9

The Gorkov Approach

Abstract

- *The Gorkov approach to the BCS problem uses Green functions constructed on the mean-field Hamiltonian*

$$\tilde{H}^{(MF)} = \tilde{H}_0 + V_{BCS}^{(MF)},$$

with $\tilde{H}_0 = \sum_{\mathbf{k}s} \xi_{\mathbf{k}} a^\dagger_{\mathbf{k}s} a_{\mathbf{k}s}$. *The reduced BCS potential* V_{BCS} *is replaced by its mean-field approximation,*

$$V_{BCS}^{(MF)} = -\mathcal{V} \sum_{\mathbf{k}\mathbf{k}'} w_{\mathbf{k}} w_{\mathbf{k}'} \Big(\langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} \rangle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} + a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \rangle \\ - \langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} \rangle \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \rangle \Big),$$

with $\langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} \rangle$ *and* $\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \rangle$ *ultimately calculated in a self-consistent way.*

- *The zero-temperature standard Green function* $\mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, \omega)$ *and the anomalous Green function* $\mathcal{F}_{\uparrow\downarrow}(\mathbf{k}, \omega)$ *are introduced through*

$$\mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, t; \mathbf{k}, t') = -i \langle \mathrm{T}\big(a_{\mathbf{k}\downarrow}(t) a^\dagger_{\mathbf{k}\downarrow}(t')\big)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, \omega),$$

$$\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k}, t; \mathbf{k}, t') = -i \langle \mathrm{T}\big(a^\dagger_{-\mathbf{k}\uparrow}(t) a^\dagger_{\mathbf{k}\downarrow}(t')\big)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \mathcal{F}_{\uparrow\downarrow}(\mathbf{k}, \omega).$$

They are found to obey the two coupled equations

$$(\omega - \xi_{\mathbf{k}})\, \mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, \omega) + \Delta_{\mathbf{k}} \mathcal{F}_{\uparrow\downarrow}(\mathbf{k}, \omega) = 1,$$

$$(\omega + \xi_{\mathbf{k}})\, \mathcal{F}_{\uparrow\downarrow}(\mathbf{k}, \omega) + \Delta^*_{\mathbf{k}} \mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, \omega) = 0,$$

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where $\Delta^*_{\mathbf{k}} = w_{\mathbf{k}}\Delta^*$*, with*

$$\Delta^* = -\mathcal{V}\sum_{\mathbf{k}'} w_{\mathbf{k}'}\langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow}\rangle.$$

- *Resolution of these Gorkov equations leads to the "gap equation"*

$$1 = \mathcal{V}\sum_{\mathbf{k}} \frac{w_{\mathbf{k}}}{2\sqrt{\xi^2_{\mathbf{k}} + |\Delta|^2}}.$$

- *Extension to finite temperature gives the ratio of the zero-temperature gap* $|\Delta|$ *and the critical temperature* T_c *for gap disappearance as*

$$\frac{|\Delta|}{k_B T_c} \simeq \pi e^{-\gamma} \approx 1.76.$$

This ratio, independent of any physical parameter, is in good agreement with experiments, in spite of numerous approximations included in the BCS model for superconductivity.

The Gorkov approach to the BCS problem is a mean-field theory. Like the Bogoliubov approach, the Gorkov approach transforms the two-body reduced BCS potential into a one-body operator. Yet, the Gorkov approach uses Green functions to self-consistently determine the expectation values introduced in the mean-field Hamiltonian. One advantage of the Gorkov approach is that it easily extends to finite temperature (Gorkov 1958; Eliashberg 1961). Electromagnetic effects (London and London 1935; Pippard 1953) also are easy to include, through the substitution of $-i\hbar\nabla$ by $-i\hbar\nabla + |e|\mathbf{A}/c$.

In this chapter, we derive the zero-temperature gap equation by solving the two coupled Gorkov equations for standard and anomalous Green functions. Then, we briefly show how to extend the procedure to $T \neq 0$ in order to get the finite-temperature gap equation from which the transition temperature T_c for gap disappearance can be obtained.

9.1 The mean-field Hamiltonian

We start with the Hamiltonian in the grand canonical ensemble considered by Bardeen, Cooper, and Schrieffer, namely,

$$\tilde{H}_{BCS} = \tilde{H}_0 + V_{BCS}. \tag{9.1}$$

The one-body part of this Hamiltonian is given by

$$\tilde{H}_0 = \sum_{\mathbf{k},s=(\uparrow,\downarrow)} \xi_{\mathbf{k}} a^\dagger_{\mathbf{k}s} a_{\mathbf{k}s}, \tag{9.2}$$

with $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$, where μ here is the chemical potential for the N electrons in the potential layer plus the N_0 electrons of the frozen Fermi sea; V_{BCS} is the usual reduced BCS potential

$$V_{BCS} = -\mathcal{V} \sum_{\mathbf{k}\mathbf{k}'} w_{\mathbf{k}} w_{\mathbf{k}'} a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \tag{9.3}$$

but with $w_{\mathbf{k}}$ defined for convenience as $w_{\mathbf{k}} = 1$ for $\mu - \omega_c \leq \varepsilon_{\mathbf{k}} \leq \mu + \omega_c$, and zero otherwise. In previous chapters, $w_{\mathbf{k}}$ was taken equal to 1 in the energy layer $\varepsilon_F \pm \omega_c$, and μ was ultimately found equal to ε_F in the BCS configuration.

In a spirit similar to the Bogoliubov approach, the product of electron operators appearing in V_{BCS} is written as

$$\left(a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} - \langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow}\rangle + \langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow}\rangle\right)\left(a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} - \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\rangle + \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\rangle\right). \tag{9.4}$$

This leads us to split the BCS potential as $V_{BCS} = V^{(MF)}_{BCS} + W_G$, where the one-body (mean-field) part reads

$$\begin{aligned} V^{(MF)}_{BCS} = -\mathcal{V} \sum_{\mathbf{k}\mathbf{k}'} w_{\mathbf{k}} w_{\mathbf{k}'} \Big(&\langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow}\rangle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} + a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\rangle \\ &- \langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow}\rangle \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\rangle \Big). \end{aligned} \tag{9.5}$$

The resulting mean-field Hamiltonian then reads

$$\tilde{H}^{(MF)} = \tilde{H}_0 + V^{(MF)}_{BCS}. \tag{9.6}$$

The two-body part of the V_{BCS} potential appears through

$$W_G = -\mathcal{V} \sum_{\mathbf{k}\mathbf{k}'} w_{\mathbf{k}} w_{\mathbf{k}'} \left(a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} - \langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow}\rangle\right)\left(a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} - \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\rangle\right), \tag{9.7}$$

where W_G is just the W operator of the Bogoliubov procedure with $z_{\mathbf{k}}$ taken as $\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\rangle$. In the Gorkov approach, the two-body potential W_G is simply neglected. This approximation, expected to be valid for appropriate $\langle a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}\rangle$'s, is conceptually similar to what is done in the Bogoliubov approach, which takes these mean values as free parameters ultimately chosen for the W contribution to the energy to be negligible in the large sample limit.

The mean values introduced in Eq. (9.4) are defined for finite temperature as

$$\langle a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} \rangle_T = \frac{\mathrm{Tr}\left(e^{-\beta \tilde{H}^{(MF)}} a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow}\right)}{\mathrm{Tr}\ e^{-\beta \tilde{H}^{(MF)}}}, \tag{9.8}$$

with $\beta = 1/k_B T$, the trace being taken over the eigenstates of the mean-field Hamiltonian $\tilde{H}^{(MF)}$. For $T = 0$, these eigenstates reduce to the mean-field ground state $|\Psi_0\rangle$; so,

$$\langle a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} \rangle_{T=0} = \frac{\langle \Psi_0 | a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}. \tag{9.9}$$

These mean values are self-consistently determined, as shown below. Note that $\langle a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} \rangle$ does not reduce to zero because the mean-field Hamiltonian is taken in the grand canonical ensemble; so, it does not conserve the particle number.

9.2 Gorkov equations for $T = 0$

(i) We first derive particle equations of motion. By turning to Heisenberg operators which, for $\hbar = 1$, read

$$a^{\dagger}_{\mathbf{k}\uparrow}(t) = e^{it\tilde{H}^{(MF)}} a^{\dagger}_{\mathbf{k}\uparrow} e^{-it\tilde{H}^{(MF)}}, \tag{9.10}$$

we get

$$\begin{aligned} \frac{\partial a^{\dagger}_{\mathbf{k}\uparrow}(t)}{\partial t} &= e^{it\tilde{H}^{(MF)}} \left[i\tilde{H}^{(MF)}, a^{\dagger}_{\mathbf{k}\uparrow} \right]_- e^{-it\tilde{H}^{(MF)}} \\ &= i e^{it\tilde{H}^{(MF)}} \Big(\xi_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow} - \mathcal{V} w_{\mathbf{k}} a_{-\mathbf{k}\downarrow} \sum_{\mathbf{k}'} w_{\mathbf{k}'} \langle a^{\dagger}_{\mathbf{k}'\uparrow} a^{\dagger}_{-\mathbf{k}'\downarrow} \rangle \Big) e^{-it\tilde{H}^{(MF)}}, \end{aligned} \tag{9.11}$$

which leads to

$$\frac{\partial a^{\dagger}_{\mathbf{k}\uparrow}(t)}{i\partial t} = \xi_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow}(t) - \mathcal{V} w_{\mathbf{k}} a_{-\mathbf{k}\downarrow}(t) \sum_{\mathbf{k}'} w_{\mathbf{k}'} \langle a^{\dagger}_{\mathbf{k}'\uparrow} a^{\dagger}_{-\mathbf{k}'\downarrow} \rangle. \tag{9.12}$$

In the same way, as $\left[\tilde{H}_0, a_{\mathbf{k}\downarrow}\right]_- = -\xi_{\mathbf{k}} a_{\mathbf{k}\downarrow}$, we find that

$$\frac{\partial a_{\mathbf{k}\downarrow}(t)}{i\partial t} = -\xi_{\mathbf{k}} a_{\mathbf{k}\downarrow}(t) - \mathcal{V} w_{\mathbf{k}} a^{\dagger}_{-\mathbf{k}\uparrow}(t) \sum_{\mathbf{k}'} w_{\mathbf{k}'} \langle a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow} \rangle. \tag{9.13}$$

(ii) Next, we introduce zero-temperature (standard) Green functions defined in terms of the $|\Psi_0\rangle$ mean-field ground state, $\big(\tilde{H}^{(MF)} - \mathcal{E}^{(MF)}\big)|\Psi_0\rangle = 0$, as

$$\mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, t; \mathbf{k}, t') = -i\langle \mathrm{T}\big(a_{\mathbf{k}\downarrow}(t)a^{\dagger}_{\mathbf{k}\downarrow}(t')\big)\rangle \equiv -i\frac{\langle\Psi_0|\mathrm{T}\big(a_{\mathbf{k}\downarrow}(t)a^{\dagger}_{\mathbf{k}\downarrow}(t')\big)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}, \tag{9.14}$$

the time-ordering operator T being defined as

$$\mathrm{T}\big(a_{\mathbf{k}\downarrow}(t)a^{\dagger}_{\mathbf{k}\downarrow}(t')\big) = \Theta(t-t')a_{\mathbf{k}\downarrow}(t)a^{\dagger}_{\mathbf{k}\downarrow}(t') - \Theta(t'-t)a^{\dagger}_{\mathbf{k}\downarrow}(t')a_{\mathbf{k}\downarrow}(t), \tag{9.15}$$

where $\Theta(t)$ is the Heaviside step function, that is, $\Theta(t) = 1$ for $t \geq 0$, and 0 otherwise. The time derivative of this Green function reads

$$\frac{\partial}{\partial t}\mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, t; \mathbf{k}, t') = -i\delta(t-t')\langle a_{\mathbf{k}\downarrow}(t)a^{\dagger}_{\mathbf{k}\downarrow}(t) + a^{\dagger}_{\mathbf{k}\downarrow}(t)a_{\mathbf{k}\downarrow}(t)\rangle$$
$$-i\langle \mathrm{T}\Big(\Big(\frac{\partial}{\partial t}a_{\mathbf{k}\downarrow}(t)\Big)a^{\dagger}_{\mathbf{k}\downarrow}(t')\Big)\rangle. \tag{9.16}$$

The mean value in the first term reduces to 1 because of the anticommutation relation between electron operators. Calculating the second term using Eq. (9.13) gives

$$\frac{\partial}{i\partial t}\mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, t; \mathbf{k}, t') = -\delta(t-t') - \xi_{\mathbf{k}}\mathcal{G}_{\downarrow\downarrow}(\mathbf{k}, t; \mathbf{k}, t')$$
$$-\mathcal{V}w_{\mathbf{k}}\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k}, t; \mathbf{k}, t')\sum_{\mathbf{k}'} w_{\mathbf{k}'}\langle a_{-\mathbf{k}'\downarrow}a_{\mathbf{k}'\uparrow}\rangle, \tag{9.17}$$

where $\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k}, t; \mathbf{k}, t')$ is the so-called anomalous Green function defined as

$$\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k}, t; \mathbf{k}, t') \equiv -i\langle \mathrm{T}\big(a^{\dagger}_{-\mathbf{k}\uparrow}(t)a^{\dagger}_{\mathbf{k}\downarrow}(t')\big)\rangle. \tag{9.18}$$

This anomalous Green function, which accounts for the BCS superconducting state, is linked to the gap, as we now show. The time derivative of $\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k}, t; \mathbf{k}, t')$ appears as

$$\frac{\partial}{\partial t}\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k}, t; \mathbf{k}, t') = -i\delta(t-t')\langle a^{\dagger}_{-\mathbf{k}\uparrow}(t)a^{\dagger}_{\mathbf{k}\downarrow}(t) + a^{\dagger}_{\mathbf{k}\downarrow}(t)a^{\dagger}_{-\mathbf{k}\uparrow}(t)\rangle$$
$$-i\langle \mathrm{T}\Big(\Big(\frac{\partial}{\partial t}a^{\dagger}_{-\mathbf{k}\uparrow}(t)\Big)a^{\dagger}_{\mathbf{k}\downarrow}(t')\Big)\rangle. \tag{9.19}$$

The mean value in the first term reduces to 0 because of the anticommutation relation between electron operators; so, using Eq. (9.12), we find

$$\frac{\partial}{i\partial t}\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k},t;\mathbf{k},t') = \xi_{-\mathbf{k}}\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k},t;\mathbf{k},t') \\ -\mathcal{V}w_{-\mathbf{k}}\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},t;\mathbf{k},t')\sum_{\mathbf{k}'}w_{\mathbf{k}'}\langle a^\dagger_{\mathbf{k}'\uparrow}a^\dagger_{-\mathbf{k}'\downarrow}\rangle. \tag{9.20}$$

(iii) To get "Gorkov equations" that couple standard and anomalous Green functions, we rewrite the $\mathbf{k}'$ sum appearing in Eqs. (9.17, 9.20) as

$$-\mathcal{V}w_{\mathbf{k}}\sum_{\mathbf{k}'}w_{\mathbf{k}'}\langle a^\dagger_{\mathbf{k}'\uparrow}a^\dagger_{-\mathbf{k}'\downarrow}\rangle = w_{\mathbf{k}}\Delta^* \equiv \Delta^*_{\mathbf{k}}. \tag{9.21}$$

The mean values $\langle a^\dagger_{\mathbf{k}'\uparrow}a^\dagger_{-\mathbf{k}'\downarrow}\rangle$, introduced at the beginning of the procedure, only appear through this $\mathbf{k}'$ sum. We will show that $|\Delta|$ is just the zero-temperature superconducting gap. As $\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$ and $w_{\mathbf{k}} = w_{-\mathbf{k}}$, Eqs. (9.17, 9.20) then read

$$\left(\frac{\partial}{i\partial t}+\xi_{\mathbf{k}}\right)\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},t;\mathbf{k},t') - \Delta_{\mathbf{k}}\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k},t;\mathbf{k},t') = -\delta(t-t'), \tag{9.22a}$$

$$\left(\frac{\partial}{i\partial t}-\xi_{\mathbf{k}}\right)\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k},t;\mathbf{k},t') - \Delta^*_{\mathbf{k}}\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},t;\mathbf{k},t') = 0. \tag{9.22b}$$

(iv) The last step is to note that, since $\tilde{H}^{(MF)}$ does not depend on time, Green functions only depend on the time difference t–t'. We then perform Fourier transform according to

$$\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},t;\mathbf{k},t') = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},\omega), \tag{9.23a}$$

$$\mathcal{F}_{\uparrow\downarrow}(-\mathbf{k},t;\mathbf{k},t') = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\mathcal{F}_{\uparrow\downarrow}(\mathbf{k},\omega). \tag{9.23b}$$

The Gorkov equations then take a nicely compact form,

$$(\omega-\xi_{\mathbf{k}})\,\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},\omega) + \Delta_{\mathbf{k}}\mathcal{F}_{\uparrow\downarrow}(\mathbf{k},\omega) = 1, \tag{9.24a}$$

$$(\omega+\xi_{\mathbf{k}})\,\mathcal{F}_{\uparrow\downarrow}(\mathbf{k},\omega) + \Delta^*_{\mathbf{k}}\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},\omega) = 0, \tag{9.24b}$$

with similar coupled equations between $\mathcal{G}_{\uparrow\uparrow}(\mathbf{k},\omega)$ and $\mathcal{F}_{\downarrow\uparrow}(\mathbf{k},\omega)$. In the absence of spin-dependent interaction, these two sets of equations are equivalent.

9.3 The energy gap

It is easy to check that the solution of the above equations reads

$$\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},\omega) = \frac{\omega+\xi_{\mathbf{k}}}{\omega^2-E_{\mathbf{k}}^2}, \tag{9.25a}$$

$$\mathcal{F}_{\uparrow\downarrow}(\mathbf{k},\omega) = -\frac{\Delta_{\mathbf{k}}^*}{\omega^2-E_{\mathbf{k}}^2}, \tag{9.25b}$$

where $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$. Such a solution however forces $\omega \neq \pm E_{\mathbf{k}}$. To give meaning to this solution for all ω, we use a trick (Liftshitz and Pitaevskii 1999): we introduce a small imaginary part $i\eta$ into $E_{\mathbf{k}}$ with an as yet arbitrary η sign. We will show that η must be taken positive, in agreement with the imaginary part of standard Green function poles. In this trick, $1/(\omega^2 - E_{\mathbf{k}}^2)$ is replaced with

$$-\frac{1}{2E_{\mathbf{k}}}\left(\frac{1}{\omega+E_{\mathbf{k}}-i\eta} - \frac{1}{\omega-(E_{\mathbf{k}}-i\eta)}\right). \tag{9.26}$$

Inserting this substitution into Eqs. (9.25a, b) gives

$$\mathcal{G}_{\downarrow\downarrow}(\mathbf{k},\omega) = \frac{1}{2}\left(1+\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)\frac{1}{\omega-E_{\mathbf{k}}+i\eta} + \frac{1}{2}\left(1-\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right)\frac{1}{\omega+E_{\mathbf{k}}-i\eta}, \tag{9.27a}$$

$$\mathcal{F}_{\uparrow\downarrow}(\mathbf{k},\omega) = -\frac{\Delta_{\mathbf{k}}^*}{2E_{\mathbf{k}}}\left(\frac{1}{\omega-E_{\mathbf{k}}+i\eta} - \frac{1}{\omega+E_{\mathbf{k}}-i\eta}\right). \tag{9.27b}$$

To get $\Delta_{\mathbf{k}}^*$, we note, using Eqs. (9.18, 9.21), that Δ^* is related to the anomalous Green function through

$$\Delta^* = -i\mathcal{V}\sum_{\mathbf{k}'} \mathcal{F}_{\uparrow\downarrow}(\mathbf{k}', 0_+; -\mathbf{k}', 0), \tag{9.28}$$

where 0_+ is a small positive time. The Fourier transform defined in Eqs. (9.23a, b) then gives Δ^* as

$$\begin{aligned}\Delta^* &= -i\mathcal{V}\sum_{\mathbf{k}'} w_{\mathbf{k}'}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega 0_+}\mathcal{F}_{\uparrow\downarrow}(\mathbf{k}',\omega) \qquad (9.29)\\ &= -\mathcal{V}\sum_{\mathbf{k}'} w_{\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}^*}{2E_{\mathbf{k}'}}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}e^{-i\omega 0_+}\left(\frac{1}{\omega-E_{\mathbf{k}'}+i\eta} - \frac{1}{\omega+E_{\mathbf{k}'}-i\eta}\right).\end{aligned}$$

To go further, we note that $\Delta^*_{\mathbf{k}'}$ can be replaced by Δ^*, the factor $w_{\mathbf{k}'}$ being already present in the $\mathbf{k}'$ sum. The ω integral is calculated using the residue theorem. The factor $e^{-i\omega 0_+}$ forces us to choose the integration contour over the lower half complex plane. So, the integral in Eq. (9.29) gives (−1) for $\eta > 0$, and (+1) for $\eta < 0$, from which we get

$$1 = \text{sgn}(\eta)\mathcal{V}\sum_{\mathbf{k}'} \frac{w_{\mathbf{k}'}}{2\sqrt{\xi^2_{\mathbf{k}'} + |\Delta|^2}}. \tag{9.30}$$

As the $\mathbf{k}'$ sum is positive, this imposes to take $\text{sgn}(\eta) = +1$ in Eqs. (9.27a, b). So, the above equation ultimately reduces to the gap equation for $T = 0$.

9.4 Gorkov equations and the energy gap for $T \neq 0$

As this book does not focus on finite-temperature effects, let us just outline how the Gorkov formalism nicely extends to finite temperature and conclude this chapter by deriving one of the most important relations in BCS superconductivity, namely, the link between the zero-temperature energy gap and the critical temperature T_c for gap disappearance, which made the BCS model so famous.

The procedure to derive Gorkov equations for $T \neq 0$ is just the same as the one for $T = 0$. The Gorkov equations for finite-temperature Green functions read just as Eqs. (9.24a, b), provided that the real frequency ω is replaced, via the Matsubara trick (Matsubara 1955), by the imaginary frequency $i\omega_n$, with discrete values $\omega_n = (2n+1)\pi/\beta$ for fermions. So, to get the gap as a function of temperature, we replace ω in Eq. (9.29) by $i\omega_n$, and the integral $(2\pi i)^{-1}\int d\omega$ by the discrete sum $\beta^{-1}\sum_{\omega_n}$. Equation (9.29) then transforms into

$$\begin{aligned}\Delta^* &= \mathcal{V}\sum_{\mathbf{k}} w_{\mathbf{k}} \frac{1}{\beta}\sum_n \mathcal{F}_{\uparrow\downarrow}(\mathbf{k}, i\omega_n)\\ &= \mathcal{V}\sum_{\mathbf{k}} w_{\mathbf{k}} \frac{1}{\beta}\sum_n \frac{\Delta^*_{\mathbf{k}}}{\omega_n^2 + E^2_{\mathbf{k}}}.\end{aligned} \tag{9.31}$$

Since $\Delta^*_{\mathbf{k}} = w_{\mathbf{k}}\Delta^*$, the following identity,

$$\sum_n \frac{1}{(2n+1)^2\pi^2 + a^2} = \frac{1}{2a}\tanh\frac{a}{2}, \tag{9.32}$$

when used in the above equation, gives the gap equation for $T \neq 0$ as

$$1 = \mathcal{V}\sum_{\mathbf{k}} \frac{w_{\mathbf{k}}}{2E_{\mathbf{k}}}\tanh\frac{\beta E_{\mathbf{k}}}{2}. \tag{9.33}$$

In the $T \to 0$ limit, $\beta \to \infty$, and $\tanh(\beta E_{\mathbf{k}}/2)$ approaches 1; so, the above equation reduces to Eq. (9.30). In the $T \to \infty$ limit, $\beta \to 0$, and $\tanh(\beta E_{\mathbf{k}}/2)$ approaches 0. As the sum over $\mathbf{k}$ in Eq. (9.33) stays equal to 1, the gap $|\Delta|$, hidden in $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$, must decrease with T. A detailed analysis of Eq. (9.33) shows that $|\Delta|$ rapidly drops to zero when the temperature approaches a critical value T_c. Above T_c, the gap is equal to zero, and superconductivity disappears.

The critical temperature is defined as the temperature at which $|\Delta|$ vanishes. By again taking a constant density of states ρ in the potential layer and by noting that $E_{\mathbf{k}} = |\xi_{\mathbf{k}}|$ for $|\Delta| = 0$, we find that Eq. (9.33) reduces to

$$1 = \frac{\rho\mathcal{V}}{2}\int_{\mu-\omega_c}^{\mu+\omega_c} \frac{d\xi_{\mathbf{k}}}{|\xi_{\mathbf{k}}|} \tanh\frac{|\xi_{\mathbf{k}}|}{2k_B T_c} = \frac{\rho\mathcal{V}}{2}\int_{-\omega_c}^{\omega_c} \frac{d\varepsilon_{\mathbf{k}}}{|\varepsilon_{\mathbf{k}}|} \tanh\frac{|\varepsilon_{\mathbf{k}}|}{2k_B T_c}. \tag{9.34}$$

As the integrand is an even function of $\varepsilon_{\mathbf{k}}$, we can rewrite this equation as

$$1 = \rho\mathcal{V}\int_0^{\omega_c} \frac{d\varepsilon_{\mathbf{k}}}{\varepsilon_{\mathbf{k}}} \tanh\frac{\varepsilon_{\mathbf{k}}}{2k_B T_c} = \rho\mathcal{V}\int_0^{\frac{\omega_c}{2k_B T_c}} \frac{dx}{x}\tanh x. \tag{9.35}$$

We then note that, for $\rho\mathcal{V} \simeq 0$, the integral upper boundary must go to infinity, that is, T_c must go to 0, in order for the RHS to stay equal to 1. So, for $\rho\mathcal{V}$ small, this upper boundary must be much larger than 1. The integral in Eq. (9.35), performed through an integration by parts, then gives

$$\frac{1}{\rho\mathcal{V}} = (\ln x)\tanh x\Big|_0^{\frac{\omega_c}{2k_B T_c}} - \int_0^{\frac{\omega_c}{2k_B T_c}} dx\frac{\ln x}{\cosh^2 x}. \tag{9.36}$$

As $1/\cosh x$ is exponentially small for $x \gg 1$, we can replace the integral upper boundary with infinity. This integral then gives $-\ln(4e^{\gamma}/\pi)$, where $\gamma \approx 0.577$ is the Euler constant. Since $\tanh x \simeq 1$ for large x while $(\ln x)\tanh x \simeq 0$ for small x, we end with a critical temperature given by

$$k_B T_c = \frac{e^{\gamma}}{\pi} 2\omega_c e^{-1/\rho\mathcal{V}}. \tag{9.37}$$

As the zero-temperature gap is given for small $\rho\mathcal{V}$ by $|\Delta| \simeq 2\omega_c e^{-1/\rho\mathcal{V}}$, the above equation shows that the ratio

$$\frac{|\Delta|}{k_B T_c} \simeq \pi e^{-\gamma} \approx 1.76 \tag{9.38}$$

does not depend on any physical parameter. Such a prediction imposes a strong constraint between the superconducting gap at $T = 0$ and the critical temperature T_c for gap disappearance. It is quite remarkable that experimental data (see Kittel 1996, p. 336) on metallic superconductors support this prediction, in spite of numerous approximations contained in the BCS model for superconductivity.