BdG(Bogoliubov-de-Gennes) Equations

Giovanni Benedetti da Rosa

1 Deriving BdG(Bogoliubov-de-Gennes) Equations

1.1 Introduction

The BCS (Bardeen-Cooper-Schrieffer) theory marked a significant milestone in the advancement of a comprehensive microscopic framework for understanding superconductivity. However, the BCS theory is constrained to investigating the ground state of these systems at low temperatures. Conversely, the Bogoliubov-de Gennes (BdG) formalism transcends such limitations, allowing for the exploration of properties beyond the ground state, including scenarios involving finite temperatures and out-of-equilibrium conditions. This document aims to elucidate the derivation of the Bogoliubov-de Gennes equations.

1.2 BCS Hamiltonian

First, let's define the BCS(Bardeen-Cooper-Schrieffer) Hamiltonian. To this, it's appropriate to define using second quantization operators:

$$H_{BCS} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} \left(V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k},\uparrow} c^{\dagger}_{-\mathbf{k},\downarrow} c_{-\mathbf{k}',\uparrow} c_{\mathbf{k}',\downarrow} \right) \tag{1}$$

where: - $\xi_{\mathbf{k}}$ represents the kinetic energy of the electrons, - $c^{\dagger}_{\mathbf{k},\sigma}$ and $c_{\mathbf{k},\sigma}$ are the creation and annihilation operators for an electron with momentum $\mathbf{k}$ and spin σ.

The first term of (1) is the kinetic energy of the electrons, while the second represents the translation of the phonon mediated electron-electron interaction into this framework.

As a consequence of of the Pauli exclusion principle the anti-commutation relationship between the operators can be defined as: $\{c_{\mathbf{k},\sigma}, c^{\dagger}_{\mathbf{k}',\sigma'}\} = c_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k}',\sigma'} + c^{\dagger}_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'}$

Remembering the definitions: $c^{\dagger}_{\mathbf{k},\sigma}|0\rangle = |\mathbf{k},\sigma\rangle$ and $c_{\mathbf{k},\sigma}|\mathbf{k},\sigma\rangle = |0\rangle$. It's easy to see that: $\{c^{\dagger}_{\mathbf{k},\sigma}, c^{\dagger}_{\mathbf{k}',\sigma'}\} = \{c_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}\} = 0$.

1.3 Mean Field approximation

The Hamiltonian described in equation (1) is difficult to solve. So, it's possible to perform a Mean Field approximation. In the mean-field theory, we only consider the average of the operators. So, we can redefine the electron-electron term:

$$\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \left\langle c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} \right\rangle c_{-k'\downarrow} c_{k'\uparrow} + c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} \left\langle c_{-k'\downarrow} c_{k'\uparrow} \right\rangle - \left\langle c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} \right\rangle \left\langle c_{-k'\downarrow} c_{k'\uparrow} \right\rangle$$

Using the operator's anti-commutation relationship, we can easily see that the last term equals zero. Now, we can define the order parameter of the superconductivity that appears naturally when doing the mean-field approximation, superconductor gap:

$$\Delta_k = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \left\langle c_{-k'\downarrow} c_{k'\uparrow} \right\rangle \tag{2}$$

Finally, we can rewrite the BCS Hamiltonian taking into account the Mean Field approximation:

$$H^{(MFA)}_{BCS} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} \Delta_k c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} - \Delta^*_k c_{-k\downarrow} c_{k\uparrow} \tag{3}$$

1.4 Bogoliubov transformation

To diagonalize exactly the Hamiltonian described by (3), we can perform a Bogoliubov transformation. In order to do this, we define new quasi-particles operators that represent the collective excitations of the system:

$$\begin{cases} \gamma_{\mathbf{k},\uparrow} = u^*_{\mathbf{k}} c_{\mathbf{k},\uparrow} + v_{\mathbf{k}} c^{\dagger}_{-\mathbf{k},-\downarrow} \\ \gamma^{\dagger}_{-\mathbf{k},\downarrow} = -v^*_{\mathbf{k}} c_{\mathbf{k},\uparrow} + u_{\mathbf{k}} c^{\dagger}_{-\mathbf{k},\downarrow} \end{cases} \tag{4}$$

such that $u_{\mathbf{k}} u^*_{\mathbf{k}} + v_{\mathbf{k}} v^*_{\mathbf{k}} = 1$

With this unitary transformation, we can rewrite the Hamiltonian (3) like:

$$\begin{aligned} H = \sum_k \Big\{ \xi_{\mathbf{k}} \Big(\left(|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 \right) \left(\gamma^{\dagger}_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\uparrow} + \gamma^{\dagger}_{-\mathbf{k}\downarrow} \gamma_{-\mathbf{k}\downarrow} \right) \; + 2\left|v_{\mathbf{k}}\right|^2 + 2u^*_{\mathbf{k}} v^*_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow} \gamma_{\mathbf{k}\uparrow} + 2u_{\mathbf{k}} v_{\mathbf{k}} \gamma^{\dagger}_{\mathbf{k}\uparrow} \gamma^{\dagger}_{-\mathbf{k}\downarrow} \Big) \\ \Big(\left(\Delta_{\mathbf{k}} u_{\mathbf{k}} v^*_{\mathbf{k}} + \Delta^*_{\mathbf{k}} u^*_{\mathbf{k}} v^*_{\mathbf{k}} \right) \left(\gamma^{\dagger}_{\mathbf{k}\uparrow} \gamma_{\mathbf{k}\uparrow} + \gamma^{\dagger}_{-\mathbf{k}\downarrow} \gamma_{-\mathbf{k}\downarrow} - 1 \right) + \left(\Delta_{\mathbf{k}} \left(v_{\mathbf{k}}\right)^* - \Delta^*_{\mathbf{k}} \left(u_{\mathbf{k}}\right)^* \right) \gamma_{-\mathbf{k}\downarrow} \gamma_{\mathbf{k}\uparrow} \\ + \left(\Delta^*_{\mathbf{k}} v^2_{\mathbf{k}} - \Delta_{\mathbf{k}} u^2_k \right) \gamma^{\dagger}_{\mathbf{k}\uparrow} \gamma^{\dagger}_{-\mathbf{k}\downarrow} + \Delta_{\mathbf{k}} b^*_{\mathbf{k}} \Big) \Big\} \end{aligned} \tag{5}$$

Then, as we want a Hamiltonian in a diagonal form $H_{\mathrm{BdG}} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} \gamma^{\dagger}_{\mathbf{k},\sigma} \gamma_{\mathbf{k},\sigma} +$ *const*, we require that the other terms combine to zero: -

$$2\xi_k u_k v_k + \Delta^*_k u^2_k - \Delta_k v^2_k = 0$$

Multiplying both sides by $\frac{\Delta_k^*}{u_k^2}$:

$$\frac{\Delta_{\mathbf{k}}^* v_{\mathbf{k}}}{u_k} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} - \xi_{\mathbf{k}} \equiv E_{\mathbf{k}} - \xi_{\mathbf{k}}$$

where

$$E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}.$$

Finally, we can find the same relations of the BCS theory: $\begin{cases} |u_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \\ |v_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \end{cases}$

1.5 Superconductor gap

Using the definition of Δ, we rewrite in terms of the Bogoliubov operators(4):

$$c_{-k\downarrow}c_{k\uparrow} = u_k v_k \gamma^\dagger_{\mathbf{k},\uparrow}\gamma_{\mathbf{k},\uparrow} - u_k v_k \gamma_{-\mathbf{k},\downarrow}\gamma^\dagger_{-\mathbf{k},\downarrow} + u_k^2 \gamma_{-\mathbf{k},\downarrow}\gamma_{\mathbf{k},\uparrow} - v_k^2 \gamma^\dagger_{\mathbf{k},\uparrow}\gamma^\dagger_{-\mathbf{k},\downarrow}$$

Once the two last terms do not conserve the operator number for the Bogoliubov operators, their expected value will be zero. So:

$$\langle c_{-k\downarrow}c_{k\uparrow}\rangle = \langle \gamma^\dagger_{\mathbf{k},\uparrow}\gamma_{\mathbf{k},\uparrow}\rangle + \langle \gamma_{-\mathbf{k},\downarrow}\gamma^\dagger_{-\mathbf{k},\downarrow}\rangle - 1 \implies$$

$$\Delta_k = \sum_{\mathbf{k}'} (V_{\mathbf{k},\mathbf{k}'}(1 - n_f(E_k))$$

in which $n_f(E_k)$ is the Fermi-Dirac distribution. Thus:

$$\Delta_k = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} tanh(\frac{\beta E_k}{2}) \tag{6}$$