PAIRING IN THE BOGOLIUBOV-de GENNES EQUATIONS

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Abstract

It is shown that the Bogoliubov-de Gennes equations pair the electrons in states which are linear combinations of the normal states. Accordingly, the BCS-like reduction procedure is required to choose a correct pairing. For a homogeneous system, we point out that the kernel of the self-consistency equation derived from the Bogoliubov-de Gennes equations needs to be constrained by the BCS pairing condition. In the presence of ordinary impurities, on the other hand, the Bogoliubov-de Gennes equations should be supplemented by Anderson's pairing condition to obtain the correct vacuum state by the corresponding unitary transformation. This results in localization correction to the phonon-mediated interaction.

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1. Introduction

Recently it was shown[1,2] that the Abrikosov and Gor'kov's[3,4] Green's function theory of impure superconductors is in serious conflict with Anderson's theorem.[5] (Strong coupling theory of impure superconductors was discussed elsewhere.[6]) For magnetic impurity effects, Kim and Overhauser[7] (KO) proposed a BCS type theory with different predictions from the pair-breaking theory of Abrikosov and Gor'kov.[3] In fact, there have been several experiments[8−12] which agree with KO's predictions. It was also pointed out[13] that the failure of Green's function theory comes from the intrinsic pairing problem in Gor'kov's formalism.[14] The self-consistency equation needs to be supplemented by a pairing condition derived from the physical constraint of the Anomalous Green's function. The resulting equation is nothing but another form of the BCS gap equation. Then the discrepancy disappears.

In this letter we show that the same pairing constraint is required in the Bogoliubov-de Gennes (BdG) equations.[15] The equations are obtained by a real space version of the Bogoliubov-Valatin (BV) transformation,[16,17] which is a generalization[18,19] of the BV transformation. In this case, the pairing constraint is determined to find a correct vacuum state by the corresponding unitary transformation. The resulting pairing condition is the same as that obtained from the physical constraint of the Anomalous Green's function.[13]

For a homogeneous system, choosing a constant pair potential gives rise to the BCS pairing. However, the kernel of the self-consistency equation has not been fixed by the BCS pairing condition. In the presence of ordinary impurities, Anderson's pairing between time-reversed states is not obtained from the BdG equations because the pair potential depends on the position. Alternatively, pairing occurs between the states which are the linear combination of the scattered states. Consequently, the BdG equations predict incorrectly that T_c doesn't change even if the scattered states are localized. Note that the linear combination of localized states becomes extended one. Magnetic impurities will be considered elsewhere.

2. Homogeneous System

2.1 Bogoliubov-de Gennes Equations

Let's consider a homogeneous system. We follow first de Gennes' derivation.[15] The Hamiltonian is given

$$H = \int d\mathbf{r} \sum_{\alpha} \Psi^{\dagger}(\mathbf{r}\alpha)[\frac{\vec{p}^2}{2m}]\Psi(\mathbf{r}\alpha) - \frac{1}{2}V \int d\mathbf{r} \sum_{\alpha\beta} \Psi^{\dagger}(\mathbf{r}\alpha)\Psi^{\dagger}(\mathbf{r}\beta)\Psi(\mathbf{r}\beta)\Psi(\mathbf{r}\alpha), \tag{1}$$

where the field operator $\Psi(\mathbf{r}\alpha)$ is expanded by plane wave basis set $\phi_{\vec{k}}(\mathbf{r}) = e^{i\vec{k}\cdot\mathbf{r}}$, that is,

$$\Psi(\mathbf{r}\alpha) = \sum_{\vec{k}} \phi_{\vec{k}}(\mathbf{r}) a_{\vec{k}\alpha}, \tag{2}$$

where $a_{\vec{k}\alpha}$ is a destruction operator for an electron with spin α. Using the Gor'kov's factorization[14], we may get an effective Hamiltonian of the form

$$H_{eff} = \int d\mathbf{r} \{\sum_{\alpha} \Psi^{\dagger}(\mathbf{r}\alpha)[\frac{\vec{p}^2}{2m}]\Psi(\mathbf{r}\alpha) + \Delta(\mathbf{r})\Psi^{\dagger}(\mathbf{r}\uparrow)\Psi^{\dagger}(\mathbf{r}\downarrow) + \Delta^*(\mathbf{r})\Psi(\mathbf{r}\downarrow)\Psi(\mathbf{r}\uparrow)\}, \tag{3}$$

where

$$\Delta(\mathbf{r}) = -V < \Psi(\mathbf{r}\downarrow)\Psi(\mathbf{r}\uparrow) > . \tag{4}$$

$\Delta(\mathbf{r})$ is called by the pair potential at the position $\mathbf{r}$.

In order to find the eigenstates and corresponding energies, we perform a unitary transformation

$$\begin{aligned} \Psi(\mathbf{r}\uparrow) &= \sum_n (\gamma_{n\uparrow} u_n(\mathbf{r}) - \gamma^{\dagger}_{n\downarrow} v^*_n(\mathbf{r})), \\ \Psi(\mathbf{r}\downarrow) &= \sum_n (\gamma_{n\downarrow} u_n(\mathbf{r}) + \gamma^{\dagger}_{n\uparrow} v^*_n(\mathbf{r})), \end{aligned} \tag{5}$$

where the γ and $\gamma^{\dagger}$ are quasiparticle operators satisfying the fermion commutation relations

$$\begin{aligned} &\{\gamma_{n\alpha}, \gamma^{\dagger}_{m\beta}\} = \delta_{mn}\delta_{\alpha\beta}, \\ &\{\gamma_{n\alpha}, \gamma_{m\beta}\} = 0. \end{aligned} \tag{6}$$

By the transformation (5), the effective Hamiltonian may be diagonalized, that is,

$$H_{eff} = E_g + \sum_{n,\alpha} \epsilon_n \gamma^{\dagger}_{n\alpha}\gamma_{n\alpha}, \tag{7}$$

where E_g is the ground state energy of H_{eff} and ϵ_n is the energy of the excitation n. ¿From the condition (7), we obtain the well-known Bogoliubov-de Gennes equations:

$$\begin{aligned} \epsilon u(\mathbf{r}) &= H_e u(\mathbf{r}) + \Delta(\mathbf{r}) v(\mathbf{r}), \\ \epsilon v(\mathbf{r}) &= -H_e^* v(\mathbf{r}) + \Delta^*(\mathbf{r}) u(\mathbf{r}), \end{aligned} \tag{8}$$

where $H_e = \frac{\vec{p}^2}{2m}$. These equations can be written compactly in a matrix form

$$\epsilon \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} H_e & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -H_e^* \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}. \tag{9}$$

Notice that different eigenfunctions are orthogonal and $\begin{pmatrix} u \\ v \end{pmatrix}$ is orthogonal to $\begin{pmatrix} -v^* \\ u^* \end{pmatrix}$.

Substituting Eq. (5) into Eq. (4) we find

$$\Delta(\mathbf{r}) = V \sum_n v_n^*(\mathbf{r}) u_n(\mathbf{r})(1 - 2f_n), \tag{10}$$

where $f_n = \frac{1}{\exp(\beta\epsilon_n)+1}$. Eq. (10) is the self-consistency equation for the pair potential.

2.2 Vacuum State

Now we analyze the derivation. It is important to note that the unitary transformation (5) is in fact a generalization[18,19] of the BV transformation,

$$\begin{aligned} a_{\vec{k}\uparrow} &= u_k \gamma_{\vec{k}\uparrow} + v_k \gamma^\dagger_{-\vec{k}\downarrow}, \\ a_{\vec{k}\downarrow} &= u_k \gamma_{\vec{k}\downarrow} - v_k \gamma^\dagger_{-\vec{k}\uparrow}, \end{aligned} \tag{11}$$

where

$$u_k^2 + v_k^2 = 1. \tag{12}$$

Inserting Eq. (2) into Eq. (5) we obtain

$$\begin{aligned} \sum_{\vec{k}'} \phi_{\vec{k}'}(\mathbf{r}) a_{\vec{k}'\uparrow} &= \sum_n (\gamma_{n\uparrow} u_n(\mathbf{r}) - \gamma^\dagger_{n\downarrow} v_n^*(\mathbf{r})), \\ \sum_{\vec{k}'} \phi_{\vec{k}'}(\mathbf{r}) a_{\vec{k}'\downarrow} &= \sum_n (\gamma_{n\downarrow} u_n(\mathbf{r}) + \gamma^\dagger_{n\uparrow} v_n^*(\mathbf{r})). \end{aligned} \tag{13}$$

If we multiply the left side of Eq. (13) with $\phi^*_{\vec{k}}(\mathbf{r})$ and integrate over the position, we find

$$
\begin{aligned}
a_{\vec{k}\uparrow} &= \sum_n (\gamma_{n\uparrow} u_{n,\vec{k}} - \gamma^\dagger_{n\downarrow} v_{n,\vec{k}}), \\
a_{\vec{k}\downarrow} &= \sum_n (\gamma_{n\downarrow} u_{n,\vec{k}} + \gamma^\dagger_{n\uparrow} v_{n,\vec{k}}),
\end{aligned}
\tag{14}
$$

where

$$
\begin{aligned}
u_{n,\vec{k}} &= \int \phi^*_{\vec{k}}(\mathbf{r}) u_n(\mathbf{r}) d\mathbf{r}, \\
v_{n,\vec{k}} &= \int \phi^*_{\vec{k}}(\mathbf{r}) v^*_n(\mathbf{r}) d\mathbf{r}.
\end{aligned}
\tag{15}
$$

Let's compare Eqs. (11) and (14). Only if both $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ are proportional to the normal state wavefunction $\phi_{\vec{k}}(\mathbf{r})$, then the transformation (14) becomes the same as the BV transformation.

To understand the physical meaning of the unitary transformation (5), we express $\gamma_{n\uparrow}$ by the creation and destruction operators for an electron. If we multiply $u^*_{n'}(\mathbf{r})$ to the first equation of Eq. (13) and integrate over the position, we find

$$
\sum_{\vec{k}} u^*_{n',\vec{k}} a_{\vec{k}\uparrow} = \sum_n \Big(\gamma_{n\uparrow} \int u_n(\mathbf{r}) u^*_{n'}(\mathbf{r}) d\mathbf{r} - \gamma^\dagger_{n\downarrow} \int u^*_{n'}(\mathbf{r}) v^*_n(\mathbf{r}) d\mathbf{r} \Big). \tag{16}
$$

By a similar process to the second equation, we also find

$$
\sum_{\vec{k}} v_{n',\vec{k}} a^\dagger_{\vec{k}\downarrow} = \sum_n \Big(\gamma^\dagger_{n\downarrow} \int u^*_n(\mathbf{r}) v^*_{n'}(\mathbf{r}) d\mathbf{r} + \gamma_{n\uparrow} \int v_n(\mathbf{r}) v^*_{n'}(\mathbf{r}) d\mathbf{r} \Big). \tag{17}
$$

Adding Eqs. (16) and (17) and by the orthogonality condition of eigenfunctions, one can get

$$
\gamma_{n'\uparrow} = \sum_{\vec{k}} (u^*_{n',\vec{k}} a_{\vec{k}\uparrow} + v_{n',\vec{k}} a^\dagger_{\vec{k}\downarrow}). \tag{18}
$$

Similarly it is given

$$
\gamma_{n'\downarrow} = \sum_{\vec{k}} (u^*_{n',\vec{k}} a_{\vec{k}\downarrow} - v_{n',\vec{k}} a^\dagger_{\vec{k}\uparrow}). \tag{19}
$$

Let's define $\Phi_n(\mathbf{r})$ and $\Phi_{\bar{n}}(\mathbf{r})$ by

$$\Phi_n(\mathbf{r}) = \frac{1}{U_n} u_n(\mathbf{r}) = \frac{1}{U_n} \sum_{\vec{k}} u_{n,\vec{k}} \phi_{\vec{k}}(\mathbf{r}), \tag{20}$$

and

$$\Phi_{\bar{n}}(\mathbf{r}) = \frac{-1}{V_n} v_n^*(\mathbf{r}) = \frac{-1}{V_n} \sum_{\vec{k}} v_{n,\vec{k}} \phi_{\vec{k}}(\mathbf{r}), \tag{21}$$

where

$$|U_n|^2 = \int u_n^*(\mathbf{r}) u_n(\mathbf{r}) d\mathbf{r}, \tag{22}$$

and

$$|V_n|^2 = \int v_n^*(\mathbf{r}) v_n(\mathbf{r}) d\mathbf{r}. \tag{23}$$

Notice that $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ were expanded by the plane wave basis $\phi_{\vec{k}}(\mathbf{r})$ in Eqs. (20) and (21). Then we find

$$\begin{aligned} a_{n\alpha} &= \frac{1}{U_n} \sum_{\vec{k}} u_{n,\vec{k}}^* a_{\vec{k}\alpha}, \\ a_{\bar{n}\alpha} &= \frac{-1}{V_n^*} \sum_{\vec{k}} v_{n,\vec{k}}^* a_{\vec{k}\alpha}. \end{aligned} \tag{24}$$

Finally, by substituting Eq. (24) into Eqs. (18) and (19), we obtain

$$\begin{aligned} \gamma_{n\uparrow} &= U_n a_{n\uparrow} - V_n a_{\bar{n}\downarrow}^\dagger, \\ \gamma_{n\downarrow} &= U_n a_{n\downarrow} + V_n a_{\bar{n}\uparrow}^\dagger. \end{aligned} \tag{25}$$

Note that we pair $\Phi_n(\mathbf{r})[= \frac{1}{U_n} u_n(\mathbf{r})] \uparrow$ and $\Phi_{\bar{n}}(\mathbf{r})[= -\frac{1}{V_n} v_n^*(\mathbf{r})] \downarrow$ (instead of $\phi_{\vec{k}}(\mathbf{r}) \uparrow$ and $\phi_{-\vec{k}}(\mathbf{r}) \downarrow$) by the unitary transformation (5). The generated vacuum state is

$$\tilde{\phi}_{BdG} = \prod_n (U_n + V_n a_{n\uparrow}^\dagger a_{\bar{n}\downarrow}^\dagger)|0>, \tag{26}$$

instead of the BCS ground state[20]

$$\tilde{\phi}_{BCS} = \prod_{\vec{k}} (u_{\vec{k}} + v_{\vec{k}} a_{\vec{k}\uparrow}^\dagger a^\dagger_{-\vec{k}\downarrow})|0> . \tag{27}$$

Therefore a pairing constraint is necessary for the unitary transformation (5) to generate the BCS ground state; that is, both $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ should be proportional to the normal state wavefunction $\phi_{\vec{k}}(\mathbf{r})$ in order to pair $\vec{k}\uparrow$ and $-\vec{k}\downarrow$. For the current-carrying state, we can pair $\vec{k}+\vec{q}\uparrow$ and $-\vec{k}+\vec{q}\downarrow$. Then, $u_n(\mathbf{r}) = U_{\vec{k}} e^{i(\vec{k}+\vec{q})\cdot\mathbf{r}}$ and $v_n^*(\mathbf{r}) = V_{\vec{k}} e^{i(-\vec{k}+\vec{q})\cdot\mathbf{r}}$.

2.3 Pairing Constraint on the Self-consistency Equation

The pairing constraint should be also supplemented in the self-consistency equation

$$\Delta(\mathbf{r}) = V \sum_n v_n^*(\mathbf{r}) u_n(\mathbf{r})(1-2f_n). \tag{10}$$

However, u_n and v_n are usually expanded as a power series in Δ[15]

$$\begin{aligned} u_n &= u_n^o + u_n^1 + \cdots, \\ v_n &= v_n^o + v_n^1 + \cdots, \end{aligned} \tag{28}$$

where

$$\begin{aligned} &u_n^o = \phi_{\vec{k}}, \quad v_n^o = 0 \quad (\xi_{\vec{k}} > 0), \\ &u_n^o = 0, \quad v_n^o = \phi_{\vec{k}}^* \quad (\xi_{\vec{k}} < 0), \end{aligned} \tag{29}$$

and

$$\begin{aligned} u_n^1 &= \sum_{\vec{k}'} e_{n\vec{k}'} \phi_{\vec{k}'}, \\ v_n^1 &= \sum_{\vec{k}'} d_{n\vec{k}'} \phi_{\vec{k}'}^*. \end{aligned} \tag{30}$$

$e_{n\vec{k}'}$ and $d_{n\vec{k}'}$ are given

$$\begin{aligned} (|\xi_n| - \xi_{\vec{k}'}) e_{n\vec{k}'} &= \int \Delta(\mathbf{r}) \phi_{\vec{k}'}^*(\mathbf{r}) v_n^o(\mathbf{r}) d\mathbf{r} \\ (|\xi_n| + \xi_{\vec{k}'}) d_{n\vec{k}'} &= \int \Delta^*(\mathbf{r}) \phi_{\vec{k}'}(\mathbf{r}) u_n^o(\mathbf{r}) d\mathbf{r}, \end{aligned} \tag{31}$$

with $\xi_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m} - E_F$. In that case both u_n and v_n are the linear combiantion of the normal state wavefunction, which violates the pairing constraint. If we substitute Eq. (28) to the self-consistency equation Eq. (10), we obtain

$$\Delta(\mathbf{r}) = \int K(\mathbf{r},\mathbf{l})\Delta(\mathbf{l})d\mathbf{l}, \tag{32}$$

where

$$K(\mathbf{r},\mathbf{l}) = VT\sum_{\omega}\sum_{\vec{k}\vec{k}'}\frac{\phi^*_{\vec{k}}(\mathbf{l})\phi^*_{\vec{k}'}(\mathbf{l})\phi_{\vec{k}}(\mathbf{r})\phi_{\vec{k}'}(\mathbf{r})}{(\xi_{\vec{k}}-i\omega)(\xi_{\vec{k}'}+i\omega)}. \tag{33}$$

The ω's are $\omega_n = (2n+1)\pi T$ for all integer n. Consequently, this equation should be corrected by a pairing constraint. Then we find

$$\Delta(\mathbf{r}) = \int K^c(\mathbf{r},\mathbf{l})\Delta(\mathbf{l})d\mathbf{l}, \tag{34}$$

where

$$K^c(\mathbf{r},\mathbf{l}) = VT\sum_{\omega}\sum_{\vec{k}\vec{k}'}\frac{\phi^*_{\vec{k}}(\mathbf{l})\phi^*_{\vec{k}'}(\mathbf{l})\phi_{\vec{k}}(\mathbf{r})\phi_{\vec{k}'}(\mathbf{r})}{(\xi_{\vec{k}}-i\omega)(\xi_{\vec{k}'}+i\omega)}\delta_{\vec{k}'=-\vec{k}}. \tag{35}$$

Note that Eq. (32) is the Gor'kov's self-consistency equation

$$\Delta(\mathbf{r}) = VT\sum_{\omega}\int\Delta(\mathbf{l})G_{\omega}(\mathbf{r},\mathbf{l})G_{-\omega}(\mathbf{r},\mathbf{l})d\mathbf{l}. \tag{36}$$

The revised self-consistency equation (34) can be written

$$\Delta(\mathbf{r}) = VT\sum_{\omega}\int\Delta(\mathbf{l})\{G_{\omega}(\mathbf{r},\mathbf{l})G_{-\omega}(\mathbf{r},\mathbf{l})\}_{p.p.}d\mathbf{l}, \tag{37}$$

where p.p. means proper pairing constraint which dictates pairing between $\vec{k}\uparrow$ and $-\vec{k}\downarrow$. It was pointed out[13] that Eq. (36) was obtained from the Anomalous Green's function $F(\mathbf{r},\mathbf{r}')$ which includes the terms violating the homogeneity constraint $F(\mathbf{r},\mathbf{r}') = F(\mathbf{r}-\mathbf{r}')$. Accordingly, the same pairing constraint may be obtained from the homogeneity constraint of the Anomalous Green's function.[13]

3. Inhomogeneous System: Nonmagnetic impurity case

3.1 Correct Vacuum State

In the presence of ordinary impurities, Anderson[5] proposed a BCS type theory which employs time-reversed scattered state pairs. The exact scattered states ψ_n satisfy the equation

$$[\frac{p^2}{2m} + U(\mathbf{r})]\psi_n(\mathbf{r}) = \xi_n \psi_n(\mathbf{r}), \tag{38}$$

where

$$U(\mathbf{r}) = \sum_i V_o \delta(\mathbf{r} - \mathbf{R}_i). \tag{39}$$

$\{\mathbf{R}_i\}$ are the impurity sites. Accordingly, the ground state is[15]

$$\tilde{\phi}_{Anderson} = \prod_n (u_n + v_n c^\dagger_{n\uparrow} c^\dagger_{\bar{n}\downarrow})|0>, \tag{40}$$

where $c^\dagger_{\bar{n}\downarrow}$ is the creation operator for an electron in the state $\psi^*_n(\mathbf{r})|\downarrow>$.

On the other hand, it has been claimed[15] that the energy is lowered if we pair states $\tilde{\Phi}_n$ which are better choices than ψ_n by using the Bogoliubov-de Gennes equations. The state $\tilde{\Phi}_n$ is basically a linear combination of the normal scattered states. The coupling comes from the pair potential. However, we show that pairing $\tilde{\Phi}_n \uparrow$ and $\tilde{\Phi}_{\bar{n}} \downarrow$ leads to the violation of the physical constraint of the system.

The effective Hamiltonian is given

$$H'_{eff} = \int d\mathbf{r}\{\sum_\alpha \Psi^\dagger(\mathbf{r}\alpha)[\frac{\vec{p}^2}{2m} + U(\mathbf{r})]\Psi(\mathbf{r}\alpha) + \Delta(\mathbf{r})\Psi^\dagger(\mathbf{r}\uparrow)\Psi^\dagger(\mathbf{r}\downarrow) + \Delta^*(\mathbf{r})\Psi(\mathbf{r}\downarrow)\Psi(\mathbf{r}\uparrow)\}, \tag{41}$$

where

$$\Delta(\mathbf{r}) = -V < \Psi(\mathbf{r}\downarrow)\Psi(\mathbf{r}\uparrow) > . \tag{42}$$

As in Sec. 2.1, the unitary transformation

$$\begin{aligned} \Psi(\mathbf{r}\uparrow) &= \sum_n (\gamma_{n\uparrow} u_n(\mathbf{r}) - \gamma^\dagger_{n\downarrow} v^*_n(\mathbf{r})), \\ \Psi(\mathbf{r}\downarrow) &= \sum_n (\gamma_{n\downarrow} u_n(\mathbf{r}) + \gamma^\dagger_{n\uparrow} v^*_n(\mathbf{r})), \end{aligned} \tag{43}$$

leads to the following Bogoliubov-de Gennes equations

$$\begin{aligned} \epsilon u(\mathbf{r}) &= [H_e + U(\mathbf{r})]u(\mathbf{r}) + \Delta(\mathbf{r})v(\mathbf{r}), \\ \epsilon v(\mathbf{r}) &= -[H^*_e + U(\mathbf{r})]v(\mathbf{r}) + \Delta^*(\mathbf{r})u(\mathbf{r}). \end{aligned} \tag{44}$$

To find the vacuum state for γ particles, we expand the field operator by the scattered states:

$$\Psi(\mathbf{r}\alpha) = \sum_n \psi_n(\mathbf{r}) c_{n\alpha}. \tag{45}$$

Then it can be shown

$$\begin{aligned}\gamma_{n\uparrow} &= \sum_{n'} (u^*_{n,n'} c_{n'\uparrow} + v_{n,n'} c^\dagger_{n'\downarrow}), \\ \gamma_{n\downarrow} &= \sum_{n'} (u^*_{n,n'} c_{n'\downarrow} - v_{n,n'} c^\dagger_{n'\uparrow}),\end{aligned} \tag{46}$$

where

$$\begin{aligned}u_{n,n'} &= \int \psi^*_{n'}(\mathbf{r}) u_n(\mathbf{r}) d\mathbf{r}, \\ v_{n,n'} &= \int \psi^*_{n'}(\mathbf{r}) v^*_n(\mathbf{r}) d\mathbf{r}.\end{aligned} \tag{47}$$

For the states $\tilde{\Phi}_n$ and $\tilde{\Phi}_{\bar{n}}$ defined by

$$\begin{aligned}\tilde{\Phi}_n(\mathbf{r}) &= \frac{1}{U_n} u_n(\mathbf{r}) = \frac{1}{U_n} \sum_{n'} u_{n,n'} \psi_{n'}(\mathbf{r}), \\ \tilde{\Phi}_{\bar{n}}(\mathbf{r}) &= \frac{-1}{V_n} v^*_n(\mathbf{r}) = \frac{-1}{V_n} \sum_{n'} v_{n,n'} \psi_{n'}(\mathbf{r}),\end{aligned} \tag{48}$$

it is given

$$\begin{aligned}b_{n\alpha} &= \frac{1}{U_n} \sum_{n'} u^*_{n,n'} c_{n'\alpha}, \\ b_{\bar{n}\alpha} &= \frac{-1}{V^*_n} \sum_{n'} v^*_{n,n'} c_{n'\alpha}.\end{aligned} \tag{49}$$

$b_{\bar{n}\alpha}$ is the destruction operator for an electron in the state $\tilde{\Phi}_n\alpha$.

Finally, we obtain

$$\begin{aligned}\gamma_{n\uparrow} &= U_n b_{n\uparrow} - V_n b^\dagger_{\bar{n}\downarrow}, \\ \gamma_{n\downarrow} &= U_n b_{n\downarrow} + V_n b^\dagger_{\bar{n}\uparrow},\end{aligned} \tag{50}$$

and

$$\tilde{\phi}_{BdG} = \prod_n (U_n + V_n b^\dagger_{n\uparrow} b^\dagger_{\bar{n}\downarrow}) |0> . \tag{51}$$

Note that the Bogoliubov-de Gennes equations, Eq.(44) correspond to the vacuum state where $\tilde{\Phi}_n(\mathbf{r})[= \frac{1}{U_n} u_n(\mathbf{r})] \uparrow$ and $\tilde{\Phi}_{\bar{n}}(\mathbf{r})[= -\frac{1}{V_n} v_n^*(\mathbf{r})] \downarrow$ (instead of $\psi_n(\mathbf{r}) \uparrow$ and $\psi_{\bar{n}}(\mathbf{r}) \downarrow$) are paired.

Now we must decide which is the correct ground state in the presence of impurities. Above all, the correct ground state should satisfy the physical constraint of the system. If we average over the impurity positions, the system becomes homogeneous. Consequently, the pair potential should be a constant after the impurity average, i.e.,

$$\overline{\Delta(\mathbf{r})}^{imp} = \text{constant}. \tag{52}$$

$\overline{}^{imp}$ means an average over impurity positions $\vec{R}_i$.

Let's first check the constraint for the state $\tilde{\phi}_{BdG}$. Eq. (42) leads to the pair potential at $T = 0$,

$$\begin{aligned} \Delta(\mathbf{r}) &= V \sum_n v_n^*(\mathbf{r}) u_n(\mathbf{r}) \\ &= -V \sum_n U_n V_n \tilde{\Phi}_n(\mathbf{r}) \tilde{\Phi}_{\bar{n}}(\mathbf{r}). \end{aligned} \tag{53}$$

In terms of the scattered states, it is rewritten

$$\Delta(\mathbf{r}) = -V \sum_n \sum_{m,m'} u_{n,m} \psi_m(\mathbf{r}) v_{n,m'} \psi_{m'}(\mathbf{r}). \tag{54}$$

Subsequently it is given

$$\overline{\Delta(\mathbf{r})}^{imp} \sim \overline{\psi_m(\mathbf{r}) \psi_{m'}(\mathbf{r})}^{imp}. \tag{55}$$

Note that

$$\begin{aligned} \overline{\psi_{m(\vec{k})\uparrow}(\mathbf{r}) \psi_{m'(\vec{k}')\downarrow}(\mathbf{r})}^{imp} &= e^{i(\vec{k}+\vec{k}')\cdot\mathbf{r}} [1 + V_o^2 \sum_{\vec{q},i} \frac{1}{(\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}})(\epsilon_{\vec{k}'} - \epsilon_{\vec{k}'-\vec{q}})} + \cdots] \\ &\neq \text{constant}, \end{aligned} \tag{56}$$

and

$$\begin{aligned} \overline{\psi_{m(\vec{k})\uparrow}(\mathbf{r}) \psi_{\bar{m}(-\vec{k})\downarrow}(\mathbf{r})}^{imp} &= [1 + V_o^2 \sum_{\vec{q},i} \frac{1}{(\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}})^2} + \cdots] \\ &= \text{constant}. \end{aligned} \tag{57}$$

In deriving these relations, we used the scattered states $\psi_{m(\vec{k})}(\mathbf{r})$,

$$\psi_{m(\vec{k})}(\mathbf{r}) = e^{i\vec{k}\cdot\mathbf{r}} + \sum_{\vec{q}} \frac{V_o}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}}} [\sum_i e^{-i\vec{q}\cdot\vec{R}_i}] e^{i(\vec{k}+\vec{q})\cdot\mathbf{r}} + \cdots. \tag{58}$$

Consequently the state $\tilde{\Phi}_{BdG}$ gives the 'averaged' pair potential

$$\overline{\Delta(\mathbf{r})}^{imp} \neq \text{constant}, \tag{59}$$

which violates the physical constraint of the system.

¿From Eq. (57), it is clear that the state $\tilde{\Phi}_{Anderson}$ gives the correct 'averaged' pair potential which satisfy the physical constraint of the system. Therefore the correct ground state is $\tilde{\Phi}_{Anderson}$. To obtain $\tilde{\Phi}_{Anderson}$ from the Bogoliubov-de Gennes equations, we need a pairing constraint:

$$\tilde{\phi}_{BdG} = \tilde{\phi}_{Anderson}, \tag{60}$$

which gives

$$\begin{aligned} u_n(\mathbf{r}) &\propto \psi_n(\mathbf{r}), \\ v_n^*(\mathbf{r}) &\propto \psi_{\bar{n}}(\mathbf{r}). \end{aligned} \tag{61}$$

3.2 Localization Correction

It has been a common practice to assume a constant pair potential to derive Anderson's theorem.[15,21,22] For the constant pair potential Δ_o, we can also choose

$$\begin{aligned} u(\mathbf{r}) &= \psi_n(\mathbf{r}) u_n, \\ v(\mathbf{r}) &= \psi_n(\mathbf{r}) v_n. \end{aligned} \tag{62}$$

Then Eq. (44), or Eq. (10) leads to

$$\Delta_o = V \sum_n u_n v_n \psi_n(\mathbf{r}) \psi_n^*(\mathbf{r})(1 - 2f_n). \tag{63}$$

To be consistent, the right hand side is substitituted by the impurity average of the square of wavefunction, i.e.,

$$\Delta_o = V\overline{N_o}\int d\xi_n u_n v_n(1-2f_n), \tag{64}$$

where

$$\overline{N_o} = \sum_n \delta(\xi_n)\overline{\psi_n(\mathbf{r})\psi_n^*(\mathbf{r})}^{imp}. \tag{65}$$

Eq. (64) is the same form as that of the homogeneous case. Consequently, the transition temperature doesn't change in the presence of nonmagnetic impurities, which is called by Anderson's theorem.

However, we should not assume a constant pair potential to derive Eq. (62), which is just Anderson's pairing constraint. Then, we obtain the self-consistency equation

$$\Delta(\mathbf{r}) = V\sum_n u_n v_n \psi_n(\mathbf{r})\psi_n^*(\mathbf{r})(1-2f_n), \tag{66}$$

instead of Eq. (63) which is inconsistent. Multiplying the both sides of Eq. (66) by $\psi_m^*(\mathbf{r})\psi_{\bar{m}}^*(\mathbf{r})$, one finds that

$$\Delta_m = \sum_n V_{mn} u_n v_n(1-2f_n), \tag{67}$$

where

$$V_{mn} = V\int \psi_m^*(\mathbf{r})\psi_{\bar{m}}^*(\mathbf{r})\psi_n(\mathbf{r})\psi_{\bar{n}}(\mathbf{r})d\mathbf{r}. \tag{68}$$

And it is given

$$\begin{aligned} u_n &= \frac{1}{2}(1+\frac{\xi_n}{\sqrt{\xi_n^2+\Delta_n^2}}), \\ v_n &= \frac{1}{2}(1-\frac{\xi_n}{\sqrt{\xi_n^2+\Delta_n^2}}). \end{aligned} \tag{69}$$

Comparing Eqs. (67) and (64), we find that Anderson's theorem is valid only when V_{mn} is not much different from V, which is the effective interaction without impurities. It was pointed out that this quantity is almost the same as V up to the first order of the impurity concentration.[1,2]

Now it is clear that localization correction is important in Eq. (68). For the strongly localized states, the effective interaction is exponentially small,[1,6] like the conductance.[23,24] It is, then, expected that the same weak localization correction terms occur both in the conductance and the effective interaction. Recently weak localization correction to the phonon-mediated interaction was reported.[13] The results are the following:

$$V_{nn'}^{3d} \cong -V[1 - \frac{1}{(k_F\ell)^2}(1 - \frac{\ell}{L})], \tag{70}$$

$$V_{nn'}^{2d} \cong -V[1 - \frac{2}{\pi k_F \ell} ln(L/\ell)], \tag{71}$$

$$V_{nn'}^{1d} \cong -V[1 - \frac{1}{(\pi k_F a)^2}(L/\ell - 1)], \tag{72}$$

where ℓ and L are the elastic and inelastic mean free paths and a is the radius of the wire. For thin films, the empirical formula is given[25]

$$\frac{T_{co} - T_c}{T_{co}} \propto R_{sq}, \tag{73}$$

where T_{co} is the unperturbed value of T_c and R_{sq} is the resistance of a square sample. Notice that this formula is obtained if we substitute Eq. (71) into the BCS gap equation. More details will be published elsewhere.

4. Conclusion

It is shown that the Bogoliubov-de Gennes equations need a pairing constraint to obtain a correct vacuum state by the corresponding transformation. The constraint is the same as that obtained from the physical constraint of the Anomalous Green's function.

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