unitary transformation is referred to as the (reduced) Bogoliubov transformation in 3. This is an example of the Bogoliubov transformation with $N=3$ discussed in 2. Since the conditions in (v) are apparently satisfied, all the general properties derived in 2 hold in this system.

In order to investigate the improper transformation, let us consider two extreme cases of the transformation, (a) $k \to \infty$ and (b) $k \to 0$. The former corresponds to $a_k \to c_k$,

\begin{equation}
u_k \to 0 \text{ and } \nu_k \to 0 ,
\end{equation}

\textsuperscript{4)} In what follows we omit the Lagrange multiplier for the color singlet condition. If we take into account this condition, our conclusions mentioned below are not changed at all.
which leads to a proper transformation, $\det U_k = 1$. The latter transformation corresponds to $a_k \to c_k^\dagger$, that is,

$$u_k \to 0 \quad \text{and} \quad \nu_k \to 1.$$  

(22)

This does lead to an improper transformation, $\det U_k = -1$, from the property (iv). There are now two kinds of Bogoliubov transformations: (a) the proper transformation ($\det u_k \neq 0$) and (b) the improper one ($\det \nu_k \neq 0$). These are represented as follows:

$$
U_k^{(a)} = \begin{pmatrix}
1 & -ix_k \bar{c}

ix_k \bar{c} & 1
\end{pmatrix}
\begin{pmatrix}
S_k & 0
0 & S_k
\end{pmatrix}
\quad \text{and} \quad
U_k^{(b)} = \begin{pmatrix}
x_k \bar{c} & -i
i & x_k \bar{c}
\end{pmatrix}
\begin{pmatrix}
S_k & 0
0 & S_k
\end{pmatrix},

(23)

(\det U_k^{(b)} = -\det U_k^{(a)}).$ The real variable $x_k$ and real matrix $S_k$ in both cases are determined by the same equations except for the sign of $\bar{c}$. The energy of the gapless quasi-particle is given by $E_k = e_k$ for (a) and $E_k = -e_k$ for (b), respectively. Taking into account the assumption that the quasi-particle energy is positive, the following selection is evident. The proper transformation (a) should be chosen for the particle state ($e_k > \mu$) and the improper one (b) for the hole state ($e_k < \mu$). Note that this doublet structure is characteristic of $N = \text{odd}$ systems and does not exist in the $N = \text{even}$ systems. The Fermi energy $\mu$ should be determined by the total number condition of our quark system.

Now there is sudden change of the determinant across the Fermi surface, which will bring about singularities in various physical quantities. In fact, the particle occupation number in the ground (BCS) state is given by

$$
\langle c_{k^*a} c_{k^*a} \rangle = (\nu_k \nu_{k'}^{\dagger})_{a,a}.
$$

(24)

The quantity on the right-hand side is dependent on the coefficients of the Bogoliubov transformation so that it has a discontinuity across the Fermi surface. From the detailed calculation done in Ref. 4), the jump of the occupation number becomes 1/3. On the other hand, the gap parameter (17) is not changed.

Finally it is instructive to comment on the relation between the present Bogoliubov transformation and that appearing in usual electron superconductors. The usual Bogoliubov transformation is written as

$$
\begin{pmatrix}
c_{k^*t}
c_{k^*i}
c_{-k^*_i}
c_{-k^*_t}
\end{pmatrix} = \begin{pmatrix}
u_k & 0 & 0 & \nu_k^*
0 & -\nu_k^* & 0 & \nu_k
0 & \nu_k & 0 & -\nu_k
-\nu_k & 0 & 0 & -\nu_k
\end{pmatrix}\begin{pmatrix}
a_{k^*t}
a_{k^*i}
a_{-k^*_i}
a_{-k^*_t}
\end{pmatrix},
$$

(25)

This transformation has just the same form as that in Eq. (4). Thus it is reduced to the transformations

$$
\begin{pmatrix}
c_{k^*t}
c_{k^*_i}
\end{pmatrix} = \begin{pmatrix}
u_k & \nu_k^*
-\nu_k & \nu_k^*
\end{pmatrix}\begin{pmatrix}
a_{k^*t}
a_{k^*_i}
\end{pmatrix},
$$

(26)

which is familiar form in electron superconductors. It is evident that the determinant
of this matrix is always unity irrespective of the single particle state, due to the minus sign appearing in the non-diagonal element. This sign originates from the fact that the Cooper pair is in the spin-singlet state. Thus we are not worried about the improper transformation. We must, however, be careful about the presence of the improper one when the number of the single-particle state is odd.

In conclusion, we have investigated the general properties of the Bogoliubov transformations $SO(2N)$ with odd $N$. It is shown that improper transformations appear naturally and some quasi-particles are gapless. This leads to the property that some physical quantities have singularities across the Fermi surface in momentum space.4)

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