Quasiclassical Green’s functions and superconducting non-equilibrium Fermi systems

Janne Viljas

1Low Temperature Laboratory, Helsinki University of Technology,
P.O.Box 2200, FIN-02015 HUT, Finland

(Dated: March 3, 2013)

Message to reader: These are my personal notes on how to derive the basic results of "quasi-classical theory" of degenerate, superconducting Fermi systems in nonequilibrium. The derivation involves perturbative methods of quantum statistical mechanics applied to many-body Green’s functions, so this topic has to be dealt with first. The approach is very traditional, making no use of path integral methods. The notes, written mostly in fall 2002 while working on my doctoral thesis at Helsinki University of Technology, grew out of a need to introduce myself to the nonequilibrium (i.e., Keldysh) methods, having no previous knowledge of them and no-one to teach me. As such, they were never intended to be actually read by anyone, perhaps including myself. If you read them anyway, be aware that I have avoided technical difficulties and exact proofs as far as possible, preferring to use words (a lot of them!) and diagrammatig visualizations instead. As a result, I expect some of my statements, as well as some of the diagrams, to be simply wrong: they only reflect my level of (mis)understanding at the time of writing. I hope that someday I will find enough time and motivation to clean things up and turn the notes into a more useful reference text.

CONTENTS

I. Green’s functions in normal systems, general notions 2
A. Green’s functions $G$, $G^{R,A,K}$, and statistical ensembles 3
B. Quantum-mechanical pictures and equations of motion 3
II. Normal systems: zero-temperature formalism 4
A. Lehmann representation, spectral functions, and the quasiparticle concept 4
   1. Lehmann representation 4
   2. The retarded, advanced and Keldysh functions $G^{R,A,K}$, and further relations for $G$ 6
   3. Quasiparticles 7
   4. Coherent and incoherent vs. low and high energy 9
B. Perturbation theory at zero temperature 9
   1. Wick’s theorem and contractions of operators 9
   2. Adiabatic “switching on and off” at zero temperature 10
   3. Some results from perturbation theory for the single-particle propagator 11
C. The two-particle function 12
III. Normal systems: finite temperatures and nonequilibrium 13
A. Equilibrium at finite temperatures, comments about perturbation theory 13
B. Nonequilibrium and the Keldysh contour 14
   1. Interaction picture for $K_0 = T - \mu N$, “adiabatic switching on”, and the Keldysh contour 14
   2. Contour-ordered functions, the Keldysh space, and perturbation theory at finite temperatures 16
   3. Symmetry properties, definition of the Keldysh function $G^K$, and rotations in Keldysh space 17
   4. Equations of motion in Keldysh space and symmetries of self energies 18
   5. Further relations 19
C. Explicit expressions for the propagators 20
   1. Noninteracting nonequilibrium 20
   2. Generalized Lehmann representation in equilibrium 20
IV. Generalization to systems with Cooper-pair condensates 22
A. Introduction to the “F functions” 22
B. Exact results from spectral decompositions 23
   1. Lehmann representation for $F$ at zero temperature 23
   2. Unperturbed propagators in the BCS model 24
   3. Functions $F^{R,A,K}$, symmetries, and finite-temperature results 25
C. Construction of Nambu matrices and the particle-hole space 26
   1. Matrix propagator and particle-hole space 26
   2. Equation of motion for the unperturbed Nambu propagator 27
D. Perturbation theory approach for superconductors 28
   1. Discussion 28
   2. Diagrammatic analysis 29
V. Derivation of the nonequilibrium equations 30
A. Form of the Hamiltonian operator 31
B. Separation of low and high energy parts of the propagator 32
The original purpose of writing these notes was to gain a sufficient background for understanding the so-called “quasiclassical theory” of superconductivity. In the general nonequilibrium case the central equations of this theory are known as the Eilenberger-Larkin-Ovchinnikov-Eliashberg (ELOE) equations [1]. Our main goal here is to sketch their derivation. To begin this effort, the following three sections discuss some aspects of the calculation of many-body Green’s functions in the case of “normal” Fermi systems. Applications are given in the many references which I have provided, and we do not worry about them here. The notation is kept at a very condensed level: in particular, ℏ = 1 in most places, unless special clarity is required.

Much of the initial discussion is based on the book of Nozieres [2], which concentrates on developing the theoretical formalism. In Nozieres’ book, particular emphasis is put on defining the concept of quasiparticles and related issues. This is also a good source for many of the more complicated diagrammatic nontrivialities encountered in Fermi-liquid theory, including a discussion of the energy functionals and their variational principles. Here one usually refers to certain original articles by deDominics and Martin or Luttinger and Ward, both of which are practically unreadable to a beginner. The classic book of Fetter and Walecka [3] is also a very nice introduction to the basic concepts of many-body quantum theory. The other classic of Abrikosov, Gorkov, and Dzyaloshinski [4] is a bit tough as an introduction, but is very compact and covers some topics not addressed by Fetter and Walecka. Yet another classic that is often useful is the book of Doniach and Sondheimer [5].

The pre-1980’s literature, however, rarely discusses the nonequilibrium formalism, although it was developed already in the 1960’s by Kadanoff and Baym [6] and by Keldysh [7]. At least one mid-1980’s review paper by Rammer and Smith [8] contains a rather good general account, but is hopelessly complicated as an introduction. (See also the book by Rammer [9].) Fortunately, the book by Zagoskin [10] turned out to be simple enough, and it is therefore the other reference which I have used widely. However, I have since learned that a very readable and compact description of the general nonequilibrium Green-function formalism is given in the book of Haug and Jauho [11], which basically builds on the review of Rammer and Smith. Also the original book of Kadanoff and Baym is actually very readable, although it does not directly contain the idea of the “Keldysh contour”, which has now become the standard tool for describing nonequilibrium. The book of Mahan [12] (2nd ed.) also has a brief discussion of these issues. Furthermore, I should mention the papers of Danielewicz [13] and Wagner [14], the latter of which introduces a neat generalization of the Keldysh technique. An excellent modern introduction to the topics of many-body theory.
is given by the recent book of Bruus and Flensberg [15], although it does not cover the nonequilibrium theory. In fact, new presentations just keep popping up all the time: see also Refs. 16 and 17, which deal with time-dependent density-functional theory. Finally, the notes by Kamenev [21] represent a more “modern” path-integral approach to non-equilibrium Green functions.

However, a comprehensive treatment of the basic formalism and perturbation theory for superconductors (which are “non-normal”) by using the nonequilibrium concepts is still missing in all of the above references. For the case of conventional (singlet) superconductivity the perturbation theory is somehow covered in Refs. 8, 10, and 18. Also the book of Kopnin [19] covers mostly conventional superconductors. In contrast, we are particularly interested in the general pairing case, since this type includes also the triplet-paired superfluid $^3$He [1, 20]. Thus, in Sec. IV where I turn to discuss BCS superconductors and superfluids, I am forced to use varied references and attempt to fill in the remaining gaps by myself. I have found the appendixes in the review of Serene and Rainer [1] particularly useful.

A. Green’s functions $G$, $G^{R,A,K}$, and statistical ensembles

We start off by giving the general definitions of four useful single-particle (or two-point) propagators of a many-body system: These are the time-ordered (or causal) function $G$, the retarded (advanced) function $G^R$ ($G^A$), and the “Keldysh” function $G^K$. These functions are related to each other in ways which will become clear later on. Choosing the signs according to the conventions used in Refs. [3, 10], their expressions are

$$
G(x_1, x_2) = -i\langle T\psi(x_1)\psi(x_2)\rangle
$$

$$
G^R(x_1, x_2) = -i\langle [\psi(x_1)\psi(x_2)]_\oplus \theta(t_1 - t_2)\rangle
$$

$$
G^A(x_1, x_2) = i\langle [\psi(x_1)\psi(x_2)]_\ominus \theta(t_2 - t_1)\rangle
$$

$$
G^K(x_1, x_2) = -i\langle [\psi(x_1)\psi(x_2)]_\ominus \rangle
$$

We use a notation where $[\cdot, \cdot]_\oplus = [\cdot, \cdot]$ is a commutator and $[\cdot, \cdot]_\ominus = \{\cdot, \cdot\}$ an anticommutator. We are mainly interested in fermions, but sometimes note how expressions should be modified for the case of bosons. Thus, whenever a sign appears circled ($\oplus$ or $\ominus$), then it should be changed when bosons rather than fermions are concerned. We also denote $x_i = (x_i, \sigma_i, t_i)$, where $\sigma_i$ includes spin ($\uparrow$ or $\downarrow$) and possibly other relevant single-particle quantum numbers, and $T$ is the time-ordering ($t$-ordering) operator [3]. (Sometimes we explicitly separate the time variables $t_i$ in which case $x_i = (x_i, \sigma_i)$, and on occasion the $\sigma_i$ are further separated such that $\psi(x_i) = \psi_\sigma(x_i \beta_i)$. Furthermore, the spin indices may be dropped from time to time.) In addition to $G$ and $G^{R,A,K}$ also a number of other types of real-time propagators are often introduced, as will be discussed further below. (In addition, in the finite-temperature equilibrium formalism a and “imaginary-time”, or “Matsubara” function $G^M$ may be defined.) However, initially we only need the time-ordered function, whose properties we shall be discussing throughout the beginning sections.

The statistical average is defined as $\langle \cdots \rangle = Tr[\rho \cdots]$, where the statistical operator (density matrix) $\rho$ is arbitrary in general, but is normalized according to $Tr\rho = 1$. When the system is in thermodynamic equilibrium with a heat and particle bath, $\rho = \exp[\beta(\Omega - K)] = Z^{-1}\sum_n \exp(-\beta K_n)|\Psi_n\rangle\langle\Psi_n|$, where $K = H - \mu N = T + V - \mu N$ is the time-independent grand-canonical Hamiltonian, $|\Psi_n\rangle$ and $K_n$ are its eigenstates and eigenvalues, and $Z = \exp(-\beta\Omega) = \text{Tr}[\exp(-\beta K)]$ defines the thermodynamic potential $\Omega$ of the grand-canonical ensemble. As an important special case, at zero temperature only the (interacting) ground state $|\Psi_0\rangle$ of $K$ is occupied, and $\rho$ reduces to $\rho = |\Psi_0\rangle\langle\Psi_0|$. We adopt the use of $K$ in the definition of the field operators and $G$, but the relation between our $G$ and that defined with $H = T + V$ is simple, the main difference being in the choice for the zero of energy which can be chosen arbitrarily in the nonrelativistic limit. This is done to facilitate direct comparison with the superconductor case, where the grand-canonical ensemble will be unavoidable for technical reasons. In equilibrium the “chemical potential” $\mu$ must also be related to the average particle number $N_{ave}$ according to $\langle N \rangle_{eq} = -\partial\Omega/\partial\mu = N_{ave}$, but the actual value of $N_{ave}$ is not visible anywhere in the formalism. For our purposes, the value of $\mu$ is thus practically arbitrary and only shifts the zero point of all energies. However, at $T = 0$, for example, it is usually assumed to coincide with the Fermi energy.

B. Quantum-mechanical pictures and equations of motion

Above we have used the Heisenberg picture, where all time dependence is associated with the operators, except the statistical operator $\rho$. (In equilibrium also $K$ remains time-independent since it commutes with the time-evolution operator which is given by the constant $K$ itself). The Heisenberg, Schrödinger, and interaction pictures are related as follows. We separate the Schrödinger-picture Hamiltonian $K(t) = K_0 + K_1(t)$ so that $K_0$ is an “unperturbed” time-independent Hamiltonian (for example $K_0 = T - \mu N$, where $T$ includes kinetic energy and possibly static external potentials such as those due to an ion lattice). $K_1(t)$ is either a time-dependent (one-body) perturbation $K_1(t) = V_{ext}(t)$ due to external fields (in which case we use $K_0 = T - \mu N + V$) or the adiabatically switched-on interaction $K_1(\eta)(t) = \exp(-\eta|t|)V$ when $V_{ext} \equiv 0$. We may also consider a mixed case where $K_0 = T - \mu N$ and $K_1(\eta)(t) = \exp(-\eta|t|)(V + V_{ext}(t))$. Either way, if we choose the state vectors (density matrices) and operators in the different “pictures” to coincide at a
time \( t = t_0 \), then
\[
|\Psi_S(t)\rangle = e^{-iK_0(t-t_0)}|\Psi_I(t)\rangle = U(t,t_0)|\Psi_H\rangle
\] (2)
while the density matrices satisfy
\[
\rho_S(t) = e^{-iK_0(t-t_0)} \rho_I(t) e^{iK_0(t-t_0)} = U(t,t_0) \rho_H U^\dagger(t,t_0)
\] (3)
and the field operators (as well as all other ones) are related via
\[
\psi(x) = \psi_H(x,t) = U^\dagger(t,t_0) \psi_S(x) U(t,t_0)
= U^\dagger(t,t_0) e^{-iK_0(t-t_0)} \psi_I(x,t) e^{iK_0(t-t_0)} U(t,t_0)
\] (4)
Here \( U(t,t') = T \exp[-i \int_{t'}^t K(\tau) d\tau] \) \((t > t')\) is the time-evolution operator for Schrödinger state vectors (density matrices) and Heisenberg operators. Note that \( U(t,t') = U(t,t'') U(t'',t') \) for any intermediate time \( t'' \), and \( U^\dagger(t,t') = U(t',t) \). The time evolution of interaction-picture state vectors (density matrices) is given by
\[
S(t,t') = e^{iK_0(t-t_0)} U(t,t') e^{-iK_0(t-t_0)}
\]
and the field operators are further simplified as
\[
\psi_H(x,t) = S^\dagger(t,t_0) \psi_I(x,t) S(t,t_0)
\] (5)
which will prove useful later on. As for the equations of motion which are satisfied by the state vectors or density matrices and the operators, we note the following “Schrödinger equations”
\[
i \frac{\partial}{\partial t} |\Psi_S(t)\rangle = K(t) |\Psi_S(t)\rangle
\]
\[
i \frac{\partial}{\partial t} |\Psi_I(t)\rangle = K_{11}(t) |\Psi_I(t)\rangle
\] (6)
the “quantum Liouville equations” or “von-Neumann equations”
\[
i \frac{\partial}{\partial t} \rho_S(t) = [K(t), \rho_S(t)]
\]
\[
i \frac{\partial}{\partial t} \rho_I(t) = [K_{11}(t), \rho_I(t)]
\] (7)
and the “Heisenberg equations”
\[
i \frac{\partial}{\partial t} \psi_H(x,t) = [\psi_H(x,t), K(t)]
\]
\[
i \frac{\partial}{\partial t} \psi_I(x,t) = [\psi_I(x,t), K_0]
\] (8)

We have chosen the state vectors, density matrices, and the operators to coincide at \( t = t_0 \) : \( |\Psi_H\rangle = |\Psi_I(t_0)\rangle = |\Psi_S(t_0)\rangle \), \( \rho_H = \rho_I(t_0) = \rho_S(t_0) \), and \( \psi_H(t_0) = \psi_I(t_0) = \psi_S \). Usually we set \( t_0 = 0 \) below, but this choice is completely arbitrary. Sometimes it is more convenient to choose some other value \( t_0 \), and often \( t_0 = -\infty \), or the time where some external perturbation is switched on [8]. If the interactions are not spin-independent, then \( U \) or \( S \) will mix the spin components (i.e., rotate the spin vector), but unless otherwise stated, we assume the spin-independence below. Finally we note that the above operator relations hold for other operators as well, not just the field operators we have used.

II. NORMAL SYSTEMS:
ZERO-TEMPERATURE FORMALISM

In this Section we concentrate exclusively on discussing the zero-temperature formalism for fermions. For bosons the situation is more complicated due to the existence of Bose condensation. This would require a treatment similar to the one discussed in Sec. IV for superconducting fermion systems.

A. Lehmann representation, spectral functions, and the quasiparticle concept

1. Lehmann representation

To start with, we shall only consider translationally invariant systems with time-independent grand-canonical Hamiltonians \( K = H - \mu N \) [2, 10]. In this case \( G \) only depends on \( x = x_1 - x_2 \) and \( t = t_1 - t_2 \), and may be Fourier transformed to \( k \) and \( \omega \) space (see appendices). In our case (at \( T = 0 \)) the definition of the single-particle potential takes the \( k \)-space form (we follow Ref. [2], but the following may be done in coordinate space as well [3, 10])
\[
G_{\alpha\beta}(k,t) = -i \langle 0| T a_{\alpha k}(t)a_{\beta k}^\dagger(0) |0\rangle
\] (9)
However, we drop the spin indices “\( \alpha,\beta \)” in the following since they would only add a diagonal “\( \delta_{\alpha\beta} \)” factor. Indeed, if there is no preferred direction, then \( G = a_1 + b \sigma \cdot k \), where \( a \) and \( b \) are functions of \( |k| \) and \( \omega \). If the Hamiltonian is invariant under spatial reflections, so must \( G \) be, and \( b \) vanishes because \( \sigma \cdot k \) a pseudoscalar under reflections [3]. Thus below \( \text{Tr} \langle \text{spin} | G | 2 \rightarrow G \). We note that our results for the grand-canonical \( G \) are related to the fixed-\( N \) functions \( G_N \), where energies are calculated relative to the vacuum state of bare particles and not \( \mu \). By \( G_N(t) = \exp(-i\mu t) G(t) \) or \( G_N(\omega) = G(\omega - \mu) \). With this replacement all results below should agree with Refs. [2, 3], apart from the different overall sign definition in the latter reference.

We assume that the full Hamiltonian \( H = H - \mu N \) has the eigenstates \( |\Psi_s\rangle \) and corresponding eigenvalues \( K_s = E_s - \mu N_s \). Translational invariance implies that the total momentum operator commutes with the Hamiltonian \( \{P,K\} = 0 \) and thus these energy eigenstates are also momentum eigenstates. Using this basis to insert \( 1 = \sum_s |\Psi_s\rangle\langle\Psi_s| \) in between the operators in Eq. (9) we
Here we have chosen the excitation energies \( \xi_{n0}^{(+)} \) and \( \xi_{m0}^{(-)} \) to be positive. A Fourier transformation with respect to time (substitute, for example, the contour representations of \( \theta(t) \) and change frequency variables; see Appendix D) then gives

\[
G(k, \omega) = \int_0^\infty d\omega' \left\{ \frac{A_+(k, \omega')}{\omega - \omega' + i\eta} + \frac{A_-(k, \omega')}{\omega + \omega' - i\eta} \right\}
\]

This is the so-called Lehmann (or Källen-Lehmann, or spectral) representation of \( G \).

The meaning of the excitation energies is explained as follows. We see that if the ground state \( |\Psi_0\rangle \) contains \( N_0 = N \) particles, then the states labeled with “\( n \)” or “\( m \)” must contain \( N_n = N + 1 \) or \( N_m = N - 1 \) particles, respectively. Thus the corresponding eigenvalues \( K_s(N_s) = E_s(N_s) - \mu N_s \) for \( s = n, m, 0 \) must be given by

\[
\begin{align*}
K_n(N + 1) &= E_n(N + 1) - \mu N + \mu \\
K_m(N - 1) &= E_m(N - 1) - \mu N + \mu \\
K_0(N) &= E_0(N) - \mu N
\end{align*}
\]

We now define the excitation energies as energy differences between excited and ground states in systems with fixed particle number: thus we let \( \xi_{n0}^{(+)} \equiv E_n(N + 1) - E_0(N + 1) > 0 \) (excitations in an \( N + 1 \) particle system) and \( \xi_{m0}^{(-)} \equiv E_m(N - 1) - E_0(N - 1) > 0 \) (excitations in an \( N - 1 \) particle system). Imagining that the excited states are created by adding or removing one particle from the \( N \) particle system (these are the elementary “particle” or “hole” excitations), they correspond to total energy differences \( \omega_{n0}^{(+)} = E_n(N + 1) - E_0(N) = \xi_{n0}^{(+)} + \mu > 0 \) and \( \omega_{m0}^{(-)} = E_m(N - 1) - E_0(N) = \xi_{m0}^{(-)} - \mu < 0 \). Here we used \( E_0(N + 1) - E_0(N) = \partial E_0/N = \mu \), which is always independent of \( N \) to order \( N^{-1} \), and is assumed to be fixed in the grand-canonical ensemble. In this way we see that

\[
\begin{align*}
K_n(N + 1) - K_0(N) &= E_n(N + 1) - E_0(N) - \mu \\
&= \xi_{n0}^{(+)} + E_0(N + 1) - E_0(N) - \mu = \xi_{n0}^{(+)} \\
K_m(N - 1) - K_0(N) &= E_m(N - 1) - E_0(N) + \mu \\
&= \xi_{m0}^{(-)} + E_0(N - 1) - E_0(N) + \mu = \xi_{m0}^{(-)}
\end{align*}
\]

and thus we immediately see why the quantities \( \xi_{n0}^{(+)} \) and \( \xi_{m0}^{(-)} \) should appear in Eq. (11), when we use \( a_k(t) = e^{iKt} a_k(0)e^{-iKt} \) in the expectation values \( \langle \Psi_0 | a_k(t) | \Psi_n \rangle \) and similar ones.

In different references slightly different choices are made concerning the signs of the “excitation energies” in Eq. (11) or the signs of the integration variables and \( \omega' \) and thus also the range of integration in the two different terms of Eqs. (10) and (12). Strictly speaking, the \( n \) and \( m \) sums in Eq. (11) should also include factors \( V_{\delta_{kk},p_n} \) and \( V_{\delta_{kk},-p_n} \), where \( p_{n,m} \) are the momenta of the energy eigenstates, but above it is assumed that the sums have already been restricted accordingly — see Refs. [3, 10] for alternative treatments. From Eq. (12) we see that \( G \) is a meromorphic function, having only isolated poles of finite order. We stress that the poles of \( G \) on the real axis correspond to the exact eigenstates of \( K \). In the above expansion the imaginary parts \( \pm i\eta \) cause these poles to be shifted from the real axis by an infinitesimal amount. The imaginary parts which they introduce to the excitation energies are purely technical artifacts which render the integrals in Eq. (10) convergent in the correct time regimes. Since they are infinitesimal, the corresponding states still have infinite lifetimes as they should.

Let us now consider a system of non-interacting fermions. In this case we have \( |\Psi_0\rangle = |\Phi_0\rangle \) which is just the Fermi sea, and upon extracting the time dependence from the Heisenberg operators \( G(k, t) \) becomes simply [2, 3]

\[
G^0(k, t) = -i\theta(t)\theta(|k| - k_F) \exp[-i\xi^0_k t/\hbar] \\
+ i\theta(-t)\theta(k_F - |k|) \exp[-i\xi^0_k t/\hbar]
\]

where \( \xi^0_k = \langle \Phi_0 | a_k^\dagger a_k | \Phi_0 \rangle = \theta(k_F - |k|) \) is just the bare-particle distribution function, whereas \( 1 - m_k = \theta(|k| - k_F) \) is the distribution function for bare holes. The interpretation is obvious: an additional particle (hole) inserted into the system may only propagate where the particle (hole) states are not already occupied. Assuming noninteracting, free particles we have \( \xi^0_k = \hbar^2 k^2/2m \) for the energy of a bare particle, and we define \( \xi_k = \xi^0_k - \mu \approx \hbar^2 F(k - k_F) \), where we used \( \xi^0_k = \hbar^2 k^2/2m \) for the energy of a bare particle.
and we see that the particle energies \( \xi_k^0 = |\xi_k^0| = |\xi_k^0 - \mu| \). A further time transformation of \( G^0 \) gives

\[
G^0(k, \omega) = \frac{\theta(\omega - \omega_k^0) + \theta(\omega_k^0 - \omega)}{\omega - \omega_k^0 + \mu/h + i\eta} + \frac{\theta(\omega - \omega_k^0) + \theta(\omega_k^0 - \omega)}{\omega - \omega_k^0 + \mu/h - i\eta} \tag{16}
\]

and we see that the particle energies \( \xi_k^0 = h\omega_k^0 - \mu \) appear as the poles, whose residues are equal to unity. It is very interesting to note that using the formulas in the Appendix, this may be cast in the form

\[
G^0(k, \omega) = \frac{1}{\omega - \omega_k^0 + \mu/h + i\eta} + 2\pi i \delta(\omega - \omega_k^0 + \mu/h) m_k
\]

\[
= \frac{\mathcal{P}}{\omega - \omega_k^0 + \mu/h - i\eta} - i\pi \delta(\omega - \omega_k^0 + \mu/h)(1 - 2m_k) \tag{17}
\]

where the distribution function \( m_k \) appears. This way of thinking will be useful later on, since it generalizes straightforwardly to nonequilibrium situations. Note that since \( k_F \) is by definition the k value, where \( \omega = \omega_k^0 - \mu/h = 0 \), and \( k \geq k_F \) correspond to \( \omega \geq 0 \), we could equally well replace \( m_k = \theta(k_F - |k|) \) here with the energy distribution \( \theta(\omega) \), and so on. This form should probably remain valid even when a more complicated energy spectrum \( \xi_k^0 = \hbar\omega_k^0 - \mu \) were considered. This would be the case if we took into account, say, the effects of a periodic ion lattice: the Fermi surface determined by \( \xi_k^0 = \nabla \) would be anisotropic, \( \nu_F \) would not be parallel to \( k_F \) everywhere, the mass \( m \) would be band-renormalized, etc. Gladly, these are not a problem in superfluid \( ^3 \)He, where no ion lattice exists.

2. The retarded, advanced and Keldysh functions \( G^{R, A, K} \), and further relations for \( G \)

Let us now return to the fully interacting case, and add some details. Similarly as above, we obtain for the retarded \( G^R \) and advanced \( G^A \) the forms

\[
G^R(k, t) = -i\theta(t) \int_0^\infty [A_+(k, \omega) \exp(-i\omega t) + A_-(k, \omega) \exp(+i\omega t)] d\omega \tag{18}
\]

\[
G^A(k, t) = +i\theta(-t) \int_0^\infty [A_+(k, \omega) \exp(-i\omega t) + A_-(k, \omega) \exp(+i\omega t)] d\omega
\]

Fourier transformation yields the Lehmann expansions

\[
G^R(k, \omega) = \int_0^\infty d\omega' \left\{ \frac{A_+(k, \omega')}{\omega - \omega' + i\eta} + \frac{A_-(k, \omega')}{\omega + \omega' + i\eta} \right\} \tag{19}
\]

\[
G^A(k, \omega) = \int_0^\infty d\omega' \left\{ \frac{A_+(k, \omega')}{\omega - \omega' - i\eta} + \frac{A_-(k, \omega')}{\omega + \omega' - i\eta} \right\}
\]

They are thus obtained from that of \( G \) by shifting all the poles of \( G \) to the lower \( \omega \) half-plane \((R)\), or to the upper half-plane \((A)\). In the opposite parts of the plane the functions are analytic. The functions \( G^{R, A} \) satisfy the “Kramers-Kronig” relation \[3\]

\[
\text{Re} G^{R, A}(k, \omega) = \mp \frac{1}{\pi} \int_{-\infty}^\infty \frac{d\omega'}{\omega - \omega'} \text{Im} G^{R, A}(k, \omega') \tag{20}
\]

and thus \( \text{Re} G^R \) and \( \text{Im} G^R \) are said to be “Hilbert-transform” pairs. (This is a consequence of the “causality” property, that \( G^R(t, t') \) vanishes for \( t - t' < 0 \).) For real \( \omega \) we also have the important relations

\[
\text{Re} G(k, \omega) = \text{Re} G^R(k, \omega) = \text{Re} G^A(k, \omega)
\]

\[
\text{Im} G(k, \omega) = \text{Im} G^{R, A}(k, \omega) \quad \text{for } \omega \geq 0
\]

\[
G^R(k, \omega) = [G^A(k, \omega)]^* \tag{21}
\]

In the special case of noninteracting particles we have

\[
G^R_0(k, t) = -i\theta(t) \exp[-i\xi^0 K t/\hbar]
\]

\[
G^A_0(k, t) = +i\theta(-t) \exp[-i\xi^0 K t/\hbar] \tag{22}
\]

or

\[
G^R_0(k, \omega) = \frac{1}{\omega - \omega_k^0 + \mu/h + i\eta}
\]

\[
G^A_0(k, \omega) = \frac{1}{\omega - \omega_k^0 + \mu/h - i\eta} \tag{23}
\]

Finally we discuss the interpretation of the spectral functions. By integrating Eqs. (11) over frequencies, and comparing the result with the expectation value of the (anti)commutator \([a_{k\alpha}, a^\dagger_{k'\beta}]_\bullet = \delta_{\alpha\beta}\delta_{k, k'}\) we find that the spectral functions are normalized according to \[3\]

\[
\int_0^\infty d\omega [A_+(k, \omega) + A_-(k, \omega)] = 1 \tag{24}
\]

Using Eq. (24) we then find that

\[
G(k, \omega) = G^R(k, \omega) = G^A(k, \omega)
\]

\[
\sim \frac{1}{\omega} \int_0^\infty d\omega' [A_+(k, \omega') + A_-(k, \omega')] \tag{25}
\]

\[
\sim \frac{1}{\omega} \quad |\omega| \to \infty
\]

which is important for applying Jordan’s lemma for neglecting contour integrals over paths which are taken to
infinity. Using the formulas of Appendix D we also obtain
\[ i[G^R(k, \omega) - G^A(k, \omega)] \]
\[ = 2\pi \int_0^\infty d\omega' [A_+(k, \omega')\delta(\omega - \omega') + A_-(k, \omega')\delta(\omega + \omega')] \]
\[ = 2\pi[A_+(k, \omega)\theta(\omega) + A_-(k, -\omega)\theta(-\omega)] \equiv \rho(k, \omega) \]
(26)
where \( \rho(k, \omega) \) is the spectral density function. It satisfies the normalization condition (or sum rule)
\[ \int_{-\infty}^\infty \frac{d\omega}{2\pi} \rho(k, \omega) = 1 \]  
(27)
Using Eq. (26) \( G^{R,A} \) may be also written [10]
\[ G^{R,A}(k, \omega) = \int_{-\infty}^\infty \frac{d\omega'}{2\pi} \frac{\rho(k, \omega')}{\omega - \omega' \pm i\eta} \]  
(28)
We also note that the Keldysh function may be written as
\[ G^K(k, \omega) = -i(1 - 2\theta(\omega))\rho(k, \omega), \]
(29)
which is thus related to \( G^{R,A} \) via Eq. (26).

For noninteracting particles the density of states (DOS) for one spin species and for given volume \( V \) of the system \( \tilde{N}_0(\omega) = V N_0(\omega) \equiv \sum_k \delta(\omega - \xi_k^0) \) may obviously be expressed with \( \rho_0(k, \omega) = i(G^R_0(k, \omega) - G^A_0(k, \omega)) \)
\[ = -2\mathrm{Im} G_0^R(k, \omega) = 2\pi\delta(\omega - \xi_k^0) \]  
(30)
More generally \( \sum_k \) would be replaced by a trace over spatial and spin coordinates; adding the spin sum here will only multiply the result by 2. For interacting particles the expression
\[ \tilde{N}(\omega) = \frac{1}{2\pi} \sum_k \rho_0(k, \omega) = -\frac{1}{\pi} \sum_k \mathrm{Im} G^R(k, \omega) \]  
(31)
does not give the true density of eigenstates, but something related to it. We may analyze the meaning of \( A_{\pm} \) as follows. We denote the true densities of “particle” and “hole” type states (per one spin direction) with \( dn/d\omega' = \sum_k \delta(\omega' - \xi_m) \) and \( dm/d\omega' = \sum_m \delta(\omega' - \xi_m) \), whose sum gives the total density of states. If it is not important to resolve the individual poles in these functions (observation timescale too short, or if we are in the thermodynamic limit) we may smooth out these expressions and think of them as continuous functions of \( \omega \). We can then write
\[ A_+(k, \omega) \approx \int_0^\infty d\omega' |a_+(k, n(\omega'))|^2 \frac{dn}{d\omega'} \delta(\omega - \omega') \]
\[ = |\bar{a}_+(k, \omega)|^2 \frac{dn}{d\omega} \]  
(32)
\[ A_-(k, \omega) \approx \int_0^\infty d\omega' |a_-(k, m(\omega'))|^2 \frac{dm}{d\omega'} \delta(\omega - \omega') \]
\[ = |\bar{a}_-(k, \omega)|^2 \frac{dm}{d\omega} \]
where \( a_+(k, n) = \langle \Psi_n | a_k^\dagger \Psi_0 \rangle, \ a_-(k, m) = \langle \Psi_m | a_k \Psi_0 \rangle \) etc. (In case of “particle-hole symmetry” \( dn/d\omega \) and \( dm/d\omega \) are equal.) Thus the poles of \( G \) will merge into continuous branch cuts along the real \( \omega \) axis. We note that while \( dn/d\omega \) and \( dm/d\omega \) are the true densities of states of the interacting system, \( \sum_k A_+ \) and \( \sum_k A_- \) are proportional to some sort of weighted, or renormalized, densities. In fact, we interpret \( \tilde{N}(\omega) \) in Eq. (31) as a “quasiparticle” density of states. So what the devil is a quasiparticle?

3. Quasiparticles

Apart from the branch cut singularities right on the real \( \omega \) axis the Green’s functions are well-behaved, since Eq. (12) may be used to analytically continue \( G \) to imaginary \( \omega \) values, where no other singularities appear (7). However, the analytical continuations of the smoothed-out spectral functions \( A_{\pm} \) may have isolated poles off the real axis, and it can be shown that these lead to “approximate” poles of \( G \) also. These poles have the important property that they do not merge into the continuous branch cuts in the thermodynamic limit, but remain isolated [10]. They also have a well-defined dispersion relation, i.e. energy-momentum relation, and therefore correspond to “single-particle” states.

Suppose now that one of these postulated poles of \( A_{\pm} \) has a small imaginary part \( -\Gamma_k \) (see Fig. 1). This is reflected on the real axis as a more-or-less sharp peak of \( A_{\pm} \) whose area is proportional to the residue of the pole, as we shall see. Assuming the density of states to be relatively constant, or at most linear, in \( \omega \), the peaks can only be due to peaks in \( a_{\pm}(k, \omega) \) distributions, whose positions \( \omega_k \) depend smoothly on \( k \). They correspond to approximate single-particle eigenstates, to which many real eigenstates of \( K \) contribute collectively. (Note that in an interacting system exact single-particle eigenstates are not well defined, since particles continually exchange momentum with each other.) Such single-particle excitations are generally called quasiparticles, and the energy dispersion relation (with respect to the Fermi surface) of the quasiparticle is given by \( \xi_k = \hbar \omega_k \) (with respect to the chemical potential \( \mu \)). Since exciting only a single real eigenmode requires an infinitely well defined energy, i.e., small frequency band for the perturbation, it is the quasiparticles which are the true elementary excitations of the system. (This is also why we were satisfied with the smoothed version of the spectral function in the first place.) Note that according to the above “definition” the quasiparticles are completely delocalized in space, like the usual (box-normalized) plane-wave states of noninteracting particles. Localized states and hence approximations for classical particles may be created by constructing wave packets with several \( k \) components around some \( k_F \) on the Fermi surface.

We shall now make the previous discussion more mathematical [2]. Suppose an extra bare particle with wave
vector $k$ ($k > k_F$) is added to the ground state at $t = 0$, thus creating an excited state $a_k^\dagger\Psi_0$ of the system. For $t > 0$, the subsequent time-development of this excitation is described by the propagator $G(k, t) = \langle \Psi_0 | a_k(t) a_k^\dagger | \Psi_0 \rangle$. We may now deform the contour of integration as indicated in Fig. 2 so that

$$-iG(k, t) = -\int_0^\infty A_+(k, \omega)e^{-i\omega t}d\omega + 2\pi \sum_j \zeta_j e^{-i\omega_j t},$$

(33)

where $\zeta_j$ are the residues of the assumed poles of $A_+$ at complex-valued positions $\omega = \omega_j = \zeta_j$. The integration along the lower part of the contour was neglected assuming $\alpha \gg 1/t$ so that $e^{-\alpha t}$ is negligible. One of the poles, of frequency $\omega = \xi_k - i\Gamma_k$ and residue $\xi_k$, is located very close to the real axis (above the dotted line in Fig. 2). This gives rise to the peak of width $\sim 2\Gamma_k$ in $A_+$ indicated in the figure, and the area of the peak is roughly equal to $z_k = -2\pi \xi_k \equiv z_+$. The integral over the rest of $A_+e^{-i\omega t}$ in Eq. (33) averages to zero for any nonzero $t$ due to the large range of frequencies with equal weights. If $t$ is large, but satisfying $\alpha \gg 1/t \gtrsim \Gamma_k$ (thus $t \lesssim \Gamma_k^{-1}$) then the principal contribution to Eq. (33) comes from the pole $\xi_k - i\Gamma_k$, which we call a \textit{quasiparticle pole}. The propagator then becomes

$$G(k, t) \approx -iz_+ \exp\left(-i\xi_k t/\hbar\right), \quad t > 0, \quad |k| > k_F$$

(34)

which is exactly of the same form as Eq. (15) for noninteracting particles, except for the \textit{quasiparticle renormalization factor} $z_+$, and the damping timescale $\Gamma_k^{-1}$, which we interpret as an intrinsic \textit{quasiparticle lifetime}. For times $t \lesssim \Gamma_k^{-1}$ the propagator oscillates coherently with the frequency $\xi_k = h\omega_k$. A similar analysis may be done for the $t < 0$ side ($k < k_F$), where instead of a particle excitation, the propagation of a hole from a given $t < 0$ to $t = 0$ is studied. The pole $\xi_k - i\Gamma_k$ must then be above the $\omega$ axis and below the Fermi surface, with a corresponding $A_-$ peak area $z_-$.)

 Plenty of more discussion of these interesting things may be found in Ref. [2]. It may for example be seen that as $k$ passes $k_F$, the quasiparticle pole $\xi_k - i\Gamma_k$ crosses the point $\omega = 0 + i0$ continuously so that $\xi_k \approx \hbar v_F(k - k_F)$ and $\Gamma_k \approx \pm u(k - k_F)^2$, as indicated schematically in Fig. 1. The quadratic $k$ dependence of $\Gamma_k$ actually follows from the properties of the density of single-particle states close to the Fermi surface. The signs are such that $\xi_k, \Gamma_k$ are $\gtrsim 0$ for $k \gtrsim k_F$, i.e., $v_F$, and $u$ are positive real constants. We see that as $k = k_F$, the lifetime $\Gamma_k^{-1}$ of the elementary excitations in infinite: they are almost exact eigenstates of the system, and the peak in $A_\pm$ approaches $z_k \delta(\omega - \xi_k)$. Furthermore, as we cross the Fermi surface $z_k \approx z_\pm$ is continuous and roughly constant; therefore we write $z_+ = z_- \equiv a$. This constant gives the jump of the bare-particle distribution function $m_k = \langle \Psi_0 | a_k^\dagger a_k | \Psi_0 \rangle = -iG(k, 0)$, at the Fermi surface: $\Delta m_k = -i[G(k_F^+, 0^-) - G(k_F^+, 0^-)] = a$, and thus $0 < a < 1$. This should be compared with the noninteracting case [Eq. (15)], where $a = 1$ — see Fig. 3.

In general the propagator is thus of the form

$$G(k, t) = G_{\text{inc}}(k, t) - ia\theta(t)\theta(|k| - k_F)$$

$$-\theta(-t)\theta(k_F - |k|) \exp\left[-i(\xi_k + \Gamma_k)t/\hbar\right]$$

$$G(k, \omega) = G_{\text{inc}}(k, \omega) + \frac{a}{\omega - \xi_k + i\Gamma_k},$$

(35)

where the latter terms are formally equal to Eqs. (15) and (16). We call them the \textit{coherent part} $G_{\text{coh}}$ of the propagator, since they correspond to the elementary excitations which remain coherent up to times of order $\Gamma_k^{-1}$. After that their frequency components, which are in the range $[\xi_k - \Gamma_k, \xi_k + \Gamma_k]$, begin to interfere destructively and the oscillatory behavior of $G_{\text{coh}}(k, t)$ vanishes. The first term is the \textit{incoherent part} and it is mostly due to the integral along the imaginary axis in Eq. (33), and possibly due to some of the further-away poles. It includes so many frequency components that it never exhibits coherent oscillations, but instead forms a “background noise” in $G$.

From the above we see that the postulated poles (with residue $\xi_k$) of the exact spectral functions $A_\pm$ now appear
as the quasiparticle poles (with residue $z_k$) of the approximate propagator $G_{coh}$. We stress that, strictly speaking, the actual singularities at these poles must be canceled by the incoherent part $G_{inc}$ since we know from the Lehmann representation that the exact $G = G_{inc} + G_{coh}$ has poles only at the real excitation energies on the real $\omega$ axis! Thus we must interpret the “incoherent noise” in $G_{inc}$ to be due to the presence of many other elementary excitations (i.e., other poles like those shown in Fig. 2, whose residues appear in the sum of Eq. (33)) which interfere with each other in an incoherent fashion and “somehow” screen the divergence. However, what is important is that for real frequencies the above separation provides an adequate description: even if unphysical poles were introduced in $G$ at complex frequencies, they do not essentially alter the situation on the real axis, where only a finite peak in the spectral functions should be, and indeed is, observed.

4. Coherent and incoherent vs. low and high energy

In doing quasiclassical theory, another separation of the Green’s function is usually introduced [1]. Namely, $G(k, \omega)$ is split into two parts according to their frequency (or energy) range. Energies $\hbar \omega$ and $\xi_k$ below a cutoff $E_c$ belong to the low-energy regime, and those above $E_c$ to a high-energy regime. The cutoff $E_c$ is needed for technical reasons, and therefore it is artificial and even arbitrary, but some energy scale relevant to the problem may be used. Thus we have two divisions

$$G = G_{coh} + G_{inc}$$

$$G = G_{low} + G_{high}$$

and according to these, the “propagator space” is divided into four distinct parts. (Note, however, that the coherent part is probably always effective in the low-energy regime only, where the quasiparticles are well defined. Therefore, to some extent the divisions are equal!) According to the low-high division, we introduce an energy-integrated Green’s function $g$ by integrating $G_{low}$ with respect to the variable $\xi_k$,

$$g(\tilde{k}, \omega) = \frac{1}{a} \int_{-E_c}^{E_c} d\xi_k G_{low}(k, \omega) \approx \frac{1}{a} \int_{-E_c}^{E_c} d\xi_k G_{coh}(k, \omega)$$

(37)

Here we have also renormalized the propagator by dividing with the renormalization factor $a$. The tricky part related to the choice and handling of the high-energy cutoff $E_c$ shall not be touched here, but $E_c$ should also be made to vanish from all results; for discussions, see Refs. [1, 8, 37], and below.

Note that in the latter equality of Eq. (37) the incoherent part was again assumed to interfere destructively. This approximation is not strictly true, since it neglects the presence of other quasiparticles and hence collisions between them. However, if we do drop the incoherent part in Eq. (37), we see, using Eq. (35), that we end up with a propagator which is (assuming $\Gamma_k$ to be very small) equal to the propagator $G_0(k, \omega)$ of noninteracting particles! Indeed, as we already stated, the coherent low-energy part $G_{low}(k, \omega)$ is describing a system of noninteracting quasiparticles. In effective low-energy theories (like the quasiclassical approximation to be discussed below) the roles of $G_0(k, \omega)$ and $G(k, \omega)$ will more-or-less be replaced by $G_{coh}(k, \omega)$ and $G_{low}(k, \omega)$, respectively. Here $G_{low}$ already takes into account the largest part of bare-particle interactions (the lowest-order high-energy vertex part — see below and Ref. [1]), but still has a very simple functional form. The remaining effective interactions (contained in $G_{low}$) may often be neglected altogether, or they may be accounted for in a simple mean-field approximation. This simplifies calculations considerably, and it is the beauty of the quasiparticle concept — if and when it is applicable. The quasiclassical approximation procedure will be formalized below [1].

In practice, knowing the actual value of $a$ (or even if the “quasiparticle peak” in $A_\pm$ is due to one or more closely-lying poles) is not necessarily important. Neither is the exact way in which the bare-particle-energy spectrum $\xi_k^0$ is modified by interactions into the quasiparticle energy spectrum $\xi_k$. Knowledge of some more general properties is sufficient. Next we turn to discuss these issues briefly.

B. Perturbation theory at zero temperature

1. Wick’s theorem and contractions of operators

At zero temperature the time-ordered Green’s function of Eq. (1) becomes just a ground-state average

$$G(x_1, x_2) = -\frac{\langle \Psi_0 | T \psi(x_1) \psi^\dagger(x_2) | \Psi_0 \rangle}{\langle \Psi_0 | \psi(x_1) | \Psi_0 \rangle}$$

(38)

Here we keep the the normalizing denominator for reasons which will become clear. In order to do perturbation theory on $G$ in powers of the interaction term $K_{11}$, we want to be able to use Wick’s theorem [3, 24, 25], and therefore express $G$ in terms of expectation values in the unperturbed ground state $|\Phi_0\rangle$, i.e. the ground state of $K_0$. This is because the concepts of normal-ordering and contractions (or pairings) of operators can only be defined with respect to a vacuum state $|\psi\rangle$ for which $c_i|\psi\rangle = 0$ if $c_i$ is any single-excitation destruction operator. If $K_0$ is expressed in the $c_i^\dagger c_i$ operators and $c_i|\Phi_0\rangle = 0$ for all $i$, then $|\psi\rangle = |\Phi_0\rangle$. For a free electron gas $|\Phi_0\rangle$ is the Fermi sea, and the excitations whose vacuum state $|\psi\rangle$ this is, are “particles” for $k > k_F$ and “holes” for $k < k_F$. We reserve the notation $|0\rangle$ for the true vacuum state with absolutely no real particles (created with $a_i^\dagger$) in it: $a_i|0\rangle = 0$. The contraction of two operators $A$ and $B$ is then defined as

$$\langle\langle AB \rangle\rangle = T[AB] - N[AB] = \langle \Phi_0 | T[AB] | \Phi_0 \rangle$$

(39)
where the normal-ordering operator \( N \) orders all \( c_i^\dagger \) operators to the left of \( c_i \)'s. The last equality follows trivially since it may be shown that contractions are “c numbers”, and since \( \langle \Phi_0 | N (AB) | \Phi_0 \rangle = 0 \) by definition of \( N \). In particular we note that for field operators we find

\[
\psi(x_1)\psi(x_2) = \langle \Phi_0 | T \psi(x_1)\psi(x_2) | \Phi_0 \rangle = iG^0(x_1, x_2)
\]

which is the Green function for the noninteracting system. The point of perturbation theory will then be to express Eq. (38) as a sum of terms containing factors from the bare-particle interaction \( V(x_1, x_2) \) and the \( G^0(x_1, x_2) \) functions, since the form of both of these in known explicitly, as we have seen. Technically this expansion may be done with the following “adiabatic switching-on” procedure.

2. Adiabatic “switching on and off” at zero temperature

If we switch on the interaction \( V \) through \( K^{(\eta)}_1(t) \) then for given \( \eta \), the time development of an interaction-picture eigenstate \( | \Phi_0 \rangle \) of \( K_0 = T - \mu N \) is given by \( | \Psi^{(\eta)}_f(t) \rangle = S_\eta(t, -\infty)| \Phi_0 \rangle \). Here \( S_\eta(t, t') \) is the time-evolution operator corresponding to \( K^{(\eta)} = K_0 + K^{(\eta)}_1 \). The switching-on is made “adiabatic” by taking the limit \( \eta \to 0^+ \) so that for each time \( K^{(\eta)}(t) \) has a set of eigenstates which develop from \( t = -\infty \) to \( t = 0 \) as smoothly as possible, and no unwanted excitations are created. (In practice the switching-on should be adiabatic enough, if \( \hbar \eta \) is smaller than the smallest level spacing of the system?) Here we shall assume \( t_0 = 0 \) if needed. The properties of \( | \Psi^{(\eta)}_f(0) \rangle \) in the limit \( \eta \to 0^+ \) are expressed by the Gell-Mann and Low theorem [3, 5, 43]. It states that for an eigenstate \( | \Phi_0 \rangle \) of \( K_0 \), the following limit exists

\[
\lim_{\eta \to 0^+} \frac{S_\eta(0, -\infty) | \Phi_0 \rangle}{\langle \Phi_0 | S_\eta(0, -\infty) | \Phi_0 \rangle} = \frac{| \Psi^{(\eta)}_f(0) \rangle}{\langle \Phi_0 | \Psi^{(\eta)}_f(0) \rangle} \quad (41)
\]

where the generated state \( | \Psi^{(\eta)}_f \rangle \) is an eigenstate of \( K = K^{(\eta)}(0) = K^{(0)} \), i.e. \( K | \Psi^{(\eta)}_f \rangle = E | \Psi^{(\eta)}_f \rangle \). Assuming now \( K_0 | \Phi_0 \rangle = E_0 | \Phi_0 \rangle \) then \( E = E_0 + \langle \Phi_0 | K_1 | \Psi_0 \rangle / \langle \Phi_0 | \Psi_0 \rangle \) is directly obtained. If \( | \Phi_0 \rangle \) is the unperturbed ground state (or vacuum \( | \text{vac} \rangle \) as it usually is, hence the notation), then the generated state \( | \Psi^{(\eta)}_f \rangle \) may be the ground state of the interacting system (as again, it usually is), but not necessarily. For this to be so, no “level crossings” between \( E_{0i} \) and \( E_i \) of different eigenstates \( i \) must occur during the adiabatic switching on, which is the case for normal Fermi systems, but not superconductors, for example (see below). (This may in fact be taken as one definition of the “normality”?) The limits of the nominator and denominator in Eq. (41) do not exist separately due to diverging \( \sim \eta^{-1} \) phases of these expressions, but in Eq. (41) the phase factors cancel each other. If we always assume a small, but finite \( \eta \), we may forget about the complications due to the limiting procedure and write simply \( | \Psi^{(\eta)}_f \rangle = S_\eta(0, -\infty) | \Phi_0 \rangle \), which is well-defined for any finite \( \eta \).

If we continue from \( t = 0 \) to \( t = \infty \), then the interaction will be adiabatically switched off, and \( | \Psi^{(\eta)}_f(t) \rangle \) should again develop into an eigenstate of the noninteracting \( K_0 \). Defining the \( s \) matrix \( S_\eta(S_\eta, -\infty, -\infty) \) we write this state as \( | \Psi^{(\eta)}_f \rangle = | \Psi^{(\eta)}_f(\infty) \rangle = S_\eta | \Phi_0 \rangle \). If now \( | \Phi_0 \rangle \) and the intermediate state are non-degenerate, then the state \( | \Phi_0 \rangle \) should be equal to \( | \Phi_0 \rangle \), apart from a constant phase factor: \( | \Phi_0 \rangle = S_{\eta} | \Phi_0 \rangle = e^{i\alpha} | \Phi_0 \rangle \) (compare with a phase shift in a scattering problem?) Thus we have (drop \( \eta \))

\[
| \Psi^{(\eta)}_f \rangle = S(0, -\infty) | \Phi_0 \rangle = S(0, \infty) S(0, -\infty) = e^{i\alpha} S(0, \infty) | \Phi_0 \rangle \quad (42)
\]

A similar theorem as Eq. (41) thus also exists for \( | \Phi_0 \rangle \) and the “time-reversed” switching-on process from \( t = \infty \) to \( t = 0 \). The difference due to the phase factor is canceled by the denominator.

Assuming now that \( | \Psi_0 \rangle \) and \( | \Phi_0 \rangle \) are indeed the (non-degenerate) ground states of the interacting and noninteracting systems, respectively, we may express the Green’s function [Eq. (38)] as an expectation value in the \( | \Phi_0 \rangle \) state. However, to keep the time-ordering acting on all of the sandwiched operators, we must use \( \langle \Phi_0 | = \langle \Psi^{(\eta)}_f(0) | S^\dagger(0, \infty) = | \Phi_0 \rangle | S^\dagger(0, \infty) \rangle \) on the left, and \( | \Psi^{(\eta)}_f \rangle = S(0, -\infty) | \Psi^{(\eta)}_f(-\infty) \rangle = S(0, -\infty) | \Phi_0 \rangle \) on the right. Then, after using Eq. (5), the relations \( S^\dagger(t, t') = S(t', t) \) and \( S(t, t'') S(t', t') = S(t, t') \), and moving \( T \) to the left, the Green’s function becomes [remember, \( x_i = (x_i, t_i) \) ]

\[
iG(x_1, x_2) = \frac{\langle \Phi_0 | T [S(\infty, t_1) \psi^\dagger(x_1) S(t_1, t_2) \psi^\dagger(x_2) S(t_2, -\infty)] | \Phi_0 \rangle}{\langle \Phi_0 | S^\dagger | \Phi_0 \rangle} = \frac{\langle \Phi_0 | T S^\dagger | \psi^\dagger(x_1) \psi^\dagger(x_2) | \Phi_0 \rangle}{\langle \Phi_0 | T | \Phi_0 \rangle} \quad (43)
\]

To prove this in detail, some \( \eta \to 0 \) techniques should again be applied [3] — note in particular that the nominator and denominator are still not separately well defined. This form is the starting point for perturbation theory for single-particle propagators. The perturbation series is obtained by inserting the series expansion of \( S \), and using Wick’s theorem to express all expectation values as products of pairings of the operators in the unperturbed state \( | \Phi_0 \rangle \). We shall briefly discuss the results in the next section, and then generalize everything for non-equilibrium cases. A similar expression exists for the two-particle propagator, whose perturbation expansion we may discuss later.
3. Some results from perturbation theory for the single-particle propagator

Here we only briefly collect certain formal equations and ideas related to a perturbative calculation of $G$, and its relation to the concept of quasiparticles\cite{2,3}. We may return to these issues in more detail when we discuss superconductivity.

Perturbation theory is based on an expansion of Eq. (43) in powers of the interaction $K_{11}$, use of Wick’s theorem to express the expansion in terms of unperturbed Green’s function $G_0$ and the two-particle interaction potential, and a subsequent (partial) resummation. The divergences in the nominator and denominator of Eq. (43) are due to “disconnected diagrams”, which exactly cancel each other, leading to a (supposedly) well-defined and finite result, known as the Dyson equation:

$$G(k,\omega) = G_0(k,\omega) + G_0(k,\omega)\Sigma(k,\omega)G(k,\omega)$$ (44)

It is represented diagrammatically in Fig. 4. Here the self-energy $\Sigma(k,\omega)$ is in general complex-valued, and (using “skeleton diagrams”) may be considered a functional of $G$, just as $G$ is a functional of $\Sigma$: $G_0^{-1}G - \Sigma G = 1$ and thus $G = (G_0^{-1} - \Sigma[G])^{-1}$. (This formal solution shows us, by comparison with the Lehmann representation, that $\text{Sgn}[\text{Im} \Sigma(k,\omega)] = -\text{Sgn} \omega$\cite{10}. Therefore at least $\text{Im} \Sigma(k,\omega = 0) = 0$.) In this way we are led to a self-consistent set of equations, which may be solved on different levels of approximation. Often, the Hartree-Fock approximation $\Sigma = \Sigma^{HF}[G] = \Sigma^{(1)}[G]$ is used, where the bare propagator lines in the first-order approximation of Fig. 4 are replaced by the full $G$.

The excitation spectrum of the interacting system should again follow from the poles of $G = G_0^{-1} - \Sigma$.

Let us now briefly discuss its solutions. As an important property of $\Sigma(\omega)$ we note that it is usually relatively smooth since, due to time-localized interactions, the function $\Sigma(t-t')$ is strongly peaked at $t - t' \approx 0$ and goes to zero over some microscopic relaxation time $\tau_{rel}$. In the limit of large $\omega \gg \tau_{rel}$, however, we expect $\Sigma(k,\omega)$ to vanish. This behavior is sketched in Fig. 5. Now, due to this smoothness of $\Sigma(k,\omega)$ we may assume that the equation only has a single solution $\omega = \xi(k)$ for each $k$, which gives a self-consistent equation for the “quasiparticle energy” (see again Fig. 5)

$$\xi(k) = \xi_0(k) + \Sigma[k_F,\xi(k)]$$ (46)

Note that we are considering the chemical potential $\mu$ to be our zero of energy, which is unchanged by switching on interactions. What will change are the renormalization factor $\Delta\xi$, the Fermi momentum $k_F$, and the Fermi velocity $v_F$. They may be obtained as follows.

First we note that we have the relations $\xi_0(k_F) = 0$ and $\xi(k_F) = 0$, which define the Fermi surfaces of the noninteracting and interacting systems, respectively. We may approximate the dispersion relations by linearizing them as before: $\xi_0(k) \approx h v_F (k - k_F^0)$ and $\xi(k) \approx h v_F (k - k_F)$. Now we look at the implicit equation $\xi(k) - \xi_0(k) = \Sigma[k,F](\xi(k)) - \Delta \xi(k_F) = 0$ for the spectrum $\xi(k)$. For $k = k_F^0$ we obtain $\xi(k_F^0) = \Sigma[k_F^0,\xi(k_F^0)] = \Delta \xi(k_F^0)$, where $\Delta \xi(k_F^0)$ is the shift in single-particle energy for given $k$ due to the interactions. Note again that if we had fixed the particle number $N$ instead of $\mu = \epsilon_F$, then $\Delta \xi(k_F^0)$ would give a shift in Fermi energy. Now, instead, the Fermi momentum $k_F$ may change. (Is this so? See Ref. 23.) Assuming that $\Delta \xi(k_F^0)$ is positive, we find $\xi(k_F^0) \approx h v_F \cdot (k_F^0 - k_F) > 0$, which yields $k_F < k_F^0$ for a spherical Fermi surface. In terms of the self energy, for $k = k_F$ we obtain the equation

$$\xi(k_F) = \xi_0(k_F) + \Sigma[k_F,0] = 0$$ (47)
which may in principle be solved for $k_F$. (Note again that $\Sigma(k,0) = \text{Re} \Sigma(k,0).$)

Next, by equating the inverse $\Sigma^{-1}_k(\omega - \xi(k) - i\delta_k)$ of the coherent part of Eq. (35) with $\omega - \xi^0(k) - \Sigma(k,\omega)$ and differentiating, we also obtain the residue $z_k$ of the “quasiparticle pole” of $G(k, \omega)$ as

$$z_k = \frac{1}{1 - \partial \Sigma(k, \omega)/\partial \omega \bigg|_{\omega = \xi(k)}}$$  \hspace{1cm} (48)

It is seen from the sketch in Fig. (5) that $\partial \Sigma/\partial \omega |_{\omega = \xi(k)} < 0$ so that $0 < z_k < 1$ as expected. Furthermore, $z_k$ should be slowly varying in $k$, and thus $z_k \approx z_{k_F} = a = \text{const.}$

Finally, we may obtain an expression for the Fermi velocity, which is roughly equal to the group velocity of localized quasiparticle wave packets, which are formed of quasiparticle states near the Fermi surface. As usual, this is given by the slope of the quasiparticle excitation spectrum $\xi(k)$ at the Fermi surface

$$v_F = \hbar^{-1} \nabla_k \xi(k) \bigg|_{k = k_F} = \hbar^{-1} \nabla_k \{ \xi^0(k) + \Sigma(k, \xi(k)) \} \bigg|_{k = k_F}$$  \hspace{1cm} (49)

Note that $\xi(k)$, $z_k$, and $v_F$ may contain small imaginary parts due to $\text{Im} \Sigma$, but they may be eliminated by replacing $\Sigma$ with $\text{Re} \Sigma$ in the definitions.

In analogy with noninteracting particles, for which $v^0 = \hbar^{-1} \nabla_k \xi^0(k) = \hbar k/m$ we may define the effective mass $m^*$ of the quasiparticle by $v = \hbar k/m^*$. In general this makes $m^*$ dependent on $k$, but we only need its Fermi-surface value, defined via $v_F = \hbar k_F/m^*$. In general $m^*$ will be a tensor quantity, since $v_F \neq k_F$, but we consider the case of a spherical Fermi surface where $m^*$ is a scalar. In principle we could now evaluate also $m^*$ by using the above formulas for $k_F$ and $v_F$. However, such calculations [2, 3, 22] are exceedingly difficult, and in practice $m^*$ is taken from experiments on the low-temperature specific heat. This is possible since the specific heat depends on the (single-spin) Fermi-surface density of quasiparticle states per unit volume [2]

$$N(0) = \int_{S_F} \frac{d^2s}{(2\pi \hbar)^3 |v_F(s)|} = \frac{4\pi p_F^2}{(2\pi \hbar)^3 v_F} = \frac{m^* k_F}{2\pi^2 \hbar^2}$$  \hspace{1cm} (50)

Here the area of the Fermi surface in momentum space is given by $S_F = \int_{S_F} d^2S$ and the variable “$s$” which parametrizes the surface is chosen such that $d^2S = d^2s/S_F$ and hence $\int d^2s = 1$. For a spherical surface $S_F = 4\pi p_F^2$, $|v_F(s)| = v_F$, and the integral is trivial.

Indeed, none of the set of $z_k = a$, $v_F$, and $p_F = \hbar k_F$ are easy to calculate from first principles. Below they are all taken as phenomenological constants which parametrize the low-energy inverse propagator of noninteracting quasiparticles $G^{-1}_{\text{low}, \text{coh}}(k, \omega) = a^{-1} [\omega - \xi(k)] \approx a^{-1} [\omega - \hbar v_F \cdot (k - k_F)]$, which appears in many situations as a differential operator in the low-energy equations of motion. The renormalization constant “$a$” may always be made to disappear from the effective theory by embedding it into other phenomenological parameters of the so-called “normal vertices” [1]. In particular, when quasiparticle-quasiparticle interactions are taken into account in a mean-field approximation, the interaction vertex is parametrized by the “Landau” parameters $F^0$ (and $F^1$, or some equivalent parameters [1]). Using arguments based on gauge and Galilean invariance, one may then confirm Landau’s famous result $m^*/m = 1 + F^1/3$.

### C. The two-particle function

We have neglected above the possibility of collisions between quasiparticles — they are not important at low temperatures. To take those into account, we have to study the two-particle Green’s function. We give the definition of the time-ordered two-particle (or four-point) function as

$$X(x_1, x_2; x_3, x_4) = (-i)^2 \langle \psi(x_1) \psi(x_2) \psi^\dagger(x_3) \psi^\dagger(x_4) \rangle$$  \hspace{1cm} (51)

Higher-order functions may be defined analogously, but they shall never be needed in practice. However, this second-order one is still very important. We now introduce a conceptually useful and intuitively plausible perturbation-theoretic result involving $X$ and $G$.

Namely, (for normal systems) it can be shown (see Refs. [2, 4, 10]) that the two-particle function $X$ may be decomposed into two parts as follows

$$X(12; 1′2′) = X^{\text{HF}}(12; 1′2′) + \delta X(12; 1′2′)$$  \hspace{1cm} (52)

Here

$$X^{\text{HF}}(12; 1′2′) = G(1′)(G(22′) - G(12′)G(21′))$$  \hspace{1cm} (53)

is the so-called free or reducible part of $X$, whereas

$$\delta X(12, 1′2′) = \int \int \int \int d^3d^3d^4d^4G(13)G(24) \times i\Gamma(34; 3′4′)G(3′1′)G(4′2′)$$  \hspace{1cm} (54)

is the bound or irreducible (or vertex) part. Equation (54) defines the so-called vertex function $\Gamma(12; 34)$, which, in some sense, describes “renormalized” interactions between the “renormalized” particles propagated by the full $G$. In the low-energy regime these are the quasiparticles, whereas in the high-energy regime they are not well defined. For noninteracting bare particles ($V = 0$), $\delta X$ vanishes exactly and only $X^{\text{HF}} = X^0$ remains, with $G = G^0$. Otherwise, neglect of the bound part $\delta X$ corresponds to the so-called Hartree-Fock approximation, which is often good for short-range interaction potentials [44]. The name derives from the fact that it reproduces the results of the elementary “Hartree-Fock” wave function theory of normal-state particles [44]. However, defined in this way, the approximation is much more general. Figure 6 depicts the decomposition of the
FIG. 6. The two-particle function may be decomposed to two parts $i^2 X = i^2 X_{HF} + i^2 \delta X$ as explained in the text.

FIG. 7. Structure of the full equation of motion $[i G^0]^{-1} i G = 1 - (-i V) i^2 X$ for the single-particle propagator, with $V(12)$ the unsymmetrized, local two-particle interaction (a). Since we also have $[i G^0]^{-1} i G = 1 + (-i \Sigma) i G$, the two-particle function $X$ and the single-particle self energy $\Sigma$ must be connected to each other as illustrated in part (b). Part (c) shows the decomposition into bound and free parts, which gives the Hartree-Fock approximation to the self energy as is should. The diagrams may be readily generalized to the case of a more general bare two-particle interaction $\Gamma_0(12,34)$. Part (d), which looks like an exchange term, shows yet another way of emphasizing the structure of the self energy.

two-particle function. Using the two-particle function or the vertex function, the equations of motion for $G$ may be written as in Fig. 7.

By the term quasiparticle lifetime one usually means the (temperature-dependent) quasiparticle-quasiparticle scattering time $\tau_{qp}$, which is associated with the mean free path $\ell_{qp} = v_F \tau_{qp}$. This lifetime arises from the bound part $\delta X$ [Eq. (54)] which gives rise to an imaginary part in the quasiparticle (self) energy, and hence results in damping of the quasiparticle states. (Note that quasiparticle-quasiparticle collisions are “inelastic”, meaning that in this process there can be energy transfer between the quasiparticles.) (What precisely is the relation of this lifetime to the “intrinsic” lifetime $\Gamma_k^{-1}$ defined above? Are they the same?)

III. NORMAL SYSTEMS: FINITE TEMPERATURES AND NONEQUILIBRIUM

This Section discusses the generalizations of the above ideas to finite temperatures and to the case of nonequilibrium. Again, the emphasis is kept on fermions, but the discussion is mostly applicable also to bosons.

A. Equilibrium at finite temperatures, comments about perturbation theory

We shall not discuss the finite-temperature equilibrium case in detail here. Very good accounts of it can be found in the literature [3, 8, 15]. One central result in the finite-temperature case is the so-called Kubo-Martin-Schwinger (KMS) [10] relation

$$\langle A(t) B(t') \rangle^eq = \text{Tr}\{e^{\beta(1-K)} e^{i K t} A(0) e^{-i K t'} B(t')\}$$

$$= \text{Tr}\{e^{\beta(1-K)} B(t') e^{-\beta K} e^{i K t} A(0) e^{-i K t'} e^{\beta K}\}$$

$$= \langle B(t') A(t + i\beta) \rangle^eq$$

This relation, which follows from the formal similarity of the equilibrium density matrix $e^{-\beta K}$ and the unitary time-evolution operator $e^{-i K t'}$, suggests the introduction of imaginary times. If we are only interested in calculating equilibrium averages of observables, we may indeed get rid of explicit real times altogether by performing an analytic continuation from real times $t$ to imaginary times $i$ (or from real to imaginary frequencies), a procedure known as Wick’s rotation [10, 29]. One must then define new field operators $\psi_M(x, \tau) = \psi(x, -i \tau)$ and $\bar{\psi}_M(x, \tau) = \bar{\psi}(x, -i \tau)$ which depend on $\tau$, and temperature (or Matsubara) Green’s functions

$$G(x_1, x_2, \tau) = -\langle T_\tau \psi_M(x_1, \tau) \bar{\psi}_M(x_2, 0) \rangle$$

where a $\tau$-ordering operator $T_\tau$ is introduced. The KMS relation implies that $G(\tau)$ has the antiperiodicity $G(\tau + \beta) = -G(\tau)$ which leads to a discrete set of “Matsubara frequencies” $\epsilon_m = \pi \beta^{-1} (2m + 1)$ when $G(\tau)$ is expanded into a Fourier series. The following connections (through analytical continuation) between the real and imaginary times and frequencies exist: $t \leftrightarrow \tau$ and $\omega \leftrightarrow i \epsilon_m$.

For the imaginary-time Matsubara Green function, it is possible to construct a perturbation theory whose form is very similar to the $T = 0$ case. The “difficulty” arises from a need for a new version of Wick’s theorem, since the expectation values are not to be taken in the noninteracting ground state (i.e. the vacuum state), but over a thermal ensemble including all eigenstates of $K_0(3)$. The pairing of operators is thus no longer defined as in Eq. (39) since normal ordering has no meaning, but directly as

$$\overline{A B} = \langle T_\tau [A B] \rangle^eq$$

(57)
where \(\langle \cdots \rangle_0 = \text{Tr}[\rho \cdots]\), \(\rho_0 = e^{\beta(H_0 - K_0)}\). For \(A = \psi(\tau)\) and \(B = \bar{\psi}(0)\) this defines the non-interacting temperature function \(-G^0(\tau)\). Furthermore, the adiabatic switching-on is now done with respect to imaginary time \(\tau\) and the role of

\[
\langle \Phi_0 | T A(t_1) B(t_2) \cdots | \Phi_0 \rangle \tag{58}
\]

in perturbation expansions is basically taken by

\[
\langle T A(\tau_1) B(\tau_2) \cdots \rangle_{eq}^{\psi} = \frac{\text{Tr}[e^{-\beta K_0} T A(\tau_1) B(\tau_2) \cdots]}{\text{Tr}[e^{-\beta K_0}]} \tag{59}
\]

and the new “Wick’s theorem” says that this may be written as a sum of products of the two-operator pairings in Eq. (57) [3]. It is important here that \(K_0\) is a quadratic operator. This form of the theorem is no longer a pure operator identity — it is a “weaker” statistical form concerning the thermal averages, and strictly valid only in the thermodynamic limit [10]. The imaginary-time calculation leads to a similar Dyson’s equation as for the thermodynamic limit [10]. The imaginary-time calculation leads to a similar Dyson’s equation as for the thermodynamic limit [10].

We index the propagators with “eq” to remind that we are dealing with thermodynamic equilibrium.

We note that it is possible to define a Wick decomposition in cases where the density matrix is not of the equilibrium form. However, it must be an exponential of a quadratic operator [13]. This version of the Wick decomposition can be used also for real-time Green’s functions. The statistical versions of the Wick decomposition are analogous to a certain Gaussian integral identity which also carries the name of “Wick’s theorem” [27, 43].

One of the above Wick’s theorems may be used whenever one manages to write the expectation values in the ground state or over the noninteracting ensemble. This includes nonequilibrium cases, to which we turn next. Note, however, that there are still other ways of creating the same perturbation series for \(G\) than a direct application [8] of Wick’s theorem. One such method proceeds by using variational derivatives and iterating an integro-differential equation for \(G\) [1, 6, 13, 29, 30].

B. Nonequilibrium and the Keldysh contour

Now we turn to discuss situations where the system is neither in its ground state, nor otherwise in thermal equilibrium. If the time-dependent fields driving the system away from equilibrium are small, then it may be possible to do response theory to linear order in the fields by using only equilibrium \((T = 0\) or \(T \neq 0\)) averages [3, 10]. This is the field of the elegant “Kubo formalism”, which leads to important concepts like the fluctuation-dissipation theorem, and all sorts of relations between god-knows-what correlation functions [32, 34]. For more general nonequilibrium situations this is not enough. Below we follow the simple treatment of Zagoskin [10]. A more complete but also more formal development is found in Refs. [8, 11].

1. Interaction picture for \(K_0 = T - \mu N\), “adiabatic switching on”, and the Keldysh contour

The reason why the nonequilibrium Green’s function theory becomes much more complicated than the equilibrium one can be seen as follows. To start with, consider the time-ordered Green’s function which is evaluated in an arbitrary pure state \(|\Psi\rangle\) of the system

\[
G(x_1, x_2) = -i \frac{\langle \Phi \mid T \psi(x_1) \psi^\dagger(x_2) \mid \Psi \rangle}{\langle \Psi \mid \Psi \rangle} \tag{61}
\]

Statistical averaging over some \(\rho\) could easily be added anywhere below, since \(\text{Tr}(\rho A) = \sum \phi \phi \langle \Psi | A | \Psi \rangle\) is a linear operation — we return to this case later. Equation (61) is in the Heisenberg picture, but the state \(|\Psi\rangle\) is equal to the Schrödinger or interaction picture states at \(t = t_0 = 0\). We now assume that the time-dependent Hamiltonian is of the form \(K(t) = K_0 + K_1(t)\), where \(K_0 = T - \mu N\) and \(K_1(t) = e^{-\eta |t|}(V + V_{ext})\), with \(\eta = 0+\) so that the interactions \(V\) between particles and the time-dependent external one-particle potential \(V_{ext}(t)\) are turned on slowly, starting from \(t = -\infty\). [14, 15] Again we drop \(\eta\) and neglect all convergence discussions involving the normalization denominator, which are similar to those in subsection II B 2. Furthermore, we assume that the state \(|\Psi\rangle\) is such that it can be generated from a state of the non-interacting system at \(t = -\infty\) by the switching-on procedure, i.e., \(|\Psi\rangle = S(0, -\infty) |\Phi_0\rangle\). Here \(|\Phi\rangle\) is not necessarily the ground state \(|\Phi_0\rangle\) (or even an eigenstate) of the non-interacting system, but we shall assume it to be so — otherwise perturbation theory will not be well-defined. Thus from here on we set \(|\Phi\rangle = |\Phi_0\rangle\), and assume all interacting nonequilibrium states to be generated by starting from this noninteracting equilibrium state. We wish to express \(G\) in the interaction picture, and thus use

\[
e^{iK_0 t} U(t, 0) |\Psi\rangle = |\Psi_I(t)\rangle = S(t, -\infty) |\Phi_0\rangle \tag{62}
\]

where \(|\Psi_I(t \to -\infty)\rangle \equiv |\Phi_0\rangle\). At \(t = 0\) the interactions are fully turned on, and as we approach \(t = +\infty\), they will be slowly turned off again. The resulting interaction-picture state vector is

\[
|\Phi'_0\rangle \equiv |\Phi_I(\infty)\rangle = S(\infty, -\infty) |\Phi_0\rangle \tag{63}
\]

However, this time the state \(|\Phi'_0\rangle = S(\Phi_0)\) is in no simple way related to \(|\Phi_0\rangle\), as it was before. Even if the system started from the noninteracting ground state at \(t = -\infty\), it will not return to the ground state at \(t = +\infty\). The reason is that the explicitly time-dependent \(V_{ext}(t)\) may cause transitions to excited states, which will not relax
to the ground state unless we introduce some mechanism for this to happen. Thus the state $|\Phi_n\rangle = S|\Phi_0\rangle$ will be some complicated superposition of the eigenstates $|\Phi_n\rangle$ of $K_0$ for all $n$, whose coefficients depend on the form of $V_{ext}(t)$ around $t \approx 0$. Using Eq. (5), $|\Psi\rangle = S(0, -\infty)|\Phi_0\rangle$ and $|\Psi\rangle = (\Phi_0|S(0, -\infty) = (\Phi_0|S(\infty, 0)$ and upon moving $T$ as far to the left as possible, we obtain the intuitively reasonable result

$$iG(x_1, x_2) = \frac{\langle \Phi_0|S^\dagger T[S(\infty, t_1)\psi_1(x_1)S(t_1, t_2)\psi_2^\dagger(x_2)S(t_2, -\infty)]|\Phi_0\rangle}{\langle \Phi_0|S^\dagger S|\Phi_0\rangle}$$

and the returning path with “+” (sometimes “2” or “−”). We see that if, instead of $T$ and $\tilde{T}$, we introduce an operator $T_c$ which orders the operators along the contour, then Eq. (64) may be written as

$$iG_{\ldots}(x_1, x_2) = \frac{\langle \Phi_0|\tilde{T}[S^\dagger T[S(\psi_1(x_1)\psi_2^\dagger(x_2)]|\Phi_0\rangle}{\langle \Phi_0|\tilde{T}[S]|\Phi_0\rangle}$$

Also the symbol $T_c$ has the familiar (anti)symmetry characteristics for interchange of operators subjected to it. Here we introduced the “contour s matrix”

$$S_c = T_c \exp \left[ -\frac{i}{\hbar} \int_{c_1}^{c_2} dr K_{11}(r) \right]$$

and added indices “−−” to $G$ since both times $t_{1,2}$ appear on the forward-part of the contour $c = c_- + c_+$. The time variables under the $T_c$ operator should be interpreted as complex variables and the contour as a contour in the complex time plane, infinitesimally close to the real axis [11]. Note that on the $c_-$ part $T_c = \tilde{T}$ and on the $c_+$ part $T_c = \tilde{T}$. If $t_1$ comes after $t_2$ along the contour, we write $t_3 > t_2$. Furthermore, if $t_{\infty}$ is the turning point, then for $c_-$ and $c_+$ we have $t < t_{\infty}$ for $c_-$ and $t > t_{\infty}$ for $c_+$, respectively. To be more general, we allow for the possibility that the contour runs along some more general closed time path $t_{\infty} \rightarrow t_{\infty} \rightarrow t_{\infty}$, where $t_{\infty}$ may be different from $\pm \infty$.

If we denote with the first and second indices the contour parts of $t_1$ and $t_2$, respectively, then we may define altogether four functions for the interacting nonequilibrium system: $G_{+\ldots}$, $G_{-\ldots}$, $G_{\ldots+}$, and $G_{\ldots-}$. We saw that $G_{-\ldots}$ is just the causal function $G$, but it is not clear what the interpretation of the other three could be, and why they should be defined. However, if we now apply Wick’s theorem to a perturbation expansion of Eq. (66) with the contraction redefined as $A^\star B^\star = T_c[AB] - A^\star [AB]$, we do obtain four types of pairings in the state $|\Phi_0\rangle$. Denoting $\langle \cdots | = \langle \Phi_0| \cdots |\Phi_0\rangle$ these are of the form $(\psi_\pm)$ are obvious shorthands, still in the interaction picture

$$\langle T_c \psi_\pm \psi_\pm^\dagger \rangle_0, \langle T_c \psi_+ \psi_-^\dagger \rangle_0, \langle T_c \psi_- \psi_+^\dagger \rangle_0, \langle T_c \psi_+^\dagger \psi_-^\dagger \rangle_0$$

or equivalently

$$\langle T \psi_\pm \psi_\pm^\dagger \rangle_0, \langle T \psi_+ \psi_-^\dagger \rangle_0, \langle T \psi_- \psi_+^\dagger \rangle_0, \langle T \psi_+^\dagger \psi_-^\dagger \rangle_0$$
since contour ordering is trivial if \( t_{1,2} \) are on different parts of \( c \). Now, assuming the left-side (right-side) operators in Eqs. (68) to occur with coordinates \( x_1 (x_2) \), we take these four pairings as the definitions of the functions \( \mathbf{iG}_{0,-}^0, \mathbf{iG}_{0,+}^0, \mathbf{iG}_{0,-}^1 \), and \( \mathbf{iG}_{++}^0 \) for the non-interacting equilibrium (\( T = 0 \)) system.

As mentioned in passing, we could have defined all the expectation values using statistical ensemble averages due to their linearity. Above we generated the pure “nonequilibrium state” \( \langle \Psi \rangle \) at “zero temperature” by starting from the equilibrium state \( \langle \Phi_0 \rangle \) of the non-interacting system. This state must furthermore be the ground (or vacuum) state, in order for some form of operator Wick’s theorem to be useful for generating the perturbation series. Similarly, at finite temperatures a mixed nonequilibrium state with statistical operator \( \rho \) must be generated by assuming that at \( t = -\infty \) the system was at thermodynamic equilibrium and with all interactions turned off. Only in this way (i) the “temperature” becomes well-defined, and (ii) we get to use the statistical version of Wick’s theorem valid for averaged with respect to a quadratic \( K_0 \) (see subsection III A).

Thus \( \rho(t) = S(t, -\infty) \rho_0 S^\dagger(t, \infty) \), where \( S(t, \infty) \) is as above, and \( \rho_0 = e^{\beta(b_0 - K_0)} \). The new time-contour functions of Eq. (68) then follow in a very similar fashion, with \((\cdots)_{\rho}\) being the average with respect to \( \rho_0 \). Below we shall be discussing mainly the finite-temperature case, and as the next step we repeat some of the above using the density-matrix picture.

2. Contour-ordered functions, the Keldysh space, and perturbation theory at finite temperatures

Having gained some insight from the previous discussion, we may now attempt a somewhat more systematic approach, and begin with general definitions. As usual, the \( \psi \) are Heisenberg operators for the full \( K \), and expectation values are over arbitrary statistical ensembles. First of all, as a generalization of the functions \( G_{\pm \pm} \) above we define, for the interacting non-equilibrium system,

\[
\begin{align*}
G_{-}^e(x_1, x_2) &= -i\langle T \psi(x_1) \psi^\dagger(x_2) \rangle \\
G_{+}^e(x_1, x_2) &= -i\langle \bar{T} \psi(x_1) \psi^\dagger(x_2) \rangle \\
G_{-}^\pm(x_1, x_2) &= \pm i\langle \psi^\dagger(x_2) \psi(x_1) \rangle \\
G_{+}^\pm(x_1, x_2) &= -i\langle \psi(x_1) \psi^\dagger(x_2) \rangle 
\end{align*}
\]  

We have we added here a superscript “\( e \)”, which will be important for distinguishing between different representations below — in this respect we follow the notation of Ref. [1]. Sometimes also the additional notations are used: \( G^S = G^e_+ \), and \( G^\pm = G_{\pm}^\pm \). These definitions may be neatly combined into a definition of the contour-ordered Green’s function

\[
G_{ij}^e(x_1, x_2) = -i\langle T_c \psi(x_1) \psi^\dagger(x_2) \rangle_{ij} 
\]  

Here the indices \( i, j = \pm \) denote the contour parts which \( t_{1,2} \) occupy. We give the name Keldysh space for the two-dimensional space whose basis vectors these \( + \) and \( - \) enumerate. We call matrices with such a \( 2 \times 2 \) structure laxly “Keldysh space matrices”. (No accent notation like “\( \tilde{\cdot} \)” is introduced at this point, since they are used to distinguish between certain choices for the basis.) Note that they are additionally 2 \( \times \) 2 spin matrices, and thus the spin-Keldysh direct-product space is four dimensional. (Below, in the case of superconductivity, we multiply this dimensionality by yet another factor of 2.)

Similarly as in Sec. III B for \( G = G_{-}^e \), we may do perturbation theory for the whole \( G^e \) matrix function. To do this one usually proceeds slightly differently from what was done above [8, 11]. Namely, one first transforms to an interaction picture where only the external driving is separated. In this way one relates \( G \) to an interacting equilibrium state. In the next step, in order to use the statistical Wick theorem, one makes another transformation to an interaction picture with respect to the noninteracting time-independent Hamiltonian. The rest of this subsection is very sketchy — a more detailed discussion is found in Refs. [8, 11].

We assume the that before some time \( t = t_{int} \) (for example \( t_{int} = t_{-\infty} = -\infty \), which we assume) the nonequilibrium term \( V_{ext}(t) = 0 \), and thus the system is in thermodynamic equilibrium determined by the time-independent Hamiltonian \( K = T - \mu N + V \). Thus for \( t_{1,2} < t_{int} \) the function \( G^e \) must satisfy the boundary condition requiring it to be equal to the temperature Green’s function (via analytic continuation) [Sec. (III A)]. The temperature function must furthermore satisfy the KMS boundary condition, which now reads

\[
G_{+}^e(x_1, t_1; x_2, t_2) = -G_{-}^e(x_1, t_1; x_2, t_2 - i\beta) 
\]  

For \( t > t_{int} \) the system starts to be driven out of equilibrium by the explicitly time-dependent term \( V_{ext}(t) \). We describe this by using an interaction picture where only \( V_{ext}(t) \) is separated from the other terms in the full Hamiltonian \( K(t) \). Most importantly, no artificial adiabatic switching on is introduced at this point. Thus we write \( \tilde{K}_0 = T - \mu N + V \) and \( \tilde{K}_0^{(\eta)}(t) = V_{ext}(t) \). We set \( V_{ext}(t) = 0 \) for \( t < t_{int} \). We obtain [8, 11]

\[
G_{ij}^e(x_1, x_2) = -i\langle T_c S_c \psi(x_1) \psi^\dagger(x_2) \rangle_{ij}^{eq} \langle T_c S_c \rangle^{eq} 
\]  

where the average \( \langle \cdots \rangle^{eq} = \text{Tr}[\rho \cdots] \) is a finite-temperature equilibrium average with respect to \( \rho = e^{\beta(\tilde{K}_0 - K_0)} \), where \( K_0 = T - \mu N + V \), \( e^{-\beta K_0} = \text{Tr}[e^{-\beta \tilde{K}_0}] \). The operator \( S_c \) is as before, but in the different interaction picture. With the \( T, \bar{T} \) and \( S, S^\dagger \) operators these may be written just as in Eq. (66) (we drop the denomi-
Furthermore, we find the relation
\[ G_{-+}^c(x_1, x_2) = -i\langle [\mathcal{T}[\psi(x_1)\psi^\dagger(x_2)]\rangle \] ^eq
\[ G_{++}^c(x_1, x_2) = -i\langle [\mathcal{T}[\psi(x_1)\psi^\dagger(x_2)]\rangle \] ^eq
\[ G_{--}^c(x_1, x_2) = \pm i\langle [\mathcal{T}[\psi(x_1)\psi^\dagger(x_2)]\rangle \] ^eq
\[ G_{+-}^c(x_1, x_2) = -i\langle [\mathcal{T}[\psi(x_1)\psi^\dagger(x_2)]\rangle \] ^eq
(74)

Starting from Eq. (73), there are different ways of creating the perturbation series in powers of the two-body interaction \( V \) and \( V_{\text{ext}} \). One way is to employ the functional derivative method (see Ref. [1]), and another is to use the statistical Wick’s theorem. The latter method is explained in Refs. [8, 11]. In this case a further transformation to the interaction picture of the quadratic Hamiltonian \( K_0 = T-\mu N \), and use of the KMS relation is needed to be able to express \( G^c \) as an average \( \langle [\cdots [\rho_0 \cdots] \rangle \] with respect to \( \rho_0 = e^{i(\delta_0-K_0)} \). (At this point a formal adiabatic switching on of \( V \) may again be needed.) Both ways are a little bit tricky and we pass the derivations here. As a result one obtains a Dyson’s equation for \( G^c \), which is of the usual form \( G^c = G^c_0 + G^c_0 SS^c G^c \), but with matrix products between the whole 4 × 4 spin-Keldysh matrices. However, for certain purposes it will be more convenient to write the equation of motion for different Keldysh-space representations than what is used above. We shall discuss these next.

3. Symmetry properties, definition of the Keldysh function
\( G^K \), and rotations in Keldysh space

At this point we also introduce a useful shorthand notation which gets rid of the increasing number of indices. We define
\[ G^c(1, 2) = G^c_{i_1 i_2}(x_1, x_2) = -i\langle T[\psi(x_1)\psi^\dagger(x_2)] \] ^eq
\[ \] ^eq
so that all coordinates \( i \) (Keldysh), \( x \) (spin-space-time), and possibly some additional ones, are grouped under one index. We may then write convolution ("folding") products like \( G(1, 3) = \int d2G(1, 2)G(2, 3) \) etc. if needed. Also partial shorthand like \( G_{\pm\pm}(1, 2) \) are used, so that the Keldysh index is specified separately. From the definitions of Eq. (70) it follows that
\[ G_{-+}(1, 2) = -[G_{++}(2, 1)]^* \]
\[ G_{--}(1, 2) = -[G_{+-}(2, 1)]^* \]
\[ G_{+-}(1, 2) = -[G_{--}(2, 1)]^* \]
(76)

Furthermore, we find the relation
\[ G_{-+}^c(1, 2) + G_{+-}(1, 2) = G_{--}^c(1, 2) + G_{+-}^c(1, 2) \]
(77)

Therefore, the functions \( G_{\pm\pm} \) are not all independent — only three of them are, and the fourth is given by Eq. (77). We may also choose some convenient linear combinations of \( G_{\pm\pm} \) as the independent functions. If we take into use the familiar retarded and advanced functions \( G^{R,A} \) plus in addition the Keldysh function \( G^K \) defined in Eq. (1) of Sec. I, then we find that they may be expressed by the combinations
\[ G^R = G^c_{--} - G^c_{--} = G^c_{++} - G^c_{++} \]
\[ G^A = G^c_{--} - G^c_{+-} = G^c_{++} - G^c_{++} \]
\[ G^K = G^c_{--} + G^c_{++} = G^c_{++} + G^c_{++} \]
(78)

It is these three functions which we take as the independent components. Expressing \( G_{\pm\pm} \) with \( G^{R,A,K} \) we find
\[ G_{--} = (G^R + G^A + G^K)/2 \]
\[ G_{+-} = (-G^R + G^A + G^K)/2 \]
\[ G_{++} = (G^R - G^A + G^K)/2 \]
\[ G_{--} = (G^R - G^A + G^K)/2 \]
(79)

For reasons which will become clearer shortly, it will be more convenient to deal with the Keldysh-space matrix defined as \( \hat{G} = \sigma_3 G^c \), where \( \sigma_3 \) is the Pauli matrix in Keldysh space — it has nothing to do with spin! Componentwise this is written \( G_{ij} = \sigma_3 G^c_{ij} \) and by using matrices we have
\[ G^c = \begin{bmatrix} G_{--} & G_{+-} \\ G_{+-} & G_{++} \end{bmatrix} \]
\[ \hat{G} = \begin{bmatrix} \sigma_3 G^c_{--} & \sigma_3 G^c_{+-} \\ \sigma_3 G^c_{+-} & \sigma_3 G^c_{++} \end{bmatrix} \]
(80)

Thus the only change so far is the signs of two matrix components. Note that we denoted the new representation with an accent "\( \cdot \)", now following the definition of Ref. [8]. (The reason for doing this redefinition is that the equations of motion for the Keldysh matrix \( \hat{G} \) will be formally more similar to those of the usual \( G \).) Having done this, we may furthermore perform a similarity transformation (or "basis change") of \( \hat{G} \) with the rotation matrix
\[ R = (\sigma_0 + i\sigma_2)/\sqrt{2} = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \]
(81)

which satisfies \( R^{-1} R = R^\dagger = R^T \). This transformation yields
\[ \hat{G} = R^{-1} \hat{G} R = R^{-1} [\sigma_3 G^c] R = \begin{bmatrix} G^R & G^K \\ 0 & G^A \end{bmatrix} \]
(82)

where now the independent \( G^{R,A,K} \) appear as components, and a new accent "\( \cdot \)" is introduced. Also another type of transformation may be found in the literature. This is apparently the one used originally by Keldysh [8]. It consists of the same rotation on \( G^c \) as was done above on \( \hat{G} \). We denote the result with the accent "\( \cdot \)";
\[ \tilde{G} = R^{-1} G^c R = \begin{bmatrix} 0 & G^A \\ G^R & G^K \end{bmatrix} \]
(83)
We reserve the accents “*^*” and “*~*” etc. for another type of matrix to be encountered below, the “Nambu” matrix, and possibly (yet I hope not) something else. As an important property of the upper-triangular matrices $\hat{G}$ is that they form a group with respect to matrix multiplication. In simpler terms, the product of two such matrices remains upper-triangular:

$$
\begin{bmatrix}
B^R & B^K \\
0 & B^A
\end{bmatrix}
\begin{bmatrix}
C^R & C^K \\
0 & C^A
\end{bmatrix} =
\begin{bmatrix}
B^R C^R & B^R C^K + B^K C^A \\
0 & B^A C^A
\end{bmatrix}
$$

and so does the inverse matrix, assuming it exists:

$$
\bar{B} = \begin{bmatrix}
B^R & B^K \\
0 & B^A
\end{bmatrix}
\Rightarrow \bar{B}^{-1} = \begin{bmatrix}
(B^R)^{-1} & -(B^R)^{-1} B^K (B^A)^{-1} \\
0 & (B^A)^{-1}
\end{bmatrix}
$$

We should also observe that the “$R$” and “$A$” parts on the diagonal do not mix with each other nor with the off-diagonal “$K$” parts. This is perhaps the most convenient property of this particular representation.

4. Equations of motion in Keldysh space and symmetries of self-energies

We now take the symmetry discussion one step further. The equations of motion for the noninteracting propagators are easily found. If we define $G_0^{-1}(1) = i\hbar \partial/\partial t - K_0(x_1)$ where $\langle x'|K_0|x \rangle = \delta(x - x')K_0(x)$, then

$$
\begin{align*}
G_0^{-1}(1)G_{0c}^{0c}(1,2) &= \hbar\delta(1-2) \\
G_0^{-1}(1)G_{0-}^{0+}(1,2) &= 0 \\
G_0^{-1}(1)G_{0+}^{0-}(1,2) &= 0 \\
G_0^{-1}(1)G_{0+}^{0+}(1,2) &= -\hbar\delta(1-2)
\end{align*}
$$

Here the $-\hbar\delta(1-2)$ the last equation follows from differentiation with respect to anti-time ordering. Using matrix notation we have (1, 2 do not include Keldysh indices)

$$
G_0^{-1}(1)G_{0c}^{0c}(1,2) = \sigma_3\hbar\delta(1-2)
$$

or in shorthand $\bar{G}_0^{-1}G_{0c}^{0c} = \sigma_3$. We see that the noninteracting inverse propagator $G_{0c}^{-1}$, which satisfies $G_{0c}^{-1}G_{0c} = 1$, must be of the form $G_{0c}^{-1} = \sigma_3 \bar{G}_0^{-1}$.

Acting with the operator $\bar{G}_0^{-1}$ on the Dyson equations from the left, and using Eq. (87) we obtain a set of integro-differential equations

$$
[(\bar{G}_0^{-1} - \sigma_3 G^c)G^c](1,2) = \hbar\delta(1-2)\sigma_3
$$

or $\bar{G}_0^{-1} - \sigma_3 = \Sigma^c$ from the right. The simplification due to multiplications by $\sigma_3$ is again visible. Just like $G^c$, $\hat{G}$, and $G$, the self-energies $\Sigma^c$, $\hat{\Sigma}$, and $\Sigma$ are also Keldysh matrices. We denote their components with

$$
\Sigma^c = \begin{bmatrix}
\Sigma_{cc} & \Sigma_{c+} \\
\Sigma_{c+} & \Sigma_{++}
\end{bmatrix},
\hat{\Sigma} = \begin{bmatrix}
\Sigma_{cc} & \Sigma_{c-} \\
\Sigma_{c+} & \Sigma_{++}
\end{bmatrix} = \Sigma^c\sigma_3 = \begin{bmatrix}
\Sigma_{cc} & -\Sigma_{c+} \\
-\Sigma_{c-} & \Sigma_{++}
\end{bmatrix}
$$

At this point we do not specify the details of these functions, but their symmetry properties with respect to the Keldysh indices follow directly from those of $G^c$ or $\hat{G}$ through the Dyson equation. Most important, by writing down the transformation from $G^c, \Sigma^c$ to the representation $\hat{G}, \hat{\Sigma}$ and using the condition $\hat{G}_{++} = 0$ (which we already proved with Eqs. (77) and (82)), one finds

$$
\Sigma^c_{c-} + \Sigma^c_{c+} = -\Sigma^c_{c+} + \Sigma^c_{c-}
$$

It is thus immediately seen that only three components of the self energy are again independent. In the third representation we then have

$$
\hat{\Sigma} = R^{-1}\Sigma R = R^{-1}[\Sigma^c\sigma_3]R = \begin{bmatrix}
\Sigma^R & \Sigma^K \\
0 & \Sigma^A
\end{bmatrix}
$$

where we define the three independent components

$$
\begin{align*}
\Sigma^R &= \Sigma^c_{c-} + \Sigma^c_{c+} = -\Sigma^c_{c+} - \Sigma^c_{c-} \\
\Sigma^A &= \Sigma^c_{c+} + \Sigma^c_{c+} = -\Sigma^c_{c-} - \Sigma^c_{c+} \\
\Sigma^K &= \Sigma^c_{c-} + \Sigma^c_{c+} = -\Sigma^c_{c-} - \Sigma^c_{c-}
\end{align*}
$$

Note that (check this...)

$$
\hat{\Sigma} = R^{-1}\Sigma R = \begin{bmatrix}
\Sigma^K & \Sigma^R \\
\Sigma^A & 0
\end{bmatrix}
$$
As a final ingredient to a full set of equations, we still invert these
\[
\begin{align*}
\Sigma_{c-} &= (\Sigma^R + \Sigma^A + \Sigma^K)/2, \\
\Sigma_{c+} &= (\Sigma^R - \Sigma^A - \Sigma^K)/2, \\
\Sigma_{c+} &= (-\Sigma^R + \Sigma^A - \Sigma^K)/2, \\
\Sigma_{c+} &= (-\Sigma^R - \Sigma^A + \Sigma^K)/2
\end{align*}
\]  
(95)

We now note a second good reason for defining the representation with \(\tilde{G}\) and \(\tilde{\Sigma}\) — this is the more important one. If the symmetries of Eqs. (78) or (79) and Eqs. (93) or (95) are written by using the components of \(\tilde{G}\) and \(\tilde{\Sigma}\), the two sets of equations become formally equivalent. Thus in that representation the Green functions and the self-energies satisfy exactly the same Keldysh-space symmetries. The transformation which shows this is trivial and we shall not display it here. Let us mention, however, that when all Keldysh-space matrices satisfy the same symmetries, one can use the very useful “Langreth rules” for manipulating expressions involving products of such matrices [11, 33].

While the retarded and advanced components satisfy separate Dyson equations,
\[
G^{R,A} = G^{R,A}_0 + G^{R,A}_0 \Sigma^{R,A} G^{R,A}
\]  
(96)

the Keldysh \((K, +, -\), or \(-)\) components do not. Instead, they satisfy the so-called Keldysh equations, for example
\[
\begin{align*}
G^+ - (1 + G^R \Sigma^R) G^{-} = (1 - G^A \Sigma^A) - G^R \Sigma^+ - G^A \\
G^c - (1 + G^R \Sigma^R) G^c = (1 - G^A \Sigma^A) - G^R \Sigma^c - G^A \\
G^K = (1 + G^R \Sigma^R) G^K (1 - G^A \Sigma^A) + G^R \Sigma^K G^A
\end{align*}
\]  
(97)

where one should note that \((1 + G^R \Sigma^R) = G^R(\Sigma^R)^{-1}\), for example. Then, if the unperturbed state is in equilibrium, one may show that \(G^K = G^R \Sigma^K G^A\) to zeroth order in \((\Sigma^R)^{-1} - (\Sigma^A)^{-1}\), which is the form usually applied to transport problems. Note: Despite the apparent closedness of the Dyson equations (96), the self-energies \(\Sigma^{R,A}\) depend in general also on the \(G^K\) function! Thus, the Eqs. (96) and (97) must be solved together.

Finally, let us make a note on another widely used set of definitions, which involve the “greater and lesser” functions [6]. The connection of these to our notation is the following: \(G^c = G^c_{+}, G^c = G^c_{-}, G^T = G^T_{-}, G^T = G^T_{+}\), and \(\Sigma^c = -\Sigma^c_{+}, \Sigma^c = -\Sigma^c_{-}, \Sigma^T = \Sigma^T_{+}, \Sigma^T = \Sigma^T_{-}\). Their Keldysh-space Dyson equation then looks like
\[
\begin{bmatrix}
G^T & -G^c \\
G^c & -G^T
\end{bmatrix}
= \begin{bmatrix}
G^T & -G^c \\
G^c & -G^T
\end{bmatrix}
\times \begin{bmatrix}
\Sigma^T & -\Sigma^c \\
\Sigma^c & -\Sigma^T
\end{bmatrix}
\]
(98)

With these conventions, to go to the \(R, A, K\) representation, a different rotation matrix than the \(R\) defined above is needed. However, the minus signs could also be assigned also to the bottom row. Then the rotation would be the same. Also in this case, the Green functions and self-energies satisfy the same symmetries, namely those of Eqs. (78) and (79), and the “Langreth rules” should work.

5. Further relations

As shown above, all the symmetries of the self-energies follow from the symmetries of the Green functions through the Dyson equation. In this way, the self-energies inherit very similar Keldysh-space properties as the Green functions. Some such relations still remain to be explained. For example, it may also be shown that the “(anti)causality” of \(G^{R(A)}(t, t')\), i.e., the fact that it vanishes for \(t < t' (t > t')\), is also transferred to the self-energy \(\Sigma^{R(A)}\) [8]. This can be seen as follows. Consider the Dyson equation
\[
G^R(1') = g^R(1') + \int d2 \int d3 g^R(12) \Sigma^R(23) G^R(31')
\]  
(99)

For \(t_1 < t_1'\) this yields
\[
0 = \int_{t_1}^{t_2} d2 \int d3 g^R(12) \Sigma^R(23) G^R(31')
\]  
(100)

where the restrictions \(t_3 > t_1\) and \(t_1 > t_2\) together with \(t_1' > t_1\) imply \(t_3 > t_2\). Thus we must have \(\Sigma^R(1, 1') = 0\) for \(t_1 < t_1'\). Similarly \(\Sigma^A(1, 1') = 0\) for \(t_1' < t_1\), which may be seen for example from the fact that
\[
G^A = [G^R]^\dagger \implies \Sigma^A = [\Sigma^R]^\dagger
\]  
(101)

Now, using Eqs. (93) these also imply that
\[
\Sigma^c_{-}(1, 1') = -[\Sigma^c_{+}(1, 1')] \text{ for } t_1 < t_1' \quad \text{ and } \quad -[\Sigma^c_{-}(1, 1')] \text{ for } t_1 > t_1',
\]  
(102)

and they may be combined into
\[
\Sigma^R(1, 1') = -\theta(t_1 - t_1') [\Sigma^c_{-}(1, 1') - \Sigma^c_{+}(1, 1')]
\]  
(103)

Due to the (anti)causality properties, in stationary state the real and imaginary parts of \(\Sigma^{R(A)}(\epsilon)\) are Hilbert-transform pairs in a similar way as those of \(G^{R(A)}\) — see Eq. (20). Notice that in general the \(\Sigma^{R(A)}(1, 1')\) may also contain singular terms proportional to \(\delta(t_1 - t_1')\), such as in the case of the Hartree-Fock approximation for the instantaneous Coulomb interaction, or any single-particle potential. For more, see Refs. 8 and 13, for example.
The above symmetries follow directly from the most general definitions, and are thus always satisfied. However, often there exist some additional “symmetries”. For example, in equilibrium a relation of the form \( G^K = h(G^R - G^A) \) will always exist, where \( h(\omega) \) is a real scalar function (This is the “fluctuation-dissipation theorem” — see below). In this case, an application of the Dyson equation shows us that
\[
G^K = h(G^R - G^A) \implies \Sigma^K = h(\Sigma^R - \Sigma^A) \tag{104}
\]

Finally we stress that the Keldysh-space symmetries which we have presented are not modified even in the presence of superconductivity. In that case the propagators and self-energies will simply be replaced by the “Nambu matrices” — see below. This concludes our symmetry discussion. For more of it, see Ref. [1] and other references. As the final step we shall check whether the general symmetries work in some simple situations, where the propagators have simple expressions.

C. Explicit expressions for the propagators

1. Noninteracting nonequilibrium

Let us write down the expressions of the many propagators for a translationally invariant noninteracting system. As in Sec. II A, we again neglect the spin structure, which should only add \( \delta_{\alpha\beta} \) factors to them. Assuming the system is in a stationary pure state \( |\Phi\rangle \), we find directly from the definitions [10]
\[
G_{--}^{0c}(k, \omega) = \frac{1}{\omega - \omega_k^0 + \mu/h + i\eta} + 2\pi i\delta(\omega - \omega_k^0 + \mu/h)m_k \\
G_{++}^{0c}(k, \omega) = -\frac{1}{\omega - \omega_k^0 + \mu/h - i\eta} + 2\pi i\delta(\omega - \omega_k^0 + \mu/h)m_k \\
G_{+-}^{0c}(k, \omega) = -2\pi i(1 \otimes m_k)\delta(\omega - \omega_k^0 + \mu/h) \\
G_{-+}^{0c}(k, \omega) = 2\pi i m_k \delta(\omega - \omega_k^0 + \mu/h)
\]
where \( m_k = \langle \Phi | a_k^\dagger a_k | \Phi \rangle \). These are also solutions of Eq. (86), which is, in principle, another route for arriving at the expressions. Then, using Eq. (78) we obtain
\[
G_0^R(k, \omega) = \frac{1}{\omega - \omega_k^0 + \mu/h + i\eta} \\
G_0^A(k, \omega) = \frac{1}{\omega - \omega_k^0 + \mu/h - i\eta} \\
G_0^K(k, \omega) = -2\pi i(1 \otimes m_k)\delta(\omega - \omega_k^0 + \mu/h)
\]
where we repeat the content of Eq. (23). We are happy to see that Eqs. (105) and (106) satisfy all the general symmetries of Sec. III B 3 as they should. Among other things, it should be noted that \( G_0^{R,A} \) carry no information about the state: they are exactly the same here, as they were for the zero-temperature ground-state system of Sec. (II A). The only information about the state of the system is in the (nonequilibrium) distribution function \( m_k \) appearing in \( G^K \). For fermions in equilibrium at zero temperature \( m_k = \theta(k_F - |k|) \). At general \( T \neq 0 \) it is equal to the Fermi function \( m_k = [\exp(\beta(k_F - \mu)) + 1]^{-1} \) — see below.

In the interacting \( T = 0 \) case we may proceed to write the usual Lehmann expansions for \( G_{\pm,\pm} \) and \( G^K \) also, but rather than do that, it is more sensible to use the symmetries. For example we directly obtain the Lehmann expansion for \( G^K \) by using \( G^K = 2G - G^R - G^A \), since we already know them for \( G \) and \( G^{R,A} \). However, for the nonequilibrium formalism the most interesting cases are those with \( T \neq 0 \), interactions present, and, of course, where no equilibrium exists. At least for the general equilibrium case there exists a generalized Lehmann expansion, which we explain shortly [10]. But for realistic nonequilibrium calculations we must resort to the most general expressions and their equation of motion — the Dyson equation. Luckily, the quasiparticle concept will allow one to return to work mostly with propagators which are of the noninteracting form, and thus Eqs. (105) and (106) are very important. Next we shall consider their form in general equilibrium states.

2. Generalized Lehmann representation in equilibrium

In this section I will present the results for the generalized Lehmann expansion for normal, translationally invariant equilibrium systems with a grand-canonical Hamiltonian \( K = H - \mu N \) at general \( \beta^{-1} = k_B T \neq 0 \). The assumption of translational invariance is by no means necessary, and most of the following results may be straightforwardly generalized to the inhomogeneous equilibrium case. In fact, it may be done for any response functions of the type \( G_{AB}(t) = -i\langle TA(t)B(0)\rangle \), \( G_{AB}^R(t) = -i\partial_t\langle [A(t), B(0)]_\beta \rangle \), etc., in which case the derivation essentially gives the fluctuation-dissipation theorem — see Appendix 2 or Ref. [5]. Here I follow Ref. [10], but with a modified notation to be more consistent with our \( T = 0 \) case. The fluctuation-dissipation relations actually follow more easily from the KMS relation, but the Lehmann expansion is perhaps more instructive here.

The time-ordered equilibrium propagator is defined as
\[
G_{eq}(k, t) = -i\langle a_k(t)a_k^\dagger(0)\rangle_{eq} = \int d^3x \int dt e^{-ik\cdot x} e^{i\omega t}(-i) = \langle T\psi(x,t)\psi^\dagger(0,0)\rangle_{eq} \tag{107}
\]
where \( \langle \cdots \rangle_{eq} = \text{tr}[\rho_{eq} \cdots] \), \( \rho_{eq} = e^{\beta H} \), and \( e^{-\beta H} = \text{tr}[e^{-\beta K}] \). In a representation where the basis states \( |\Psi_n\rangle \) are eigenstates of “canonical” energy \( H \) and par-
ticle number \(N\), i.e.,

\[
K|\Psi_n\rangle = (\mathcal{H} - \mu N)|\Psi_n\rangle = K_n|\Psi_n\rangle = (E_n - \mu N_n)|\Psi_n\rangle
\]

the statistical operator is diagonal: \(\rho_{\alpha\beta}^m_n = \rho_n^\alpha \delta_{m_n}\), where \(\rho_n^\alpha = e^{-\beta E_n - \mu N_n}\). The major difference here, as compared with the \(T = 0\) case, is that all eigenstates — not just the one with \(n = 0\) — are occupied with finite probabilities, and thus all transition amplitudes \(|\langle \Psi_m|\psi_\alpha(0)|\Psi_n\rangle|\) and energies \(\xi_{mn}\) play a role. In this eigenbasis the generalized Lehmann expansion takes the form

\[
G_{eq}(k, \omega) = \int_{-\infty}^{\infty} d\omega' A_{eq}(k, \omega') \left\{ \frac{1}{\omega - \omega' + i\eta} \right\}
\]

where we define

\[
A_{eq}(k, \omega') = \left[ \frac{1}{2} \sum_\alpha \sum_n \sum_m \rho_n^\alpha |\langle \Psi_n|\psi_\alpha(0)|\Psi_m\rangle|^2 \right] \times V_{\theta k, \mathbf{p}, m_n} \delta(\omega' - \xi_{mn}),
\]

\[
\xi_{mn} = E_m - \mu N_m - (E_n - \mu N_n)
\]

The derivation of this is just as easy as in the zero-temperature case. Note that there is an idea of detailed balance of reversed transition rates associated with the exponential factor [35]. It follows from the recognition that \(\rho_m = \rho_n e^{-\beta \xi_{mn}}\). To make a closer contact with Eq. (12) we may insert \(\psi_\alpha(0) = \sum_k a_k^{\alpha*}\), and make \(\delta_{\theta k, \mathbf{p}, m_n}\) vanish by restricting the \(n, m\) sums so that \(|n, m| \to |n, m; k|\) [3]. The real and imaginary parts may be separated as

\[
\text{Re} G_{eq}(k, \omega) = P \int_{-\infty}^{\infty} d\omega' A_{eq}(k, \omega') \left( 1 \oplus e^{-\beta \omega'} \right) \frac{1}{\omega - \omega'} \tag{109}
\]

\[
\text{Im} G_{eq}(k, \omega) = -\pi \int_{-\infty}^{\infty} d\omega' A_{eq}(k, \omega') \times \left( 1 \oplus e^{-\beta \omega'} \right) \delta(\omega - \omega') = -\pi A_{eq}(k, \omega) \left( 1 \oplus e^{-\beta \omega} \right) \tag{110}
\]

For the retarded and advanced functions we obtain similarly

\[
G_{eq}^{R}(k, \omega) = \int_{-\infty}^{\infty} d\omega' A_{eq}(k, \omega') \left\{ \frac{1 \oplus e^{-\beta \omega'}}{\omega - \omega' + i\eta} \right\} \tag{111}
\]

\[
G_{eq}^{A}(k, \omega) = \int_{-\infty}^{\infty} d\omega' A_{eq}(k, \omega') \left\{ \frac{1 \oplus e^{-\beta \omega'}}{\omega - \omega' - i\eta} \right\}
\]

and

\[
\text{Re} G_{eq}^{R,A}(k, \omega) = \text{Re} G_{eq}(k, \omega)
\]

\[
\text{Im} G_{eq}^{R,A}(k, \omega) = \mp \pi A_{eq}(k, \omega) \left( 1 \oplus e^{-\beta \omega} \right)
\]

Upon defining the spectral density

\[
\rho_{eq}(k, \omega) = i[G_{eq}^{R}(k, \omega) - G_{eq}^{A}(k, \omega)] = 2\pi A_{eq}(k, \omega)(1 \oplus e^{-\beta \omega}) \tag{113}
\]

Eqs. (112) may again we written as

\[
G_{eq}^{R,A}(k, \omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \rho_{eq}(k, \omega') \pm i\eta \tag{115}
\]

The equilibrium density of states may still be defined with Eqs. (31) and (114), but we shall not repeat the expression here. (Note: no confusion should arise from the double use of the symbol \(\rho_{eq}\) here.) From the above expressions for \(G\) and \(G^{R,A}\) we may again derive some important symmetry relations, valid at real frequencies [10]:

\[
\text{Re} G_{eq}^{R,A}(k, \omega) = \text{Re} G_{eq}(k, \omega)
\]

\[
\text{Im} G_{eq}^{R,A}(k, \omega) = \pm \text{Im} G_{eq}(k, \omega) \frac{1 \oplus e^{-\beta \omega}}{1 \oplus e^{-\beta \omega}} \tag{116}
\]

\[
G_{eq}^{R}(k, \omega) = \left[ G_{eq}^{A}(k, \omega) \right]^* \tag{117}
\]

Compare these with Eq. (21), with which they should coincide in the limit \(\beta \to \infty\). In fact, all of the present results should simplify to the \(T = 0\) results of Sec. II A 1. Equation (116) may be used to obtain the functions \(G^{R,A}\) if \(G\) is known. Indeed, there is no regular perturbation theory for calculating \(G^{R,A}\) directly like there is for \(G\) in equilibrium (namely, the Matsubara formalism), and for \(G\) in general [10]. The Matsubara functions (i.e., \(G\) at imaginary times) have a simple perturbation expansion, and \(G^{R,A}\) may be obtained from this by analytic continuation. However, we shall not discuss the Matsubara technique here; see Refs. [3, 10] for example.

We have not yet discussed the form of the Keldysh function. This may be obtained by using the symmetry \(G_K = 2G - G^R - G^A\) or by an explicit calculation, either of which which yields

\[
G_K(k, \omega) = -2\pi i A_{eq}(k, \omega)(1 \oplus e^{-\beta \omega}). \tag{118}
\]

In this way we find the very important relation

\[
G_{eq}^{K}(k, \omega) = \frac{1 \oplus e^{-\beta \omega}}{1 \oplus e^{-\beta \omega}} \left[ G_{eq}^{R}(k, \omega) - G_{eq}^{A}(k, \omega) \right]
\]

\[
= -i \frac{1 \oplus e^{-\beta \omega}}{1 \oplus e^{-\beta \omega}} \rho_{eq}(k, \omega) \tag{119}
\]

Thus in equilibrium the Keldysh function is redundant, since it is obtainable from the retarded and advanced functions and the known distribution function \(h(\omega) = (1 - e^{-\beta \omega})/(1 + e^{-\beta \omega}) = \tanh(\beta \omega)/2\) (in case of fermions). This is related to the usual Fermi function \(f(\omega) = [\exp(\beta \omega) + 1]^{-1}\) by \(h = 1 - 2f\). All other \(G_{\pm \pm}\) may be obtained as well. For example the off-diagonal components of the original (contour-ordered) Keldysh representation become \(G_{\pm \pm}(k, \omega) = -f(\omega)[G^A(k, \omega) - G^R(k, \omega)] = if(\omega)\rho_{eq}(k, \omega)\) and \(G_{\pm \pm}(k, \omega) = [1 - f(\omega)]G^R(k, \omega) -
\( G^A(k, \omega) \) = \(-i[1 - f(\omega)]\rho_{eq}(k, \omega) \). Thus we see that the delta functions \( 2\pi \delta(\omega - \omega_0^0 + \mu/h) \) in Eqs. (105) have been replaced by the more general spectral functions \( \rho_{eq}(k, \omega) \), and the bare-particle distributions \( m_k \) by \( f(\omega) \).

We note that in the limit \( \beta \to \infty \) Eq. (118) simplifies to \( G^K = i \text{Im} G^K = (1 - 2\theta(\omega))(G^R - G^A) \). This is obtainable directly from Eqs. (12) and (19) or from Eq. (21), as was done in Eq. (29).

It should be noted here that the the above equilibrium relations for the contour-ordered and the Keldysh functions can be more straightforwardly derived by using the Fourier-transformed KMS relation, derived above.

As we know, in the quasiparticle picture we may return from the full \( G \) and \( G^{R,A} \) in terms of the spectral functions to “coarse-grained” Green’s functions which are of the noninteracting form apart from a renormalization of the spectrum etc. Therefore we still reproduce explicitly the results for the noninteracting fermion system in equilibrium [10]:

\[
G_{eq}^0(k, \omega) = \frac{1 - f(\omega)}{\omega - \omega_k^0 + \mu + i\eta} + \frac{f(\omega)}{\omega - \omega_k^0 + \mu - i\eta}
\]

\[
G_{eq}^{R,A}(k, \omega) = \frac{1}{\omega - \omega_k^0 + \mu \pm i\eta} - \frac{i \pi \delta(\omega - \omega_k^0 + \mu)}{\omega - \omega_k^0 + \mu \pm i\eta}
\]

These should agree with the general symmetries of Eqs. (116). Again we easily find that \( G^K_{eq}(\omega) = \tanh(\beta \omega/2)(G^R_{eq}(\omega) - G^A_{eq}(\omega)) \).

IV. GENERALIZATION TO SYSTEMS WITH COOPER-PAIR CONDENSATES

In this section we shall consider the case of Fermi systems where the Fermi surface of the noninteracting ground state has collapsed due to the presence of effectively attractive interactions. The collapse is associated with the formation of the so-called Cooper pairs, and at \( T = 0 \) all particles are in the Cooper-paired condensate.

There is an energy gap \( 2\Delta \) for single-particle excitations above the ground state, and this is interpreted roughly as the minimum energy needed for breaking up a Cooper pair. The new ground state does not exhibit discontinuities at \( k = k_F \) (in the bare-particle distribution functions, for example), and the separation between particle and hole excitations has become vague. In (conventional) superconducting metals the effective pairing interaction follows from interactions between electrons and the lattice phonons [36], whereas in superfluid \(^3\)He from more complicated \(^3\)He atom “paramagnon” interactions mediated by the fluid itself [20].

A. Introduction to the “\( F \) functions”

Different simplified models may be constructed to describe these phenomena, but they are all plagued by annoying difficulties in interpretation, even if they would be very successful in reproducing experimental results. This is because the condensation into bound pairs of particles is manifestly a many-particle phenomenon, and any model based on single particle quantities cannot be correct in a strict sense. In the language of Green’s functions this means that single-particle (or two-point) propagators alone are not sufficient. We should work with two-particle (four-point) functions and possibly higher-order ones in order keep things better defined. If we attempt to do without them by factorizing “\( \langle \psi \psi \psi \psi \rangle \to \langle \psi \psi \rangle \langle \psi \psi \rangle \rangle”, we must give up conservation of particle number in one way or another. And yet this is exactly what is always done, since working with the two-particle functions or any equivalent description is mathematically very complicated. With perturbation theory in mind, there is also another (although related) complication to be faced, which may be seen as follows.

In the case of normal systems, the Gell-Mann and Low theorem shows that an adiabatic switching-on of the interactions generates from the non-interacting ground state an eigenstate of the interacting system, which may well be the ground state (and usually is). But for superconductors the true ground state can not be generated adiabatically from the non-interacting Fermi sea. This is because we know that the ground-state energy cannot have a series expansion in the electron-phonon coupling constant \( g \) (due to the \( 2E_F - 2E_c \exp[-2/gN(0)] \) dependence of the energy of a Cooper-pair on the Fermi surface, with a surprisingly similar BCS result for \( k_BT_c \)), whereas the Gell-Mann and Low theorem gives the energy of the resulting eigenstate explicitly as \( E = E_0 + \langle \Phi_0 | K_1 | \Phi_0 \rangle / \langle \Phi_0 | \Phi_0 \rangle \), if \( K_0 | \Phi_0 \rangle = E_0 | \Phi_0 \rangle \). The state which is adiabatically generated from the Fermi sea is an eigenstate of the interacting superconductor, but not the ground state. In different terms, for some \( \lambda(t) = e^{-\eta(t)} \) between \( 0 < \lambda(t) < 1 \) during the switching on a “level crossing” occurs where the original ground state switches position with another state. Therefore, we should really start from a “noninteracting” ground state which already has the condensate, an associated energy gap, and other superconducting properties. (Or at least the model which we choose should result in these ground-state properties when the real interactions are turned on.) A non-interacting condensate is contradictory is a strict sense, but we may, for example, assume the presence of an infinitesimally small attractive interaction to start with. After all, due to presence of the Fermi sea and the Pauli exclusion principle, pairing on the Fermi surface is indeed possible for arbitrarily small attractive forces. This is in contrast to pairs of particles in empty space.

We start by following the usual practice of using single-particle propagators. In order to describe superconduc-
tivity, it turns out that we must introduce new types of “off-diagonal” or “anomalous” propagators, which are usually denoted with the letter $F$. The time-ordered, retarded, advanced, and Keldysh “$F$ functions” are defined symmetrically with the $G$ functions in Eq. (1)

$$
F(x_1, x_2) = -i\langle T \psi(x_1)\psi(x_2) \rangle
$$

$$
F^R(x_1, x_2) = -i\langle \psi(x_1)\psi(x_2) \rangle\theta(t_1 - t_2)
$$

$$
F^A(x_1, x_2) = i\langle \psi(x_1)\psi(x_2) \rangle\theta(t_2 - t_1)
$$

$$
F^K(x_1, x_2) = -i\langle \psi(x_1)\psi(x_2) \rangle
$$

(120)

Here the labels $x_i = (x_i, \sigma_i, t_i)$ have a similar, varying interpretation as before. Similar definitions exist for the path ordered, and Matsubara functions, etc. At this point we do not worry about the details of how to calculate any of these, nor the reason for doing it in the first place — the symmetric definitions are required by aesthetics, if nothing else! However, we mention that anomalous averages of the type $\langle \psi\psi \rangle$, $\langle \psi^\dagger\psi^\dagger \rangle$, may be attributed to the presence of so-called off-diagonal (in the density matrix) long-range order (ODLR) in the condensate [10]. With perturbation theory in mind, we attempt to introduce the anomalous functions for both interacting ($F$) and non-interacting ($F^0$) systems. In the latter case certain models for the unperturbed Hamiltonian (the BCS model, say) will have to be assumed to obtain explicit results. Nevertheless, in a perturbative approach it is not particularly important which model is chosen, as we shall discuss later on.

As was pointed out in the introductory section, finding good sources for the perturbative treatment of (triplet) superconductors appears to be difficult. Consequently, some of the discussion below is subject to some doubt. However, in the beginning sections we concentrate on the case of a singlet-paired superfluid, for which better references are available. Thus we only consider first the properties of the function $F(x_1, x_2) \equiv F_{11}(x_1t_1, x_2t_2)$. Generalizations to more general cases should be straightforward, or so it seems to me. Again, I begin with Ref. [2], and then move on to concoct the story as best I can.

### B. Exact results from spectral decompositions

#### 1. Lehmann representation for $F$ at zero temperature

If we want to work with states of well-defined particle number, then the only reasonable way to define the “anomalous propagator” $F$ (at $T = 0$) is the following [2]:

$$
F(x_1, x_2) = -i\langle \Psi_0(N)|T\psi_1(x_1)\psi_1(x_2)\Psi_0(N + 2) \rangle
$$

(121)

Here $\Psi_0(M)$ is the interacting ground state of the particle-conserving Hamiltonian $K$ for a superconductor with $M$ particles ($M/2$ pairs). The amplitude must be calculated between states with different $M$ (thus it is off-diagonal in Fock, or occupation number space), which leads to some ambiguity with respect to the interpretation, but this is unavoidable. Note, for example, that we cannot add a normalization denominator $\langle \Psi_0(N + 2)|\Psi_0(N) \rangle$ since this vanishes — something else must be done. Actually, a similar “problem” of interpretation occurred already with the Lehmann expansion of $G$ in normal systems, where off-diagonal expectation values were also essential. This expansion may now be done for $F$ also. Assuming (space and time) translational invariance, then, by Fourier transforming Eq. (121), the propagator may be written

$$
F(k, t) = -i\langle \Psi_0(N)|T a_{k\uparrow}(t)a_{-k\downarrow}(0)|\Psi_0(N + 2) \rangle
$$

(122)

The signs of the momentum indices $\pm k$ of the $a_k$ and $a^\dagger_{-k}$ operators must be opposite because of conservation of total momentum. If the condensate were moving with momentum $q$ per pair, then the indices would be $q/2 \pm k$, but this gives a phase $e^{iqR}$ which varies with position $R = (x_1 + x_2)/2$ — in contradiction to our assumption of translational invariance. We shall not worry about this supercurrent-carrying case here.

Now, assuming the existence of a complete set of eigenvectors $|\Psi_n \rangle$ and eigenvalues $K_n = E_n - \mu N_n$ of $K$ (for system of $N_n = N + 1$ particles) $F$ may be decomposed as

$$
F(k, t) = -i\int_0^\infty A(k, \omega) \exp[-i\omega|t|]
$$

(123)

where we define only one spectral function

$$
A(k, \omega) = \sum_n \langle \Psi_0(N)|a_{k\uparrow}\Psi_n \rangle \times \langle \Psi_n|a_{-k\downarrow}\Psi_0(N + 2) \rangle \delta(\omega - \xi_n)
$$

(124)

$$
= -\sum_n \langle \Psi_0(N)|a_{-k\downarrow}\Psi_n \rangle \times \langle \Psi_n|a_{k\uparrow}\Psi_0(N + 2) \rangle \delta(\omega - \xi_n)
$$

The second equality in Eq. (124) follows simply from the equal-time commutation relation. As before, the positive excitation energies $\xi_n$ are given by $E_n(N + 1) - E_0(N) = \xi_n + \mu$ (cf. discussion for the normal case). By assuming time-reversal symmetry and using Eq. (124) it may be shown that $A = A^*$ and thus $A$ is a real function [2]. We shall assume this below for simplicity, but it is not true in general. If we make a global gauge transformation on all destruction operators $a_{\pm k, \uparrow}$ with the phase factor $e^{i\phi/2}$, then $A$ obtains a factor $e^{i\phi}$. We call this phenomenon broken gauge symmetry. In the $G$ functions this would not happen since they contain an equal number of creation and destruction operators.

The time Fourier transform of Eq. (123) is

$$
F(k, \omega) = \int_0^\infty d\omega' A(k, \omega') \left\{ \frac{1}{\omega - \omega' + i\eta} - \frac{1}{\omega + \omega' - i\eta} \right\}
$$

(125)
and this is the Lehmann representation of $F$. Since we have not specified the properties of the Hamiltonian $K$, there is little to be said about the excitation energies $\xi_{0\alpha}$ — we cannot even see directly if there is a gap or not. However, note that the poles of $F$ occur in pairs, symmetrically with respect to the origin of complex $\omega$ plane. The retarded and advanced functions $F^{R,A}$ may thus be defined in a similar fashion as for normal systems, by shifting the poles between upper and lower half-planes, and the Keldysh function is obtained with the symmetry $F^{K} = 2F - F^{R} - F^{A}$. We return to discuss these below. The $G$ and $G^{R,A,K}$ functions remain formally the same as in normal systems — only the excitation spectrum has supposedly been changed (Sec. II A 1).

For the noninteracting case $|\Psi_0\rangle = |\Phi_0\rangle$ and by extracting the time dependence from the Heisenberg operators (by using the formulas in the Appendix), assuming $K_0$ to be quadratic and particle-conserving and with the eigen-energies changing sign at $|k| = k_F$ as before, we find (cf Eq. (15))

$$G^{0}(k,t) = -i\theta(t)A_{+}(k)\exp(-iE_{k}t) + i\theta(-t)A_{-}(k)\exp(iE_{k}t)$$

$$F^{0}(k,t) = -iA(k)\exp[-iE_{k}|t|]$$

where the prefactors are again simply the bare-hole and bare-particle distribution functions $A_{+}(k) = \langle \Phi_{0}(N)|a_{k\uparrow}\Phi_{0}(N)\rangle$, $A_{-}(k) = \langle \Phi_{0}(N)|a_{k\downarrow}\Phi_{0}(N)\rangle$, $= 1 - A_{+}(k)$ and the “particle-hole” distribution, or pair amplitude $A(k) = \langle \Phi_{0}(N)|a_{k\uparrow}a_{-k\downarrow}|\Phi_{0}(N + 2)\rangle$. A time transformation gives

$$G^{0}(k,\omega) = \frac{A_{+}(k)}{\omega - E_{k} + i\eta} + \frac{A_{-}(k)}{\omega + E_{k} - i\eta}$$

$$F^{0}(k,\omega) = \frac{A(k)}{\omega - E_{k} + i\eta} - \frac{A(k)}{\omega + E_{k} - i\eta}$$

The result for $G^{0}$ is similar to Eq. (16) but with $A_{\pm}$ in the nominator instead of unity. Thus we see that the distribution functions $A_{\pm}$ and $A$ appear as the residues of poles of these propagators, and $A_{\pm}$ are not necessarily equal to step functions $\theta(\pm|k| - k_F)$ (in fact they are not even discontinuous, since there is no Fermi surface anymore — see below).

Now as you realize, the distributions and the excitation energies $E_{k}$ grow $0$ are still undetermined, and we cannot proceed further unless we know the non-interacting Hamiltonian $K_0$ and its ground state $|\Phi_0\rangle$ explicitly. If we take $K_0$ to be the Hamiltonian of a non-interacting electron system, then $|\Phi_0\rangle$ is the Fermi sea, $F^{0}$ vanishes (in the thermodynamic limit, at least?) and $G^{0}$ reduces to the result of the previous section — and this conclusion is absolutely correct! But as we said, the Fermi sea is not a good starting point for perturbation theory, since the latter is supposed to construct a finite $F$ for the interacting system from $F^{0}$ of the noninteracting system, and this is not possible if $F^{0} = 0$. Therefore we must use some kind of a model Hamiltonian, which would give us the energies $E_{k}$ and finite values for all of the three amplitudes. An important requirement for the model is that the resulting $E_{k}$’s should exhibit an energy gap, i.e., a nonzero minimum. This may be achieved at least with the “BCS model”, where we allow for a particle non-conserving Hamiltonian, and an associated ground state which is a superposition of many states with differing particle numbers. We now turn to explain this model.

2. Unperturbed propagators in the BCS model

As an explicitly calculable model, we consider the following “off-diagonal” or “anomalous” (or ”BCS”) mean-field Hamiltonian $K_{0} = T + V_{mf}$ for a singlet-paired superconductor

$$K_{0} = \sum_{k\alpha} \int d^{3}x \varphi_{\alpha}(x) \left[ -\frac{\hbar^{2}\nabla^{2}}{2m} - \mu \right] \psi_{\alpha}(x)$$

$$+ \int d^{3}x d^{3}y [\Delta^{0}(x,y)\varphi_{\uparrow}(x)\varphi_{\downarrow}(y)$$

$$+ \Delta^{0\ast}(x,y)\psi_{\uparrow}(y)\psi_{\downarrow}(x)]$$

(The constant term proportional to $|\Delta^{0}|^2$ often appearing in the end is dropped along with any ”diagonal” mean-field contributions. See below for more discussion.) In the momentum representation (assuming translational invariance, and a real $\Delta^{0}(x - y)$), we get something like

$$K_{0} = \sum_{k\alpha \sigma} (\epsilon_{k}^{0} - \mu) a_{k\alpha\sigma}^{\dag} a_{k\alpha\sigma} + \sum_{k\sigma} \Delta_{k}^{0}(a_{k\uparrow\sigma}^{\dag} a_{-k\downarrow\sigma}^{\dag} + a_{-k\downarrow\sigma} a_{k\uparrow\sigma})$$

This can be diagonalized with the canonical Bogoliubov transformation $a_{k\sigma}^{\dag} = u_{k} a_{k\sigma}^{\dag} + v_{k} a_{-k\sigma}$ or

$$a_{k\uparrow}^{\dag} = u_{k} a_{k\uparrow}^{\dag} + v_{k} a_{-k\downarrow}$$

$$a_{-k\downarrow} = -v_{k} a_{k\uparrow}^{\dag} + u_{k} a_{-k\downarrow}$$

so that

$$K_{0} = \sum_{k\sigma} E_{k} u_{k\sigma}^{\dag} a_{k\sigma} + \sum_{k\sigma} \xi_{k}^{0} v_{k}^{2}$$

if we choose $u_{k}$ and $v_{k}$ such that

$$u_{k} = \sqrt{\frac{1}{2} + \frac{\epsilon_{k}^{0}}{2E_{k}}}$$

$$v_{k} = \sqrt{\frac{1}{2} - \frac{\epsilon_{k}^{0}}{2E_{k}}}$$

$$\xi_{k}^{0} = \epsilon_{k}^{0} - \mu, \quad E_{k} = \sqrt{(\xi_{k}^{0})^2 + (\Delta_{k}^{0})^2}.$$
where \( |0\rangle \) is the vacuum state for the bare particles created by \( a^\dagger \) (i.e., state with no particles at all). These choices give the noninteracting propagators, Eqs. (126) and (127), with the amplitudes \( A_+ (k) = u_k^2 \), \( A_-(k) = v_k^2 \), and \( A(k) = u_k v_k \). Written explicitly they are

\[
\begin{align*}
G^0(k, t) &= -i \theta(t) u_k^2 \exp(-i E_k t) + \theta(-t) v_k^2 \exp(i E_k t) \\
F^0(k, t) &= -i u_k v_k \exp[-i E_k |t|]
\end{align*}
\] (134)

and in frequency space

\[
\begin{align*}
G^0(k, \omega) &= \frac{u_k^2}{\omega - E_k + i\eta} + \frac{v_k^2}{\omega + E_k - i\eta} \\
F^0(k, \omega) &= \frac{u_k v_k}{\omega - E_k + i\eta} - \frac{u_k v_k}{\omega + E_k - i\eta}
\end{align*}
\] (135)

As an exercise you may now write the corresponding expressions for \( F^{R,A,K}_{R,A} \) and use the excitation spectrum \( E_k \) to obtain the density of states \( N_0(\omega) \) for the BCS model [45]. The gap \( |\Delta| \) should be visible there also. In the quasiparticle picture of an interacting system this corresponds to the DOS of elementary excitations, not the full density of eigenstates.

Although this procedure gives us what we wanted, it should be kept in mind that it is only a crude model — one out of many possible, in principle at least. For perturbation theory it is only important to know that nonzero \( F^0 \) functions may be defined, and that contractions may be generalized to include pairs of \( a \) or \( a^\dagger \) operators. For this we must re-define the meaning of normal ordering, and with the \( \alpha \) operators this is easy. A normal-ordered product \( \mathcal{N}(a_{1}a_{2}\cdots a_{i}a_{i}^\dagger a_{2}\cdots) \) of operators is such that all \( a^\dagger \) operators are on the left, whereas \( a \)’s are on the right: after all \( a|0\rangle = 0 \). When re-expressed again with the bare-particle operators we have

\[
\begin{align*}
\mathcal{N}(a_{\alpha}^\dagger a_{\alpha}) &= a_{\alpha}^\dagger a_{\alpha} - u_k^2 \\
\mathcal{N}(a_{\alpha} a_{-\alpha}) &= a_{\alpha} a_{-\alpha} - \sigma u_k v_k \tag{136}
\end{align*}
\]

If the contraction is defined as usual \( \langle UV \rangle = U^{**}V^{*} = \mathcal{T}(UV) - \mathcal{N}(UV) \), so that \( U^{**}V^{*} = \langle \Phi_0|T(UV)|\Phi_0 \rangle \), then

\[
\begin{align*}
a_{\alpha\sigma}(t) a_{\alpha^\prime\sigma^\prime}(t') &= i G_{\alpha\beta}^0(k, t, t') \\
a_{\alpha\sigma}(t) a_{\alpha^\prime\sigma^\prime}(t') &= i F_{\alpha\beta}^0(k, t, t') \tag{137}
\end{align*}
\]

As you see, this no longer makes any reference to the parameters of the model, \( u_k, v_k, \Delta_0^k \), or the Bogoliubov operators. We may thus forget about the details (including the actual form of the noninteracting ground state) and use these contractions in perturbation expansions in a completely formal way. Below we generalize the mean-field Hamiltonian of Eq. (128) to include general pairing. In that case we no longer need to go into such practical details as above.

3. Functions \( F^{R,A,K} \), symmetries, and finite-temperature results

Here we briefly collect some further results. The details in many cases would be very similar to the corresponding results for \( G \) which were discussed previously. The retarded and advanced functions have the decompositions

\[
\begin{align*}
F^{R,A}(k, \omega) &= \int_0^\infty d\omega' A(k, \omega') \\
&\quad \times \left\{ \frac{1}{\omega - \omega' \pm i\eta} - \frac{1}{\omega + \omega' \pm i\eta} \right\} \tag{138}
\end{align*}
\]

whereas in the unperturbed system

\[
F^{R,A}_0(k, \omega) = \frac{A(k)}{\omega - E_k \pm i\eta} - \frac{A(k)}{\omega + E_k \pm i\eta} \tag{139}
\]

The Keldysh function is obtained with \( F^K = 2F - F^R - F^A \) and is easily found to satisfy \( F^K(k, \omega) = \theta(\omega) F^R(k, \omega) - \theta(-\omega) F^A(k, \omega) = [1 - 2\theta(\omega)][F^R(\omega) - F^A(\omega)] \). If the spectral function \( A(k, \omega) \) [or pair amplitude \( A(k) \)] is assumed to be real, then for real frequencies we again have

\[
\begin{align*}
\text{Re} F(k, \omega) &= \text{Re} F^R(k, \omega) = \text{Re} F^A(k, \omega) \\
\text{Im} F(k, \omega) &= \text{Im} F^{R,A}(k, \omega) \quad \text{for } \omega \geq 0 \\
F^R(k, \omega) &= [F^A(k, \omega)]^* \tag{140}
\end{align*}
\]

The spectral function \( A(k, \omega) \) is normalized to the pair amplitude \( A(k) \equiv \langle \Psi_0(N)|a_{k\uparrow} a_{-k\downarrow}|\Psi_0(N+2) \rangle \)

\[
\int_0^\infty d\omega A(k, \omega) = \langle \Psi_0(N)|a_{k\uparrow} a_{-k\downarrow}|\Psi_0(N+2) \rangle = A(k) \tag{141}
\]

We may also define the “anomalous spectral density”

\[
\rho_F(k, \omega) \equiv i [F^R(k, \omega) - F^A(k, \omega)]
= 2\pi \int_0^{\infty} [A(k, \omega') \theta(\omega) - A(k, -\omega') \theta(-\omega)] \tag{142}
\]

which is normalized to zero

\[
\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \rho_F(k, \omega) = 0 \tag{143}
\]

For completeness, we may also define the “anomalous density of states” or “Cooper-pair density of states”

\[
N_F(\omega) \equiv \frac{1}{2\pi} \sum_k \rho_F(k, \omega) \tag{144}
\]

Never mind what the interpretation of all of these should be. Finally we note that in equilibrium at finite temperatures, there exists a similar “generalized Lehmann representation” as for \( G_{\alpha\beta} \) in Eq. (109). The main difference is that the transition probability \( |\langle \Psi_m|\Psi_\alpha(0)|\Psi_n \rangle|^2 \)
will be replaced by \( \langle \Psi_m \mid \psi_t(0) \mid \Psi_n \rangle \langle \Psi_n \mid \psi_0(0) \mid \Psi_m \rangle \). Apparently, based on this analysis, we should again find all the results of Sec. III C 2 for \( F \). In particular, we mention

\[
F_{eq}^K(k, \omega) = \tanh(\beta \omega/2) \left[ F_{eq}^R(k, \omega) - F_{eq}^A(k, \omega) \right].
\]  

All in all, we see that the \( F, F^{R,A,K} \) functions satisfy exactly the same relations between each other as the \( G, G^{R,A,K} \) functions do.

C. Construction of Nambu matrices and the particle-hole space

1. Matrix propagator and particle-hole space

If we write down the equations of motion for \( G(x_1,x_2) \) and \( F(x_1,x_2) \), using the Hamiltonian (128), it turns out that we are led introduce two new time-ordered propagators

\[
\hat{G}(x_1,x_2) = -i \langle T \psi^\dagger(1) \psi(2) \rangle \quad \hat{F}(x_1,x_2) = -i \langle T \psi^\dagger(1) \psi(2) \rangle
\]

where \( \hat{G}(x_1,x_2) = -G(x_2,x_1) \). Similar definitions exist for \( \hat{G}^{R,A,K} \) and \( \hat{F}^{R,A,K} \). When we write the EOM's for these new propagators also, we find a closed system of equations, which may be written in matrix form by combining the four propagators \( G, F, \hat{G}, \) and \( \hat{F} \) into a matrix propagator

\[
\hat{G}(x_1,x_2) = \left[ \begin{array}{cc} G(x_1,x_2) & F(x_1,x_2) \\ \hat{F}(x_1,x_2) & \hat{G}(x_1,x_2) \end{array} \right] 
\]

\[
= -i \langle T \left[ \psi(1) \psi^\dagger(2) \quad \psi(1) \psi^\dagger(2) \right] \psi^\dagger(1) \psi(2) \rangle
\]

\[
\hat{G}_{eq}(x_1,x_2;\omega) = \tanh(\beta \omega/2) \left[ \hat{G}_{eq}^R(x_1,x_2;\omega) - \hat{G}_{eq}^A(x_1,x_2;\omega) \right]
\]

at real frequencies \( \omega \). Most of the other results and definitions Sec. III C 2 are also easily generalized for the full Nambu matrices.

The above definition [Eq. (147)] may be made more transparent by introducing yet another two-dimensional degree of freedom (in addition to spin and the Keldysh index) to the field operators, namely the particle-hole index. Thus \( \hat{G} \) is said to be a matrix in particle-hole space, or Nambu space [18]. We shall also call matrices of the type in Eq. (147) \( \text{Nambu matrices} \). The present approach is my own, so beware. Let us first define the nonlocal “pseudospinor” [42] operators

\[
\hat{\Psi}(x_1, x_2) = \left[ \begin{array}{c} \psi_{\tau_1}(x_1,t_1) \\ \psi_{\tau_2}^\dagger(x_2,t_2) \end{array} \right], \quad \hat{\Psi}^\dagger(x_1, x_2) = \left[ \begin{array}{c} \psi_{\tau_1}^\dagger(x_1,t_1) \\ \psi_{\tau_2}(x_2,t_2) \end{array} \right]
\]

Using these we set \( \Psi(x) \equiv \hat{\Psi}(x,x), \Psi^\dagger(x) \equiv \hat{\Psi}^\dagger(x,x) \). The components \( \Psi_l(x) \) of this field are numbered with the “particle-hole” index \( l = p, n = +1, -1 \) so that \( \Psi_{\uparrow}(x) = \psi(x) \) and \( \Psi_{\downarrow}(x) = \psi^\dagger(x) \) and so on. Using these operators the Nambu matrix propagator may be written as

\[
\hat{G}_{eq}(x_1,x_2) = -i \langle T \Psi_l(x_1) \Psi^\dagger_l(x_2) \rangle
\]

Obviously we may also define

\[
\hat{F}_{eq}(x_1,x_2) = -i \langle T \Psi^\dagger_l(x_1) \Psi_l(x_2) \rangle
\]

and so on, but these definitions are redundant. They only correspond to different “representations” of the particle-hole space: \( \hat{F} = \hat{G}_{\uparrow}, \hat{F} = \hat{G}_{\downarrow}, \hat{G} = \hat{G}_{\uparrow}, \hat{G} = \hat{G}_{\downarrow}. \) Note Sometimes [1] we may use \( \Psi_n \) with the Nambu index \( n = 1, 2, 3, 4 \) to cover the whole four-dimensional spin-Nambu space so that \( \Psi_1 = \psi_1, \Psi_2 = \psi_4, \Psi_3 = \psi_1^\dagger, \) and \( \Psi_4 = \psi_4^\dagger \).

The original field operators \( \psi, \psi^\dagger \) must satisfy the Fermionic equal-time commutation relations as usual \( \{ \psi_\alpha(x,t), \psi^\dagger_\beta(y,t) \} = \delta_\alpha_\beta \delta(x - y), \)}
and \( \{ \psi_\alpha(x,t), \psi_\beta(y,t) \} = 0 \). However, defined as above, the “pseudospinor” operators only satisfy \( \{ \Psi_\alpha(x,t), \Psi_\beta(y,t) \} = \delta_{\alpha\beta} \delta(x-y) \), and \( \{ \Psi_j(x,t), \Psi_j(y,t) \} = (1 - \delta_{j\ell}) \delta(x-y) \), where \( x, y \) include the spin variables. Therefore we must be careful not to assume too much when manipulating expressions containing these operators. One way to get over this potential difficulty seems to be via the redefinitions \( \Psi(x) \equiv \Psi^+(x^+,x^-) \), \( \Psi^+(x) \equiv \Psi^+(x^+,x^-) \). Thus \( \Psi_j(x) = \psi(x^+) \) and \( \Psi_k(x) = \psi(x^-) \) and so on. Here \( x^\pm \) means that \( t_{1,2} = t, \sigma_{1,2} = \sigma, \ x_{1,2} = x \pm \eta a \), where \( a \) is arbitrary and \( \eta \to 0 \) after calculations. Using these we obtain the normal commutation relations: \( \{ \Psi_j(x,t), \Psi_{j'}^+(y,t) \} = \delta_{jj'} \delta(x-y) \), and \( \{ \Psi_j(x,t), \Psi_{j'}(y,t) \} = 0 \). For the latter of these to be valid we must note the difference between the expressions \( \delta(x - y^+) = 0 \) and \( \delta(x^\pm - y^\pm) = \delta(x - y) \). The limiting procedure is therefore essential if we wish to write the commutation relations in the familiar form, but it is not otherwise necessary.

The above pseudospinor fields are most commonly introduced only for singlet pairing in the absence of magnetic effects. The definition is more straightforward then: \( \Psi(x) = [\psi_\uparrow(x) \psi_\downarrow(x)]^T \), \( \Psi^+(x) = [\psi_\uparrow(x) \psi_\downarrow(x)]^T \), and the Fermionic commutation relations are preserved without problems [18]. Furthermore, expectation values of the type \( \langle \Psi \Psi^\dagger \rangle \) vanish automatically, since they correspond to triplet amplitudes \( \langle \psi_\uparrow \psi_\downarrow \rangle \) or spin-flip amplitudes \( \langle \psi_\uparrow \psi_\downarrow \rangle \) [10]. These make the handling of perturbation theory formally analogous to the normal-state case, there being no need to refer to the original operators \( \psi, \psi^\dagger \). Similar definitions may also be done in K space. As an example for a singlet [10] we define \( A_k(\omega) = [a_{k\uparrow}^\dagger(\omega) a_{-k\downarrow}(\omega)]^T \), and \( A_{-k}(\omega) = [a_{k\downarrow}^\dagger(\omega) a_{-k\uparrow}(\omega)]^T \). For the general (triplet) case, see Ref. [47].

2. Equation of motion for the unperturbed Nambu propagator

We now derive an equation of motion for the time-ordered Nambu matrix propagator, Eq. (150), in the noninteracting (and equilibrium) case. To this end, we start with the generalized mean-field Hamiltonian in Schrödinger picture

\[
K_0(t) = \int \int dx dy \psi_\uparrow(x)^T [T(x,y,t) + U^0(x,y,t)] \psi_\downarrow(y) + \int \int dx dy \Delta^0(x,y,t) \psi_\uparrow(y) \psi_\downarrow(x) \]

(152)

where \( T(x,y,t) = \delta(x - y) \xi^0(-i \hbar \nabla_y - q A(y,t)) \), while \( U^0(x,y,t) \) and \( \Delta^0(x,y,t) \) are some single-particle and “particle-hole” potentials which are in nonlocal in space, but not in time. However, since we are now discussing an equilibrium system, \( K_0(t) \) should have at most an adiabatic explicit time dependence. Furthermore, \( U^0 \) and \( \Delta^0 \) should always be considered as infinitesimal “generating fields” in any case — all external potentials \( U = V_{ext} \), time-dependent or not, will generally be introduced separately whenever needed. The general form of the equations will, however, be clearer if we include \( U^0 \) and \( \Delta^0 \) explicitly, and with the time dependences included. For certain purposes we may also need to introduce time-nonlocal generating fields \( U^0(x,t,y,t') \) and \( \Delta^0(x,t,y,t') \), but this generalization is rather trivial. Note again that \( x \) and \( y \) contain the spin variables, so that the integrals include a spin sum.

By transforming to the Heisenberg picture and using the Heisenberg equation of motion \( i \hbar \partial \psi(t)/\partial t = [\psi(t), K_{H0}(t)] \) we easily find

\[
i \hbar \partial \psi(t) = \int dy [T(x,y,t) + U^0(x,y,t)] \psi(y,t) - \int dy \Delta^0(x,y,t) \psi(y,t)
\]

(153)

By making use of the Nambu operators these may be written compactly in the form

\[
i \hbar \partial \Psi(t) = \int dy [i \hbar \tilde{K}_0(x,y,t) \Psi(y,t) \]

(154)

\[
i \hbar \partial \Psi_1(t) = -\int dy [K_0(x,y,t)^* \Psi(y,t)
\]

where we introduced the Nambu matrix operator

\[
\tilde{K}_0(x,y,t) = \begin{bmatrix} T(x,y,t) + U^0(x,y,t) & -\Delta^0(x,y,t) \\ \Delta^0(x,y,t) & -T^*(x,y,t) + U^0(x,y,t) \end{bmatrix}
\]

(155)

and a matrix multiplication of \( \tilde{K}_0 \) and \( \Psi \) is implied. Equation (155) is a Nambu and position-space representation of the Hermitian operator \( K_0 \). Indeed, the Schrödinger Hamiltonian of Eq. (152) itself may be written as

\[
K_0(t) = \int \int dx dy [\Psi_1^\dagger(x) \tilde{K}_0(x,y,t) \Psi_1^\dagger(y,t) + \text{const}]
\]

(156)

and using this with the anticommutation relations for \( \Psi \) and \( \Psi_1 \). Eq. (154) may be directly reproduced from the Heisenberg equation \( i \hbar \partial \Psi_1(t)/\partial t = [\Psi_1(t), K_{H0}(t)] \). The Hamiltonian may furthermore be diagonalized with a generalized Bogoliubov transformation. This transformation is a unitary “rotation” of the Nambu space coordinates, rather similar to that done in Keldysh space.
before [10, 48]. Now, if we differentiate Eq. (150) with respect to the first time coordinate \( t_1 \), and use Eq. (154) along with the commutation relations, we obtain

\[
\begin{align*}
\imath \hbar \left( \frac{\partial}{\partial t_1} \hat{G}^0_{t_1}(x_1 t_1, x_2 t_2) \right) &= + \hbar \delta(t_1 - t_2) \langle \{ \Psi_t(x_1 t_1), \Psi_t^\dagger(x_2 t_2) \} angle \\
&= - \imath \langle T \hbar \left( \frac{\partial}{\partial t_1} \Psi_t(x_1 t_1) \right) \Psi_t^\dagger(x_2 t_2) \rangle \\
&= + \hbar \delta(t_1 - t_2) \delta(x_1 - x_2) \\
&\quad + \sum_{m=p, h} \int \! dt \tilde{K}_{tm}(x_1, y_t) \hat{G}^0_{mt}(y_t, x_2 t_2)
\end{align*}
\]

which is obtained by differentiating with respect to \( t_2 \), and we shall need them later on. However, Eqs. (157,158,159) represent the first and most important step toward what we set out to do. Below they will be supplemented with similar equations for the \( \hat{G}^+, \hat{G}_{0+}^-, \) and \( \hat{G}^+, \hat{G}^- \) alone and everything gets more complicated.

We may transform Eq. (157) to a more transparent form \( \hat{G}^{-1} \hat{G} = \hat{1} \), or more explicitly

\[
\int \! dx \int \! dt \hat{G}^{-1}(x_1 t_1, x_3 t_3) \hat{G}^0(x_3 t_3, x_2 t_2) = \hbar \hat{1} \delta(x_1 - x_2) \delta(t_1 - t_2)
\]

if we define the (left) inverse operator of \( \hat{G}^0 \) with

\[
\hat{G}^{-1}(x_1 t_1, x_3 t_3) = \delta(t_1 - t_3) \left[ \hat{1} - \hat{K}_0(x_1, x_3; t_3) \right]
\]

Here \( \hat{1} \) is the unit matrix in Nambu space. Using the specific form \( T(x, y; t) = \delta(x - y) \xi_0 (-i \hbar \nabla_y - q \mathbf{A}(y, t)) \) and \( T^*(x, y) \) this operator may be written as

\[
\hat{G}^{-1}(x_1 t_1, x_3 t_3) = \delta(t_1 - t_3) \xi_0 \left[ \hat{1} + \frac{\delta(t_1 - x_3)}{\partial t_3} + \delta(t_1 - x_3) \xi_0 \nabla x_3 - q \mathbf{A} \right]
\]

where \( \xi_0 \) is the Pauli matrix in Nambu space, and where we defined the Nambu matrix potential

\[
\hat{\Sigma}^0(x, y; t) = \begin{bmatrix} U^0_{\psi}(x, y; t) & - \Delta^0_{\psi}(x, y; t) \\ \Delta^0_{\psi}(x, y; t) & - U^0_{\psi}(x, y; t) \end{bmatrix}
\]

(Note in passing: the sign in the definition of \( \hat{\Sigma}^0 \) has been chosen correctly to comply with the sign of the self-energy \( \hat{\Sigma} \) in \( \hat{G} = \hat{G}^0 + \hat{G}^0 \hat{\Sigma} \) and thus \( \hat{G}^{-1} - \hat{\Sigma} \hat{G} = \hat{1} \) — see below.)

Similar “right-handed” equations \( \hat{G}_0 \hat{G}_0^{-1} = \hat{1} \) may be obtained by differentiating with respect to \( t_2 \), and we shall need them later on. However, Eqs. (157,158,159) represent the first and most important step toward what we set out to do. Below they will be supplemented with similar equations for the \( \hat{G}^+, \hat{G}_{0+}^-, \) and \( \hat{G}^+, \hat{G}^- \) alone and everything gets more complicated. We may transform Eq. (157) to a more transparent form \( \hat{G}^{-1} \hat{G} = \hat{1} \), or more explicitly

\[
\int \! dx \int \! dt \hat{G}^{-1}(x_1 t_1, x_3 t_3) \hat{G}^0(x_3 t_3, x_2 t_2) = \hbar \hat{1} \delta(x_1 - x_2) \delta(t_1 - t_2)
\]

if we define the (left) inverse operator of \( \hat{G}^0 \) with

\[
\hat{G}^{-1}(x_1 t_1, x_3 t_3) = \delta(t_1 - t_3) \left[ \hat{1} - \hat{K}_0(x_1, x_3; t_3) \right]
\]

Here \( \hat{1} \) is the unit matrix in Nambu space. Using the specific form \( T(x, y; t) = \delta(x - y) \xi_0 (-i \hbar \nabla_y - q \mathbf{A}(y, t)) \) and \( T^*(x, y) \) this operator may be written as

\[
\hat{G}^{-1}(x_1 t_1, x_3 t_3) = \delta(t_1 - t_3) \xi_0 \left[ \hat{1} + \frac{\delta(t_1 - x_3)}{\partial t_3} + \delta(t_1 - x_3) \xi_0 \nabla x_3 - q \mathbf{A} \right]
\]

where \( \xi_0 \) is the Pauli matrix in Nambu space, and where we defined the Nambu matrix potential

\[
\hat{\Sigma}^0(x, y; t) = \begin{bmatrix} U^0_{\psi}(x, y; t) & - \Delta^0_{\psi}(x, y; t) \\ \Delta^0_{\psi}(x, y; t) & - U^0_{\psi}(x, y; t) \end{bmatrix}
\]

(Note in passing: the sign in the definition of \( \hat{\Sigma}^0 \) has been chosen correctly to comply with the sign of the self-energy \( \hat{\Sigma} \) in \( \hat{G} = \hat{G}^0 + \hat{G}^0 \hat{\Sigma} \) and thus \( \hat{G}^{-1} - \hat{\Sigma} \hat{G} = \hat{1} \) — see below.)

Similar “right-handed” equations \( \hat{G}_0 \hat{G}_0^{-1} = \hat{1} \) may be obtained by differentiating with respect to \( t_2 \), and we shall need them later on. However, Eqs. (157,158,159) represent the first and most important step toward what we set out to do. Below they will be supplemented with similar equations for the \( \hat{G}^+, \hat{G}_{0+}^-, \) and \( \hat{G}^+, \hat{G}^- \) alone and everything gets more complicated.

We may transform Eq. (157) to a more transparent form \( \hat{G}^{-1} \hat{G} = \hat{1} \), or more explicitly

\[
\int \! dx \int \! dt \hat{G}^{-1}(x_1 t_1, x_3 t_3) \hat{G}^0(x_3 t_3, x_2 t_2) = \hbar \hat{1} \delta(x_1 - x_2) \delta(t_1 - t_2)
\]

if we define the (left) inverse operator of \( \hat{G}^0 \) with

\[
\hat{G}^{-1}(x_1 t_1, x_3 t_3) = \delta(t_1 - t_3) \left[ \hat{1} - \hat{K}_0(x_1, x_3; t_3) \right]
\]

Here \( \hat{1} \) is the unit matrix in Nambu space. Using the specific form \( T(x, y; t) = \delta(x - y) \xi_0 (-i \hbar \nabla_y - q \mathbf{A}(y, t)) \) and \( T^*(x, y) \) this operator may be written as

\[
\hat{G}^{-1}(x_1 t_1, x_3 t_3) = \delta(t_1 - t_3) \xi_0 \left[ \hat{1} + \frac{\delta(t_1 - x_3)}{\partial t_3} + \delta(t_1 - x_3) \xi_0 \nabla x_3 - q \mathbf{A} \right]
\]

where \( \xi_0 \) is the Pauli matrix in Nambu space, and where we defined the Nambu matrix potential

\[
\hat{\Sigma}^0(x, y; t) = \begin{bmatrix} U^0_{\psi}(x, y; t) & - \Delta^0_{\psi}(x, y; t) \\ \Delta^0_{\psi}(x, y; t) & - U^0_{\psi}(x, y; t) \end{bmatrix}
\]

(Note in passing: the sign in the definition of \( \hat{\Sigma}^0 \) has been chosen correctly to comply with the sign of the self-energy \( \hat{\Sigma} \) in \( \hat{G} = \hat{G}^0 + \hat{G}^0 \hat{\Sigma} \) and thus \( \hat{G}^{-1} - \hat{\Sigma} \hat{G} = \hat{1} \) — see below.)
orem, in the perturbation expansions. They may be interpreted as describing momentum-conserving conversion between particle and hole type excitations through the condensate (cf. “Andreev reflection”).

Nevertheless, we know that superconductivity should exist also when the particle number is conserved, and it should be possible to make the theory reflect this fact. As already mentioned, one way of keeping the conservation of particle number would be to consider only two-particle Green’s functions $\langle \psi \psi \bar{\psi} \bar{\psi} \rangle$ (and higher-order ones), since they are able to describe the coherent propagation of two-particle bound states as well as single-particle excitations [2, 5, 10]. It is in the factorization of the two-particle functions to products of one-particle functions where the interpretational difficulties appear [10]. However, although the concept of four-point functions is important for perturbation theory (see below), they are mathematically rather complicated and unintuitive to handle. Therefore one rather breaks them up into a sum of products of two-point functions by introducing the small term $V_{mf}$ and by applying Wick’s theorem, and accepts the accompanying difficulties with the apparent non-conservation of particles in the intermediate steps of propagation. Besides, the factorization must be done at some point in any case, to cut off the infinite hierarchy of equations which is generated by writing equations of motion for multiparticle Green’s functions [2, 10], and thus enable an approximate self-consistent theory. But even if the factorization is done, it is possible to formally retain particle conservation. The idea is that in turning on the interactions (screened Coulomb repulsion and the real pairing interaction etc.) in $K_1(t)$ adiabatically, one simultaneously subtracts $V_{mf}$ to make the final Hamiltonian (and the ground state) particle conserving again [2, 18]. Or, rather equivalently, one may simply set $\Delta^0 = 0$ after partially summing the infinite perturbation expansion for the Nambu matrix propagator [1]. This is the way of thinking we have chosen.

2. Diagrammatic analysis

Now we demonstrate briefly how the perturbation theory must be generalized in the presence of $V_{mf}$ in $K_0$. We assume $T = 0$, although the general equilibrium case may be treated similarly with the temperature Green’s functions. To be specific, we refer to the discussion of Sec. 3.9 of Ref. [3]. When anomalous pairings are taken into account, then the first-order expansion of Eq. (9.1) in that reference becomes

\[
iG^{(1)}_{\alpha \beta}(x, y) = -\frac{1}{\hbar} \sum_{\lambda \lambda', \mu \mu'} \int d^4x_1 d^4x_1' V(x_1, x_1') \lambda \lambda': \mu \mu' \\
\left\{ iG^0_{\alpha \beta}(x, y) [iG^0_{\mu \lambda}(x_1', x_1') G^0_{\lambda \lambda}(x_1, x_1) - iG^0_{\mu \lambda}(x_1', x_1) iG^0_{\lambda \lambda}(x_1, x_1') - iF^0_{\mu \lambda}(x_1', x_1) iF^0_{\lambda \lambda}(x_1, x_1')] \right. \\
+ iG^0_{\alpha \lambda}(x, x_1) [iG^0_{\mu \beta}(x_1', x_1') G^0_{\lambda \beta}(x_1, x_1) - iG^0_{\mu \beta}(x_1', x_1) iG^0_{\lambda \beta}(x_1, x_1') - iF^0_{\mu \beta}(x_1', x_1) iF^0_{\lambda \beta}(x_1, x_1')] \\
+ iG^0_{\alpha \mu}(x, x_1') [iG^0_{\lambda \lambda}(x_1, x_1) iG^0_{\beta \lambda}(x_1', x_1') - iF^0_{\mu \beta}(x_1', x_1) iF^0_{\lambda \beta}(x_1', x_1') - iG^0_{\lambda \lambda}(x_1, x_1') iG^0_{\beta \lambda}(x_1', x_1') - iF^0_{\mu \beta}(x_1', x_1) iF^0_{\lambda \beta}(x_1', x_1')] \\
+ iF^0_{\alpha \lambda}(x, x_1) [iF^0_{\beta \lambda}(x_1, x_1) iG^0_{\mu \beta}(x_1', x_1') - iF^0_{\mu \beta}(x_1', x_1) iG^0_{\lambda \beta}(x_1', x_1')] \\
\left. + iF^0_{\alpha \mu}(x, x_1') [iF^0_{\lambda \lambda}(x_1, x_1) iG^0_{\beta \lambda}(x_1', x_1') - iF^0_{\mu \beta}(x_1', x_1) iG^0_{\lambda \beta}(x_1', x_1')] \right\} \\
\tag{162}
\]

In this mess, the line pairs 3&4 and 5&6 are equal since $V(x, y)_{\mu \mu', \nu \nu'} = V(x)_{\nu \nu', \mu \mu'}$. The second line includes the disconnected vacuum diagrams, which are canceled by the denominator in $IG = IG'/\langle S(\infty, -\infty) \rangle$. The terms in Eq. (162) may be represented by the diagrams shown in Fig. 9.

The summation of $G$ with skeleton diagrams is described in Fig. 10, and similar analysis may be done for the other Nambu components. After the summations have been done, we set $\Delta_0 = 0$. At this point all the terms with bare $F^0$ or $\hat{\mathcal{F}}^0$ functions will vanish, which reduces the number of possible diagrams considerably. In the end, one finds that the expansions may be written in the form shown in Fig. 11. Actually, Fig. 11 represents the equations of motion, but that is equivalent. These may further be put in the Nambu matrix form

\[
\hat{G}_1^{-1} \hat{G} = 1 + \hat{\mathcal{S}} \hat{G} 
\]

Finally, Fig. 12 represents the “Hartree-Fock” approximation to the matrix self-energy. Note that the diagonal parts include both “direct” and “exchange” terms, whereas the off-diagonal parts (which are responsible for the superfluidity) have only an exchange-type diagram.

A similar analysis may be done for $T > 0$, and thus in general equilibrium situations we have a Dyson’s equation of the familiar form

\[
\hat{G}_{eq} = \hat{G}_{eq}^0 + \hat{G}_{eq}^0 \hat{\mathcal{S}}_{eq} \hat{G}_{eq} 
\]

Here $\hat{G}_{eq}^0$ is the noninteracting propagator in Eq. (157), with, however, $U = 0$ and $T(x, y; t) = T(x, y)$ since equilibrium is assumed. The diagrammatic calculations, whose details we skip, are most conveniently done in the
imaginary-time Matsubara formalism [3]. Initially one starts with \( \Delta^0 \neq 0 \), and thus with the off-diagonal components \( F^0 \), \( F^{0}\) of \( \hat{G}_{eq} \) present. If they were not present, then the off-diagonal components would obviously never be generated in \( \hat{G}_{eq} \) and \( \Sigma_{eq} \) either. However, once the expansion is made, the terms of the infinite series are then rearranged and summed so that \( \Sigma_{eq} \) in Eq. (163) may be interpreted as a functional \( \hat{\Sigma}_{eq}[\hat{G}_{eq}] \) of \( \hat{G}_{eq} \). The so-called “skeleton diagrams” are needed for this [2]. After this point we may formally set “\( \Delta^0 = 0 \)”, and remove \( F^0 \), \( F^{0}\) from \( \hat{G}_{eq} \) without affecting the existence of the off-diagonal components in \( \hat{\Sigma}_{eq} \), and hence a finite superconducting “order parameter” \( \Delta \). The result then correctly describes the intuitive requirement that there is no superconductivity in the noninteracting system. It is only generated when the full interactions are taken into account. Note again that is absolutely essential to sum the whole infinite series in terms of the skeleton diagrams first, and only then take \( \Delta^0 = 0 \). In any finite approximation, \( \Sigma \) may only be a functional \( \Sigma_{eq}(n)[\hat{G}_{eq}] \) of \( \hat{G}_{eq} \), and the off-diagonal self-energies will vanish if we set “\( \Delta^0 = 0 \)” [10]. However, the when the full Dyson equation, Eq. (163), is written as “\( \hat{G}_{eq}^{-1}\hat{G}_{eq} = 1 \)”, where \( \hat{G}_{eq}^{-1} = \hat{\Sigma}_{eq}^{-1} - \hat{\Sigma}_{eq} \), it will be of exactly the same form as Eq. (158). The function \( \Delta^0 \) are simply replaced by the off-diagonal self energy \( \Delta \), and the external potential \( U \) is supplemented by the diagonal self-energy.

The choice \( U = 0 \) etc. is needed because the perturbation expansion for \( \hat{G} \) (or Wick’s theorem) is well-defined only for equilibrium averages as discussed above on several occasions. For \( U(t) \neq 0 \) we must resort to a perturbation expansion of the full contour-ordered Nambu-Keldysh matrix \( \hat{G}_{cij} \), and this we shall discuss below in Sec. V.

**V. DERIVATION OF THE NONEQUILIBRIUM EQUATIONS**

The rest of this article is devoted to a study of the different stages for “deriving” the nonequilibrium quasi-classical equations. This is only a complicated technical
procedure, which should not involve distracting physical interpretations. It is just a chaos of equations.

A. Form of the Hamiltonian operator

We start off the way any self-respecting theorist always does, that is, by defining the properties of the Hamiltonian. We do not attempt to be completely general, assuming, among other things, the interactions to be local in time albeit nonlocal in space. We remind that, whenever the variable \( x_1 \) stands alone, it refers to the position \( x_1 \) and all other coordinates (spin, time, Nambu, Keldysh — usually in this order of importance) which have not been separately specified. The same goes for the even more condensed notation “1”.

We assume the (grand-canonical) Schrödinger-picture Hamiltonian to be of the form

\[
K = T + U + V_{mf} + V
\]

As representatives for one-body and two-body terms we have chosen

\[
T(t) = \int \int dx dy \psi^\dagger(x) T(x, y; t) \psi(y)
\]

\[
U(t) = \int \int dx dy \psi^\dagger(x) U(x, y; t) \psi(y)
\]

\[
V_{mf} = \int \int dx dy [\Delta^{a}(x, y; t) \psi(x) \psi(y)
+ \Delta^{0}(x, y; t) \psi^\dagger(y) \psi^\dagger(x)]
\]

\[
V = \frac{1}{4} \int \int \int dx_1 dx_2 dx_3 dx_4 \psi^\dagger(x_1) \psi^\dagger(x_2) \times \Gamma_0(x_1, x_2; x_3, x_4) \psi(x_3) \psi(x_4)
\]

Here \( T(x, y; t) = \delta(x - y) \bar{T}(y, t) \), and \( \bar{T}(y, t) = \xi(-i \hbar \nabla_y - qA(y, t)) \) which is the “kinetic energy” of (bare or quasi) particles with respect to the chemical potential, \( U(x, y; t) \) represents (time-localized) one-body potentials like an external perturbation \( V_{ext} \) or some technical “generator field” \( V^0(x, y; t) \), and the term \( V_{mf} \) creates and/or destroys pairs of particles. Thus \( T + U^0 + V_{mf} = K_0 \) is the non-interacting equilibrium mean-field Hamiltonian of Eq. (152). Finally, \( V \) is the general operator for an (instantaneous) interaction between of two particles. The usual unsymmetrized spin-independent local interaction

and the exchange-symmetrized spin-independent local interaction used in Ref. [1] are obtained with the substitutions

\[
\Gamma_0(12; 34) = 28(1 - 3)\delta(2 - 4)V(x_1, x_2) \quad \text{and}
\]

\[
\Gamma_0(12; 34) = [\delta(1 - 3)\delta(2 - 4)
- \delta(1 - 4)\delta(2 - 3)]V(x_1, x_2),
\]

respectively. The latter is depicted diagrammatically if Fig. 13. Spin-dependent potentials are also possible, but we neglect them here. Due to the Hermiticity of \( V \), and whatever else (TR symmetry?), we must generally have \( \Gamma_0(12; 34) = \Gamma_0(21; 43) = \Gamma_0(34; 12) \). In addition, there is the fermionic exchange symmetry \( \Gamma_0(12; 34) = -\Gamma_0(21; 43) = -\Gamma_0(12; 43) \). Many diagrammatic expressions are greatly simplified and clarified when we use \( \Gamma_0(12, 34) \) instead of \( V(12) \). For example, Fig. 14 shows the resulting structure of the normal-state equations of motion for \( G \).

In equations of motion, we need the commutators of the above potentials with field operators. By using \[ [A, B^\dagger C] = [A, B^\dagger]C + [B^\dagger, A]C = [A, B^\dagger]C - [B^\dagger]A, C \]
and \[ [A, B^\dagger C^\dagger D^\dagger E] = [A, B^\dagger C^\dagger]D^\dagger E + B^\dagger C^\dagger[A, D^\dagger E] = ([A, B^\dagger]C^\dagger - B^\dagger[A, C^\dagger])D^\dagger E - B^\dagger C^\dagger{[A, D^\dagger E - D{A, E}]} \] we obtain

\[
[\psi(xt), T_H(t)] = + \int dyT(x, y; t)\psi(yt)
\]

\[
= + \bar{T}(x, t)\psi(xt)
\]

\[
[\psi(xt), U_H(t)] = + \int dy U(x, y; t)\psi(yt)
\]

\[
[\psi(xt), V^B_{CS}(t)] = - \int dy \Delta^0(x, y; t)\psi^\dagger(yt)
\]
In case of \( V \), in the last equation the symmetry \( \Gamma_0(12;34) = \Gamma_0(21;43) = \Gamma_0(34;12) \) was used. Since \( T, V_{mf} \) and \( V \) must be Hermitian, we obtain the commutators with creation operators as follows: \([\psi^\dagger(x), T] = -[\psi^\dagger(x), T]^\dagger = -T^\ast(x, t)\psi^\dagger(x), \]

\([\psi^\dagger(x), V_{mf}] = -[\psi^\dagger(x), V_{mf}]^\dagger \), and \([\psi^\dagger(x), V_H(t)] = -[\psi^\dagger(x), V_H(t)]^\dagger \). To derive the first of these directly we must use partial integration. We sketch the procedure here for some arbitrary functions \( f \) and \( g \). If we expand \( \xi(-i\nabla - qA) = \sum_{n=0}^\infty \xi(n)(-i\nabla - qA)^n \) then, assuming surface terms to vanish, we obtain

\[
\int dy f^\ast(y)\xi(-i\nabla_y - qA)g(y) = \sum_n \frac{1}{n!}\xi^{(n)}(0) \int dy f^\ast(y)(-i\nabla_y - qA) \times (-i\nabla_y - qA)^{n-1}g(y) \\
= \sum_n \frac{1}{n!}\xi^{(n)}(0) \int dy (i\nabla_y - qA)f^\ast(y) \times (-i\nabla_y - qA)^{n-1}g(y) \\
= \cdots = \int dy [\xi(\nabla_y - qA)f^\ast(y)]g(y) \\
= -\int dy f^\ast(y)\xi(\nabla_y - qA)g(y)
\]

Thus integration by parts is equivalent to the replacement \( \nabla \rightarrow -\nabla \), where \( \nabla \) operates to the left. Using this we may write

\[
T = \int \int dx dy \psi^\dagger(x)T(x, y)\psi(y) \\
= \int \int dx dy \psi^\dagger(x)\delta(x - y)\xi(-i\nabla_y - qA)\psi(y) \\
= \int dy \psi^\dagger(y)\xi(-i\nabla_y - qA)\psi(y) \\
= \int dx \psi^\dagger(x)\xi(\nabla_x - qA)\psi(x) \\
= \int \int dx dy \psi^\dagger(x)\xi(\nabla_x - qA)\delta(x - y)\psi(y) \\
= \int \int dx dy [T(y, x)\psi(x)]^\dagger\psi(y) = T^\dagger
\]

where \([T(y, x)]^\dagger = T(y, x)^\ast \), while \( T^\dagger \) is the Hermitian conjugate of \( T \). For the position-representations \( T(x, y) = \langle x | T | y \rangle \) and \( T^\dagger(x, y) = \langle x | T^\dagger | y \rangle = \langle y | T^\ast | x \rangle \) we obtain from Eq. (170) the useful relation \( T(x, y) = \delta(x - y)\xi(-i\nabla_y - qA) = \xi(i\nabla_y - qA)\delta(x - y) = T^\dagger(x, y) \). These are simply continuum versions of \( A_{ij} = A_{ji} = [A^\dagger]_{ij} \) or \( u^\dagger Au = u^\dagger A^\dagger u = (Av)^\dagger v \) valid for Hermitian matrices \( A \). If in some equations we write \( T(x, y) \) or \( T^\dagger(x, y) \), it is assumed that these differential operators operate to the right or to the left, respectively.

Note: Above \( \xi(k) \) is actually the energy of Bloch electrons in the conduction band, assuming the band to consist of one branch. Its treatment as a single-particle Hamiltonian with (kinetic) momentum \( \hbar k \) already constitutes a semiclassical approximation, that is, assumes the use of wave packets (see Ref. [44], App. H) Here we furthermore replace the (canonical) momentum by the operator \(-\hbar \nabla \). This is related to what is sometimes called a “Peierls substitution”, and is not a rigorous procedure.

### B. Separation of low and high energy parts of the propagator

Here we briefly comment on the very important issue of separating \( G \) to low and high-energy parts: \( G = G^{low} + G^{high} \). This technique is required to systematize the classification of different diagrams in powers of “small” parameters, as explained in Ref. [1]. We shall not explicitly use this trick but it is good to note some of its practical consequences on the equations motion.

Part (a) of Fig. 15 represents the usual Hartree-Fock
approximation to the normal-state equation of motion which was depicted exactly in Fig. 14. A slightly different mean-field approximation is obtained by taking $G^{\text{high}}$ into account to all orders, and by making the “HF” approximation only in $G^{\text{low}}$. The result is shown in part (c) of Fig. 15. The important point is that the form of the EOM is not changed — the bare-particle interaction vertex $\tilde{\Gamma}_0$ has only been replaced by some renormalized interaction vertex $\bar{T}$. It is actually an example of what Ref. [1] calls “normal vertices”, but the details of their construction are not important for us. It is enough to know that these vertices may often be parametrized by a finite number of phenomenological parameters, like the “Landau parameters” or equivalent ones. The most important low-energy diagrams involving normal vertices are collected in Fig. 17. Diagram (b) gives just the mean-field self-energy appearing in Fig. 15.

For the case of superconductivity, these issues become a bit more complicated, but not too much. The “normal vertices” may still involve only normal-state propagators (hence the name), while the $F$ functions only appear in the low-energy part of the Nambu matrix propagator.

C. Contour-ordered Nambu space Green’s functions

As the next step in our discussion we give the most general definitions of the two types of Green’s function we shall ever need. These are the contour-ordered one-particle and two-particle functions in Nambu space. We define the contour-ordered single-particle Nambu-space Green’s function as

$$\hat{G}^c(x_1, x_2)_{ij} = -\langle T_c \Psi(x_1) \Psi^\dagger(x_2) \rangle_{ij} \quad (171)$$

where $ij$ are Keldysh indices. In terms of Nambu components $ll'$ we have

$$\hat{G}^c_{ll'}(x_1, x_2)_{ij} = -\langle T_c \Psi_l(x_1) \Psi_{l'}^\dagger(x_2) \rangle_{ij} \quad (172)$$

Here we choose to show Nambu indices and Keldysh indices in different positions to avoid confusion. However, this order seems to be exactly the opposite to what is used in Ref. [1], for example.

We also define the contour-ordered two-particle Green’s function as

$$\hat{X}^c(x_1, x_2; x_3, x_4)_{ij,kl} = (-i)^2 \langle T_c \Psi(x_1) \Psi(x_2) \Psi(x_4) \Psi(x_3) \rangle_{ij,kl} \quad (173)$$

or again in terms of Nambu components

$$\hat{X}^c_{mm',n'n'}(x_1, x_2; x_3, x_4)_{ij,kl} = (-i)^2 \langle T_c \Psi_m(x_1) \Psi_n(x_2) \Psi_{n'}^\dagger(x_4) \Psi_{m'}^\dagger(x_3) \rangle_{ij,kl} \quad (174)$$

The multiple products between $\Psi$ and $\Psi^\dagger$ are to be understood as tensor products, sometimes denoted with $\Psi \otimes \Psi^\dagger$ and so on. The single-particle function has a simple matrix representation in terms of the components of the tensor $\Psi \otimes \Psi^\dagger$, as discussed in previous sections. In the case of the two-particle function it becomes very complicated, although it is possible by using direct-product (Kronecker-product, tensor-product,...) matrices $[A \otimes B]_{ij,kl} = A_{ik}B_{jl}$. However, we reserve the multiplication symbol $\otimes$ for another purpose. Higher-order functions $G^{(n)}$ where $n \geq 3$ ($n=$number of propagated particles) could be introduced with trivial generalizations, but we shall hardly ever need $G^{(2)} = X$, let alone the higher ones. The contour-ordered quantities $G^c$ and $X^c$ should have well-defined perturbation expansions, although we shall not discuss them here [8].

The two-particle function may again be decomposed into free and bound parts. However, in the superconducting case the free part $X^{HF}$ should be supplemented the anomalous-average term so that

$$X^{HF}(12; 1'2') = G(11')G(22') - G(12')G(21') + F(12')\hat{F}(21') \quad (175)$$

See p. 112 of the book of Nozieres [2] for some discussion. This approximation then corresponds to the weak-coupling or BCS theory of superconductivity [18], and it should be exact if we use the mean-field Hamiltonian $K_0$ [Eq. (152)] as such. We shall not discuss the bound part here, but may return to these issues below.

D. Equations of motion for the noninteracting equilibrium propagators in Keldysh space

1. Left-handed equations

Here we generalize the discussion of Sec. IV C 2 to include all Keldysh-space functions. However, we still consider equilibrium, where time-dependent external potentials are absent. Let us take the noninteracting BCS (or anomalous Hartree-Fock) Hamiltonian $K_0$ of Eq. (152). Following the example of Eq. (157) which uses the relation

$$i\hbar \frac{\partial}{\partial t} \Psi_t(x, t) = \int dy \hat{K}_0^0(x, y; t) \Psi_t(y, t) \quad (176)$$

where

$$\hat{K}_0(x, y; t) = \left[ T(x, y; t) + U^0(x, y; t) \Delta^0(x, y; t) -[T^*(x, y; t) + U^0(x, y; t)] \right] \quad (177)$$
and $T(x, y; t) = \delta(x - y)e^{(i)\nabla_y - qA(y, t)}$, we obtain the full set

$$
\begin{align*}
\text{i}h \frac{\partial}{\partial t_1} & \mathcal{G}^{oc}_{-\sigma}(x_1t_1, x_2t_2) = +\hbar \delta(t_1 - t_2)\delta(x_1 - x_2) \\
& + \int dy \hat{K}^{oc}(x_1y; t_1)\mathcal{G}^{oc}_{-\sigma}(yt_1, x_2t_2) \\
\text{i}h \frac{\partial}{\partial t_1} & \mathcal{G}^{oc}_{\sigma}(x_1t_1, x_2t_2) = -\hbar \delta(t_1 - t_2)\delta(x_1 - x_2) \\
& + \int dy \hat{K}^{oc}(x_1y; t_1)\mathcal{G}^{oc}_{\sigma}(yt_1, x_2t_2)
\end{align*}
\tag{178}
$$

where matrix multiplication with respect to the Nambu indices is assumed. Now we redefine the linear operator $\mathcal{L}_0 = \mathcal{G}^{-1}_{0}$ of Eq. (159), namely

$$
\mathcal{L}_0(x_1t_1, x_3t_3)
= \delta(t_1 - t_3) \left[ \delta(x_1 - x_3)\text{i}h \frac{\partial}{\partial t_3} - \mathcal{K}_0(x_1, x_3; t_3) \right]
\tag{179}
$$

or

$$
\begin{align*}
\mathcal{L}_0(x_1t_1, x_3t_3)
& = \delta(t_1 - t_3)\delta(x_1 - x_3) \\
& \times \left[ \text{i}h \frac{\partial}{\partial t_3} - \tilde{\gamma}_3\Sigma(0) - \nabla_x - qA \right] \\
& - \delta(t_1 - t_3)\Sigma(0)(x_1, x_3; t_3)
\end{align*}
\tag{180}
$$

where the Nambu matrix potential

$$
\tilde{\Sigma}(x, y; t) = \begin{bmatrix} U_0(x, y; t) & -\Delta_0(x, y; t) \\ \Delta_0^*(x, y; t) & -U_0(x, y; t) \end{bmatrix}
\tag{181}
$$

was defined. We continue to include $\Delta_0$ as well as $U_0$ in the definition of the noninteracting equilibrium inverse propagator $\mathcal{G}^{-1}_{0}$, but at least $\Delta_0$ should be considered as infinitesimal, and, as stated before, the time explicit dependence of $\tilde{K}_0(t)$ as a whole should be at most adiabatically slow. The real nonequilibrium external potential $U(t) = V_{ext}(t)$ shall always be introduced separately with the inter-particle interactions. Using these definitions we may write Eqs. (178) in a Keldysh-matrix form

$$
\int dx_3 \int dt_3 \mathcal{L}_0(x_1t_1, x_3t_3)
\times \begin{bmatrix} \mathcal{G}^{oc}_{-\sigma}(x_3t_3, x_2t_2) & \mathcal{G}^{oc}_{\sigma}(x_3t_3, x_2t_2) \\ \mathcal{G}^{oc}_{\sigma}(x_3t_3, x_2t_2) & \mathcal{G}^{oc}_{-\sigma}(x_3t_3, x_2t_2) \end{bmatrix}
\tag{182}
$$

or

$$
\int dx_3 \int dt_3 \mathcal{L}_0(x_1t_1, x_3t_3) \mathcal{G}^{oc}_{\sigma}(x_3t_3, x_2t_2)_{ij}
= \hbar \left[ \delta(x_1 - x_2)\delta(t_1 - t_2) \right]
\tag{183}
$$

Compare this with the symbolic equation (87), which is more or less the same, but now the components of the Keldysh-space matrices are all $4 \times 4$ Nambu matrices. All the symmetry discussions of Sec. III B 3 then follow in a similar fashion. We note that $\mathcal{G}^{-1}_{oc} = \mathcal{L}_0$ is the left inverse operator of the Keldysh matrix $\mathcal{G}^{oc}$, and it is diagonal in the Keldysh indices.

**Note:** Although $\Sigma(0)(t)$ and $\mathcal{G}^{-1}_{oc}$ above are diagonal in Keldysh space (since they correspond to equilibrium), this will not be true for the real nonequilibrium self energy $\Sigma(t, t)'_{ij}$ and $\mathcal{G}^{-1}_{c}$, which have all Keldysh components present when a time-dependent external potential $U(t) = V_{ext}(t)$ is applied. Finally note again that we should have been using the more consistent notation $\mathcal{G}_{eq}$ instead of $G^{c}$, etc. The distinction will be essential later on, but as long as there is no room for misunderstandings, we shall stick to the shorthand $G^{c}$ since we have enough indices, sub/superscripts, and accents appearing on the propagators already.

2. **Right-handed equations**

Analogously to the above discussion, we may now write the equations of motion which follow from differentiating the propagators with respect to the second time argument. This time we need

$$
\text{i}h \frac{\partial}{\partial t} \Psi^\dagger_t(x, t) = - \int dy \hat{K}^{oc}_{\sigma}(x, y; t)^*\Psi^\dagger_t(y, t)
\tag{184}
$$

Here we use $\hat{K}^{oc}_{\sigma}(x, y; t)^* = \langle x|\hat{K}_0^\dagger|y\rangle^* = \langle y|\hat{K}_0^\dagger_0|\rangle = \hat{K}_0^\dagger(y, x)$ where

$$
\hat{K}_0^\dagger(y, x; t)
= \begin{bmatrix} T^\dagger(y, x; t) + U_0(y, x; t) & -\Delta_0(y, x; t) \\ \Delta_0^*(y, x; t) & -T^\dagger(y, x; t)^* + U_0(y, x; t) \end{bmatrix}
\tag{185}
$$

where $T^\dagger(y, x; t) = \xi_0(0) + \tilde{\nabla}_x - qA(y, t))\delta(x - y)$ and $\Delta_0^\dagger(y, x; t) = \Delta_0^\dagger(y, x; t)^*$, $\Delta_0^\dagger(y, x; t) = -\Delta_0^\dagger(y, x; t)$, as required by the Hermiticity of the mean-field Hamiltonian and the commutation relations for field operators. As an explicit example we first deal with the case analo-
gous to Eq. (157), namely

\[ \begin{align*}
\hbar \frac{\partial}{\partial t} \hat{G}_{tt}^0 (x_t, x_t) \\
&= - \hbar \delta(t_1 - t_2) \langle \{ \Psi_i (x_t, t_1), \Psi_i (x_t, t_2) \} \rangle \\
&\quad - i \langle \hat{\Psi}_i (x_t, t_1) \hbar \frac{\partial}{\partial t} \Psi_i (x_t, t_2) \rangle \\
&= - \hbar \delta(t_1 - t_2) \delta(x_1 - x_2) \\
&\quad - \sum_{m=p} \int d\gamma \hat{G}_{lm}^0 (x_t, y_t) \hat{K}_{ml}^0 (x_t, y_t, t_2)
\end{align*} \]

Here we used the commutation relations of \( \Psi, \Psi^\dagger \). This may now generalized to the following set of equations

\[ \begin{align*}
\hbar \frac{\partial}{\partial t} \hat{G}_{tt}^{0c} (x_t, x_t, t_2) \\
&= - \hbar \delta(t_1 - t_2) \delta(x_1 - x_2) \\
&\quad - \int d\gamma \hat{G}_{tt}^{0c} (x_t, x_t, t_2) \\
\hbar \frac{\partial}{\partial t} \hat{G}_{tt}^{0c} (x_t, x_t, t_2) \\
&= - \int d\gamma \hat{G}_{tt}^{0c} (x_t, x_t, t_2)
\end{align*} \]

Now we define another operator \( \hat{R}_0 \)

\[ \begin{align*}
\hat{R}_0 (x_t, x_t, t_2) \\
&= - \left[ i \hbar \frac{\partial}{\partial t} \hat{\Sigma}^{01} (x_t, x_t, t_3) \right] \delta(t_3 - t_2)
\end{align*} \]

or

\[ \begin{align*}
\hat{R}_0 (x_t, x_t, t_2) \\
&= - \left[ i \hbar \frac{\partial}{\partial t} \hat{\Sigma}^{01} (x_t, x_t, t_3) \right] \delta(t_3 - t_2)
\end{align*} \]

where

\[ \hat{\Sigma}^{01} (y, x; t) = \left[ U^0 (y, x; t) - \Delta^0 (y, x; t) \right] = \hat{\Sigma}^{01} (y, x; t) \]

Here we again note, formally, that \( \hat{\Sigma}^{01} (x, y; t) = \langle x | \hat{\Sigma}^{01} | y \rangle^\dagger \). (Note that the symmetries of all Nambu matrices should be compatible with the general formulas of Appendix C; you should check that this is the case.) The operator \( \hat{R}_0 \) is in fact just the Hermitian conjugate \( \hat{R}_0 \), as you must have guessed, and it is the right-hand inverse of \( \hat{G}^0 = \hat{G}^{0c} \).

We may use it to write Eqs. (187) as

\[ \int dx_3 \int dt_3 \left[ \hat{G}^{0c} (x_t, x_t, x_3, t_3) \hat{R}_0 (x_t, x_t, x_3, t_2) \right] \]

or finally

\[ \int dx_3 \int dt_3 \hat{G}^{0c} (x_t, x_t, x_3, t_3) \hat{R}_0 (x_t, x_t, x_3, t_2) \]

Now we note that \( \hat{G}^{-1} = \hat{R}_0 \sigma_3 \), diagonal in Keldysh indices, is the right-hand inverse operator of the Keldysh matrix \( \hat{G}^{0c} \). However, as we shall see, it will be more convenient to deal with the Nambu operators \( \hat{L}_0 \) and \( \hat{R}_0 \) and the Nambu components of \( \hat{G}^{0c} \) directly.

E. Self-energies and self-consistency equations

1. Anomalous Hartree-Fock approximation in the Hamiltonian

In Secs. V D 1 and V D 2 we have derived the exact equations of motion for the “noninteracting” Nambu-Keldysh propagator \( \hat{G}^{0c} \), using the BCS model mean-field Hamiltonian \( \hat{K}_0 (t) \) of Eq. (152). In the process, we never specified the meaning of the off-diagonal potential \( \Delta^0 \). It appears together with the diagonal potential \( U \), which we have interpreted as an external potential. At least in equilibrium (\( U = 0 \)), we may obtain a reasonable interpretation for \( \Delta^0 \) also by means of the so-called (anomalous) Hartree-Fock approximation of the two-body interaction \( V \) in Eq. (155). First of all we note that the usual direct and exchange HF terms give us back another nonlocal one-body mean-field potential

\[ U(x, y) = \frac{1}{2} V(x, y) \langle \psi^\dagger (x) \psi (y) \rangle_0^eq \]

This we may usually neglect, for reasons that will be explained below.

To obtain \( V_{mf} \), we must include the anomalous terms where the product of operators \( \psi \psi \) is replaced by their equilibrium average \( \langle \psi \psi \rangle_0^eq \), neglecting a term of second order in the fluctuations \( \psi \psi - \langle \psi \psi \rangle_0^eq \). If we choose the unsymmetrized \( \Gamma_0 (12; 34) = 2 \delta (1 - 3) \delta (2 - 4) V (1, 2) \), then by comparing \( V_{mf} \) with \( V \) we set

\[ \Delta^0 (x, y) = \frac{1}{2} V(x, y) \langle \psi (x) \psi (y) \rangle_0^eq \]
For self-consistency, the averages in Eqs. (193) and (194) must be calculated in the equilibrium ensemble of the “effective Hamiltonian” $K_0 = T + V_{HF} + V_{mf}$ itself, where $V_{HF}$ is the “normal” HF interaction term involving Eq. (193) which we may neglect. Equation (194) may furthermore be written in terms of the Green’s function $G^0 = G^{0c}_c$, which closes the system of equations and makes a self-consistent solution possible. Thus in equilibrium only the diagonal “—” component in Eqs. (183) and (192) is important, and we may (and probably should) also express it in the imaginary time, or Matsumura representation. Finally, to take charge currents $j$ into account self-consistently, we should add the self-consistency equation

$$\nabla \times \nabla \times A(x) = \mu_0 j(x)$$  \hspace{1cm} (195)

for the vector potential $A$. Granted, these self-consistency tricks seem a bit ad-hoc as they stand, so we should still try to quantify somehow the amount and type of error we have made — in Appendix E1 we discuss one attempt to work in this direction. This is nevertheless one way to think about it.

However, our original aim was to discuss a systematic perturbation-theoretic approach to superconductors. In this philosophy, the anomalous term $V_{mf}$ in $K_0$ is unperturbative, and it must be eliminated in the end, as we have already explained. It was added only to enable the anomalous contractions, and hence the existence of the off-diagonal Green’s functions. For this purpose $\Delta^0$ need not be calculated self-consistently. It may be some small constant which we shall set to zero once we can safely do so. Unless, of course, we are able to show via the perturbation-theoretic approach that the results obtained by the mean-field Hamiltonian are essentially correct in some approximation. That is what we aim to demonstrate next, by making the simplest mean-field approximation to the two-particle Green function. Along similar lines it is possible to obtain a rigorous prescription for calculating the self-energies also in nonequilibrium situations. However, we shall not attempt to do perturbation theory beyond the mean field level.

2. Self-energies from full interactions: equilibrium (or MF)

We now write the equation of motion by including a real external potential $U(t) = V_{ext}(t)$ and the full two-particle interaction $V$. We proceed as follows

$$i\hbar \frac{\partial}{\partial t_i} \tilde{G}_{ij}(x_1 t_1, x_2 t_2)_{ij} = +\hbar \langle \sigma_3 \rangle_{ij} \delta(t_1 - t_2) \langle \Psi_l(x_1, t_1), \Psi^\dagger_l(x_2, t_2) \rangle - i \langle T_c \hbar \frac{\partial}{\partial t_i} \Psi_l(x_1, t_1) \Psi^\dagger_l(x_2, t_2) \rangle_{ij} + \sum_{m=p,h} \int \text{d}y \tilde{K}^0_{lm}(x_1, y; t_1) \tilde{G}_{ml'}(y t_1, x_2 t_2)_{ij} + \sum_{m=p,h} \int \text{d}y \tilde{U}_{lm}(x_1, y; t_1) \tilde{G}_{ml'}(y t_1, x_2 t_2)_{ij} - i \langle T_c \Psi_l(x_1, t_1), V_{H}(t_1) \rangle \tilde{G}_{lj}(x_2, t_2)_{ij}$$  \hspace{1cm} (196)

Here we have assigned a Keldysh index “i” to $\tilde{U}(t) \equiv \tilde{\gamma}_3 U(t)$, since separate $U(x, y; t_1)$’s for the different Keldysh contour branches may be needed to clarify the perturbation expansion. (But in physical situations $U_+ = U_-$, and in equilibrium $U_\pm = 0$.) Equation (196) is indeed basically equivalent to Eq. (B.9) of Ref. [1] but generalized for Nambu matrices. However, for the time being, we still assume equilibrium by setting $U_i = 0$, and concentrate on the last term which arises from the particle interactions $V$. It may be written as

$$-i \langle T_c \Psi_l(x_1, t_1), V_{HF}(t_1) \rangle \tilde{G}_{lj}(x_2, t_2)_{ij}$$

$$= + \frac{1}{2} \int \int \text{d}x \text{d}y \text{d}z \Gamma_0(x_1, x_2, y, z)(-i)$$

$$\times \left\langle T_c \left[ \psi_l^\dagger(x_1) \psi_l(z_1) \psi_l^\dagger(y_1) \psi_l(x_2)_{ij} \right] \psi_l^\dagger(x_1) \psi_l(z_1) \psi_l^\dagger(y_1) \psi_l(x_2)_{ij} \right\rangle_{ll'}$$

$$= + \frac{1}{2} \int \int \text{d}x \text{d}y \text{d}z \Gamma_0(x_1, x_2, y, z)(-i) \left\langle T_c \left[ \psi_l^\dagger(x_1) \psi_l^\dagger(x_1, y) \psi_l(y_1) \psi_l(x_2)_{ij} \right] \psi_l^\dagger(x_1) \psi_l(y_1) \psi_l^\dagger(x_1) \psi_l(x_2)_{ij} \right\rangle_{ll'}$$

$$= - \frac{1}{2} \int \int \text{d}x \text{d}y \text{d}z \Gamma_0(x_1, x_2, y, z) \tilde{X}_{l', l i j}(x_1, y, z, x_1, x_2, x_1)_{ij}$$

Here the superscripts $\pm l$ in the time coordinates have been added to keep track of the order of operators which occur at equal times. The upper and lower signs are for the Keldysh indices $i = - = 1$ and $i = + = 2$, respectively, while the Nambu index $l = \pm 1$ changes the order appropriately. Equation (196) may be written symbolically as “$[iG^0]^{-1}iG = 1 - (-iG_0)^2 X$” and this corresponds to the diagrammatic expression shown
in Fig. 7 for the unsymmetrized case $\Gamma_0(12;34) = 2\delta(1-3)\delta(2-4)V(x_1,x_2)$.

Now we may proceed to make some approximations to the two-particle function. As an example we choose simplest “HF” approximation which takes into account the fermionic exchange effects as well as superconductivity. Thus we decompose Eq. (197) as follows

\[
\approx -\frac{i}{2} \int \int dx dy dz \Gamma_0(x_1, x_2; y, z) \left[ - \langle T_c \Psi_i(zt) \Psi_i^\dagger(xt) \rangle_{ij} - \langle T_c \Psi_i(yt) \Psi_i^\dagger(xt) \rangle_{ij} \right] 
\]

\[
= -\frac{i}{2} \int \int dx dy dz \Gamma_0(x_1, x_2; y, z) \left[ - i\hat{G}_0(r_1, r_2; t_1, t_2) \right] 
\]

\[
+ i\hat{G}_i(yt_1, xt_1; r_1, r_2) - i\hat{G}_i(xt_1, yt_1; r_1, r_2) 
\]

\[
+ \hat{G}_i(yt_1, xt_1; r_1, r_2) - i\hat{G}_i(xt_1, yt_1; r_1, r_2) 
\]

Next we rearrange integration variables to write the expression as simple folding products:

\[
= \int dr \left\{ -\frac{i}{2} \int dr_1 dr_2 \Gamma_0(x_1, r_1, r_2; t_1, t_2) \hat{G}_i(r_1, r_2; t_1, t_2) \right\} \hat{G}_i(r_1, r_2; t_1, t_2) 
\]

\[
+ \int dr \left\{ -\frac{i}{2} \int dr_1 dr_2 \Gamma_0(x_1, r_1, r_2; t_1, t_2) \hat{G}_i(r_1, r_2; t_1, t_2) \right\} \hat{G}_i(r_1, r_2; t_1, t_2) 
\]

This is the $ll'$ component of the following matrix expression

\[
= \int dr \left\{ -\frac{i}{2} \int dr_1 dr_2 \Gamma_0(x_1, r_1, r_2; t_1, t_2) \left[ \begin{array}{cc}
G^c(r_1, r_2; t_1, t_2) & 0 \\
0 & \hat{G}^c(r_1, r_2; t_1, t_2)
\end{array} \right]_{ii} 
\]

\[
+ \int dr \left\{ -\frac{i}{2} \int dr_1 dr_2 \Gamma_0(x_1, r_1, r_2; t_1, t_2) \left[ \begin{array}{cc}
F^c(r_1, r_2; t_1, t_2) & 0 \\
0 & \hat{F}^c(r_1, r_2; t_1, t_2)
\end{array} \right]_{ii} 
\]

\[
= \int dr \left\{ -\frac{i}{2} \int dr_1 dr_2 \Gamma_0(x_1, r_1, r_2; t_1, t_2) \left[ \begin{array}{cc}
G^c(r_1, r_2; t_1, t_2) & 0 \\
0 & \hat{G}^c(r_1, r_2; t_1, t_2)
\end{array} \right]_{ii} 
\]

Here the expression inside the curly braces is just the Nambu matrix self energy $\Sigma(x_1, r_1; t_1)$ as a functional of $\hat{G}$. Thus we see that Eq. (196) is of the form

\[
\hat{G}_0^{-1} \hat{G}_i = \hat{1}[\sigma_3]_{ij} + \Sigma_i \hat{G}_i 
\]

where the products imply integration over all internal coordinates. Remember that $\hat{G}_0^{-1}$ includes the generating term $\Sigma^0$ which from here on may be set to zero. It is replaced in Eq. (200) by the formally similar $\Sigma$, which the true self-consistently calculated (HF) self-energy arising from real particle-particle interactions.

Similar equations may again be written for the other Keldysh components $G^\pm$. However, within the above equilibrium assumptions, each component will separately have a similar set of equations, independently of the other components. Thus the off-diagonal self energies vanish, i.e., $\Sigma_{+-} = \Sigma_{-+} = 0$, and different Keldysh components are not mixed in the EOM! This is in fact what happens always in the quasiclassical mean-field, or “molecular-field”, approximation which is unable to account for energy relaxation [1]. Apparently this cannot be exactly true to higher than zeroth order in the external perturbation $U(t)$, since the expansion of the $s$ matrix in Eq. (67) includes both contour parts already in first order. In general the equations of motion should thus couple the components — for example, $G_0^{-1} G_{+-} = 1 + \Sigma_{+-} G_{+-} + \Sigma_{-+} G_{-+}$ etc. We now turn to discuss the more general case briefly.
3. Self-energies: nonequilibrium effects and one-body potentials included

Here we should start by considering some systematic way of generating the perturbation series for the nonequilibrium self energies. Unfortunately that is too complicated to be attempted at this point. As already noted, there are at least two choices for doing it: Wick’s theorem [8] or the functional-derivative method [1]. However, the main points of the results may be discussed in rather simple and non-mathematical terms.

When the perturbation theory for the two-body interaction term in Eq. (197) is analyzed properly, we should end up with the left and right-handed Dyson equations

\[
\hat{G}_{ij}^c = \hat{G}_{0c}^{eq} + \sum_{k,l} \hat{G}_{0c}^{eq} \otimes (\hat{\Sigma}^c + \hat{U}^c)_{kl} \otimes \hat{G}_{ij}^c
\]

\[
\hat{G}_{ij}^c = \hat{G}_{0c}^{eq} + \sum_{k,l} \hat{G}_{0c}^{eq} \otimes (\hat{\Sigma}^c + \hat{U}^c)_{kl} \otimes \hat{G}_{ij}^c
\]

(202)

where the folding product \( \otimes \) is explained in the Appendices. The “equations of motion” then follow by multiplying with \( \hat{G}_{0c}^{eq} \) from the left or right — see Sec. V F 1 below. In the self-energy

\[
\hat{\Sigma}^c(x, y') + \hat{U}^c(x, y')\]

(203)

we have kept separate the term \( \hat{U}^c \) arising directly from the nonequilibrium-driving one-body perturbation \( \hat{\tau}_3 U(x, x') \). Thus \( \hat{U}^c(x, y')\) is basically a given function, while the self-energy \( \hat{\Sigma}^c \) depends on \( \hat{U}^c \) only through \( \hat{G}^c \) via the skeleton diagrams; we return to this shortly. The function \( \hat{\Sigma}^c(x, x') \) should generally have all Keldysh components nonzero, and be nonlocal in time (at least if the effective particle-particle interactions are frequency-dependent, like in the case of retarded, phonon-mediated electronic interactions?). We note that the Dyson equations imply that the self-energy matrices \( \hat{\Sigma}^c \) and \( \hat{U}^c \) have essentially the same symmetries as \( \hat{G}^c \) does. These symmetries are presented in Appendix C.

When the separation into high and low energy parts is performed — which is essential for the quasiclassical approximation — then both of the terms in Eq. (203) become “renormalized” to \( \hat{U}^{low} + \hat{\Sigma}^{low} \); see Ref. [1] and Sec. V G below. However, in order for this to be possible, \( \hat{U} \) must be “weak” so that \( |U| \ll E_F \). It is also possible to include strong (\( \sim E_F \)) one-body potentials, but some new tools are needed for this. Next we briefly discuss the inclusion of localized scattering potentials \( V_{\text{imp}} \). For simplicity we only deal with the case of equilibrium where \( U \) is simply replaced by the static potential \( V_{\text{imp}} \). The nonequilibrium case is obtained by adding \( V_{\text{imp}} \) to \( U \) is Eqs. (202) and by following similar steps as below.

The impurity potentials that we consider are of the type \( V_{\text{imp}}(x, y') = \delta(x - y)\delta(t - t')V_{\text{imp}}(x)\hat{\tau}_3 \). First of all we note that in the presence of both two-particle interactions and a one-body perturbation \( \hat{V} = V_{\text{imp}} \) the perturbation expansion of the time-ordered function \( \hat{G} \equiv \hat{G} \)

\[
\hat{G}_{eq} \]

may be summed into two parts

\[
\hat{G} = \hat{G}_0 + [\hat{G}_0 \hat{V}] \hat{G} + [\hat{G}_0 \hat{\Sigma} \hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} + \hat{\Sigma} \hat{G} \]

(204)

where, again, the products imply integrations over internal coordinates (see Fig. 16). Here \( \hat{\Sigma} \) is the proper self-energy which includes all diagrams which cannot be separated by cutting a single fermion line. Thus it also includes contributions from \( \hat{V} \), but via a rearrangement of terms and partial resummation of “skeleton diagrams” \( \hat{\Sigma} \) may be considered a self-consistent functional \( \hat{\Sigma}[\hat{G}] \) of the full propagator \( \hat{G} \) only [2]. Next we may separate the two effects by introducing an intermediate function \( \hat{G}_1 \) as follows

\[
\hat{G} = \hat{G}_1 + \hat{G}_1 \hat{V} \hat{G}, \text{ where }
\]

\[
\hat{G}_1 = \hat{G}_0 + \hat{G}_0 \hat{\Sigma} \hat{G}_1
\]

(205)

The equivalence of this separation is easily proved:

\[
\hat{G} = \hat{G}_1 + \hat{G}_1 \hat{V} \hat{G}_1 = \hat{G}_0 + \hat{G}_0 \hat{\Sigma} \hat{G}_1 + \hat{G}_1 \hat{V} \hat{G}_1
\]

(206)

\[
= \hat{G}_0 + \hat{G}_0 \hat{\Sigma} \hat{G}_1 + \hat{G}_0 \hat{V} \hat{G}_1 + \hat{G}_0 \hat{\Sigma} \hat{G}_1 \hat{V} \hat{G}_1
\]

The first of Eqs. (205) may furthermore be split into two by writing

\[
\hat{G} = \hat{G}_1 + \hat{G}_1 \hat{V} \hat{G}_1 + \hat{G}_1 \hat{V} \hat{G}_1 \hat{V} \hat{G}_1 + \cdots
\]

(207)

\[
= \hat{G}_1 + (\hat{V} + \hat{V} \hat{G}_1 \hat{V} + \hat{V} \hat{G}_1 \hat{V} \hat{G}_1 \hat{V} + \cdots) \hat{G}_1
\]

where we defined the “\( T \) matrix” as the “Born series” [49]

\[
\hat{T} = \hat{V} + \hat{V} \hat{G}_1 \hat{T} = \hat{V} + \hat{V} \hat{G}_1 \hat{V} + \cdots
\]

(208)

Note that this also implies \( \hat{T} = \hat{V} + \hat{V} \hat{G} \hat{V} \) and useful relations like \( \hat{V} \hat{G} = \hat{T} \hat{G}_1 \). Some methods based on Eq. (208) for incorporating impurities and walls etc. into quasiclassical theory are discussed in Ref. [1].
F. Equations of motion in different Keldysh-space representations

1. Contour-ordered (or original) representation

In the contour-ordered $G^c$ representation we find from the the left-handed Dyson equation [in Eq. (202)]

$$\sum_k \int dx_3 \int dt_3 \hat{G}_{oc}^{-1}(x_1,t_1,x_3,t_3)_{ik}\hat{G}^c(x_3,t_3,x_2,t_2)_{kj}$$

$$= \hbar \delta_{ij} \hat{1} \delta(x_1 - x_2) \delta(t_1 - t_2)$$

$$+ \sum_k \int dx_3 \int dt_3 \hat{G}^c(x_1,t_1,x_3,t_3)_{ik}\hat{G}^c(x_3,t_3,x_2,t_2)_{kj}$$

(209)

where

$$\hat{G}_{oc}^{-1}(x_1,t_1,x_3,t_3)_{ij} = [\sigma_3]_{ij} \hat{L}_0(x_1,t_1,x_3,t_3) - \hat{U}^c(x_1,t_1,x_3,t_3)_{ij}$$

(210)

is the inverse Green’s function for a noninteracting nonequilibrium system while $\hat{G}_{oc,eq} = [\sigma_3] \hat{L}_0$ the inverse Green’s function for the noninteracting equilibrium system. Here we have defined $\hat{U}^c(x_1,t_1,x_3,t_3)_{ij} = [\sigma_3]_{ij} \tilde{\tau}_3 \delta(t_1 - t_3)U(x_1, x_3; t_1)_{i}$ and use the familiar operator

$$\hat{L}_0(x_1,t_1,x_3,t_3) = \delta(t_1 - t_3)\delta(x_1 - x_3)$$

$$+ \left[ \frac{i\hbar}{\partial t_3} \hat{1} - \tilde{\tau}_3 \delta^{0}(t_1 - t_3) \right]$$

(211)

The only difference is that now we have dropped the generating term $\Sigma^0$ from this since it is unnecessary after the perturbation series has been summed. Similarly, the right-handed Dyson equation yields

$$\sum_k \int dx_3 \int dt_3 \hat{G}^c(x_1,t_1,x_3,t_3)_{ik}\hat{G}_{oc}^{-1}(x_3,t_3,x_2,t_2)_{kj}$$

$$= \hbar \delta_{ij} \hat{1} \delta(x_1 - x_2) \delta(t_1 - t_2)$$

$$+ \sum_k \int dx_3 \int dt_3 \hat{G}^c(x_1,t_1,x_3,t_3)_{ik}\hat{G}^c(x_3,t_3,x_2,t_2)_{kj}$$

(212)

where the right-handed inverse operator equals

$$\hat{G}_{oc}^{-1}(x_3,t_3,x_2,t_2)_{ij}$$

$$= [\sigma_3]_{ij} \hat{R}_0(x_3,t_3,x_2,t_2)$$

$$- [\sigma_3]_{ij} \tilde{\tau}_3 \delta(t_1 - t_3)U(x_3,x_2,t_2)_{i}$$

(213)

and $\hat{G}_{oc,eq} = \hat{R}_0[\sigma_3]$. Again we have

$$\hat{R}_0(x_3,t_3,x_2,t_2)$$

$$= \left[ -i\hbar \frac{\partial}{\partial t_3} \hat{1} - \tilde{\tau}_3 \delta^{0}(t_3 - t_2) \right]$$

$$\times \delta(t_3 - t_2)\delta(x_3 - x_2)$$

(214)

Since the operators $\hat{L}_0$ and $\hat{R}_0$ appear associated with a multiplicative $\sigma_3$ factor here, this is not the representation we want to use. In the $\hat{G}$ representation it becomes eliminated.

2. Second Keldysh representation

In the Keldysh representation with $\hat{G} = \sigma_3 G^c$ and $\Sigma = \Sigma^0 \sigma_3$ etc. we find

$$\left[ i\hbar \frac{\partial}{\partial t_1} \hat{1} - \tilde{\tau}_3 \delta^{0}(t_1 - t_2) \right] \hat{G}(x_1, t_1, x_2)_{ij}$$

$$= \hbar \delta_{ij} \hat{1} \delta(x_1 - x_2) \delta(t_1 - t_2)$$

$$+ \sum_k \int dx_3 \int dt_3 \hat{G}(x_1,t_1,x_3,t_3)_{ik}\hat{G}^c(x_3,t_3,x_2,t_2)_{kj}$$

(215)

where $\hat{G}(x_1,t_1,x_3,t_3)_{ij} = \delta_{ij} \delta(t_1 - t_3)\tilde{\tau}_3 U(x_1, x_3; t_1)$ and

$$\hat{G}(x_1,t_1,x_2,t_2)_{ij}$$

$$= -i\hbar \frac{\partial}{\partial t_2} \hat{1} - \tilde{\tau}_3 \delta^{0}(t_2 - t_1)$$

$$+ \sum_k \int dx_3 \int dt_3 \hat{G}(x_1,t_1,x_3,t_3)_{ik}\hat{G}(x_3,t_3,x_2,t_2)_{kj}$$

(216)

This looks good already. One thing we might now note is that the time derivative is not explicitly in a gauge-invariant form. However, the electrostatic potential $+ e\Phi$ may be included in $U$ and moved from there into the single-particle operators $\hat{L}_0$ and $\hat{R}_0$, if so wished. Remember that the complete gauge transformation is of the form

$$q\Phi \rightarrow q\Phi' = q\Phi - q \frac{\partial \chi}{\partial t}$$

(217)

$$S \rightarrow S' = S + \frac{q}{\hbar} \chi$$

where $S$ and $S'$ are the phases of the single-particle fields $\psi = \psi_0 e^{iS}$ and $\psi' = \psi_0 e^{iS'}$. Therefore the proper gauge-invariant time derivative acting on $\psi$ is of the form $i\hbar \partial / \partial t - \Phi q$, as expected. The consequences of the gauge (as well as spin-rotation and Galilean) transformations is discussed in Ref. [1]. And now for the final stretch.

3. Representation with retarded, advanced, and Keldysh functions

Now all we have to do is to make the rotation transformations of Eqs. (82) and (92) in Eqs. (215) and (216),
and apply Eq. (84) to the folding products. By now we realize that the equations may be written in much shorter forms by using the shorthand notations for folding products — see related appendix. Thus we obtain

\[ \left[ i\hbar \frac{\partial}{\partial t} \hat{1} - \hat{\tau}_3 \xi^0 ( - \hat{\tau}_3 i\hbar \nabla_{x_1} - q \mathbf{A}) \right] \hat{G}^R(x_{1t}, x_{2t}) = \hat{1} \hbar \delta(x_1 - x_2) \delta(t_1 - t_2) \]

+ \left\{ \left[ \hat{\Sigma}^R + \hat{U}^R \right] \otimes \hat{G}^R \right\} (x_{1t_2}, x_{2t_2})

\[ \left[ i\hbar \frac{\partial}{\partial t} \hat{1} - \hat{\tau}_3 \xi^0 ( - \hat{\tau}_3 i\hbar \nabla_{x_1} - q \mathbf{A}) \right] \hat{G}^A(x_{1t}, x_{2t}) = \hat{1} \hbar \delta(x_1 - x_2) \delta(t_1 - t_2) \]

+ \left\{ \left[ \hat{\Sigma}^A + \hat{U}^A \right] \otimes \hat{G}^A \right\} (x_{1t_2}, x_{2t_2})

\[ \left[ i\hbar \frac{\partial}{\partial t} \hat{1} - \hat{\tau}_3 \xi^0 ( - \hat{\tau}_3 i\hbar \nabla_{x_1} - q \mathbf{A}) \right] \hat{G}^K(x_{1t}, x_{2t}) = \hat{1} \hbar \delta(x_1 - x_2) \delta(t_1 - t_2) \]

+ \left\{ \left[ \hat{\Sigma}^K + \hat{U}^K \right] \otimes \hat{G}^K \right\} (x_{1t_2}, x_{2t_2})

\[ (218) \]

and

\[ \left[ i\hbar \frac{\partial}{\partial t} \hat{1} - \hat{\tau}_3 \xi^0 ( + \hat{\tau}_3 i\hbar \nabla_{x_2} - q \mathbf{A}) \right] \hat{G}^R(x_{1t_1}, x_{2t_2}) = \hat{1} \hbar \delta(x_1 - x_2) \delta(t_1 - t_2) \]

+ \left\{ \left[ \hat{\Sigma}^R + \hat{U}^R \right] \otimes \hat{G}^R \right\} (x_{1t_1}, x_{2t_2})

\[ \left[ i\hbar \frac{\partial}{\partial t} \hat{1} - \hat{\tau}_3 \xi^0 ( + \hat{\tau}_3 i\hbar \nabla_{x_2} - q \mathbf{A}) \right] \hat{G}^A(x_{1t_1}, x_{2t_2}) = \hat{1} \hbar \delta(x_1 - x_2) \delta(t_1 - t_2) \]

+ \left\{ \left[ \hat{\Sigma}^A + \hat{U}^A \right] \otimes \hat{G}^A \right\} (x_{1t_1}, x_{2t_2})

\[ \left[ i\hbar \frac{\partial}{\partial t} \hat{1} - \hat{\tau}_3 \xi^0 ( + \hat{\tau}_3 i\hbar \nabla_{x_2} - q \mathbf{A}) \right] \hat{G}^K(x_{1t_1}, x_{2t_2}) = \hat{1} \hbar \delta(x_1 - x_2) \delta(t_1 - t_2) \]

+ \left\{ \left[ \hat{\Sigma}^K + \hat{U}^K \right] \otimes \hat{G}^K \right\} (x_{1t_1}, x_{2t_2})

\[ (219) \]

The equations of motion for \( \hat{G}^{R,A,K} \) [Eqs. (218) and (219)] are obtained from Eqs. (215) and (216) by the simple substitutions

\[ \hat{X}_{++} \rightarrow 0, \quad \hat{X}_{--} \rightarrow \hat{X}^R, \quad \hat{X}_{+-} \rightarrow \hat{X}^A, \quad \hat{X}_{-+} \rightarrow \hat{X}^K \]

\[ (220) \]

Good. We now have our general equations of motion for the single-particle propagator. The main assumptions which we must make are roughly the following. (i) The single-particle "Schrödinger" operators \( \hat{L}_0 \) and \( \hat{R}_0 \) are assume that there is no spin polarization. Therefore both spin species have the same chemical potential \( \mu \) and \( \xi = \epsilon - \mu \) measures the energy from this level. The generalization of this would be easy on this level, but would lead to difficulties when trying to go to the quasiclassical description. (ii) The unperturbed noninteracting system whose inverse propagators \( \hat{L}_0 \) and \( \hat{R}_0 \) represent is assumed to be translationally invariant (as well as time-independent), at least in an effective way. Thus all information about some periodic lattice and the resulting band structure etc. is taken into account only in the form of the Fermi surface in \( \mathbf{k} \) space, which, at \( T = 0 \), is defined by \( \xi_k = \epsilon_k - \mu = \epsilon_k - \epsilon_F = 0 \). Therefore band renormalization of independent-electron electron masses etc. has already been carried out. (iii) Although it is not explicitly seen here, the external potential \( U(t) \) must be "slowly varying" in both space and time, and not "too strong" (\( \ll E_F \)). Strong, localized scattering potentials must be treated separately with the scattering \( t \) matrices in the quasiclassical description.

G. Going to the quasiclassical limit

Now we shall transform the Dyson equations into quasiclassical form [1, 37, 38, 41]. This simplifying procedure is valid only under the general assumption of a degenerate Fermi system. Therefore the temperature \( k_B T \) must be much lower than the Fermi energy \( E_F \), so that there exists at least one small parameter \( k_B T / E_F \sim k_B T_c / E_F \ll 1 \). The approximation involves steps which may be taken in different orders and in different Fourier representations, and so the details may look different. However, the main features are explained as follows.

- \( \hat{G} \) is separated into low and high energy regimes, \( \hat{G} = \hat{G}^{\text{low}} + \hat{G}^{\text{high}} \). Then \( \hat{U} + \hat{\Sigma}[\hat{G}] \) is replaced by the momentum-independent Fermi-surface limits \( U^{\text{low}}[\hat{g}] + U^{\text{low}}[\hat{\xi}] \), where \( \hat{g} \) is the \( \xi \)-integrated \( \hat{G}^{\text{low}} \). This is a reasonable approximation, since \( \hat{G}^{\text{low}} \) is a strongly peaked function of \( \xi \) on the
Fermi surface, while $\hat{\Sigma}$ and $\hat{U}$ are slowly varying. The most relevant diagrams for $\hat{\Sigma}^\text{low}[g]$ are shown in parts (b) and (c) of Fig. 17, and those for $\hat{U}^\text{low}[g]$ in part (d) of the same figure. Diagrams (b) and (d) are of order (small)$^1$ whereas diagram (c) is of order (small)$^2$. This step is really the most involved one, and we skip its details.

- However, the strength of the perturbation potential $|U|$ must be small compared to $E_F$ for the above procedure to work. This means that there must exist another small parameter $|U|/E_F \ll 1$ and explains why impurity scattering potentials $|V_{imp}| \sim E_F$ etc. must be treated separately. An assumption of slow position and time variance of the perturbation must also be made, which introduces still two small parameters $\hbar |q|/|p_F| \ll 1$ and $|\hbar \omega|/E_F \ll 1$. This will allow one to expand expressions into low orders in gradients of $R = (x_1 + x_2)/2$ and possibly of $T = (t_1 + t_2)/2$.

- The first diagram (a) of Fig. 17 — which is of order (small)$^0$ — is included into the noninteracting-particle operator $\hat{G}_{0,eq}^{-1} = \epsilon - i\gamma \xi^0(p)$ (i.e., $\hat{L}_0$ and $\hat{R}_0$), thereby renormalizing it to the inverse noninteracting-quasiparticle propagator $\hat{G}_{\text{coh},eq}^{-1} = a^{-1}[\epsilon - i\gamma \xi(p)]$ as explained in Secs. II A 3, II B 3 and in the Appendices. This involves introduction of the quasiparticle renormalization factor “$a$”, a new Fermi momentum $p_F$ ($\mu$ is fixed in grand-canonical ensemble), and a renormalization of the single-(quasi)particle excitation spectrum $\xi(p)$ (hence also the Fermi velocity $v_F = \nabla_p \xi|_{p=p_F}$). In this way one switches from a “particle picture” to a “quasiparticle picture”.

- The quasiparticle excitation spectrum $\xi(p)$ is linearized around the Fermi surface such that $\xi(p) = v_F(s) \cdot (p - p_F(s))$. Here $s$ parametrizes the Fermi surface, and for sufficiently well-behaved cases $s$ may be replaced by $p = p_F/p_F$. This, in addition to assuming a constant normal-state density of (quasiparticle) states, amounts to so-called particle-hole symmetry. This step depends, in part, on slow $R$-dependence of $\hat{G}^\text{low}$.

- The left and right Dyson equations are subtracted and integrated over $\xi_p$ in order to obtain an equation for $\hat{g}$ in terms of $\hat{\Sigma}^\text{low}[g]$ and $\hat{U}^\text{low}[g]$. This is possible only because $\hat{\Sigma}^\text{low}[g]$ and $\hat{U}^\text{low}[g]$ were assumed to be $\xi_p$-independent in the low-$\xi_p$ regime. In this way a closed system of self-consistent equations for $\hat{g}$ is obtained, where no explicit dependence on the cutoff $E_c$ appears. The subtraction results in a linear, homogeneous set of equations, and therefore a separate set of normalization conditions must be introduced.

All these steps depend somewhat on each other, and the logical order in which they should be taken is a bit vague. We take them all in any case, so this is not a problem. The above quasiclassical approximation is completely independent of the Keldysh (or Nambu) space structures, and so transformations between different representations may be done equally well before or after it.

1. Derivation of the quasiclassical equations

We proceed by using the $\tilde{G}$ representation in order to treat all components simultaneously. As is evident from Secs. V F 2 and V F 3, equations for the $R, A, K$ functions then follow by the simple substitutions

\[ \hat{x}_+ \to 0, \quad \hat{x}_- \to \hat{x}^R, \quad \hat{x}_+^A \to \hat{x}_-^A, \quad \hat{x}_-^K \to \hat{x}_-^K \]

(222)

where $\hat{x}$ stands for the quasiclassical propagators or self energies, to be defined shortly. At any time we may also switch between different Fourier representations, but we prefer to keep the space and time variables as far as possible. The “gradient expansion” approximations may be done more generally by using the formulas in a related appendix, but we proceed via a more elementary route. From here on we explicitly incorporate spin indices into the Nambu matrices from the combination $x = (x, \sigma)$. We start from Eqs. (215) and (216), and perform two steps: taking the low energy approximation and a “renormalization” of the equilibrium propagator (here $\xi^0 \to \xi$). We also assume the (time-reversal) symmetry $\xi(-p) = \xi(p)$, which allows us to write $\xi(\epsilon - i\hbar \nabla_x - qA(x)) = \xi(\epsilon - i\hbar \nabla_x - qgA(x))$ and so on. On the purely technical side, we introduce the coordinate transformation $r = x_1 - x_2, R = (x_1 + x_2)/2, \sigma = R + r/2, x_2 = R - r/2$, as discussed in the appendices. This leads us to replace $\nabla_{x_1} = \nabla_r + \nabla_R/2$, etc.
\[ \nabla x_2 = -\nabla r + \nabla \mathbf{R}/2. \] Doing these we find
\[
\left[ i\hbar \frac{\partial}{\partial t_1} \hat{\tau}_3 \right. - i\hbar \frac{\partial}{\partial t_2} \hat{\tau}_3 \nabla r - \hat{\tau}_3 g \mathbf{A}(x_1, t_1) \right]
\times \hat{G}_{\text{low}}^\text{flow}(\mathbf{r}, \mathbf{R}; t_1, t_2)_{ij}
+ a \sum_k \left\{ \hat{\Sigma}_{ik}^\text{low} \otimes \hat{U}_{kj}^\text{low} \right\} (\mathbf{r}, \mathbf{R}; t_1, t_2)
\]
and
\[
\hat{G}_{\text{low}}^\text{flow}(\mathbf{r}, \mathbf{R}; t_1, t_2)_{ij}
\times \left[ -i\hbar \frac{\partial}{\partial t_2} \hat{\tau}_3 - i\hbar \frac{\partial}{\partial t_2} \nabla r - \hat{\tau}_3 g \mathbf{A}(x_2, t_2) \right]
= a \hbar \delta_{ij} \hat{1} \delta(t_1 - t_2)
\]
\[
+ a \sum_k \left\{ \hat{\Sigma}_{ik}^\text{low} \otimes \hat{U}_{kj}^\text{low} \right\} (\mathbf{r}, \mathbf{R}; t_1, t_2)
\]
(223)
where the factors "a" come from the bracketed differential operators which are equal to \( a G_{\text{coh,eq}}^{-1} \). We kept the notations \( x_{1,2} = \mathbf{R} \pm \mathbf{r}/2 \) in the argument of \( \mathbf{A} \) for brevity.

So far we have not made any crucial approximations, but here are two: we linearize the dispersion relation as
\[
\frac{\partial}{\partial t_2} \hat{\tau}_3 - i\hbar \frac{\partial}{\partial t_2} \nabla r - \hat{\tau}_3 g \mathbf{A}(x_2, t_2)
\]
and in addition we approximate
\[
\hat{\Sigma}_{ik}^\text{low} \otimes \hat{U}_{kj}^\text{low}
\]
(224)
where the delta functions which make Eqs. (223) and (224) unique. In the "left-right subtraction" process we lost
\[
\delta(t_1 - t_2)
\]
and
\[
\delta(t_1 + t_2)
\]
Furthermore, we Fourier transform with respect to \( r \) to go to the mixed representation.

Thus we obtain
\[
\left[ i\hbar \frac{\partial}{\partial t_2} \hat{\tau}_3 - i\hbar \frac{\partial}{\partial t_2} \nabla r - \hat{\tau}_3 g \mathbf{A}(\mathbf{R}, t_1) \right]
\times \hat{G}_{\text{low}}^\text{flow}(\mathbf{p}, \mathbf{R}; t_1, t_2)_{ij}
= a \hbar \delta_{ij} \hat{1} \delta(t_1 - t_2)
\]
\[
+ a \sum_k \left\{ \hat{\delta} \mathbf{p} \mathbf{R}^\text{low} \right\} (\mathbf{p}, \mathbf{R}; t_1, t_2)
\]
(225)
and
\[
\hat{G}_{\text{low}}^\text{flow}(\mathbf{p}, \mathbf{R}; t_1, t_2)_{ij}
\times \left[ -i\hbar \frac{\partial}{\partial t_2} \hat{\tau}_3 - i\hbar \frac{\partial}{\partial t_2} \nabla r - \hat{\tau}_3 g \mathbf{A}(\mathbf{R}, t_2) \right]
= a \hbar \delta_{ij} \hat{1} \delta(t_1 - t_2)
\]
\[
+ \sum_k \left\{ \hat{\delta} \mathbf{p} \mathbf{R}^\text{low} \right\} (\mathbf{p}, \mathbf{R}; t_1, t_2)
\]
(226)
Finally we subtract the equations, and integrate over \( \xi_\mathbf{p} \)
in the low-energy regime \([-E_c, E_c]\). Since \( \hat{\delta} + \hat{u} \) is inde-
where, furthermore, \( e^{R,A}(\hat{p}, \epsilon) \) is unknown. Clearly some information is thus lost in the subtraction process. Fortunately, it may be shown that the most essential information can be regained by introduction of separate normalization conditions [37, 38]. We shall not derive these conditions here properly. Actually a proper “proof” of them does not even exist (or else I am unaware of it), but according to some rather convincing arguments they should be valid “almost always”. We may try to point the way to a derivation as follows.

As a first step, in the previously considered case of homogeneous equilibrium we should be able to calculate the propagator \( \hat{g}(\hat{p}, \epsilon) \) from Eq. (228) directly by \( \xi_{\hat{p}} \) - integrating the low-energy quasiparticle propagator \( \hat{G}_{low}^{R,A}(\hat{p}, \epsilon) \). The latter may be found by solving the Dyson (or Gorkov) equation, Eq. (223). We solve it here in the absence of \( A \) (and \( U \)), and by considering only the off-diagonal self energy \( a \Sigma_{low}^{R,A}(\hat{p}, \epsilon) = a \Sigma_{low}(\hat{p} \hat{p}) \equiv \Delta(\hat{p}) \tau_3 \), which, furthermore, is assumed to be unitary; in the case of singlet s-wave pairing this means \( \langle a \Sigma_{low}^{2} \rangle = -\Delta^2 = |\Delta|^2 I \). In this case Eq. (223) yields

\[
[(\pm i \eta) - \hat{\tau}_3 \xi(\hat{p}) - a \Sigma_{low}^{R,A}] \hat{G}_{low,eq}^{R,A}(\hat{p}, \epsilon) = ha I
\]  

(231)

and by using the the property \( \{a \Sigma_{low}^{R}, \hat{\tau}_3\} = 0 \) (which is a consequence of \( a \Sigma_{low}^{R,A} \) being off-diagonal in Nambu space) we find the solutions [45]

\[
\hat{G}_{low,eq}^{R,A}(\hat{p}, \epsilon) = -ha \frac{\xi(\hat{p}) - a \Sigma_{low}^{R,A}}{\xi(\hat{p}) - a \Sigma_{low}^{R,A}} = -\frac{\xi(\hat{p}) - a \Sigma_{low}^{R,A}}{\xi(\hat{p}) - a \Sigma_{low}^{R,A}} \equiv \hat{G}_{low,eq}^{R,A}(\hat{p}, \epsilon)
\]  

(232)

Now from Eq. (228) we find by using \( \int d\xi(a + b \xi^2)^{-1} = \arctan(x)/\sqrt{ab} + C \)

\[
\hat{g}_{eq}^{R,A}(\epsilon) = \frac{1}{ha} \hat{\tau}_3 \int_{-E_c}^{E_c} d\xi_{\hat{p}} \hat{G}_{low,eq}^{R,A}(\hat{p}, \epsilon)
\]  

\[
= \int_{E_c}^{E_v} d\xi_{\hat{p}} \left( -\frac{\xi(\hat{p}) - a \Sigma_{low}^{R,A}}{\xi(\hat{p}) - a \Sigma_{low}^{R,A}} \right)
\]  

\[
= \int_{-E_v}^{-E_c} d\xi_{\hat{p}} \left( -\frac{\xi(\hat{p}) - a \Sigma_{low}^{R,A}}{\xi(\hat{p}) - a \Sigma_{low}^{R,A}} \right)
\]  

\[
= \int_{-E_v}^{E_v} d\xi_{\hat{p}} \left( -\frac{\xi(\hat{p}) - a \Sigma_{low}^{R,A}}{\xi(\hat{p}) - a \Sigma_{low}^{R,A}} \right)
\]  

\[
= \frac{\pi}{\sqrt{\Delta^2 - (\epsilon \pm i \xi)^2}}
\]  

Thus we have found which of the solutions in Eq. (230) is the correct one, and what the normalization constant is. We may now see that \( \hat{g}_{eq}^{R,A}(\epsilon) \) formed from Eq. (233) and the function \( \hat{g}^{R,A}_{eq}(\epsilon) = \text{tanh}(\beta \epsilon / 2)[\hat{g}^{R,A}_{eq}(\epsilon) - \hat{g}^{R,A}_{eq}(\epsilon)] \), satisfies \( \hat{g}_{eq} \circ \hat{g}_{eq}^{R,A}(\hat{p}, \epsilon) = -\pi^2 I \) or in component form

\[
\hat{g}_{eq}^{R,A}(\hat{p}, \epsilon) = -\pi^2 I
\]  

(234)

The second step is, roughly, to show from the general non-equilibrium quasiclassical equation [Eq. (227) or its simplified forms; see below] that the product \( \hat{g} \circ \hat{g} \) is “always” proportional to the unit Nambu matrix and hence invariant along a trajectory. (Note that if \( \hat{g}_1 \) and \( \hat{g}_2 \) are solutions of Eq. (227), then also \( \hat{g}_1 \circ \hat{g}_2 \) is a solution.) Then, if at any location the system may be considered to be in homogeneous equilibrium, the value of the product \( \hat{g} \circ \hat{g} \) may be calculated there, giving the result which we just derived in Eq. (234). Therefore \( \hat{g} \circ \hat{g}(\hat{p}, A, \epsilon, T) = -\pi^2 I \) is satisfied also for the full nonequilibrium \( \hat{g}(\hat{p}, R, \epsilon, T) \) of the mixed representation (see Appendix A). Thus we state without further proof that Eq. (227) for the original \( \hat{g}(\hat{p}, R; t_1, t_2) \) must be supplemented with the condition

\[
(\hat{g} \circ \hat{g})(\hat{p}, R; t_1, t_2) = -\delta(t_1 - t_2)\pi^2 I
\]  

(235)

For more discussions, see Refs. [37–41] and [1, 45, 46, 51, 52] for example.

3. General structure of the quasiclassical equations

Equation (227) together with Eq. (235) looks very complicated, written out in all detail. We now aim to simplify its appearance and therefore clarify its formal structure. First of all, we cease to index coordinate points with numbers! Second, we define the Nambu matrices [note that factors of \( \delta(t - t') \) satisfy \( f(t') = f(t) = f(t + t')/2) \]

\[
\hat{a}_{ij}(\hat{p}, R; t, t') = -\delta(t - t')\delta_{ij} q N(\hat{p}) \cdot A(\hat{R}, t') \hat{\tau}_3
\]  

\[
\hat{e}_{ij}(t, t') = i\hbar \delta'(t - t') \delta_{ij} \hat{\tau}_3
\]  

(236)

\[\hat{a}_{ij}(\hat{p}, R; t, t') = \delta(t - t')\delta_{ij} a t_{low}^{R,A}(\hat{p}, R; t') \hat{\tau}_3\]

where \( \hat{a}_{ij} \) and \( \hat{a}_{ij} \) are external scalar and vector potentials acting on the quasiparticles. They may be summed together, and thus we define the new potential term \( \hat{v} = \hat{v} + \hat{v} + \cdots \) which includes all (renormalized) one-body interactions. Using these definitions, Eqs. (227) and (235) may be written very compactly as

\[
[\hat{\epsilon} - \hat{v} - \hat{\sigma}, \hat{g} \circ \hat{g}]_0 + i\hbar \nabla_F \cdot \nabla \hat{g} = 0
\]  

\[
\hat{g} \circ \hat{g} = -\pi^2 I
\]  

(237)

Since \( \hat{\epsilon}_{++} = \hat{\epsilon}_{--}, \hat{v}_{++} = \hat{v}_{--}, \) and \( \hat{\epsilon}_{+} = \hat{\epsilon}_{-} = 0, \) it follows that \( \hat{g}^{R,A} = \hat{v} \) and \( \hat{g}^{R,A} = \hat{v}, \) while \( \hat{g}^{K} = \hat{v} \) and \( \hat{g}^{K} = \hat{v} \). Thus for the \( \hat{g}^{R,A,K} \) components of \( \hat{g} \) the equations become [50]

\[
[\hat{\epsilon} - \hat{v} - \hat{\sigma}^{R,A}, \hat{g}^{R,A}]_0 + i\hbar \nabla_F \cdot \nabla \hat{g}^{R,A} = 0
\]  

\[
[\hat{\epsilon} - \hat{v}, \hat{g}^{K}]_0 - \hat{\sigma}^{R} \circ \hat{g}^{K} + \hat{g}^{K} \circ \hat{\sigma}^{A}
\]  

\[
- \hat{\sigma}^{K} \circ \hat{g}^{A} + \hat{g}^{R} \circ \hat{g}^{K} + i\hbar \nabla_F \cdot \nabla \hat{g}^{K} = 0
\]  

(238)

\[
\hat{g}^{R,A} \circ \hat{g}^{R,A} = -\pi^2 I
\]  

\[
\hat{g}^{R} \circ \hat{g}^{K} + \hat{g}^{K} \circ \hat{g}^{A} = 0
\]  

(239)

We notice that the normalization condition may always be satisfied if we write

\[
\hat{g}^{K} = \hat{g}^{R} \circ \hat{h} - \hat{h} \circ \hat{g}^{A}
\]
where $\hat{h}$ is an arbitrary quasiclassical Nambu matrix [1, 8, 39]. One physical requirement on $\hat{h}$ is that it must yield the correct equilibrium limit. As we recall, this is given by $\hat{g}^K = h_{eq}(\hat{g}^R - \hat{g}^A)$, where $h_{eq}(\epsilon) = \tanh(\beta \epsilon/2)$ is related to the Fermi distribution function $f(\epsilon)$ by $h_{eq} = 1 - 2f$. Thus we call $h_{eq}(\epsilon)$ and the nonequilibrium functions $\hat{h}$ also “distribution functions”. Further restrictions on $\hat{h}$ are discussed in Appendix C. In general, two spin-matrix functions are required to parametrize $\hat{h}$, one for describing “particles” and the other for “holes”, for example [1]. However, there is no unique way to make this choice [1, 46]. There also exist some rather different, yet essentially equivalent, ways of introducing the distribution functions, which use a separation different from Eq. (239) [51, 52].

The equations (237) and (238) are now in a form which is independent of the Fourier representation. They are a good starting point for deriving all the explicit expressions, as long as it is understood what the symbolic notations mean. In particular, the meaning of “1” in the normalization condition in Eq. (237) must be reinterpreted in each case, so that we have

\[
\begin{align*}
(\hat{g} \circ \hat{g})(\hat{p}, \hat{R}; t, t') &= -\delta(t - t')\pi^2 \hat{I} \\
(\hat{g} \circ \hat{g})(\hat{p}, \hat{R}; \epsilon, \epsilon') &= -2\pi \hbar \delta(\epsilon - \epsilon')\pi^2 \hat{I} \\
(\hat{g} \circ \hat{g})(\hat{p}, \hat{R}; \epsilon, T) &= -\pi^2 \hat{I}
\end{align*}
\]

Here the constant $-\pi^2$ may be replaced by $-(\hbar \pi)^2$, $-\hbar^2$, $-1$, or something else, depending on the choices made in Eq. (228) or the Fourier transforms, and whether “$\hat{h} = 1$” or not. We must also transform Eqs. (236) to the different cases. For $\hat{g}(\hat{p}, \hat{R}; \epsilon, \epsilon')$ we have

\[
\begin{align*}
\hat{a}_{ij}(\hat{p}, \hat{R}; \epsilon, \epsilon') &= -\delta_{ij} 2\pi \hbar \delta(\epsilon - \epsilon') \epsilon_3 \\
\hat{a}_{ij}(\hat{p}, \hat{R}; \epsilon, \epsilon') &= \delta_{ij} aU_{low}(\hat{p}, \hat{R}; \epsilon - \epsilon') \epsilon_3 \\
\hat{a}_{ij}(\hat{p}, \hat{R}; \epsilon, T) &= \delta_{ij} aU_{low}(\hat{p}, \hat{R}; T) \epsilon_3
\end{align*}
\]

whereas for $\hat{g}(\hat{p}, \hat{R}; \epsilon, T)$ (where $T = (t + t')/2$ and and $t - t' \to \epsilon/\hbar$)

\[
\begin{align*}
\hat{a}_{ij}(\hat{p}, \hat{R}; \epsilon, T) &= -\delta_{ij} 2\pi \hbar \delta(\epsilon - \epsilon') \epsilon_3 \\
\hat{a}_{ij}(\hat{p}, \hat{R}; \epsilon, T) &= \delta_{ij} aU_{low}(\hat{p}, \hat{R}; T) \epsilon_3 \\
\hat{a}_{ij}(\hat{p}, \hat{R}; \epsilon, T) &= \delta_{ij} aU_{low}(\hat{p}, \hat{R}; T) \epsilon_3
\end{align*}
\]

The transformations for the folding product $\circ$ are explained in Appendix B.

Note that to get here we have not made any major approximations concerning the time or frequency variables. Indeed, while the “low-momentum” approximation in quasiclassical theory follows naturally from the degeneracy of the low-temperature Fermi system, no such natural approximations exist for the frequency variables. The validity of any low-frequency approximations thus depends on the properties of the particular physical system being studied. (The same goes for any assumptions of small gradients with respect to $\hat{R}$.)

Finally we note that there are other, perhaps more physical, ways of deriving the the quasiclassical equations and normalization conditions. See for example Ref. [51], where the same results are obtained without explicit integration with respect to $\xi_p$.

4. Observables: current density

Now, to actually use the solutions of the quasiclassical equations for something useful, values of some observables need to be calculated from them. We do not go into details of derivations here. As an example, the current density (for charge $q$ per fermion) in the case of a spherical Fermi surface ($v_F = v_F \hat{p}$) can be written as

\[
j(\hat{R}, t) = \hbar q v_F N(0) \frac{1}{2i} \int \frac{d\Omega_p}{4\pi} \text{Tr}[\hat{\tau}_3 \hat{g}^K(\hat{p}, \hat{R}, t, t)]
\]

(243)

where $\hat{g}^K = [\hat{g}]^K$. Here $N(0)$ is the single-spin quasiparticle density of states at Fermi energy [Eq. (50)] and the normalization $\hat{g} \circ \hat{g} = -\pi^2 \hat{I}$ is used. Note: The do not trust the prefactors without checking them.

5. Dirty limit: Usadel’s equation

Here we give a very concise derivation of the “Usadel equation”, which is a simplification of the above Eilenberger equation for superconducting metals in the dirty or disordered limit, i.e., in the presence of strong impurity scattering. To this end, consider

\[
[\hat{\epsilon} - \sigma, \hat{g}]_\circ + i\hbar v_F \cdot \nabla \hat{g} = 0,
\]

(244)

\[
\hat{g} \circ \hat{g} = -\pi^2 \hat{I},
\]

(245)

where $\sigma$ is the impurity self energy

\[
\sigma = \frac{\hbar}{2\pi \tau} \langle \hat{g} \rangle_{\hat{p}}, \quad \langle \cdots \rangle_{\hat{p}} = \int \frac{d\Omega_p}{4\pi} \cdots
\]

(246)

with $\tau$ being an impurity scattering time. We are assuming, for simplicity, a spherical Fermi surface, where $v_F = v_F \hat{p}$. The angular average then satisfies

\[
\langle v_F \rangle_{\hat{p}} = 0, \quad \langle v_F v_F \rangle_{\hat{p}} = \frac{v_F^2}{3} \tau^2
\]

(247)

In the case of a non-spherical Fermi surface, $v_F$ would an average over the Fermi surface.

Now, we expand the angular dependence is to lowest (“$p$ wave”) order so that

\[
\hat{g} = \hat{g}_0 + v_F \cdot \hat{g}
\]

(247)

where $\hat{g}_0$ and $\hat{g}$ are independent of $\hat{p}$. It can apparently be shown that this approximation is sufficient in the limit $\epsilon \ll \hbar/\tau$. So, inserting the expansion (and simplifying
notation by dropping hats and folding symbols)
\[ i\hbar v_F \cdot \nabla g_0 + i\hbar (v_F \cdot \nabla)v_F \cdot g = \]
\[ -\frac{\hbar}{2\pi^2} [g_0 + (v_F \cdot g_0 + v_F \cdot [\epsilon, g_0 + v_F \cdot g] = 0 \tag{248} \]
and
\[ i\hbar v_F \cdot \nabla g_0 + i\hbar (v_F \cdot \nabla)v_F \cdot g = \]
\[ -\frac{\hbar}{2\pi^2} [g_0 + (v_F \cdot g_0 + (v_F \cdot g_0 + [\epsilon, g_0 + v_F \cdot g] = 0 \tag{249} \]
The normalization condition gives
\[ gg = g_0 g_0 + (v_F \cdot g_0 + (v_F \cdot g_0 + \text{small}^2 = -\pi^2 \tag{250} \]
and, upon applying \( g_0 g_0 = -\pi^2 \),
\[ g_0 (v_F \cdot g) = -(v_F \cdot g_0) g_0 \tag{251} \]
Next, averaging Eq. (249) with \( \langle \cdots \rangle \) gives
\[ i\hbar v_F^2 \frac{1}{3} \nabla \cdot g + [\epsilon, g_0] = 0 \tag{252} \]
On the other hand, multiplying Eq. (249) first with \( v_F g_0 \) and only then averaging gives
\[ \langle i\hbar g_0 (v_F \cdot \nabla) g_0 \rangle \]
\[ -\frac{\hbar}{2\pi^2} (v_F g_0 g_0 v_F \cdot g - v_F g_0 v_F \cdot g_0) = 0 \tag{253} \]
The last term can be simplified with Eq. (251). Then, completing the averages yields
\[ \hbar v_F^2 \frac{1}{3} i g_0 \nabla g_0 = -\pi^2 \frac{\hbar}{3} v_F^2 g \tag{254} \]
and thus
\[ g = -i\frac{\tau}{\hbar} g_0 \nabla g_0 \tag{255} \]
Inserting this into Eq. (252) finally gives
\[ D \frac{\pi}{\hbar} \nabla \cdot (g_0 \nabla g_0) + [\epsilon, g_0]_0 = 0, \quad g_0 \nabla g_0 = -\pi^2 \frac{\hbar}{3} v_F^2 \nabla \]
where \( D = \frac{1}{4} v_F^2 \tau \) is a diffusion constant (and we reinstated the hats and folding products). This equation is the Usadel equation. Other perturbations than the impurities could straightforwardly be added to the equation as angle-averaged self energies.

6. Observables in dirty limit: current density

The current density of Eq. (243) can now also be adapted to the Usadel case. Using \( v_k = v_F \frac{\hbar p}{2m}, \langle \hat{p} \rangle_p = 0, \langle \hat{p} \hat{p} \rangle_p = \frac{1}{3} \frac{\hbar^2}{2m} \) and Eq. (255) one immediately finds that
\[ j(R, t) = -\hbar q N(0) \frac{D}{2\pi} \text{Tr} \left[ \hat{\tau}_3 [g_0 \nabla g_0]^K (R, t, t) \right], \tag{257} \]

The Usadel equation is apparently a realistic approximation in typical metallic systems, which tend to have a lot of disorder unless specially prepared. In any case, it is so much easier to solve than the Eilenberger equation that it tends to be used as a first approximation in any case. For superfluid \(^3\)He, on the other hand, the Usadel approximation tends to be quite useless.

7. Epilogue: where to go from here?

Even after all this trouble we have, of course, not done much more but scratched the surface of the quasiclassical theory. Most importantly, we should now begin to consider in more detail (i) how to solve the equations for the propagators (e.g., using the "Riccati parametrization"), and then (ii) how calculate physical observables from the solutions. Also important is (iii) to consider how the calculations may be simplified with the so-called Matsubara technique in the important case of thermodynamic equilibrium. In equilibrium we also need to consider (iv) the calculation of thermodynamic potentials. Furthermore, we might consider discussing (v) how the Ginzburg-Landau theory is derived from these equilibrium considerations in the limit \( T \to T_c \). These considerations we postpone for some later time. Meanwhile, Ref. [1] should give a reasonable starting point for most of them.

Appendix A: Fourier transform relations

All the time we must deal with quantities \( f(x, x'+t') \) which depend on two positions and times or \( f(k, \omega,k',\omega') \) which depend on two momenta and energies. In the normal-state Green’s functions these coordinate dependencies arise from expectation values of two field operators, one of which is a destruction operator \( \psi(x,t) \), and the other a creation operator \( \psi^\dagger(x,t') \). If these field operators are expanded in a box-normalized plane-wave basis \( \phi_k(x) = \exp(ik \cdot x) / \sqrt{V} \) then we are in a natural way led to make the following definitions. (Note that we always take “\( \hbar = 1 \)” to simplify presentation.)

First of all, the following “completeness relations” are important
\[ \int_V d^3x e^{-i(k-k') \cdot x} = V \delta_{kk'} \]
\[ \frac{1}{V} \sum_k e^{ik \cdot (x-x')} = \delta(x-x') \tag{A1} \]
and we have for example
\[ f(x) = \frac{1}{V} \sum_k f_k e^{ik \cdot x}, \quad f_k = \int_V d^3x f(x) e^{-ik \cdot x} \tag{A2} \]
In the thermodynamic limit \( (V \to \infty, N/V = \text{const.}) \) the following replacements must be made
\[ V \delta_{kk'} \to (2\pi)^3 \delta(k-k'), \quad \frac{1}{V} \sum_k \to \int \frac{d^3k}{(2\pi)^3} \tag{A3} \]
since the density of states in $k$ space is $V/(2\pi)^3$. In this limit we adopt the following basic definitions for the Fourier transforms of two-point propagators

$$f(x,x') = \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} e^{ik \cdot x} e^{-ik' \cdot x'} f(k,k')$$

$$f(k,k') = \int d^3x d^3x' e^{-ik \cdot x} e^{ik' \cdot x'} f(x,x')$$

(A4)

Now we introduce the coordinate transformation $r = x - x'$ and $R = (x + x')/2$, with the inverse $x = R + r/2$, $x' = R - r/2$. This transformation has unit Jacobian. Thus we may rearrange the previous equation

$$f(k,k') = \int d^3r d^3R e^{-ik \cdot (R+r/2)} e^{ik' \cdot (R-r/2)}$$

$$\times f(R + r/2, R - r/2)$$

$$= \int d^3r d^3R e^{-i(k+k') \cdot r} e^{-i(k-k') \cdot R} f(r, R)$$

$$= \int d^3r d^3R e^{-ip \cdot r} e^{-iQ \cdot R} f(r, R) \equiv f(p, q)$$

(A5)

where we defined new momentum variables $p = k + k')/2$ and $Q = k - k'$, which have the inverses $k = p + Q/2$ and $k' = p - Q/2$. All of these have obvious inverses. We also note the useful chain rule results $\nabla_x = \nabla_r + \nabla_{R/2}$, and $\nabla_{x'} = -\nabla_r + \nabla_{R/2}$ which often appear in connection with the Fourier transforms.

Now we introduce the corresponding transformations for the time and energy (frequency) variables. Suppose we have the function $f(t,t')$. Then

$$f(t,t') = \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} e^{-i\omega t} e^{i\omega' t'} f(\omega, \omega')$$

$$f(\omega, \omega') = \int dt \int dt' e^{i\omega t} e^{-i\omega' t'} f(t, t')$$

(A6)

which now have opposite sign definitions so that the position and time transformations may be combined in a relativistically covariant way. Also here we define new coordinates $\tilde{t} = t - t'$, and $\tilde{T} = (t + t')/2$, along with inverses $\tilde{t} = T + \tilde{t}/2$, $\tilde{T} = \tilde{t}/2$, and write

$$f(\omega, \omega') = \int d\tilde{t} \int d\tilde{T} e^{i\omega (T + \tilde{t}/2)} e^{-i\omega' (T - \tilde{t}/2)}$$

$$\times f(T + \tilde{t}/2, T - \tilde{t})$$

$$= \int d\tilde{t} \int d\tilde{T} e^{i[\omega + \omega']/2} e^{i(\omega - \omega')\tilde{T}} f(\tilde{t}, \tilde{T})$$

$$= \int d\tilde{t} \int d\tilde{T} e^{i\tilde{t}} e^{i\tilde{t}E \tilde{T}} f(\tilde{t}, \tilde{T}) \equiv f(\epsilon, E)$$

(A7)

Here we again defined $\epsilon = (\omega + \omega')/2$, and $E = \omega - \omega'$, and the inverses $\omega = \epsilon + E/2$, and $\omega' = \epsilon - E/2$ Note that $\partial_\tilde{t} = \partial_t + \partial_T/2$, and $\partial_\tilde{T} = -\partial_\tilde{t} + \partial_T/2$.

The partial transformation of $f(xt, x't')$ to the “mixed” representation

$$F(p, R; \epsilon, T) = \int d^3r d^\epsilon d\epsilon' e^{-ik \cdot r + i\tilde{t}}$$

$$\times f(R + r/2, T + \tilde{t}/2; R - r/2, T - \tilde{t}/2)$$

$$= \int d^3r d^\epsilon d\epsilon' f(r, R; \tilde{t}, T)$$

(A8)

This is sometimes called a Wigner transformation, because if $f(x, x')$ is a density matrix, then $F(p, R)$ is what is known as a Wigner function [10]. Functions of the form $F(p, R)$ may be interpreted as “pseudo-classical” distribution functions for particles of position $R$ and momentum $p$, and this is why the representation of Eq. (A8) is convenient for the quasiclassical approximation.

Sometimes we may also need the “trace” of $f(xt, x't')$, which we define in the coordinate and mixed representations as

$$Spf = \int d^3x \int dt f(xt, xt)$$

$$= \int d^3R \int \frac{d^3p}{(2\pi)^3} \int dt \int \frac{d\epsilon}{2\pi} F(p, R; \epsilon, T)$$

(A9)

Partial traces over the spatial (and momentum) coordinates only are even more useful.

Appendix B: Properties of folding products

1. Folding products in coordinate and mixed (“Wigner”) representations

We define the “folding” product $C = A \circ B$ by

$$(\hat{A} \otimes \hat{B})(xt, x't') = \int d^3x_3 \int d^3t_3 \hat{A}(xt, x_3t_3) \hat{B}(x_3t_3, x't')$$

(B1)

or in momentum-frequency representation

$$(\hat{A} \otimes \hat{B})(k\omega, k'\omega') = \int \frac{d^3k_3}{(2\pi)^3} \int \frac{d\omega_3}{2\pi} \hat{A}(k\omega, k_3\omega_3) \hat{B}(k_3\omega_3, k'\omega')$$

(B2)

Here the integrations could also include the spin summation, but it is more convenient to group them with the Nambu indices. Thus the spin-Nambu summation is here taken care of by a the matrix product of $4 \times 4$ Nambu matrices $\hat{A}$ and $\hat{B}$ which may both be (folding) products of some propagator and self-energy expressions. We could also include summation over the Keldysh indices in the definition of the folding product, but we prefer to display the Keldysh indices explicitly when needed. Nevertheless, sometimes we may write for example $\hat{A} \otimes \hat{B}$, where an additional matrix product over the Keldysh indices is then implied. Everywhere in this section we follow the Fourier transform definitions of Appendix A.
For many purposes it will be convenient to switch from \( \mathbf{x}, \mathbf{x}' \) to the center-of-mass coordinates \( \mathbf{r} = \mathbf{x} - \mathbf{x}' \) and \( \mathbf{R} = (\mathbf{x} + \mathbf{x}')/2 \), and furthermore Fourier transform from \( \mathbf{r} \) to the variable \( \mathbf{p} \). In this mixed (or “Wigner”) representation for \( \hat{A} \) and \( \hat{B} \) the folding product of Eq. (B1) becomes

\[
(\hat{A} \otimes \hat{B})(\mathbf{p}, \mathbf{R}; t, t') = \int dt_3 \hat{A}(\mathbf{p} + \frac{1}{2i} \nabla \mathbf{R}_2, \mathbf{R}_1; t, t_3) \times \hat{B}(\mathbf{p} - \frac{1}{2i} \nabla \mathbf{R}_1, \mathbf{R}_2; t_3, t') \bigg|_{\mathbf{R}_1 = \mathbf{R}_2 = \mathbf{R}}
\]

(B3)

In the middle row \( \nabla \mathbf{R}_2 \) is assumed to operate to the left, although we now drop the notation \( \overrightarrow{\nabla} \) for simplicity. The same center-of-mass transformation may be done for the time points \( t, t' \) by defining \( t = t - t' \) and \( T = (t + t')/2 \). If, again we replace the time \( t \) with the energy \( \epsilon \) via a Fourier transformation, then Eq. (B3) takes the form

\[
(\hat{A} \otimes \hat{B})(\mathbf{p}, \mathbf{R}; \epsilon, T) = \hat{A}(\mathbf{p} + \frac{1}{2i} \nabla \mathbf{R}_2, \mathbf{R}_1; \epsilon - \frac{1}{2i} \frac{\partial}{\partial T_1}, T_1) \times \hat{B}(\mathbf{p} - \frac{1}{2i} \nabla \mathbf{R}_1, \mathbf{R}_2; \epsilon + \frac{1}{2i} \frac{\partial}{\partial T_1}, T_2) \bigg|_{\mathbf{R}_1 = \mathbf{R}_2, T_1 = T_2 = T}
\]

(B4)

Let us now present the transformation leading to Eq. (B3) in more detail, although in the backward direction. Time variables and Nambu accents are suppressed for simplicity. We write

\[
C(\mathbf{r}, \mathbf{R}) = \int \frac{d^3 p}{(2\pi)^3} e^{i \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} (A \otimes B)(\mathbf{p}, \mathbf{R})
\]

\[
= \int \frac{d^3 p}{(2\pi)^3} e^{i \mathbf{p} \cdot \mathbf{r}} A(\mathbf{p} + \frac{1}{2i} \nabla \mathbf{R}_2, \mathbf{R}_1) \times B(\mathbf{p} - \frac{1}{2i} \nabla \mathbf{R}_1, \mathbf{R}_2) \bigg|_{\mathbf{R}_1 = \mathbf{R}_2 = \mathbf{R}}
\]

(B5)

and then insert the expressions

\[
A(\mathbf{p} + \frac{1}{2i} \nabla \mathbf{R}_2, \mathbf{R}_1) = e^{-\frac{1}{2} \nabla \mathbf{R}_2 \cdot \nabla \mathbf{R}_1} A(\mathbf{p}, \mathbf{R}_1)
\]

\[
= \int d^3 r_1 e^{-i \mathbf{p} \cdot \mathbf{r}_1} e^{i \frac{1}{2} \nabla \mathbf{R}_2 \cdot \mathbf{r}_1} A(\mathbf{r}_1, \mathbf{R}_1)
\]

\[
B(\mathbf{p} - \frac{1}{2i} \nabla \mathbf{R}_1, \mathbf{R}_2) = e^{\frac{1}{2} \nabla \mathbf{R}_1 \cdot \nabla \mathbf{p}} B(\mathbf{p}, \mathbf{R}_2)
\]

\[
= \int d^3 r_2 e^{-i \mathbf{p} \cdot \mathbf{r}_2} e^{i \frac{1}{2} \nabla \mathbf{R}_1 \cdot \mathbf{r}_2} B(\mathbf{r}_2, \mathbf{R}_2)
\]

(B6)

Using \( \int d^3 p \exp[i \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')] = (2\pi)^3 \delta^{(3)}(\mathbf{r} - \mathbf{r}') \) and assuming \( \mathbf{R}_1 = \mathbf{R}_2 = \mathbf{R} \) we find

\[
C(\mathbf{r}, \mathbf{R}) = \int \int d^3 r_1 d^3 r_2 \int \frac{d^3 p}{(2\pi)^3} e^{i \mathbf{p} \cdot (\mathbf{r}_1 - \mathbf{r}_2)}
\]

\[
\times e^{-\frac{1}{2} \nabla \mathbf{R}_2 \cdot \mathbf{r}_1} e^{\frac{1}{2} \nabla \mathbf{R}_2 \cdot \mathbf{r}_2} A(\mathbf{r}_1, \mathbf{R}_1) B(\mathbf{r}_2, \mathbf{R}_2)
\]

\[
= \int d^3 r_1 e^{-\frac{1}{2} \nabla \mathbf{R}_2 \cdot \mathbf{r}_1} e^{\frac{1}{2} \nabla \mathbf{R}_2 \cdot (\mathbf{r}_1 - \mathbf{r}_2)} A(\mathbf{r}_1, \mathbf{R}_1) B(\mathbf{r}_1 - \mathbf{r}_2) = \int d^3 r_1 A(\mathbf{r}_1, \mathbf{R}_1 + \frac{1}{2}(\mathbf{r}_1 - \mathbf{r}_2)) B(\mathbf{r}_1 - \mathbf{r}_2)
\]

\[
= \int d^3 r_1 A(\mathbf{r}_1, \mathbf{R}_1 + \frac{1}{2} \mathbf{r}_1) + \frac{1}{2} \mathbf{r}_1 - \mathbf{r}_1
\]

\[
= \int d^3 r_1 A(\mathbf{r}_1, \mathbf{R}_1 + \frac{1}{2} \mathbf{r}_1 - \mathbf{r}_1) = \int d^3 r_1 \tilde{A}(\mathbf{r}_1, \mathbf{R}_1 + \frac{1}{2} \mathbf{r}_1 - \mathbf{r}_1) \equiv \tilde{C}(\mathbf{x}, \mathbf{x}')
\]

(B7)

where we finally used \( \mathbf{x} = \mathbf{R} + \mathbf{r}/2 \) and \( \mathbf{x}' = \mathbf{R} - \mathbf{r}/2 \). Apart from a change of the integration variable to \( \mathbf{x}_3 = \mathbf{x} - \mathbf{r}_1 \) this is equivalent to Eq. (B1). (Note that this assumes an infinite system or periodic boundary conditions.)

2. Folding products for quasiclassical quantities

For quasiclassical, \( \xi_p \)-integrated propagators and self-energies which are only defined on the Fermi surface, the folding products simplify to

\[
(\hat{a} \otimes \hat{b})(\mathbf{p}, \mathbf{R}; t, t') = \int dt_3 \hat{a}(\mathbf{p}, \mathbf{R}; t, t_3) \hat{b}(\mathbf{p}, \mathbf{R}; t_3, t')
\]

(B8)

in the time representation, or

\[
(\hat{a} \otimes \hat{b})(\mathbf{p}, \mathbf{R}; \omega, \omega') = \int \frac{d\omega_3}{2\pi} \hat{a}(\mathbf{p}, \mathbf{R}; \omega, \omega_3) \hat{b}(\mathbf{p}, \mathbf{R}; \omega_3, \omega')
\]

(B9)

in energy representation, or

\[
(\hat{a} \otimes \hat{b})(\mathbf{p}, \mathbf{R}; \epsilon, T)
\]

\[
= \hat{a}(\mathbf{p}, \mathbf{R}; \epsilon - \frac{1}{2i} \frac{\partial}{\partial T_1}, T_1) \hat{b}(\mathbf{p}, \mathbf{R}; \epsilon + \frac{1}{2i} \frac{\partial}{\partial T_1}, T_2) \bigg|_{T_1,2=T}
\]

\[
= e^{\frac{1}{2} (\partial_{\epsilon_1} \partial_{\epsilon_2} - \partial_{\epsilon_2} \partial_{\epsilon_1})} \hat{a}(\mathbf{p}, \mathbf{R}; \epsilon_1, T_1)
\]

\[
\times \hat{b}(\mathbf{p}, \mathbf{R}; \epsilon_2, T_2) \big|_{T_1,2=T; \epsilon_1,2=\epsilon}
\]

(B10)

in the mixed time-energy representation. The last line of Eq. (B10) is useful for generating low-frequency (“gradient”) expansions. The “proof” of this equation is similar to what was shown in Eq. (B7), but note that the sign of the exponents differ. Finally, by Fourier transforming
Eq. (B10) with respect to $T$ we find

$$
(\hat{a} \circ \hat{b})(\hat{p}, \hat{R}; \epsilon, E) \propto \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} 2\pi \delta(E_1 + E_2 - E)
\times \hat{a}(\hat{p}, \hat{R}; \epsilon + \frac{E_2}{2}, E_1) \hat{b}(\hat{p}, \hat{R}; \epsilon - \frac{E_1}{2}, E_2)
$$

(B11)

where we used $\int dT \exp[i(E-E_1-E_2)T] = 2\pi \delta(E_1+E_2-E)$. A more symmetric form may still be achieved with the substitutions $E_2 = E/2 + E_2$ and $E - E_2 = E/2 - E_2$. The last line of Eq. (B11) may also be obtained from Eq. (B9) with the substitutions $\omega = \epsilon + E/2$, $\omega' = \epsilon - E/2$ and $\omega_3 = \epsilon - E/2 + E_2$.

We often use the following commutator notation

$$[\hat{A}, \hat{B}]_o = \hat{A} \circ \hat{B} - \hat{B} \circ \hat{A}$$

or even $[\hat{A}, \hat{B}]_c$, in which case an additional summation over the Keldysh indices is implied.

**Appendix C: Symmetries of Nambu matrices**

Below we discuss the symmetries which are valid for all Nambu matrix propagators, regardless of the state of the system or geometrical restrictions, etc. This is so because there is a certain amount of redundancy in the very definition of these propagators as expectation values of fermion field operators. From the Dyson equation it then follows that the same symmetries are valid also for the self-energy matrices, as discussed in the previous sections. In the final subsection we consider some small applications of the basic symmetries, and show how they may be used to obtain useful results.

Besides these obvious basic symmetries, in many cases the propagators and the self energies may satisfy additional symmetries which are related to the special symmetries of the Hamiltonian, or the equations of motion and the boundary conditions. However, such symmetries may just as well be spontaneously broken in the solutions, since nothing actually enforces them. One may hope to find such symmetries by studying the symmetries of the equations as follows. For example, let $\hat{g}(\mathbf{k}, \epsilon)$ be a solution of the quasiclassical (Eilenberger) equation, with self-energy $\hat{\sigma}(\mathbf{k}, \epsilon)$. It may be noticed that if we transform both $\hat{g}^R$ and $\hat{\sigma}^R$ with $\hat{x}(\mathbf{k}, \epsilon) = i\tau_2[\hat{x}(-\mathbf{k}, -\epsilon)]^T \tau_2$, then the resulting pair $\hat{g}^R$, $\hat{\sigma}^R$ still solves the same equation for reversed $\mathbf{k}$ and $\epsilon$. It is now reasonable to ask if, in fact, these two solutions could be one and the same, that is $\hat{g}^R = \hat{g}^R$, $\hat{\sigma}^R = \hat{\sigma}^R$. Then they would satisfy the symmetry $[\hat{x}(\mathbf{k}, \epsilon)]^T = i\tau_2 \hat{x}(-\mathbf{k}, -\epsilon)i\tau_2$. Indeed, this symmetry should be satisfied in the absence of external magnetic fields, which give rise to a term like $\mathbf{B} \cdot \mathbf{\sigma}$ in the Hamiltonian. (Reference? What is its relation to time reversal symmetry? Do we also have to assume the gap matrix to have a definite parity?) Finally, let us note again that in equilibrium the symmetries Eqs. (116), (118), (140), and (145) apply. Note, however, that Eq. (140) is only valid if a proper gauge is chosen.

1. The basic symmetry relations

Let us write down the general definitions of the contour-ordered, $R, A, K$, and Matsubara propagators (for fermions) [1]

$$
\hat{G}^{\text{ir}}(\mathbf{x}, t; \mathbf{x}', t')_{ij} = -i\langle T_\tau[\hat{\Psi}_1(\mathbf{x}, t)\hat{\Psi}^\dagger_1(\mathbf{x}', t')]\rangle_{ij}
$$

$$
\hat{G}^{\text{ir}}(\mathbf{x}, t; \mathbf{x}', t') = -i\theta(t - t')\langle \hat{\Psi}_1(\mathbf{x}, t), \hat{\Psi}^\dagger_1(\mathbf{x}', t') \rangle
$$

$$
\hat{G}^{\text{A}}(\mathbf{x}, t; \mathbf{x}', t') = i\theta(t' - t)\langle \hat{\Psi}_1(\mathbf{x}, t), \hat{\Psi}^\dagger_1(\mathbf{x}', t') \rangle
$$

$$
\hat{G}^{\text{R}}(\mathbf{x}, t; \mathbf{x}', t') = -i\langle \hat{\Psi}_1(\mathbf{x}, t), \hat{\Psi}^\dagger_1(\mathbf{x}', t') \rangle
$$

$$
\hat{G}^{\text{M}}(\mathbf{x}, t; \mathbf{x}', t') = -\langle T_\tau[\hat{\Psi}_1(\mathbf{x}, -it\tau), \hat{\Psi}^\dagger_1(\mathbf{x}', 0)]\rangle
$$

(C1)

where $l = 1, 2, 3, 4$, such that $\Psi_1 = \psi_1$, $\Psi_2 = \psi_4$, $\Psi_1 = \psi_1$, and $\Psi_4 = \psi_4$. The first and second Keldysh index $(i, j)$ denote the contour part (− or +) of the first and second time point, respectively. We shall only discuss the symmetries of the $\hat{G}^c$ and $\hat{G}^{R,A,K}$ functions here. Using $\langle \hat{A} \rangle^\ast = \langle \hat{A} \rangle^\dagger$, $\langle AB \rangle^\dagger = B^\dagger A^\dagger$, and the results $\hat{\tau}_1 \hat{\Psi} = \hat{\Psi}^\dagger$, $\hat{\tau}_1 \hat{\Psi}^\dagger = \hat{\Psi}$ (see discussion related to Eqs. (151)), we readily find the two sets of basic symmetry relations

$$
[\hat{G}^c(\mathbf{x}, t; \mathbf{x}', t')_{ij}]^T = -[\sigma_1]_{jk}[G^c(\mathbf{x}', t'; \mathbf{x}, t)]_{kl}[\sigma_1]_{li}
$$

$$
[\hat{G}^{A^R}(\mathbf{x}, t; \mathbf{x}', t')_{ij}]^T = [G^{A^R}(\mathbf{x}', t'; \mathbf{x}, t)]_{ij}
$$

(C2)

$$
[\hat{G}^{K}(\mathbf{x}, t; \mathbf{x}', t')_{ij}]^T = -[G^{K}(\mathbf{x}', t'; \mathbf{x}, t)]_{ij}
$$

and

$$
\hat{\tau}_1 \hat{G}^c(\mathbf{x}, t; \mathbf{x}', t')_{ij} \hat{\tau}_1 = -[\hat{G}^c(\mathbf{x}', t'; \mathbf{x}, t)]_{ji}^T
$$

$$
\hat{\tau}_1 \hat{G}^{A^R}(\mathbf{x}, t; \mathbf{x}', t') \hat{\tau}_1 = -[\hat{G}^{A^R}(\mathbf{x}', t'; \mathbf{x}, t)]^T
$$

(C3)

Here $T$ denotes transpose with respect to the Nambu indices and $\dagger = T\ast$. From the first set we note that the complex conjugation in $\dagger$ switches the contour part of each time point in $\hat{G}^c$, as represented with the transformation using $\sigma_1$ matrices. Thus $(tt', --) \rightarrow (t't', +)$, $(tt', ++) \rightarrow (t't', +)$ etc. We also see that the retarded and advanced functions are full Hermitian conjugates of each other. For convenience we now repeat these symmetries in various Fourier representations. We follow the Fourier transform definitions of Appendix A.

After transforming to a momentum-energy representa-
tion the symmetries take the forms

\[ [\hat{G}^c(k, \omega; k', \omega')]_i^j = -[\sigma_1]_{jk} [\hat{G}^c(k', \omega'; k, \omega)]_{kl}[\sigma_1]_{li} \]
\[ [\hat{G}^{R,A}(k, \omega; k', \omega')]_i^j = \hat{G}^{A,R}(k', \omega'; k, \omega) \]
\[ [\hat{G}^{K}(k, \omega; k', \omega')]_i^j = -\hat{G}^{K}(k', \omega'; k, \omega) \]  
(C4)

and

\[ \tilde{\tau}_1 \hat{G}^c(k, \omega; k', \omega')_{ij} \tilde{\tau}_1 = -[\hat{G}^c(-k', -\omega'; -k, -\omega)]_{ji} \]
\[ \tilde{\tau}_1 \hat{G}^{R,A}(k, \omega; k', \omega') \tilde{\tau}_1 = -[\hat{G}^{A,R}(-k', -\omega'; -k, -\omega)]_{ji} \]
\[ \tilde{\tau}_1 \hat{G}^{K}(k, \omega; k', \omega') \tilde{\tau}_1 = -[\hat{G}^{K}(-k', -\omega'; -k, -\omega)]_{ji} \]  
(C5)

whereas in the center-of-mass and difference coordinates

\[ [\hat{G}^c(r, R; t, T)]_i^j = -[\sigma_1]_{jk} [\hat{G}^c(-r, R; -t, T)]_{kl}[\sigma_1]_{li} \]
\[ [\hat{G}^{R,A}(r, R; t, T)]_i^j = \hat{G}^{A,R}(-r, R; -t, T) \]
\[ [\hat{G}^{K}(r, R; t, T)]_i^j = -\hat{G}^{K}(-r, R; -t, T) \]  
(C6)

and

\[ \tilde{\tau}_1 \hat{G}^c(r, R; t, T) \tilde{\tau}_1 = -[\hat{G}^c(-r, R; -t, T)]_i^j \]
\[ \tilde{\tau}_1 \hat{G}^{R,A}(r, R; t, T) \tilde{\tau}_1 = -[\hat{G}^{A,R}(-r, R; -t, T)]_i^j \]
\[ \tilde{\tau}_1 \hat{G}^{K}(r, R; t, T) \tilde{\tau}_1 = -[\hat{G}^{K}(-r, R; -t, T)]_i^j \]  
(C7)

Finally in the mixed representation

\[ [\hat{G}^c(p, R; \epsilon, T)]_i^j = -[\sigma_1]_{jk} [\hat{G}^c(p, R; \epsilon, T)]_{kl}[\sigma_1]_{li} \]
\[ [\hat{G}^{R,A}(p, R; \epsilon, T)]_i^j = \hat{G}^{A,R}(p, R; \epsilon, T) \]
\[ [\hat{G}^{K}(p, R; \epsilon, T)]_i^j = -\hat{G}^{K}(p, R; \epsilon, T) \]  
(C8)

and

\[ \tilde{\tau}_1 \hat{G}^c(p, R; \epsilon, T) \tilde{\tau}_1 = -[\hat{G}^c(-p, R; -\epsilon, T)]_i^j \]
\[ \tilde{\tau}_1 \hat{G}^{R,A}(p, R; \epsilon, T) \tilde{\tau}_1 = -[\hat{G}^{A,R}(-p, R; -\epsilon, T)]_i^j \]
\[ \tilde{\tau}_1 \hat{G}^{K}(p, R; \epsilon, T) \tilde{\tau}_1 = -[\hat{G}^{K}(-p, R; -\epsilon, T)]_i^j \]  
(C9)

One more representation (that is “\(\hat{G}(p; Q, \epsilon, E)^\dagger\)) and all the separate combinations of position/momentum and time/energy representation remain, but they should be easy to figure out from the above ones. Using the Dyson equation it may be shown that the same symmetries are valid for self-energy matrices \(\Sigma(p)\) as well as the propagators \(\hat{G}(p)\) themselves. For the quasiclassical matrices \(\hat{g}(p) \propto \tau_3 \int dp \hat{G}(p)\) and \(\hat{\sigma}(p) \propto \Sigma(p) \hat{g}(p)\) the relations of Eqs. (C8) and (C9) are transformed to

\[ [\hat{x}^c(p, R; \epsilon, T)]_i^j = \pm [\sigma_1]_{jk} [\hat{x}^c(-p, R; -\epsilon, T)]_{kl}[\sigma_1]_{li} \]
\[ [\hat{x}^{R,A}(p, R; \epsilon, T)]_i^j = \pm \tilde{\tau}_3 [\hat{x}^{R,A}(p, R; \epsilon, T)]_i^j \]
\[ [\hat{x}^{K}(p, R; \epsilon, T)]_i^j = \pm \tilde{\tau}_3 [\hat{x}^{K}(p, R; \epsilon, T)]_i^j \]  
(C10)

and

\[ [\hat{x}^c(p, R; \epsilon, T)]_i^j = -\hat{\tau}_2 \hat{x}^c(-p, R; -\epsilon, T)]_{ji} \]
\[ [\hat{x}^{R,A}(p, R; \epsilon, T)]_i^j = -\hat{\tau}_2 \hat{x}^{R,A}(-p, R; -\epsilon, T)]_{ji} \]
\[ [\hat{x}^{K}(p, R; \epsilon, T)]_i^j = -\hat{\tau}_2 \hat{x}^{K}(-p, R; -\epsilon, T)]_{ji} \]  
(C11)

where \(\hat{x}\) stands for either \(g\) or \(\sigma\). For \(\hat{g}\) the lower sign must be used if its definition includes a multiplication of \(\hat{G}\) by “i”. Similar relations exist for the Matsubara matrices, and all of them are neatly collected in Appendix C of Ref. [1].

2. Derived symmetries, separation of spin matrices

By combining Eqs. (C2) and (C3) we find the additional symmetries

\[ [\sigma_1]_{jk} [\hat{G}^c(x, t; x', t')]_{kl}[\sigma_1]_{li} = \tau_1 [\hat{G}^c(x, t; x', t')]_{ji} \]
\[ \hat{G}^{R,A}(x, t; x', t') = \tau_1 [\hat{G}^{R,A}(x, t; x', t')]^* \tau_1 \]
\[ \hat{G}^{K}(x, t; x', t') = \tau_1 [\hat{G}^{K}(x, t; x', t')]^* \tau_1 \]  
(C12)

Similarly, from Eqs. (C10) and (C11)

\[ \mp [\sigma_1]_{jk} [\hat{x}^c(p, R; \epsilon, T)]_{kl}[\sigma_1]_{li} = \mp \hat{\tau}_2 [\hat{x}^c(-p, R; -\epsilon, T)]_{ji} \]
\[ \pm \hat{x}^{R,A}(p, R; \epsilon, T) = \mp \hat{\tau}_2 \mp \hat{x}^{R,A}(-p, R; -\epsilon, T)]^* \tau_1 \]
\[ \mp \hat{x}^{K}(p, R; \epsilon, T) = \mp \hat{\tau}_2 \mp \hat{x}^{K}(-p, R; -\epsilon, T)]^* \tau_1 \]  
(C13)

where the signs and the meaning of \(\hat{x}\) are the same as before. Similar relations exist for the other Fourier representations, but we skip them here. It is often very useful to separate the spin matrix components of \(\hat{x} = \hat{x}^{R,A,K}(p, R; \epsilon, T)\) as follows [1]

\[ \hat{x} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} a + a \cdot \sigma & (b + b \cdot \sigma) i \sigma_2 \\ i \sigma_2 (c + c \cdot \sigma) & d + i \sigma_2 (d \cdot \sigma) i \sigma_2 \end{bmatrix} \]  
(C14)

where \(A, B, C, D\) are 2 \(\times\) 2 spin matrices, while \(a, b, c, d\) and \(a, b, c, d\) are their scalar and vector components. From the symmetries of Eqs. (C13) it follows that \(\hat{x}^{R,A,K}\) may be simplified to

\[ \hat{x}^{R,A} = \begin{bmatrix} A^{R,A} & B^{R,A} \\ \mp B^{R,A} & \mp A^{R,A} \end{bmatrix}, \quad \hat{x}^{K} = \begin{bmatrix} A^{K} & B^{K} \\ \mp B^{K} & \mp A^{K} \end{bmatrix} \]  
(C15)

where the “conjugation” operation is defined as [52]

\[ \hat{A}(p, R; t, t') = [\hat{A}(-p, R; -t, T)]^*, \quad \hat{A}(p, R; \omega, \omega') = [\hat{A}(-p, R; -\omega, -\omega')]^*, \quad \hat{A}(p, R; \epsilon, T) = [\hat{A}(-p, R; -\epsilon, T)]^* \]  
(C16)

and so on, depending on the representation. In addition, Eq. (C11) implies the symmetries

\[ [A^{R,A}]^\dagger = \pm A^{R,A}, \quad [B^{R,A}]^\dagger = -\hat{B}^{R,A}, \]
\[ [A^{K}]^\dagger = \mp A^{K}, \quad [B^{K}]^\dagger = -\hat{B}^{K} \]  
(C17)
One may also write these symmetry relations in terms of \( a, b, c, d \) and \( \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d} \). In particular, Eq. (C13) or Eq. (C15) implies \( d = \pm \mathbf{a}, \mathbf{d} = \pm \mathbf{a}, \) and \( \mathbf{c} = \mp \mathbf{b} \).

Equation (C17) then yields \( (a^R)^* = \mp a^A, (a^R)^* = \pm a^A \), \((b^R)^* = b^A, (b^R)^* = -b^A\), and so on.

Note: For a singlet-paired superconductor in the absence of magnetic effects one only needs to deal with the spin-scalar parts “\( a, b, c, d \)” of the propagators and self energies. Thus one may perform the following reduction from \( 4 \times 4 \) to \( 2 \times 2 \) Nambu matrices

\[
\begin{array}{c|c}
 a & b \\
\hline
 a & b \\
\hline
- c & d \\
\end{array} \rightarrow \begin{bmatrix} a & \pm b \\
\mp c & d \end{bmatrix} \tag{C18}
\]

where either the upper or lower signs are chosen. It must be noted that the above symmetries may not be blindly applied to these reduced matrices. In our notation \( \tilde{\tau}_j = 1^{spin} \otimes \sigma_j^{Nambu} \), whereas in the reduced singlet case one naturally defines \( \tilde{\tau}_j = \sigma_j^{Nambu} \). Therefore, in singlet notation the operation \( \tilde{\tau}_j \tilde{A}_j \tilde{r}_j \) in Eq. (C3) etc. switches the wrong off-diagonal components. It must be replaced by the operation \( \tilde{r}_j \tilde{A}_j \tilde{r}_j \tilde{r}_j = i\tilde{r}_2 \tilde{i} \tilde{r}_2 \), and the formulas of Eq. (C11) must be modified accordingly.

3. Further applications of the symmetries

As an example application of these relations, we consider the renormalization of the normal-state equilibrium propagator \( \tilde{G}_0^{-1}(\mathbf{p}, \epsilon) = \epsilon - \tilde{\tau}_3 \tilde{\xi}^0(p) \) to \( \tilde{G}_0^{-1}(\mathbf{p}, \epsilon) \), as discussed more phenomenologically in Secs. II A 3, II B 3 and VG, for example. The lowest-order normal vertex shown in Fig. 17(a) is necessarily diagonal in Nambu space, since it involves no low-energy propagators. We may also assume it to be proportional to the unit matrix in spin space and real-valued. (The small imaginary part of the lowest-order vertex gives rise to the intrinsic damping strength \( \Gamma_0 \), which we neglect for simplicity.) If we denote the self-energy with

\[
\tilde{\Sigma}^{0}_{\text{low}}(\mathbf{p}, \epsilon) = c(\mathbf{p}, \epsilon) + \tilde{\tau}_3 d(\mathbf{p}, \epsilon) \tag{C19}
\]

we find from Eq. (C9) the symmetries \( c(\mathbf{p}, \epsilon) = -c(-\mathbf{p}, -\epsilon) \) and \( d(\mathbf{p}, \epsilon) = d(-\mathbf{p}, -\epsilon) \). We furthermore assume the symmetry \( \tilde{\Sigma}^{0}_{\text{low}}(-\mathbf{p}, \epsilon) = \tilde{\Sigma}^{0}_{\text{low}}(\mathbf{p}, \epsilon) \) which is certainly valid for an isotropic normal system. Since \( c \) and \( d \) are apparently continuous across the Fermi surface, we may approximate them with \( c(\mathbf{p}, \epsilon) = c_1(\mathbf{p}) \epsilon \) and \( d(\mathbf{p}, \epsilon) = d_0(\mathbf{p}) \). We then write

\[
\tilde{G}^{-1}_{\text{coherent low}}(\mathbf{p}, \epsilon) = G^{-1}_0(\mathbf{p}, \epsilon) - \tilde{\Sigma}^{0}_{\text{low}}(\mathbf{p}, \epsilon)
= [\epsilon - c_1(\mathbf{p}) \epsilon - \tilde{\tau}_3 \tilde{\xi}^{0}(\mathbf{p}) - d_0(\mathbf{p})]
= \tilde{z}(\mathbf{p})^{-1} \{\epsilon - \tilde{\tau}_3 \tilde{z}(\mathbf{p}) \tilde{\xi}^{0}(\mathbf{p}) - d_0(\mathbf{p})\} \tag{C20}
\]

where we defined the renormalization factor with \( c_1(\mathbf{p}) = 1 - z(\mathbf{p})^{-1} \), or \( \tilde{z}(\mathbf{p}) = [1 - c_1(\mathbf{p})]^{-1} \), which is in exact accordance with the general definition given in Eq. (48). We also define the renormalized quasiparticle dispersion relation with \( \xi(\mathbf{p}) \equiv z(\mathbf{p}) \tilde{\xi}^{0}(\mathbf{p}) - d_0(\mathbf{p}) \) and thus obtain

\[
\tilde{G}^{-1}_{\text{coherent low}}(\mathbf{p}, \epsilon) = z(\mathbf{p})^{-1} \{\epsilon - \tilde{\tau}_3 \xi(\mathbf{p})\} \tag{C21}
\]

The new Fermi momentum \( \mathbf{p}_F \) is determined by the equation \( \xi(\mathbf{p}) = 0 \). Furthermore, since we have restricted to low-energy regime, we may replace \( z(\mathbf{p}) \) with \( a = z(\mathbf{p}_F) \). Thus we have established the connection between microscopic theory and the phenomenological quasiparticle parameters \( a, \mathbf{p}_F \) and \( \xi(\mathbf{p}) = v_F \cdot (\mathbf{p} - \mathbf{p}_F) \).

The actual calculation of these parameters from \( \tilde{\Sigma}^{0}_{\text{low}} \) is very difficult, but also unnecessary if their values are taken from experiments.

As yet another example we comment on the symmetries of the quasiclassical distribution function \( \tilde{h} \), defined via

\[
\tilde{g}^K = \tilde{g}^R \circ \tilde{h} - \tilde{h} \circ \tilde{g}^A \tag{C22}
\]

By applying Eqs. (C10), (C11), and (C13), we find the symmetries

\[
\tilde{h}(\mathbf{p}, \mathbf{R}; \epsilon, T) = \tilde{r}_3 \tilde{h}(\mathbf{p}, \mathbf{R}; \epsilon, T) \tilde{r}_3
\]

\[
\tilde{h}(\mathbf{p}, \mathbf{R}; \epsilon, T) = i\tilde{r}_2 \tilde{h}(\mathbf{p}, \mathbf{R}; -\epsilon, T) i\tilde{r}_2 \tag{C23}
\]

\[
\tilde{h}(\mathbf{p}; \epsilon, T) = -\tilde{r}_1 \tilde{h}(\mathbf{p}; \mathbf{R}; -\epsilon, T)^* \tilde{r}_1
\]

From the last line it follows that \( \tilde{h} \) may be written (we drop \( \mathbf{R} \) and \( T \))

\[
\tilde{h}(\mathbf{p}, \epsilon) = \begin{bmatrix}
\tilde{h}_1(\mathbf{p}, \epsilon) & \tilde{h}_2(\mathbf{p}, \epsilon) \\
-\tilde{h}_2(\mathbf{p}, \epsilon) & \tilde{h}_1(\mathbf{p}, \epsilon)
\end{bmatrix} \tag{C24}
\]

and from the first line that \( [\tilde{h}_1(\mathbf{p}, \epsilon)]^\dagger = \tilde{h}_1(\mathbf{p}, \epsilon), [\tilde{h}_2(\mathbf{p}, \epsilon)]^\dagger = \tilde{h}_2(\mathbf{p}, \epsilon) \), where the conjugation symbol is defined in Eq. (C16). From this we see that in general two independent spin-matrix functions (\( \tilde{h}_1(1), \tilde{h}_2(1) \)), and their conjugates, are required to parametrize \( h \) and hence \( \tilde{g}^K \).

Actually, it may be shown that the second function \( \tilde{h}_2 \) is redundant, so that \( \tilde{h} \) may be assumed diagonal in the particle-hole indices [39, 40, 46]. Often one writes \( \tilde{h} = f_1 + f_1 \tilde{r}_3 [39, 40, 46] \), where \( f_1, f_1 \) are related to \( \tilde{h}_1, \tilde{h}_1 \). It is therefore possible to parametrize all physically acceptable functions \( \tilde{g}^K \) by two functions \( \tilde{h}_1 \) and \( \tilde{h}_1 \), which are independent of each other on one half of the Fermi surface. They are only connected by the conjugation symmetry which acts via the second half-surface. One may give physical interpretations to this by saying that one function describes “particles” and the other describes “holes”. (But not the usual “Bogoliubov” quasiparticles [46]?) The connection between them is the particle-hole conversion due to Andreev reflection [1, 50].

More mathematical considerations on the problem of choosing distribution functions may be found in Refs.
Note that the first of these is like the chain rule of differentation, with \([A,\cdot]\) the derivative operator. Indeed, if \(x,p\) satisfy \([x,p]=\hbar\) and \(a, a^\dagger\) satisfy \([a,a^\dagger]=1\), then it follows that
\[
[p,x^n] = -\hbar nx^{n-1}, \quad [p,f(x)] = -\hbar f'(x) = -\hbar df(x)/dx,
\]
\[
[a^n, a^\dagger] = -n a a^\dagger, \quad [a^\dagger,f(a)] = -f'(a) = -df(a)/da,
\]
\[
[a^\dagger,(a \pm a^\dagger)^n] = -n(a \pm a^\dagger)^{n-1}, \quad [a^\dagger,f(a \pm a^\dagger)] = -f'(a \pm a^\dagger)
\]
where \(f\) is any (analytic) function. If \(a_j\) and \(a_j^\dagger\) satisfy \([a_j, a_j^\dagger] = \delta_{jk}\) and \([a_j, a_k] = 0\), then for example
\[
[a_k^\dagger, a_j] = \delta_{jk} a_k, \quad [a_k^\dagger, a_j^\dagger] = -\delta_{jk} a_k^\dagger
\]
\[
[n_{jk}, a_j] = [a_j^\dagger, a_k^\dagger] = 0
\]
with \(n_{jk} = a_j^\dagger a_j\). This relation is equally useful
\[
e^{itS}Oe^{-itS} = O + it[S,O] + \frac{(it)^2}{2!}[S,[S,O]] + \cdots \quad (D1)
\]
which is obtained by differentation with respect to \(t\) and using the Taylor expansion. Another very useful operator relation is the Baker-Campbell-Hausdorff formula (sometimes credited to Glauber or Feynman):
\[
\exp(F + G) = \exp(-[F,G]/2) \exp(F) \exp(G) = \exp([F,G]/2) \exp(G) \exp(F) \quad (D2)
\]
which is valid if \([F,[F,G]] = [G,[F,G]] = 0\). Simple applications of the first one are for example
\[
\begin{align*}
\cdot e^{xa^\dagger a} e^{-ia^\dagger a} &= e^{-ia^\dagger a} \\
\cdot e^{ip/\hbar x} e^{-ip/\hbar} &= x + u
\end{align*}
\]
where \([x,p] = \hbar\), \([a,a^\dagger] = \delta_{jk}\), \([a,a] = 0\), and \(\alpha, u\) commute with the other operators.

Related to the above exponential results, there are also some useful relations concerning expectation values of operators. For example
\[
\langle e^A \rangle = e^{\langle A^2 \rangle / 2} \quad (D3)
\]
is valid at least for an operator \(A\) that is linear in boson creation and annihilation operators. The average is with respect to an equilibrium-like density operator (so that the Danielewicz form of Wick’s theorem is applicable) or vacuum.

As further physically interesting examples we mention that if \(N = \int dx \psi(x)\psi(x)\) is the particle-number operator, then \([N,\psi(x)] = -\psi(x)\), and \([N,\psi(x)] = +\psi(x)\). As a second important example, suppose that in Eq. (D1) \(O = a, a^\dagger\) and \(S = K_0/\hbar\), where \(K_0 = T - \mu N\), \(\mu N = \sum_i (\epsilon_i - \mu) a_i^\dagger a_i\) is the Hamiltonian of the unperturbed translationally invariant system. Then by using \([K_0, a_k] = -(\epsilon_k - \mu) a_k\) and Eq. (D1) we find the time dependence of the interaction-picture operators
\[
a_k(t) = e^{-i(\epsilon_k - \mu)t/\hbar} a_k, \quad a_j^\dagger(t) = e^{i(\epsilon_k - \mu)t/\hbar} a_j^\dagger \quad (D4)
\]
Furthermore, since \([N, a_k] = -a_k\), we have \(\exp(-i\mu t N) a_k \exp(i\mu t N) = \exp(i\mu t) a_k\) and that is why our grand-canonical Green’s functions are formally related to those of an isolated system \(G_N\) by
\[
G(t_1-t_2) = e^{i\mu (t_1-t_2)} G_N(t_1-t_2), \quad G(\omega) = G_N(\omega + \mu) \quad (D5)
\]
These correspond to an equilibrium system, where \(G\) only depends on \(t_1-t_2\). Finally we note that, by using the definition \(P = \sum_{\omega} \int d^3x \psi_\omega^\dagger(x) (-i\hbar \nabla) \psi_\omega(x)\) it is easy to show that \([\psi_\omega(x), P] = -i\hbar \nabla \psi_\omega(x)\). By direct substitution into this one sees that
\[
\psi_{H_\alpha}(x,t) = e^{-iP \cdot x/\hbar} \psi_{H_\alpha}(0,t) e^{iP \cdot x/\hbar} \quad (D6)
\]
where one may still insert
\[
\psi_{H_\alpha}(0,t) = e^{-iKt/\hbar} \psi_{H_\alpha}(0,0) e^{iKt/\hbar} \quad (D7)
\]
These are useful for example for doing Lehmann expansions of the propagator [3].

2. Complex analysis

The following relations are very important. The delta function is represented as
\[
\delta(t-t') = \int_{-\infty}^\infty \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \quad (D8)
\]
whereas the step function may be written
\[ \theta(t-t') = \int_{-\infty}^{t} ds \delta(s-t') = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{e^{-i\omega(t-t')}}{\omega + i\eta} \] (D9)

Inversely we have the relations \( d\theta(t-t')/dt = \delta(t-t') \) and \( d\theta(t-t')/dt = -\delta(t-t') \). Finally we note the formulas
\[ \frac{1}{x \pm i\eta} = \frac{\omega}{x^2 + \eta^2} \pm i \frac{\eta}{x^2 + \eta^2} \] (D10)

All of these are needed for deriving some of the results discussed in the text.

3. Further relations with Fourier transforms

Let \( f(x) \) and \( g(x) \) be (analytic) functions and \( \tilde{f}(k) \) and \( \tilde{g}(k) \) their Fourier transforms, as defined with
\[ \tilde{f}(k) = \int_{-\infty}^{\infty} dx f(x) e^{-ikx}, \quad f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{f}(k) e^{+ikx} \] (D11)

and with similar equations for \( g \). Then the (forward or inverse) Fourier transforms of \( xf(x) \) and \( kg(k) \) are \( i\partial\tilde{f}(k)/\partial k \) and \( -i\partial \tilde{f}(x)/\partial k \), respectively. Using Taylor’s expansions these may be generalized to
\[ \tilde{f}(k)\tilde{g}(k) \rightarrow \tilde{f}(\hat{k})g(x), \quad f(x)g(x) \rightarrow f(\hat{x})g(\hat{x}), \]
where \( \hat{k} = -i\frac{\partial}{\partial x}, \quad \hat{x} = i \frac{\partial}{\partial k} \] (D12)

Note that we may similarly write
\[ \tilde{f}(k)\tilde{g}(k) \rightarrow f(x)\tilde{g}(\hat{k}), \quad f(x)g(x) \rightarrow f(\hat{x})g(k), \]
where \( \hat{k} = -i\frac{\partial}{\partial x}, \quad \hat{x} = i \frac{\partial}{\partial k} \] (D13)

Expressions of the form \( \hat{k}_x f(x, x') \) may be written as “folding products” as follows
\[ -i \frac{\partial}{\partial x} f(x, x') = \int dx_1 \delta(x-x_1) \left[-i \frac{\partial}{\partial x_1} f(x_1, x')\right] \]
\[ = \int dx_1 \left[i \frac{\partial}{\partial x_1} \delta(x-x_1)\right] f(x_1, x') \]
\[ = \int dx_1 \left[-i \frac{\partial}{\partial x} \delta(x-x_1)\right] f(x_1, x') \]
\[ = \int dx_1 K(x, x_1) f(x_1, x') \] (D14)

where the “matrix element” \( K(x, x_1) \) is defined formally as
\[ K(x, x_1) = -i \frac{\partial}{\partial x_1} \delta(x-x_1) = -i \frac{\partial}{\partial x} \delta(x-x_1) \]
\[ = -i \delta'(x-x_1) \] (D15)

Obviously the Fourier transform of Eq. (D14) is
\[ kf(k, k') = \int \frac{dk_1}{2\pi} K(k, k_1) f(k_1, k') \] (D16)

where the transform of \( K(x, x_1) \) is given by \( K(k, k_1) = 2\pi k \delta(k - k_1) \).

4. Miscellaneous

Fermi and Bose functions:
\[ \frac{1}{e^x + 1} = \frac{e^{-x/\tau}}{e^{x/\tau} + e^{-x/\tau}} \]
\[ = \frac{1}{e^{x/2} + e^{-x/2}} + \frac{1}{e^{x/2} + e^{-x/2}} \]
\[ = \left\{ \begin{array}{ll} \frac{1}{2} - \tan(x/2) & \text{Fermi}(+) \\ \frac{1}{2} \coth(x/2) - 1 & \text{Bose}(-) \end{array} \right. \] (D17)

More on delta functions: if \( x_i \) are the zeros of function \( f(f(x_i) = 0) \), then
\[ \delta[f(x)] = \sum_i \delta(x-x_i)/|f'(x_i)| \] (D18)

A result concerning the derivative of delta function: The derivative of the delta function may often be written as
\[ \delta'(x) = -\frac{\delta(x)}{x} \] (D19)

This may be verified by \( \int dx \delta'(x)f(x) = -\int dx \delta(x)[f(x) + xf'(x)] = -\int dx \delta(x)f(x) \).

Pauli matrices: The full set of Pauli matrices, which form a basis for \( 2 \times 2 \) matrices are
\[ \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \] (D20)

We use these with the labels \( \tau \) when they refer to Nambu space and with labels \( \sigma_u \) when they refer to Keldysh space. If spin-space matrices are needed, we use underlined symbols \( \underline{\sigma} \). The matrices satisfy \( [\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \) where \( i, j, k = 1, 2, 3 \), and \( \sigma_1 \sigma_2 = i\sigma_3, \sigma_3 \sigma_1 = i\sigma_2, \sigma_2 \sigma_3 = i\sigma_1 \). We also denote \( \sigma = (\sigma_1, \sigma_2, \sigma_3) \), and note the Hermiticity \( \sigma^\dagger = \sigma^T \) and \( \sigma^T = i\sigma_3 \sigma_2 \sigma_1 \). As a consequence \( [\sigma_1 \sigma_2]^T = \sigma \sigma_1 \sigma_2 \), and \( \sigma \sigma_3 = -i\sigma_2 \sigma^* \), and so on.

Time reversal: The “antiunitary” time-reversal operation \( \theta \) transforms spin-1/2 wavefunctions (i.e. complex single-particle amplitudes) and the operators \( a \) (or \( a^\dagger \)) according to the prescriptions
\[ \theta \psi_a(x, t) = e^{i(\pi/2)(1+a^\dagger)} \psi^*(x, -t) \]
\[ \theta a_{k\sigma}(t) \theta^{-1} = e^{i(\pi/2)(1+a)} a_{-k\sigma}(-t) \]
\[ \theta a_{k\sigma}^\dagger(t) \theta^{-1} = e^{i(\pi/2)(1-a)} a_{-k\sigma}(-t) \] (D21)
or more explicitly
\[
\begin{align*}
\theta \left[ \psi_1(x, t) \right] & = -i\sigma_z \left[ \psi_1(x, t) \right] = -\psi_1^\dagger(x, t), \\
\theta \left[ a_k\psi_\uparrow(t) \right] \theta^{-1} & = -a_k\psi_\uparrow(t) - a^\dagger(-k)\psi_\downarrow(t)
\end{align*}
\]

Thus for example \( \langle \Psi | a_{k\sigma} a_{-k\sigma} | \Psi \rangle \rightarrow \langle \theta \Psi | a_{k\sigma} a_{-k\sigma} | \theta \Psi \rangle \) and in particular \( \langle \Psi | a_{k\uparrow} a_{-k\downarrow} | \Psi \rangle \rightarrow \langle \theta \Psi | a_{k\uparrow} a_{-k\downarrow} | \theta \Psi \rangle^* \) for a singlet state. See for example Ref. [56].

Real and imaginary time orderings: The real-time field operators have the time dependences \( \psi(t) = U(t, 0)\psi(0)U(t, 0) \) and the Hermitian conjugate \( \psi^\dagger(t) = U^\dagger(t, 0)\psi^\dagger(0)U(t, 0) \). The imaginary-time field operators have \( \tau \) dependences \( \psi_M(\tau) = \psi(\tau) \) and \( \psi_M(\tau)^\dagger = \psi(\tau)^\dagger \). These are not Hermitian conjugates of each other; instead \( \psi_M(\tau)^\dagger = \hat{\psi}_M(-\tau) \) and \( \psi_M(\tau)^\dagger = \hat{\psi}_M(\tau) \). Thus we find the relations

\[ \{ T[A(t)B(t')] \}^\dagger = T[B(t')A(t)] \]
\[ \{ T[A(\tau)B(\tau')] \}^\dagger = T[B(\tau')A(\tau)] \]

where \( \hat{T} \) is the anti-time ordering operator, and \( A, B \) are either creation or destruction operators. We also denote \( \hat{\psi} = \psi \) etc. These are important for studying the symmetries of propagators.

Appendix E: Equilibrium properties

1. “Justification” of \( V_{mf} \) in equilibrium

Consider the grand-canonical Hamiltonian \( K = T - \mu N + V \), with full two-particle interactions \( V \) included. We assume that only the pairing-interaction part is important here. (The others may effectively only result in a shift of the chemical potential and Fermi velocity, or something — see below for discussion on the Hartree-Fock approximation.) Suppose, for example, that due to the macroscopic occupation of the condensate the field-operator pair \( \hat{S} = \psi_1 \psi_2 \) can be decomposed into a sum of (i) a part which is close to a classical complex field \( D \), a “macroscopic wave function” of the condensate, and (ii) a fluctuation. (The commutator of the near-classical part vanishes as \( \sim 1/N \) in the thermodynamic limit, as in the treatment of condensed Bose systems in Sec. 6 of Ref. [3], or in Ref. [4], or something like that — see p.292 of Ref. [4].) Thus we make in \( V = \int U_{12} \psi_1 \psi_2 \psi_1 \psi_2 \) the replacement \( \psi_1 \psi_2 \rightarrow D + \langle \psi_1 \psi_2 \rangle - D \), assuming the quantum fluctuations \( \delta = \psi_1 \psi_2 - D \) to be small, and with zero average in any case. By dropping the second-order term \( \delta^2 \) we end up with the effective Hamiltonian

\[ K_{eff} = \int dx [T - \mu] \psi^\dagger \psi + \int \int dx_1 dx_2 U[D\psi_1^\dagger \psi_2^\dagger + D^* \psi_1 \psi_2 - |D|^2] \]

It is vital to keep the “constant” term \(|D|^2\), for at this point it is unknown and is yet to be determined self-consistently. Apparently, what must be done is to set \( D = \langle \psi_1 \psi_2 \rangle \), where the expectation value has to be calculated with respect to \( \rho_{eff} = Z_{eff}^{-1} \exp(-\beta K_{eff}) \), \( Z_{eff} = \text{Tr} \exp(-\beta K_{eff}) \) to get a non-vanishing value.

A more formal way of arriving at this interpretation, and \( K_{eff} \), is as follows [10, 27]. We are assuming that below the superconducting transition, there is an extra thermodynamic (field) variable \( D \) (the order parameter of the phase transition) in addition to the usual variables \( T, V, \mu \), such that there exist many “microstates” for each “macrostate” corresponding to a given field distribution \( D \). Thus we may split the state sum in the partition function as follows:

\[ Z = e^{-\beta \Omega} = \text{Tr} e^{-\beta K} = \int \int \mathcal{D}^* \mathcal{D} e^{-\beta \Omega_{eff}[D,D^*]} \]

where a functional-integral notation is used for the sum over classical fields, and

\[ Z_{eff} = e^{-\beta \Omega_{eff}[D,D^*]} = \text{Tr}_{D^*} e^{-\beta K} = \text{Tr}[e^{-\beta K_{eff}}] \]

Here, after the first equality, \( \mathcal{Y}_D \) is a partial trace over all microstates corresponding to \( \psi_1 \psi_2 \approx D \) (in the state-space spanned by the eigenbasis of \( K \)) — never mind what this actually means. The second equality follows from a mathematically more “exact” trick known as a Hubbard-Stratonovich transformation [10, 27, 28, 53]. Based on Gaussian integral identities, it gets rid of the quartic operator term in \( K \) in favor of the classical fields \( D, D^* \) in an effective Hamiltonian \( K_{eff} \) which is exactly equal to Eq. (E1). Accordingly, the trace \( \text{Tr} \) is over the whole state-space spanned by \( K_{eff} \).

In equilibrium the thermodynamic potential \( \Omega(T, V, \mu) \) must be minimized with respect to any other thermodynamic variables [26]. The greatest contribution to \( Z \) and thus \( \Omega \) is due to the saddle point (minimum) of \( \Omega_{eff} \), \( \text{Tr}_{D^*} \exp(-\beta K_{eff}) \) with respect to \( D \) and \( D^* \). Thus by taking the variational derivative and setting it to zero

\[ \frac{\delta \Omega_{eff}}{\delta D^*} = U[(\psi_1 \psi_2) - D] = 0 \]

where \( \langle \ldots \rangle = \text{Tr}[\rho_{eff} \ldots] \), we have, upon defining \( \Delta = UD \), the BCS gap equation \( \Delta = U \langle \psi_1 \psi_2 \rangle \). With spin indices and everything in place, it reads

\[ \Delta_{\alpha\beta}(x_1, x_2) = \frac{1}{2} U_{\alpha\beta\gamma\delta}(x_1, x_2) \langle \psi_\gamma(x_1) \psi_\delta(x_2) \rangle \]

Fluctuation corrections to this saddle point result can be calculated [27].
Appendix F: Langreth rules

Note: This appendix should be cleaned up and the notation should be unified with the main text (+ vs. −, L vs. R). Langreth developed very useful “analytic continuation” rules to transform quantities from the complex ordering contour to quantities defined on the real time axis [33]. For a nice derivation of the rules, also known as the “Langreth theorem”, see the book of Haug and Jauho [11]. Here we consider only a very simplified form of the theorem, which captures the most important results.

Let’s look at the matrix (folding) product in two different representations of the Keldysh space. First $\tilde{A} = B\tilde{C}$

$$
\begin{bmatrix}
A^{++} & A^{+-} \\
A^{−+} & A^{−−}
\end{bmatrix} =
\begin{bmatrix}
B^{++} & B^{+-} \\
B^{−+} & B^{−−}
\end{bmatrix}
\begin{bmatrix}
C^{++} & C^{+-} \\
C^{−+} & C^{−−}
\end{bmatrix}
$$

(F1)

and then $\tilde{A} = B\tilde{C}$

$$
\begin{bmatrix}
A'^r & A'^k \\
0 & A^a
\end{bmatrix} =
\begin{bmatrix}
B'^r & B'^k \\
0 & B^a
\end{bmatrix}
\begin{bmatrix}
C'^r & C'^k \\
0 & C^a
\end{bmatrix}
$$

(F2)

These matrices are related via a similarity transformation $A = LBL^{-1}$, componentwise

$$
\begin{bmatrix}
A'^r & A'^k \\
0 & A^a
\end{bmatrix} = L
\begin{bmatrix}
A^{++} & A^{+-} \\
A^{−+} & A^{−−}
\end{bmatrix} L^{-1}
$$

(F3)

where the transformation matrix is

$$
L = \frac{1}{\sqrt{2}}
\begin{bmatrix}
1 & -1 \\
1 & 1
\end{bmatrix}
$$

(F4)

With these definitions the components of $\tilde{A}$ are not the contour-ordered ones ($A'^r$), but rather include the additional $\sigma_3$ factors. (It should also work with the lesser and greater functions!) In this way, one finds

$$
\begin{align*}
A'^r &= B'^r C'^r \\
A^a &= B^a C^a \\
A'^c &= B'^c C'^c + B^c C^c \\
A^c &= B^c C^c + B^c C^c
\end{align*}
$$

(F5)

These are some of the rules that result from the “Langreth theorem” [11]. Their nested application leads to further relations, such as those quoted in the text. These results can still be generalized to non-matrix products like $A_{ij}(t, t') = B_{ij}(t, t')C_{ij}(t, t')$ and $A_{ij}(t, t') = B_{ij}(t, t')C_{ij}(t', t)$, where $i$ and $j$ are Keldysh-space indices [11]. Such products often appear in self-energies.

Appendix G: Some things to be done...

- order references (BibTeX!)

- add further useful references, for example
  - ...

- derive the equilibrium relations for Green functions using the KMS relation; Note KMS references

- note that there are two additional ways of doing the Keldysh-space rotation. Note also that [check this]

$$
\tilde{\Sigma} = R^{-1} \Sigma^c R =
\begin{bmatrix}
\Sigma^R & 0 \\
0 & \Sigma^R
\end{bmatrix}
$$

(G1)

- Add discussion of the “Langreth rules”; it’s important to choose the similarity transformations correctly in order for them to work

- write all spectral decompositions etc. for the Nambu matrices:

$$
\hat{G}(\mathbf{k}, \omega_n) = \int \frac{dz}{2\pi} \frac{\hat{\rho}(\mathbf{k}, z)}{i\omega_n - z}
$$

(G2)

spectral density

$$
\hat{\rho}(\mathbf{k}, \omega) = -2 \text{Im} \hat{G}^R(\mathbf{k}, \omega) = i(\hat{G}^R - \hat{G}^A)
$$

(G3)

density of states $N(\epsilon) = \sum_{\mathbf{k}_\alpha} \delta(\epsilon - E_\mathbf{k})$ and so

$$
N(E) = \frac{1}{2\pi} \sum_{\mathbf{k}_\alpha} \rho(\mathbf{k}, E)
$$

(G4)

- derive the quasiclassical approximations for currents and perhaps other observables; note that

$$
\frac{1}{V} \sum_{\mathbf{k}} \int \frac{d^3k}{(2\pi)^3} \rightarrow N(0) \int \frac{d\Omega_k}{4\pi} \int d\xi_k
$$

(G5)

- The density is $\rho(\mathbf{r}) = \psi_+^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r})$ and the current is given by

$$
\mathbf{j}(\mathbf{r}) = \frac{\hbar}{2m^1} \{\psi_+^\dagger(\mathbf{r}) [\nabla \psi_\sigma(\mathbf{r})] - [\nabla \psi_+^\dagger(\mathbf{r})] \psi_\sigma(\mathbf{r})\}
$$

(G6)

These satisfy the continuity equation: $\dot{\rho} + \nabla \cdot \mathbf{j} = 0$.

- other relations $[\rho(\mathbf{r}), \rho(\mathbf{r}' t)] = 0$


