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Mathematical Analysis of the BCS-Bogoliubov Theory

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1 Introduction

Superconductivity is one of the historical landmarks in condensed matter physics. Since Onnes found out the fact that the electrical resistivity of mercury drops to zero below the temperature 4.2K in 1911, the zero electrical resistivity is observed in many metals and alloys. Such a phenomenon is called superconductivity, and the magnetic properties of superconductors as well as their electric properties are also astonishing. For example, the magnetic flux is excluded from the interior of a superconductor. This phenomenon was observed first by Meissner in 1933, and is called the Meissner effect. In 1957 Bardeen, Cooper and Schrieffer [1] proposed the highly successful quantum theory called the BCS theory. The superconducting state and the Hamiltonian they dealt with are called the BCS state and the BCS Hamiltonian, respectively. In 1958 Bogoliubov [2] obtained the results similar to those in the BCS theory using the canonical transformation called the Bogoliubov transformation. This theory is called the Bogoliubov theory.

The ground state of the BCS Hamiltonian is discussed by several authors. In 1961 Mattis and Lieb [5] studied the wavefunction of the ground state of the BCS Hamiltonian under the condition that in the ground state, all the electrons in the neighborhood of the Fermi surface are paired. See Richardson [7] and von Delft [3] for the ground state of the BCS Hamiltonian without the condition just above. From the viewpoint of C^*-algebra, Gerisch and Rieckers [4] studied a class of BCS-models to show that there is a unique C^*-dynamical system for each BCS-model.

In this paper, first, we reformulate the BCS-Bogoliubov theory of superconductivity from the viewpoint of linear algebra. We define the BCS Hamiltonian on $\mathbb{C}^{2^{2M}}$, where M is a positive integer. We discuss selfadjointness and symmetry of the BCS Hamiltonian as well as spontaneous symmetry breaking. Beginning with the gap equation, we give the well-known expression for the BCS state and find the existence of an energy gap. We also show that the BCS state has a lower energy than the normal state. Second, we introduce a new superconducting state explicitly and show from the viewpoint of linear algebra that this new state has a lower energy than the BCS state. Third, beginning with our new gap equation, we show from the viewpoint of linear algebra that we arrive at the results similar to those in the BCS-Bogoliubov theory. See Watanabe [8] for more details.

Let L, $K_{max} > 0$ be large enough and let us fix them. For $n_1,\, n_2,\, n_3 \in \mathbb{Z}$, set

$$\Lambda = \left\{ \frac{2\pi}{L}(n_1,\, n_2,\, n_3) \in \mathbb{R}^3 :\ \frac{2\pi}{L}\sqrt{n_1^2+n_2^2+n_3^2} \le K_{max} \right\}.$$

Here we do not let $K_{max} = \infty$ for simplicity. Let the number of all the elements of Λ be M and let wave vector k belong to Λ.

The number $n_{k\sigma}$ of electrons with wave vector k and spin σ ($\sigma =\uparrow$ (spin up), $\downarrow$ (spin down)) is equal to 0 or 1, and so the number of the states

$$|\, n_{k\uparrow},\, n_{k\downarrow},\, n_{k'\uparrow},\, n_{k'\downarrow},\, \dots\rangle, \qquad k,\, k',\, \dots \in \Lambda$$

is equal to 2^{2M}. Here, $n_{k\uparrow}$, $n_{k\downarrow} = 0,\ 1$, and the elements k and k' are arranged in a certain order.

We therefore choose, as our Hilbert space $\mathcal{H}$,

$$\mathcal{H} = \mathbb{C}^{2^{2M}}$$

and denote each standard unit vector in $\mathcal{H} = \mathbb{C}^{2^{2M}}$:

$$e_i = (0,\, \dots\, ,\, 0,\, \overset{i}{\widehat{1}},\, 0,\, \dots\, ,\, 0), \qquad i = 1,\, 2,\, \dots\, ,\, 2^{2M}$$

by each state above for simplicity.

For example, we denote

$$e_1 = (1,\, 0,\, 0, \dots\, ,\, 0), \qquad e_2 = (0,\, 1,\, 0, \dots\, ,\, 0)$$

by $|0,\, 0,\, 0,\, \dots\rangle$, $|1,\, 0,\, 0,\, \dots\rangle$, respectively. Moreover, we denote

$$e_{2^{2M}} = (0,\, 0,\, \dots\, ,\, 0,\, 1)$$

by $|1,\, 1,\, 1,\, \dots\rangle$.

Here the symbol $|0,\, 0,\, 0,\, \dots\rangle$ corresponds to the state $n_{k\uparrow} = n_{k\downarrow} = 0$ for all $k \in \Lambda$, and $|1,\, 0,\, 0,\, \dots\rangle$ to the state $n_{k\uparrow} = 1$ and $n_{k\downarrow} = n_{k'\sigma} = 0$ for all $k' \in \Lambda \setminus \{k\}$ and for all $\sigma =\uparrow,\, \downarrow$. Moreover, $|1,\, 1,\, 1,\, \dots\rangle$ corresponds to the state $n_{k\uparrow} = n_{k\downarrow} = 1$ for all $k \in \Lambda$.

We abbreviate $|0,\, 0,\, 0,\, \dots\rangle$ to $|0\rangle$ and call it the vacuum vector in $\mathcal{H} = \mathbb{C}^{2^{2M}}$. We denote by $(\cdot\, ,\, \cdot)$ the inner product of $\mathcal{H} = \mathbb{C}^{2^{2M}}$.

2 Creation and annihilation operators

We assume that each creation operator and each annihilation operator depend both on wave vector $k \in \Lambda$ and on spin σ of an electron. We denote the creation operator (resp. the annihilation operator) by $C^*_{k\sigma}$ (resp. by $C_{k\sigma}$). Note that $|\dots\, ,\, n_{k\uparrow},\, n_{k\downarrow},\, \dots\rangle$ ($n_{k\uparrow}$, $n_{k\downarrow} = 0,\ 1$) stands for the corresponding standard unit vector in $\mathcal{H} = \mathbb{C}^{2^{2M}}$, as mentioned in the preceding section.

Definition 2.1.

$$\begin{cases} C_{k\uparrow}|\dots\, ,\, n_{k\uparrow},\, n_{k\downarrow},\, \dots\rangle = (-1)^{\sharp}\delta_{1,\, n_{k\uparrow}}|\dots\, ,\, n_{k\uparrow} - 1,\, n_{k\downarrow},\, \dots\rangle, \\ C^*_{k\uparrow}|\dots\, ,\, n_{k\uparrow},\, n_{k\downarrow},\, \dots\rangle = (-1)^{\sharp}\delta_{0,\, n_{k\uparrow}}|\dots\, ,\, n_{k\uparrow} + 1,\, n_{k\downarrow},\, \dots\rangle, \end{cases}$$

where the symbol $\sharp$ denotes the number of electrons arranged at the left of the symbol $n_{k\uparrow}$ above.

$$\begin{cases} C_{k\downarrow}|\dots\, ,\, n_{k\uparrow},\, n_{k\downarrow},\, \dots\rangle = (-1)^{\sharp\sharp}\delta_{1,\, n_{k\downarrow}}|\dots\, ,\, n_{k\uparrow},\, n_{k\downarrow} - 1,\, \dots\rangle, \\ C^*_{k\downarrow}|\dots\, ,\, n_{k\uparrow},\, n_{k\downarrow},\, \dots\rangle = (-1)^{\sharp\sharp}\delta_{0,\, n_{k\downarrow}}|\dots\, ,\, n_{k\uparrow},\, n_{k\downarrow} + 1,\, \dots\rangle, \end{cases}$$

where the symbol $\sharp\sharp$ denotes the number of electrons arranged at the left of the symbol $n_{k\downarrow}$ above.

On the basis of the definition we regard each of the creation and annihilation operators as a linear operator on $\mathcal{H} = \mathbb{C}^{2^{2M}}$. The definition immediately gives the following lemma.

Lemma 2.2. (a) The annihilation operator $C_{k\sigma}$ is a bounded linear operator on $\mathcal{H} = \mathbb{C}^{2^{2M}}$, and its adjoint operator coincides with the creation operator $C^*_{k\sigma}$.
(b) The operators $C_{k\sigma}$ and $C^*_{k\sigma}$ satisfy the canonical anticommutation relations on $\mathcal{H} = \mathbb{C}^{2^{2M}}$:

$$\{C_{k\sigma},\, C^*_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}, \qquad \{C_{k\sigma},\, C_{k'\sigma'}\} = \{C^*_{k\sigma},\, C^*_{k'\sigma'}\} = 0,$$

where $\{A,\, B\} = AB + BA$.

Remark 2.3.

$$|\, n_{k\uparrow},\, n_{k\downarrow},\, n_{k'\uparrow},\, n_{k'\downarrow},\, \dots\rangle = \left(C^*_{k\uparrow}\right)^{n_{k\uparrow}} \left(C^*_{k\downarrow}\right)^{n_{k\downarrow}} \left(C^*_{k'\uparrow}\right)^{n_{k'\uparrow}} \left(C^*_{k'\downarrow}\right)^{n_{k'\downarrow}} \cdots |0\rangle.$$

3 The BCS Hamiltonian

Let m and μ stand for the electron mass and the chemical potential, respectively. Here, $m,\, \mu > 0$. Set $\xi_k = \hbar^2|k|^2/(2m) - \mu$. The BCS Hamiltonian [1] is given by

$$H = \sum_{k\in\Lambda,\,\sigma=\uparrow,\downarrow} \xi_k\, C^*_{k\sigma}C_{k\sigma} + \sum_{k,\,k'\in\Lambda} U_{k,\,k'}C^*_{k'\uparrow}C^*_{-k'\downarrow}C_{-k\downarrow}C_{k\uparrow}\,.$$

Here, $U_{k,\,k'}$ is a function of k and k', and satisfies $U_{k,\,k'} \le 0$, $U_{k',\,k} = U_{k,\,k'}$, $U_{-k,\,-k'} = U_{k,\,k'}$ and $U_{k,\,k} = 0$.

Proposition 3.1. *The BCS Hamiltonian H is a bounded, selfadjoint operator on $\mathcal{H} = \mathbb{C}^{2^{2M}}$.*

The bounded, selfadjoint operator

$$G = \sum_{k\in\Lambda,\,\sigma=\uparrow,\downarrow} C^*_{k\sigma}C_{k\sigma}$$

generates a strongly continuous unitary group $\{e^{i\alpha G}\}_{\alpha\in\mathbb{R}}$ on $\mathcal{H} = \mathbb{C}^{2^{2M}}$. As is shown just below, the transformation $e^{i\alpha G}$ gives rise to a phase transformation of the creation (the annihilation) operator.

Proposition 3.2. *Let G and H be as above. Then, for $\alpha \in \mathbb{R}$,*

$$e^{-i\alpha G}C_{k\sigma}\, e^{i\alpha G} = e^{i\alpha}C_{k\sigma}\,, \qquad e^{-i\alpha G}C^*_{k\sigma}\, e^{i\alpha G} = e^{-i\alpha}C^*_{k\sigma}\,.$$

Consequently, $\quad e^{-i\alpha G}H\, e^{i\alpha G} = H.$

Remark 3.3. The transformation $e^{i\alpha G}$ leaves the BCS Hamiltonian H invariant. In this case the BCS Hamiltonian H is said to have global U(1) symmetry.

4 Spontaneous symmetry breaking

Definition 4.1 (Nambu and Jona-Lasinio). Let G be as above. Suppose that there is the ground state $\Psi_0 \in \mathcal{H} = \mathbb{C}^{2^{2M}}$ of the BCS Hamiltonian H. The global U(1) symmetry is said to be spontaneously broken if there is a bounded linear operator A on $\mathcal{H} = \mathbb{C}^{2^{2M}}$ satisfying

$$(\Psi_0, [G, A]\,\Psi_0) \neq 0.$$

Lemma 4.2. *Set $A = C_{-k\downarrow}C_{k\uparrow}$ in the definition above. Then*

$$(\Psi_0, [G, C_{-k\downarrow}C_{k\uparrow}]\,\Psi_0) = -2\,(\Psi_0, C_{-k\downarrow}C_{k\uparrow}\Psi_0).$$

Remark 4.3. If $(\Psi_0, C_{-k\downarrow}C_{k\uparrow}\Psi_0) \neq 0$, then the global U(1) symmetry is spontaneously broken.

Remark 4.4. The concept of spontaneous symmetry breaking was introduced first by Nambu and Jona-Lasinio [6] in 1961. This plays an important role in quantum mechanics such as the BCS-Bogoliubov theory and quantum gauge field theory.

5 An energy gap for excitation from the BCS state

Let Δ_k be a function of $k \in \Lambda$. We assume the existence of the following Δ_k : Δ_k satisfies $\Delta_k \geq 0$ and $\Delta_{-k} = \Delta_k$, and is a solution to the "gap equation" ([1], [2])

$$\Delta_k = -\frac{1}{2}\sum_{k'\in\Lambda} U_{k,k'}\,\frac{\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}}\,.$$

Let θ_k be a function of $k \in \Lambda$ and let it satisfy ([1], [2])

$$\sin 2\theta_k = \frac{\Delta_k}{\sqrt{\xi_k^2 + \Delta_k^2}}\,, \qquad \cos 2\theta_k = \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta_k^2}}$$

with $0 \leq \theta_k \leq \pi/2$. Note that $\theta_{-k} = \theta_k$.

We denote by G_B the following bounded, selfadjoint operator on $\mathcal{H} = \mathbb{C}^{2^{2M}}$:

$$G_B = i\sum_{k\in\Lambda} \theta_k\left(C_{-k\downarrow}C_{k\uparrow} - C_{k\uparrow}^* C_{-k\downarrow}^*\right).$$

We set $\Psi_{BCS} = e^{iG_B}|0\rangle \in \mathcal{H} = \mathbb{C}^{2^{2M}}$ and call it the BCS state ([1], [2]).

Lemma 5.1 (BCS).

$$\Psi_{BCS} = \left\{\prod_{k\in\Lambda}\left(\cos\theta_k + \sin\theta_k\, C_{k\uparrow}^* C_{-k\downarrow}^*\right)\right\}|0\rangle.$$

Remark 5.2. In 1957 Bardeen, Cooper and Schrieffer [1] introduced the well-known expression in this lemma.

Corollary 5.3.
(a) $(\Psi_{BCS}, C_{-k\downarrow}C_{k\uparrow}\Psi_{BCS}) = \left(\Psi_{BCS}, C^*_{k\uparrow}C^*_{-k\downarrow}\Psi_{BCS}\right) = \dfrac{1}{2}\sin 2\theta_k$.
(b) $\Delta_k = -\sum_{k'\in\Lambda} U_{k,k'}\,(\Psi_{BCS}, C_{-k'\downarrow}C_{k'\uparrow}\Psi_{BCS})$.

We replace the ground state Ψ_0 of the BCS Hamiltonian by Ψ_{BCS} and set (for all $k\in\Lambda$)

$$\begin{cases} C_{-k\downarrow}C_{k\uparrow} = (\Psi_{BCS}, C_{-k\downarrow}C_{k\uparrow}\Psi_{BCS}) + b_k\,, \\ C^*_{k\uparrow}C^*_{-k\downarrow} = \left(\Psi_{BCS}, C^*_{k\uparrow}C^*_{-k\downarrow}\Psi_{BCS}\right) + b^*_k\,. \end{cases}$$

Lemma 5.4. *Set*

$$\begin{aligned} H_M &= \sum_{k\in\Lambda,\,\sigma=\uparrow,\downarrow} \xi_k\, C^*_{k\sigma}C_{k\sigma} - \sum_{k\in\Lambda}\Delta_k\left(C_{-k\downarrow}C_{k\uparrow} + C^*_{k\uparrow}C^*_{-k\downarrow}\right) \\ &\quad + \sum_{k\in\Lambda}\Delta_k\,(\Psi_{BCS}, C_{-k\downarrow}C_{k\uparrow}\Psi_{BCS})\,. \end{aligned}$$

Then the BCS Hamiltonian is rewritten as

$$H = H_M + \sum_{k,\,k'\in\Lambda} U_{k,k'}\, b^*_{k'}\, b_k\,.$$

Remark 5.5. The Hamiltonian H_M is called the mean field approximation for the BCS Hamiltonian H.

We now introduce the Bogoliubov transformation of $C_{k\sigma}$ [2]:

$$\gamma_{k\sigma} = e^{iG_B}C_{k\sigma}e^{-iG_B}.$$

Note that the operator $\gamma_{k\sigma}$ and its adjoint operator $\gamma^*_{k\sigma}$ are both bounded linear operators on $\mathcal{H} = \mathbb{C}^{2^{2M}}$.

Proposition 5.6 (Bogoliubov).

$$\begin{aligned} H_M &= \sum_{k\in\Lambda,\,\sigma=\uparrow,\downarrow} \sqrt{\xi_k^2 + \Delta_k^2}\;\gamma^*_{k\sigma}\gamma_{k\sigma} \\ &\quad + \sum_{k\in\Lambda}\left\{\xi_k - \sqrt{\xi_k^2+\Delta_k^2} + \Delta_k\,(\Psi_{BCS}, C_{-k\downarrow}C_{k\uparrow}\Psi_{BCS})\right\}. \end{aligned}$$

Corollary 5.7. (a) The BCS state Ψ_{BCS} is the ground state of H_M, and the ground state energy E_{BCS} is given by

$$E_{BCS} = \sum_{k\in\Lambda}\left\{\xi_k - \sqrt{\xi_k^2+\Delta_k^2} + \Delta_k\,(\Psi_{BCS}, C_{-k\downarrow}C_{k\uparrow}\Psi_{BCS})\right\}.$$

(b) Let E_{BCS} be as in (a). Then the spectrum of H_M is given by

$$\sigma(H_M) = \left\{ \sum_{k\in\Lambda} \sqrt{\xi_k^2 + \Delta_k^2}\,(N_{k\uparrow} + N_{k\downarrow}) + E_{BCS} \right\}_{N_{k\uparrow},\,N_{k\downarrow}=0,1}$$

Remark 5.8. The corollary above implies that it takes a finite energy $\sqrt{\xi_k^2 + \Delta_k^2}$ $(> \Delta_k)$ to excite a particle from the BCS state to an upper energy state. So the function Δ_k of $k \in \Lambda$ corresponds exactly to the energy gap, and hence Δ_k is called the gap function (see Bardeen, Cooper and Schreiffer [1], and Bogoliubov [2]).

We now study some properties of the operators $\gamma_{k\sigma}$ (see Bogoliubov [2]).

Corollary 5.9. *The operators $\gamma_{k\sigma}$ and $\gamma_{k\sigma}^*$ satisfy the following.*
(a) $\{\gamma_{k\sigma}, \gamma_{k'\sigma'}^*\} = \delta_{kk'}\delta_{\sigma\sigma'}$, $\quad \{\gamma_{k\sigma}, \gamma_{k'\sigma'}\} = \{\gamma_{k\sigma}^*, \gamma_{k'\sigma'}^*\} = 0$.
(b) $\gamma_{k\sigma}\Psi_{BCS} = 0$ for each $k \in \Lambda$ and for each $\sigma = \uparrow, \downarrow$.
(c)
$$\begin{cases} \gamma_{k\uparrow} = \cos\theta_k\, C_{k\uparrow} - \sin\theta_k\, C_{-k\downarrow}^*, \\ \gamma_{-k\downarrow} = \sin\theta_k\, C_{k\uparrow}^* + \cos\theta_k\, C_{-k\downarrow}. \end{cases}$$
(d)
$$\begin{cases} C_{k\uparrow} = \cos\theta_k\, \gamma_{k\uparrow} + \sin\theta_k\, \gamma_{-k\downarrow}^*, \\ C_{-k\downarrow} = -\sin\theta_k\, \gamma_{k\uparrow}^* + \cos\theta_k\, \gamma_{-k\downarrow}. \end{cases}$$

6 The BCS and normal states

Let $\Delta_k = 0$ for all $k \in \Lambda$. Then the BCS state Ψ_{BCS} coincides with the "Fermi vacuum" $\Psi_F \in \mathcal{H} = \mathbb{C}^{2^{2M}}$. Here the Fermi vacuum Ψ_F corresponds to the normal state and is defined by

$$\Psi_F = \left\{ \prod_{k\ (\xi_k \le 0)} C_{k\uparrow}^* C_{-k\downarrow}^* \right\} |0\rangle,$$

where the symbol k $(\xi_k \le 0)$ stands for $k \in \Lambda$ satisfying $\xi_k \le 0$.

Proposition 6.1. *The BCS state Ψ_{BCS} has a lower energy than the Fermi vacuum Ψ_F (the normal state), i.e.,*

$$\begin{aligned} (\Psi_{BCS},\, H\Psi_{BCS}) - (\Psi_F,\, H\Psi_F) &= -\frac{1}{2}\sum_{k\in\Lambda} \frac{\left(\sqrt{\xi_k^2 + \Delta_k^2} - |\xi_k|\right)^2}{\sqrt{\xi_k^2 + \Delta_k^2}} \\ &< 0. \end{aligned}$$

7 A new superconducting state

Set $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$, $k \in \Lambda$ and set $B_k = C_{-k\downarrow} C_{k\uparrow}$. We abbreviate $\sin\theta_k$ (resp. $\cos\theta_k$) to S_k (resp. to C_k). We consider the following vector in $\mathcal{H} = \mathbb{C}^{2^{2M}}$:

$$\Psi = \frac{\Psi_{BCS} + \Phi}{\sqrt{1 + (\Phi,\, \Phi)}},$$

where $\Phi = \frac{1}{2} \sum_{p,\,p' \in \Lambda} \frac{U_{p,p'} \left(C_p^2\, S_{p'}^2 + C_{p'}^2\, S_p^2\right)}{E_p + E_{p'}} \gamma_{p\uparrow}^*\, \gamma_{-p\downarrow}^*\, \gamma_{p'\uparrow}^*\, \gamma_{-p'\downarrow}^*\, \Psi_{BCS}$.

We prepare some lemmas.

Lemma 7.1. (a) $(\Psi_{BCS},\, \Phi) = 0$.
(b)

$$H_M \Phi = E_{BCS} \Phi + 2 \sum_{p,\,p' \in \Lambda} \frac{E_{p'} U_{p,p'} \left(C_p^2\, S_{p'}^2 + C_{p'}^2\, S_p^2\right)}{E_p + E_{p'}} \gamma_{p\uparrow}^*\, \gamma_{-p\downarrow}^*\, \gamma_{p'\uparrow}^*\, \gamma_{-p'\downarrow}^*\, \Psi_{BCS}.$$

(c) $$(\Psi,\, H_M \Psi) = E_{BCS} + \frac{1}{1 + (\Phi,\, \Phi)} \sum_{p,\,p' \in \Lambda} \frac{U_{p,p'}^2 \left(C_p^2\, S_{p'}^2 + C_{p'}^2\, S_p^2\right)^2}{E_p + E_{p'}}.$$

Set $H' = H - H_M$. Then

$$H' = \sum_{k,\,k' \in \Lambda} U_{k,k'} \left\{B_{k'}^* B_k - C_{k'}\, S_{k'} \left(B_k^* + B_k\right) + C_k\, S_k\, C_{k'}\, S_{k'}\right\}.$$

Lemma 7.2. *Let H' be as above.*
(a) $H' \Psi_{BCS} = - \sum_{k,\,k' \in \Lambda} U_{k,k'}\, S_k^2\, C_{k'}^2\, \gamma_{k\uparrow}^*\, \gamma_{-k\downarrow}^*\, \gamma_{k'\uparrow}^*\, \gamma_{-k'\downarrow}^*\, \Psi_{BCS}$.
(b) $(\Psi_{BCS},\, H' \Psi_{BCS}) = 0$.
(c) $(\Phi,\, H' \Psi_{BCS}) = -\frac{1}{2} \sum_{p,\,p' \in \Lambda} \frac{U_{p,p'}^2 \left(C_p^2\, S_{p'}^2 + C_{p'}^2\, S_p^2\right)^2}{E_p + E_{p'}}$.

Lemma 7.3. (a)

$$\begin{aligned} B_k \Phi \;=\; & \left(C_k\, S_k - S_k^2\, \gamma_{k\uparrow}^* \gamma_{-k\downarrow}^*\right) \Phi + C_k^2 \sum_{p \in \Lambda} \frac{U_{k,p} \left(C_k^2\, S_p^2 + C_p^2\, S_k^2\right)}{E_k + E_p} \gamma_{p\uparrow}^*\, \gamma_{-p\downarrow}^* \Psi_{BCS} \\ & -2 C_k\, S_k \sum_{p \in \Lambda} \frac{U_{k,p} \left(C_k^2\, S_p^2 + C_p^2\, S_k^2\right)}{E_k + E_p} \gamma_{k\uparrow}^*\, \gamma_{-k\downarrow}^* \gamma_{p\uparrow}^*\, \gamma_{-p\downarrow}^* \Psi_{BCS} . \end{aligned}$$

(b) $$(\Phi,\, B_k \Phi) = C_k\, S_k \left\{ (\Phi,\, \Phi) - 2 \sum_{p \in \Lambda} \frac{U_{k,p}^2 \left(C_k^2\, S_p^2 + C_p^2\, S_k^2\right)^2}{\left(E_k + E_p\right)^2} \right\}.$$

(c)

$$
\begin{aligned}
&(\Phi,\ B_{k'}^* B_k \Phi)\\
=\ & C_k\, S_k\, C_{k'}\, S_{k'} \Bigg[(\Phi,\ \Phi) \\
&\quad - 2 \sum_{p\in\Lambda} \left\{ \frac{U_{k,p}^2 \left(C_k^2\, S_p^2 + C_p^2\, S_k^2\right)^2}{\left(E_k + E_p\right)^2} + \frac{U_{k',p}^2 \left(C_{k'}^2\, S_p^2 + C_p^2\, S_{k'}^2\right)^2}{\left(E_{k'} + E_p\right)^2} \right\} \Bigg] \\
& + 4 C_k\, S_k\, C_{k'}\, S_{k'} \frac{U_{k,k'}^2 \left(C_k^2\, S_{k'}^2 + C_{k'}^2\, S_k^2\right)^2}{\left(E_k + E_{k'}\right)^2} \\
& + \left(C_k^2\, C_{k'}^2 + S_k^2\, S_{k'}^2\right) \sum_{p\in\Lambda} \frac{U_{k,p} U_{k',p} \left(C_k^2\, S_p^2 + C_p^2\, S_k^2\right) \left(C_{k'}^2\, S_p^2 + C_p^2\, S_{k'}^2\right)}{\left(E_k + E_p\right)\left(E_{k'} + E_p\right)}\,.
\end{aligned}
$$

Let

$$
\begin{aligned}
\Delta E\ =\ & \sum_{k,\,k'\in\Lambda} U_{k,k'} \frac{C_k^2\, C_{k'}^2 + S_k^2\, S_{k'}^2}{1 + (\Phi,\ \Phi)} \times \\
& \times \sum_{p\in\Lambda} \frac{U_{k,p} U_{k',p} \left(C_k^2\, S_p^2 + C_p^2\, S_k^2\right) \left(C_{k'}^2\, S_p^2 + C_p^2\, S_{k'}^2\right)}{\left(E_k + E_p\right)\left(E_{k'} + E_p\right)} \\
& + 4 \sum_{k,\,k'\in\Lambda} U_{k,k'} \frac{C_k\, S_k\, C_{k'}\, S_{k'}}{1 + (\Phi,\ \Phi)} \frac{U_{k,k'}^2 \left(C_k^2\, S_{k'}^2 + C_{k'}^2\, S_k^2\right)^2}{\left(E_k + E_{k'}\right)^2}\,.
\end{aligned}
$$

Note that $\Delta E < 0$.

Lemma 7.4. *Let H' and ΔE be as above. Then*

$$(\Phi,\ H'\Phi) = \{\,1 + (\Phi,\ \Phi)\,\}\,\Delta E.$$

We now show that the state Ψ above has a lower energy than the BCS state Ψ_{BCS} .

Theorem 7.5. *The state Ψ has a lower energy than the BCS state Ψ_{BCS}, and hence than the Fermi vacuum Ψ_F ,i.e.,*

$$(\Psi,\ H\Psi) - (\Psi_{BCS},\ H\Psi_{BCS}) = \Delta E < 0.$$

8 A new gap equation

We use the BCS state Ψ_{BCS} to deal with the expectation values of the operators $C_{-k\downarrow}C_{k\uparrow}$ and $C_{k\uparrow}^* C_{-k\downarrow}^*$.

But we originally need to use the ground state of the BCS Hamiltonian to deal with the expectation values of such operators. The ground state of the BCS Hamiltonian is studied by several authors. See Mattis and Lieb [5], Richardson [7] and von Delft [3] for example. They assumed that $U_{k,k'}$ is a negative constant if k and k' both belong to the neighborhood of the Fermi surface, and 0 otherwise. So little is known about the ground state when $U_{k,k'}$ does *not* satisfy the assumption just above.

We therefore try to use our superconducting state Ψ in the preceding section instead. This is because our state Ψ has a lower energy than the BCS state Ψ_{BCS}. To this end we begin with a new gap equation.

Let $\widetilde{\Delta}_k$ be a function of $k \in \Lambda$. We assume the existence of the following $\widetilde{\Delta}_k$: $\widetilde{\Delta}_k$ satisfies $\widetilde{\Delta}_k \geq 0$ and $\widetilde{\Delta}_{-k} = \widetilde{\Delta}_k$, and is also a solution to the new gap equation

$$\widetilde{\Delta}_k = -\frac{1}{2}\sum_{k' \in \Lambda} U_{k,k'} \frac{\widetilde{\Delta}_{k'}}{\sqrt{\xi_{k'}^2 + \widetilde{\Delta}_{k'}^2}} \left(1 - \frac{4D_{k'}}{D+2}\right),$$

where

$$\begin{aligned} D_{k'} &= \frac{1}{4}\sum_{p \in \Lambda} \frac{U_{k',p}^2}{\left(\sqrt{\xi_{k'}^2 + \widetilde{\Delta}_{k'}^2} + \sqrt{\xi_p^2 + \widetilde{\Delta}_p^2}\right)^2} \times \\ &\qquad \times \left(1 - \frac{\xi_{k'}\,\xi_p}{\sqrt{\xi_{k'}^2 + \widetilde{\Delta}_{k'}^2}\sqrt{\xi_p^2 + \widetilde{\Delta}_p^2}}\right)^2, \\ D &= \sum_{k' \in \Lambda} D_{k'}\,. \end{aligned}$$

Remark 8.1. A numerical calculation gives $4D_{k'}/(D+2) \leq O(10^{-17})$ in the case of aluminum. So it is expected that $\widetilde{\Delta}_k$ is nearly equal to Δ_k and that $\widetilde{\Delta}_k \geq 0$.

Let $\widetilde{\theta}_k$ be a function of $k \in \Lambda$ and let it satisfy

$$\sin 2\widetilde{\theta}_k = \frac{\widetilde{\Delta}_k}{\sqrt{\xi_k^2 + \widetilde{\Delta}_k^2}}, \qquad \cos 2\widetilde{\theta}_k = \frac{\xi_k}{\sqrt{\xi_k^2 + \widetilde{\Delta}_k^2}}$$

with $0 \leq \widetilde{\theta}_k \leq \pi/2$. Note that $\widetilde{\theta}_{-k} = \widetilde{\theta}_k$.

We denote by $\widetilde{G}_B$ the following bounded, selfadjoint operator on $\mathcal{H} = \mathbb{C}^{2^{2M}}$:

$$\widetilde{G}_B = i\sum_{k \in \Lambda} \widetilde{\theta}_k \left(C_{-k\downarrow}C_{k\uparrow} - C_{k\uparrow}^* C_{-k\downarrow}^*\right).$$

We set $\widetilde{\Psi}_{BCS} = e^{i\widetilde{G}_B}|0\rangle \in \mathcal{H} = \mathbb{C}^{2^{2M}}$.

Lemma 8.2. $\widetilde{\Psi}_{BCS} = \left\{ \prod_{k \in \Lambda} \left(\cos\widetilde{\theta}_k + \sin\widetilde{\theta}_k\, C_{k\uparrow}^* C_{-k\downarrow}^*\right) \right\} |0\rangle.$

Corollary 8.3.

$$\left(\widetilde{\Psi}_{BCS},\, C_{-k\downarrow}C_{k\uparrow}\widetilde{\Psi}_{BCS}\right) = \left(\widetilde{\Psi}_{BCS},\, C_{k\uparrow}^* C_{-k\downarrow}^*\widetilde{\Psi}_{BCS}\right) = \frac{1}{2}\sin 2\widetilde{\theta}_k\,.$$

We introduce another Bogoliubov transformation of $C_{k\sigma}$:

$$\widetilde{\gamma}_{k\sigma} = e^{i\widetilde{G}_B} C_{k\sigma} e^{-i\widetilde{G}_B}.$$

Note that the operator $\widetilde{\gamma}_{k\sigma}$ and its adjoint operator $\widetilde{\gamma}^*_{k\sigma}$ are both bounded linear operators on $\mathcal{H} = \mathbb{C}^{2^{2M}}$.

Corollary 8.4. *The operators $\widetilde{\gamma}_{k\sigma}$ and $\widetilde{\gamma}^*_{k\sigma}$ satisfy the following.*
(a) $\{\widetilde{\gamma}_{k\sigma}, \widetilde{\gamma}^*_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}, \qquad \{\widetilde{\gamma}_{k\sigma}, \widetilde{\gamma}_{k'\sigma'}\} = \{\widetilde{\gamma}^*_{k\sigma}, \widetilde{\gamma}^*_{k'\sigma'}\} = 0.$
(b) $\widetilde{\gamma}_{k\sigma}\widetilde{\Psi}_{BCS} = 0$ for each $k \in \Lambda$ and for each $\sigma = \uparrow, \downarrow$.
(c) $\begin{cases} \widetilde{\gamma}_{k\uparrow} = \cos\widetilde{\theta}_k\, C_{k\uparrow} - \sin\widetilde{\theta}_k\, C^*_{-k\downarrow}, \\ \widetilde{\gamma}_{-k\downarrow} = \sin\widetilde{\theta}_k\, C^*_{k\uparrow} + \cos\widetilde{\theta}_k\, C_{-k\downarrow}. \end{cases}$
(d) $\begin{cases} C_{k\uparrow} = \cos\widetilde{\theta}_k\, \widetilde{\gamma}_{k\uparrow} + \sin\widetilde{\theta}_k\, \widetilde{\gamma}^*_{-k\downarrow}, \\ C_{-k\downarrow} = -\sin\widetilde{\theta}_k\, \widetilde{\gamma}^*_{k\uparrow} + \cos\widetilde{\theta}_k\, \widetilde{\gamma}_{-k\downarrow}. \end{cases}$

Set $\widetilde{E}_k = \sqrt{\xi_k^2 + \widetilde{\Delta}_k^2}$, $k \in \Lambda$ and set $B_k = C_{-k\downarrow}C_{k\uparrow}$. We abbreviate $\sin\widetilde{\theta}_k$ (resp. $\cos\widetilde{\theta}_k$) to $\widetilde{S}_k$ (resp. to $\widetilde{C}_k$). We now consider the following vector in $\mathcal{H} = \mathbb{C}^{2^{2M}}$:

$$\widetilde{\Psi} = \frac{\widetilde{\Psi}_{BCS} + \widetilde{\Phi}}{\sqrt{1 + \left(\widetilde{\Phi}, \widetilde{\Phi}\right)}},$$

where

$$\widetilde{\Phi} = \frac{1}{2} \sum_{p,p' \in \Lambda} \frac{U_{p,p'}\left(\widetilde{C}_p^2\, \widetilde{S}_{p'}^2 + \widetilde{C}_{p'}^2\, \widetilde{S}_p^2\right)}{\widetilde{E}_p + \widetilde{E}_{p'}}\, \widetilde{\gamma}^*_{p\uparrow}\, \widetilde{\gamma}^*_{-p\downarrow}\, \widetilde{\gamma}^*_{p'\uparrow}\, \widetilde{\gamma}^*_{-p'\downarrow}\, \widetilde{\Psi}_{BCS}.$$

For all $k \in \Lambda$, set

$$\begin{cases} C_{-k\downarrow}C_{k\uparrow} = \left(\widetilde{\Psi},\, C_{-k\downarrow}C_{k\uparrow}\widetilde{\Psi}\right) + \widetilde{b}_k, \\ C^*_{k\uparrow}C^*_{-k\downarrow} = \left(\widetilde{\Psi},\, C^*_{k\uparrow}C^*_{-k\downarrow}\widetilde{\Psi}\right) + \widetilde{b}^*_k. \end{cases}$$

Corollary 8.5. $\displaystyle \widetilde{\Delta}_k = -\sum_{k' \in \Lambda} U_{k,k'} \left(\widetilde{\Psi},\, C_{-k'\downarrow}C_{k'\uparrow}\widetilde{\Psi}\right).$

Lemma 8.6. *Set*

$$\begin{aligned} \widetilde{H}_M \;=\; & \sum_{k\in\Lambda,\, \sigma=\uparrow,\downarrow} \xi_k\, C^*_{k\sigma}C_{k\sigma} - \sum_{k\in\Lambda} \widetilde{\Delta}_k \left(C_{-k\downarrow}C_{k\uparrow} + C^*_{k\uparrow}C^*_{-k\downarrow}\right) \\ & + \sum_{k\in\Lambda} \widetilde{\Delta}_k \left(\widetilde{\Psi},\, C_{-k\downarrow}C_{k\uparrow}\widetilde{\Psi}\right). \end{aligned}$$

Then the BCS Hamiltonian is rewritten as

$$H = \widetilde{H}_M + \sum_{k,\, k' \in \Lambda} U_{k,k'}\, \widetilde{b}^*_{k'}\, \widetilde{b}_k.$$

Remark 8.7. The Hamiltonian $\widetilde{H}_M$ as well as H_M is also the mean field approximation for the BCS Hamiltonian H.

Proposition 8.8.

$$\begin{aligned}\widetilde{H}_M &= \sum_{k\in\Lambda,\sigma=\uparrow,\downarrow} \sqrt{\xi_k^2+\widetilde{\Delta}_k^2}\,\widetilde{\gamma}_{k\sigma}^*\widetilde{\gamma}_{k\sigma} \\ &\quad +\sum_{k\in\Lambda}\left\{\xi_k-\sqrt{\xi_k^2+\widetilde{\Delta}_k^2}+\widetilde{\Delta}_k\left(\widetilde{\Psi},\, C_{-k\downarrow}C_{k\uparrow}\widetilde{\Psi}\right)\right\}.\end{aligned}$$

Corollary 8.9. (a) The state $\widetilde{\Psi}_{BCS}$ is the ground state of $\widetilde{H}_M$, and the ground state energy $\widetilde{E}_{BCS}$ is given by

$$\widetilde{E}_{BCS}=\sum_{k\in\Lambda}\left\{\xi_k-\sqrt{\xi_k^2+\widetilde{\Delta}_k^2}+\widetilde{\Delta}_k\left(\widetilde{\Psi},\, C_{-k\downarrow}C_{k\uparrow}\widetilde{\Psi}\right)\right\}.$$

(b) Let $\widetilde{E}_{BCS}$ be as in (a). Then the spectrum of $\widetilde{H}_M$ is given by

$$\sigma\left(\widetilde{H}_M\right)=\left\{\sum_{k\in\Lambda}\sqrt{\xi_k^2+\widetilde{\Delta}_k^2}\,\left(N_{k\uparrow}+N_{k\downarrow}\right)+\widetilde{E}_{BCS}\right\}_{N_{k\uparrow},\,N_{k\downarrow}=0,1}.$$

Remark 8.10. We see from the corollary above that it takes a finite energy $\sqrt{\xi_k^2+\widetilde{\Delta}_k^2}$ ($> \widetilde{\Delta}_k$) to excite a particle from the state $\widetilde{\Psi}_{BCS}$ to an upper energy state. So $\widetilde{\Delta}_k$ as well as Δ_k corresponds exactly to the energy gap, and hence $\widetilde{\Delta}_k$ as well as Δ_k is the gap function.

Remark 8.11. Beginning with our new gap equation we arrive at the results similar to those in the BCS-Bogoliubov theory.

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