Gor'kov Equations Extended for Anisotropic Superconductivity and Their Solutions

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1 Overview of the Derivation of the Anisotropically Extended Gor'kov Equations

We introduce the Green's function method based on the BCS theory extended to cases where the superconducting gap symmetry is non-s-wave.

First, we use a more general Hamiltonian than the BCS one, given by:

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_{\mathrm{pair}} \\ &= \sum_{\boldsymbol{k},\boldsymbol{k}',s,s'} \langle \boldsymbol{k}s|\mathcal{H}_0|\boldsymbol{k}'s'\rangle a^\dagger_{\boldsymbol{k}s} a_{\boldsymbol{k}'s'} \\ &+ \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},s_1,s_2,s_3,s_4} V_{s_1s_2s_3s_4}(\boldsymbol{k},\boldsymbol{k}') a^\dagger_{(\boldsymbol{q}/2)-\boldsymbol{k},s_1} a^\dagger_{(\boldsymbol{q}/2)+\boldsymbol{k},s_2} a_{(\boldsymbol{q}/2)+\boldsymbol{k},s_3} a_{(\boldsymbol{q}/2)-\boldsymbol{k},s_4} \quad . \end{aligned} \tag{1}$$

The first term, $\mathcal{H}_0$, represents the single-particle Hamiltonian. This term includes non-uniform effects such as impurity scattering and interface scattering. The second term, the pairing interaction, is expressed with a center-of-mass momentum $\boldsymbol{q}$ and is not constrained by anything other than momentum conservation.

We introduce the finite-temperature Green's functions in the Matsubara formalism as follows:

$$G_{ss'}(\boldsymbol{k},\boldsymbol{k}';\tau) = -\langle T_\tau\{a_{\boldsymbol{k}s}(\tau) a^\dagger_{\boldsymbol{k}'s'}(0)\}\rangle \quad , \tag{2}$$

$$F_{ss'}(\boldsymbol{k},\boldsymbol{k}';\tau) = \langle T_\tau\{a_{\boldsymbol{k}s}(\tau) a_{\boldsymbol{k}'s'}(0)\}\rangle \quad , \quad F^\dagger_{ss'}(\boldsymbol{k},\boldsymbol{k}';\tau) = \langle T_\tau\{a^\dagger_{\boldsymbol{k}s}(\tau) a^\dagger_{\boldsymbol{k}'s'}(0)\}\rangle \quad . \tag{3}$$

Here, $F^\dagger_{ss'}$ is written by convention but does not represent the Hermitian conjugate of $F_{ss'}$. It should be noted that this quantity is a c-number.

The usual Minkowski space metric, diag(-1,1,1,1), is inconvenient for calculations. We therefore perform a Wick rotation on the time axis, rotating it by $\pi/2$ in the complex plane to transform the metric from diag(-1,1,1,1) to diag(1,1,1,1), thereby converting to Euclidean space. In this case, the 0-component becomes the imaginary time $\tau = it$, and the time dependence of the creation and annihilation operators is introduced in the Heisenberg picture.

$$a_{\boldsymbol{k}s}(\tau) = e^{\mathcal{H}\tau} a_{\boldsymbol{k}s} e^{-\mathcal{H}\tau} \quad .$$

The Fourier transform from the coordinate variable τ to $i\omega_n$ is defined as follows:

$$
\begin{aligned}
G_{ss'}(\boldsymbol{k},\boldsymbol{k}';\tau) &= k_BT\sum_n G_{ss'}(\boldsymbol{k},\boldsymbol{k}';i\omega_n)e^{-i\omega_n\tau} \quad , \\
F^{(\dagger)}_{ss'}(\boldsymbol{k},\boldsymbol{k}';\tau) &= k_BT\sum_n F^{(\dagger)}_{ss'}(\boldsymbol{k},\boldsymbol{k}';i\omega_n)e^{-i\omega_n\tau} \quad . \qquad (4)
\end{aligned}
$$

Here, $\omega_n = (2n+1)\pi k_BT$, with $(n \in \mathbb{Z})$, is the fermionic Matsubara frequency.
Using the equation of motion for operators, for example,

$$
\partial_\tau a_{\boldsymbol{k}s} = [\mathcal{H}, a_{\boldsymbol{k}s}] \quad ,
$$

we obtain the Gor'kov equations for $G_{ss'}(\boldsymbol{k},\boldsymbol{k}';i\omega_n)$ and $F^{(\dagger)}_{ss'}(\boldsymbol{k},\boldsymbol{k}';i\omega_n)$:

$$
\sum_{\boldsymbol{k}'',s''}\Big[\langle\boldsymbol{k}s|i\omega_n - \mathcal{H}_0|\boldsymbol{k}''s''\rangle G_{s''s'}(\boldsymbol{k}'',\boldsymbol{k}';i\omega_n) \qquad (5)
$$

$$
-\sum_{\boldsymbol{q}''}\Delta_{ss''}(\boldsymbol{k}'',\boldsymbol{q}'')F^\dagger_{s''s'}(\frac{\boldsymbol{q}''}{2}-\boldsymbol{k}'',\boldsymbol{k}';i\omega_n)\delta_{(\boldsymbol{q}''/2)+\boldsymbol{k}'',\boldsymbol{k}}\Big] \;=\; \delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{s,s'} \quad , \qquad (6)
$$

$$
\sum_{\boldsymbol{k}'',s''}\Big[\langle\boldsymbol{k}''s''|i\omega_n + \mathcal{H}_0|\boldsymbol{k}'s'\rangle F^\dagger_{ss'}(\boldsymbol{k},\boldsymbol{k}';i\omega_n) \qquad (7)
$$

$$
-\sum_{\boldsymbol{q}''}\Delta^\dagger_{ss''}(\boldsymbol{k}'',\boldsymbol{q}'')G_{s''s'}(\frac{\boldsymbol{q}''}{2}+\boldsymbol{k}'',\boldsymbol{k}';i\omega_n)\delta_{(\boldsymbol{q}''/2)-\boldsymbol{k}'',\boldsymbol{k}}\Big] \;=\; 0 \quad , \qquad (8)
$$

$$
\sum_{\boldsymbol{k}'',s''}\Big[\langle\boldsymbol{k}s|i\omega_n - \mathcal{H}_0|\boldsymbol{k}''s''\rangle F^\dagger_{s''s'}(\boldsymbol{k}'',\boldsymbol{k}';i\omega_n) \qquad (9)
$$

$$
-\sum_{\boldsymbol{q}''}\Delta^\dagger_{ss''}(\boldsymbol{k}'',\boldsymbol{q}'')G_{s's'}(\boldsymbol{k}',\frac{\boldsymbol{q}''}{2}-\boldsymbol{k}'';i\omega_n)\delta_{(\boldsymbol{q}''/2)+\boldsymbol{k}'',\boldsymbol{k}}\Big] \;=\; 0 \quad . \qquad (10)
$$

The quartic operator form included in $\mathcal{H}_{\text{pair}}$ has been truncated using the superconducting mean-field method. The resulting pair potential is:

$$
\begin{aligned}
\Delta_{ss'}(\boldsymbol{k},\boldsymbol{q}) &= -\sum_{\boldsymbol{k}',s_1,s_2} V_{s'ss_1s_2}(\boldsymbol{k},\boldsymbol{k}')\langle a_{(\boldsymbol{q}/2)+\boldsymbol{k}',s_1}a_{(\boldsymbol{q}/2)-\boldsymbol{k}',s_1}\rangle \quad , \\
&= -k_BT\sum_n\sum_{\boldsymbol{k}',s_1,s_2} V_{s'ss_1s_2}(\boldsymbol{k},\boldsymbol{k}')\,F_{s_1s_2}(\frac{\boldsymbol{q}}{2}+\boldsymbol{k}',\frac{\boldsymbol{q}}{2}-\boldsymbol{k}';i\omega_n) \quad . \qquad (11)
\end{aligned}
$$

2 Solutions to the Gor'kov Equations for a Uniform System

In a uniform system, the two momentum variables of the Green's function $G_{ss'}(\boldsymbol{k},\boldsymbol{k}';\tau)$ are equal, meaning $\boldsymbol{k}=\boldsymbol{k}'$. For the anomalous Green's function $F_{ss'}(\boldsymbol{k},\boldsymbol{k}';\tau)$, the sign changes to $\boldsymbol{k}=-\boldsymbol{k}'$.

Looking at Equation (11), the Nambu space representation matrix for the pair potential, $\hat{\Delta}(\boldsymbol{k},\boldsymbol{q})$, becomes independent of $\boldsymbol{q}$. Furthermore, the single-particle Hamiltonian term can be simplified by extracting only the diagonal elements of the representation matrix in momentum and spin space as follows:

$$\langle \boldsymbol{k}s| \quad \mathcal{H}_0|\boldsymbol{k}'s'\rangle = \varepsilon(\boldsymbol{k})\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{s,s'}$$

Using these, the Gor'kov equations can be expressed simply as:

$$\Big[i\omega_n - \varepsilon(\boldsymbol{k})\Big]G_{ss'}(\boldsymbol{k}, i\omega_n) \; - \; \sum_{s''}\Delta_{ss''}(\boldsymbol{k})F^{\dagger}_{s''s}(\boldsymbol{k}, i\omega_n) = \delta_{s,s'} \quad , \tag{12}$$

$$\Big[i\omega_n + \varepsilon(\boldsymbol{k})\Big]F^{\dagger}_{ss'}(\boldsymbol{k}, i\omega_n) \; - \; \sum_{s''}\Delta^{\dagger}_{ss''}(\boldsymbol{k})G_{s''s}(\boldsymbol{k}, i\omega_n) = 0 \quad , \tag{13}$$

$$\Big[i\omega_n - \varepsilon(\boldsymbol{k})\Big]F_{ss'}(\boldsymbol{k}, i\omega_n) \; - \; \sum_{s''}\Delta_{ss''}(\boldsymbol{k})G_{s's''}(-\boldsymbol{k}, -i\omega_n) = 0 \quad . \tag{14}$$

Each of these equations can be solved using simple algebra. In the Nambu space representation, for the spin-singlet pair case:

$$\begin{aligned} \hat{G}(\boldsymbol{k}, i\omega_n) &= -\frac{i\omega_n + \varepsilon(\boldsymbol{k})}{\omega_n^2 + E_{\boldsymbol{k}}^2}\hat{\sigma}_0 \quad , \\ \hat{F}(\boldsymbol{k}, i\omega_n) &= \frac{\hat{\Delta}(\boldsymbol{k})}{\omega_n^2 + E_{\boldsymbol{k}}^2} \quad . \end{aligned} \tag{15}$$

In the spin-triplet pair case, including non-unitary states ($\boldsymbol{q}(\boldsymbol{k}) = i\boldsymbol{d}(\boldsymbol{k}) \times \boldsymbol{d}^*(\boldsymbol{k}) \neq 0$):

$$\begin{aligned} \hat{G}(\boldsymbol{k}, i\omega_n) &= \frac{\Big[\omega_n^2 + \varepsilon^2(\boldsymbol{k}) + |\boldsymbol{d}(\boldsymbol{k})|^2\Big]\hat{\sigma}_0 + \boldsymbol{q}\cdot\hat{\boldsymbol{\sigma}}}{(\omega_n^2 + E_{\boldsymbol{k}+}^2)(\omega_n^2 + E_{\boldsymbol{k}-}^2)}\Big[i\omega_n + \varepsilon(\boldsymbol{k})\Big] \quad , \\ \hat{F}(\boldsymbol{k}, i\omega_n) &= \frac{\Big[\omega_n^2 + \varepsilon^2(\boldsymbol{k}) + |\boldsymbol{d}(\boldsymbol{k})|^2\Big]\boldsymbol{d}(\boldsymbol{k}) - i\boldsymbol{q}\times\boldsymbol{d}(\boldsymbol{k})}{(\omega_n^2 + E_{\boldsymbol{k}+}^2)(\omega_n^2 + E_{\boldsymbol{k}-}^2)}\cdot(i\hat{\boldsymbol{\sigma}}\hat{\sigma}_y) \quad . \end{aligned} \tag{16}$$

Here, we have used the shorthand $E_{\boldsymbol{k}\pm} = \sqrt{\varepsilon^2(\boldsymbol{k}) + |\boldsymbol{d}(\boldsymbol{k})|^2 \pm |\boldsymbol{q}(\boldsymbol{k})|^2}$. $|\boldsymbol{d}(\boldsymbol{k})|^2$ represents the magnitude of the extended gap, and $|\boldsymbol{q}(\boldsymbol{k})|^2$ represents the magnitude of the gap splitting that appears when time-reversal symmetry is broken. (Note that the $\boldsymbol{q}$ from $\mathcal{H}_{\text{pair}}$ is different from the $\boldsymbol{q}$ vector that appears when time-reversal symmetry is broken. The former $\boldsymbol{q}$ was a dummy variable that vanished upon summation.)

3 Solutions to the Gor'kov Equations for a General Non-uniform System

Let's go back to Equation (10). Solving for the anomalous Green's function gives:

$$F_{ss'}(\boldsymbol{k}, \boldsymbol{k}'; i\omega_n) = \sum_{\boldsymbol{k}'', \boldsymbol{q}'', s_1, s_2} \Delta_{s_1 s_2}(\boldsymbol{k}'', \boldsymbol{q}'')G^{(0)}_{ss'}(\boldsymbol{k}, \frac{\boldsymbol{q}''}{2} + \boldsymbol{k}''; i\omega_n)G_{s's_2}(\boldsymbol{k}', \frac{\boldsymbol{q}''}{2} - \boldsymbol{k}''; -i\omega_n) \tag{17}$$

Here, the function $\hat{G}^{(0)}$ is the Green's function for the single-particle Hamiltonian $\mathcal{H}_0$, defined by:

$$\sum_{\boldsymbol{k}'', s''}\langle \boldsymbol{k}s| \quad i\omega_n - \mathcal{H}_0|\boldsymbol{k}''s''\rangle G^{(0)}_{s''s'}(\boldsymbol{k}'', \boldsymbol{k}'; i\omega_n) = \delta_{s,s'}\delta_{\boldsymbol{k},\boldsymbol{k}'} \tag{18}$$

Work in Progress...

References

[1] M. Sigrist and K. Ueda (1991) Rev. Mod. Phys.