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SCATTERING THEORY OF TRANSPORT FOR MESOSCOPIC SUPERCONDUCTORS

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January 1996

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ABSTRACT

The scattering theory of transport has been shown to provide a rigorous theoretical framework for the description of normal mesoscopic systems. This approach is based on the observation that, as long as dissipative processes in the active region can be neglected, each scattering eigenstate communicates with one and only one reservoir and as such can be assumed to be in equilibrium with that reservoir. This allows us to calculate any quantity of interest under non-equilibrium conditions using a simple extension of equilibrium statistical mechanics, without the need to solve complicated kinetic equations. In this review we discuss how the same approach can be applied to mesoscopic systems including superconducting segments and relate this approach to the commonly used Green's function formalism.

1. Introduction

The scattering theory of transport (often referred to as the Landauer-Buttiker formalism) provides a powerful theoretical framework for the description of current flow in normal mesoscopic conductors [1.1, 1.21, when there is negligible dissipation in the active region. Under these conditions, the scattering formalism has been shown (see for example, section 8.7, Ref.[1.2]) to be equivalent to the non-equilibrium Green's function (NEGF) formalism which provides a general framework for the description of quantum transport. The scattering formalism is conceptually far simpler making it a very appealing alternative in the domain where it does apply.

'Theoretical work on non-equilibrium superconductivity has traditionally been based on the Green's function formalism. From the experience with normal mesoscopic conductors, it seems natural to expect that scattering theory will also provide a simple but accurate alternative for the description of mesoscopic superconducting structures, provided the dissipation in the active region can be neglected. The purpose of this review is to provide a clear formulation of the scattering theory of transport for mesoscopic superconductors, showing the similarities and differences with normal conductors. Some of the results are simply "re-derivations" and we have tried to cite the earlier works whenever possible.

Scattering theory of transport in normal conductors

Let us briefly review the scattering theory of transport in normal conductors. The earliest work on these lines can be traced back to Frenkel in 1930 [1.3], when he derived an expression for the current, I, in a metal-insulator-metal junction in terms of the transmission probability, T :

$$I \sim \int dE\, T(E) \left[f_1(E) - f_2(E) \right] \qquad (1.1)$$

here $f_1(E)$ and $f_2(E)$ are the Fermi functions describing the electron energy distributions in the two metals. Since this early work, numerous authors have applied this approach to the description to tunneling conductors [1.4]. However, the common belief was that this was essentially a "weak-coupling approach" applicable only when the transmission probability is much less than one ($T << 1$).

Contact resistance : Landauer was probably the first to take this approach seriously even for "strong coupling" and he drew attention to the subtle questions that arise when the transmission probability is close to one [1.5]. If we linearize Eq.(1.1) to obtain an expression for the low bias conductance, G

$$I \sim \quad T(E_f)\left[\mu_1 - \mu_2\right] \qquad \rightarrow \quad G \sim \quad T(E_f) \tag{1.2}$$

we see that the conductance is finite even for ballistic conductors (T = 1). But how can a ballistic conductor have a non-zero resistance ? This led to much controversy and argument in the 1980's, till it was finally realized that this non-zero resistance was really an interface (or contact) resistance between the conductor and the large reservoirs [1.6]. The clear experimental observation of this interface resistance in 1988 [1.7] finally settled the controversy and made it clear that the scattering approach was applicable not just to weakly coupled tunneling systems but even to strongly coupled ballistic systems. In section 4 we will discuss how this contact resistance is changed in the presence of superconductors.

Exclusion principle ? Another significant development in the 1980's was Buttiker's extension of the scattering formulation to multi-terminal conductors in magnetic fields [1.8]. Eq.(1.1) is then generalized to read

$$I_i = \frac{2e}{h} \int dE \left[\sum_j T_{ji}(E)\, f_i(E) - \sum_j T_{ij}(E)\, f_j(E) \right] \tag{1.3}$$

where $f_i(E)$ is the Fermi function describing the electron energy distribution in the i^{th} terminal :

$$f_i(E) = f_0(E - \mu_i) \quad \text{where} \qquad f_0(\varepsilon) \equiv \frac{1}{e^{-\varepsilon/k_B T} + 1} \tag{1.4}$$

This extension of Eq.(1.1) raises a very important question. Why have we not included (1-f) factors in Eq.(1.3) to account for the exclusion principle ? Should we modify it to read

$$I_i = \frac{2e}{h} \int dE \left\{ \sum_j T_{ji}(E)\, f_i(E)\left[1 - f_j(E)\right] - \sum_j T_{ij}(E)\, f_j(E)\left[1 - f_i(E)\right] \right\} \qquad ??$$

If the transmission is reciprocal ($T_{ij} = T_{ji}$) then the (1-f) factors make no difference - the extra terms just cancel out. But some of the most impressive successes of Buttiker's multi-terminal formula involve non-reciprocal transmission ($T_{ij} \neq T_{ji}$) in magnetic fields, and including the (1-f) factors would change the predictions significantly. We will now present an argument which makes it clear that the (1-f) factors should not be included.

It is well-known that in equilibrium statistical mechanics we can calculate the expectation value of any one-particle operator A_{op}, if we know the eigenstates $|m)$ and the corresponding eigenenergies ε_m for the system :

$$A = \sum_m \langle m| A_{op} |m\rangle \quad f_0(\varepsilon_m - E_f) \tag{1.5}$$

Here E_f is the equilibrium Fermi energy. Under non-equilibrium conditions, however, the occupation factor for different states is not given by the Fermi function and one has to calculate it by solving some kinetic equation (in general we have to calculate the off-diagonal elements of the density matrix as well).

In open systems, the eigenstates take the form of scattering states consisting of an incident wave in one lead and scattered waves in all the leads (Fig.1.1). We assume that there are no scattering processes inside the device or at the device-contact interfaces that can transfer an electron from one scattering state to another. The scattering theory of transport is based on the observation that under these conditions, ***each scattering state remains in equilibrium with a particular reservoir.*** This is because it communicates with one and only one contact, namely the one connected to the lead from which it is incident. Consequently it can be assumed to be in equilibrium with that contact, so that its occupation factor is given by the corresponding Fermi function. This allows us to calculate non-equilibrium quantities using a simple extension of Eq.(1.5) :

$$A = \sum_m \langle m| A_{op} |m\rangle \quad f_0(\varepsilon_m - \mu_m) \tag{1.6}$$

where μ_m is the electrochemical potential in the reservoir from which the state 'm' is incident. It is apparent from this derivation why (1-f) factors should not be included. After all, no one would argue for including such factors in Eq.(1.5). As such there is really no reason to include it in Eq.(1.6) either [1.5, 1.9].

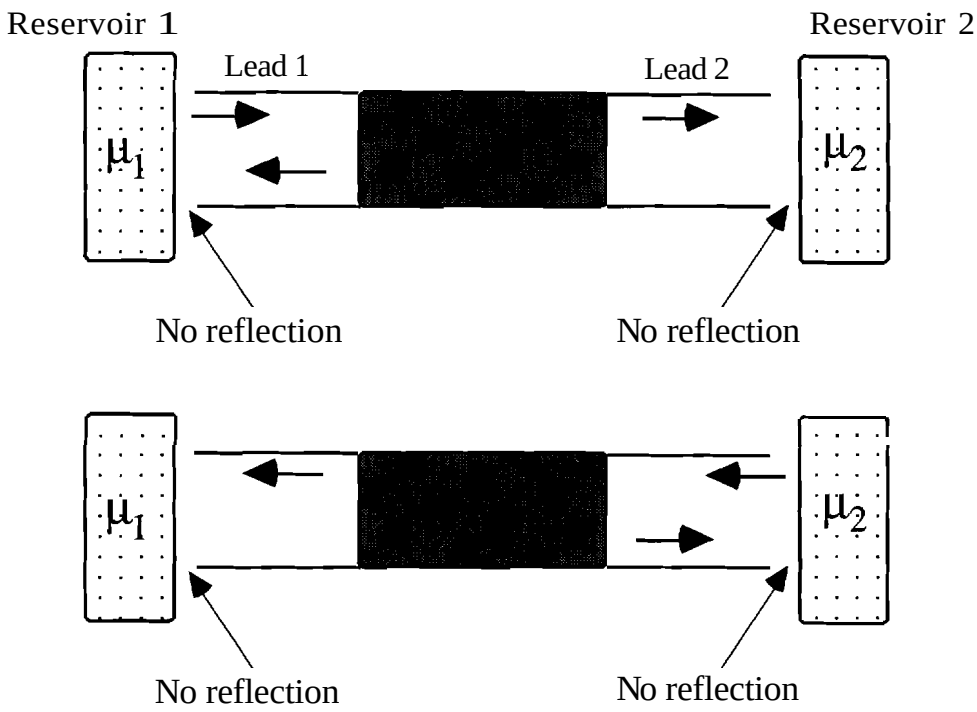


Fig.1.1. In open systems, the eigenstates take the form of scattering states consisting of an incident wave in one lead and scattered waves in all the leads. Two such scattering states incident from two different leads are shown. The scattering state shown in (a) has an electrochemical potential μ_1, while that shown in (b) has a potential μ_2.

Current formula : We can apply Eq.(1.6) to calculate any quantity of interest such as terminal currents or charge density. For example, if I_i represents the current in lead 'i', then it can be shown that

$$\langle j,k|\, I_{i,\,op}\,|j,k\rangle \;=\; \frac{ev_j(k)}{L}\left[\delta_{ij} - T_{ij}(k)\right] \tag{1.7}$$

where $|j,k\rangle$ represents an eigenstate originating in lead 'j' with wavevector 'k' and T_{ij} is the transmission probability from lead 'j' to lead 'i'. To simplify the book-keeping, we are assuming each lead to be single-moded; for multi-moded leads we could conceptually treat each mode as a separate lead, or we could add a mode index. Substituting Eq.(1.7) into Eq.(1.6) and making use of the prescription (L : normalization length, v(k): group velocity)

$$\sum_k \;\rightarrow\; 2\ (\text{for spin})\ x\ \frac{L}{2n}\int dk \;\rightarrow\; \frac{L}{\pi}\int \frac{dE}{\hbar\, v(k)} \tag{1.8}$$

to convert the summation over 'k' into an integral, we obtain

$$I_i = \frac{2e}{h}\int dE \sum_j \left[\,\delta_{ij} - T_{ij}(E)\right] f_j(E) \tag{1.9}$$

The result quoted earlier (see Eq.(1.3)) can be obtained from this expression by making use of the "sum rule"

$$\sum_j T_{ij} \;=\; \sum_j T_{ji}$$

which is a consequence of the unitarity of the scattering matrix (see Ref.[1.2], p.122).

An interesting point to note is that the transmission coefficients T_{ij} are calculated from **lead** 'i' to **lead** 'j' and not from reservoir 'i' to reservoir 'j' (see Fig.1.1). From a practical point of view this makes the job of calculating the transmission coefficients much simpler, since we do not need to worry about the detailed nature of the connection between the lead and the reservoir. From a conceptual point of view this is somewhat surprising, since the conductance given by Eq.(1.2) includes the interface resistance between the lead and the reservoir.

Summary : The modern scattering theory of transport represents a simple and elegant extension of ***equilibrium*** statistical mechanics (cf. Eq.(1.5)) that allows us to deal with ***non-equilibrium*** problems (cf. Eq.(1.6)) in mesoscopic structures where the active region is small enough that dissipative processes can be neglected. Scattering theory is based on the observation (or the 'ansatz') that as long as there are no inelastic processes, the density matrix remains diagonal in the scattering state representation :

$$\rho(m,n) = \delta_{mn}\, f_0(\varepsilon_m - \mu_m)$$

Once the density matrix is known we can of course calculate the expectation value of any one-particle operator as indicated in Eq.(1.6). We can even evaluate two-particle operators like current correlations, as we will discuss in section 6. This simple observation thus results in an enormous simplification over conventional non-equilibrium statistical mechanics where one has to solve complicated kinetic equations to obtain the density matrix.

It is important to note this subtle difference between the scattering theory of transport and theories based on the tunneling Hamiltonian. In tunneling Hamiltonian theory, electrons make transitions from one reservoir to another via the "weak link" provided by the device. It then seems natural to include the (1-f) factors to acount for the Pauli blocking. Such a viewpoint is only valid for weak coupling. The modern scattering theory of transport, on the other hand, is valid for arbitrary coupling. Here we are simply filling up one-particle eigenstates from different reservoirs, and there is no logical reason to include the (1-f) factors. This distinction was clearly noted by Blonder, Tinkham and Klapwijk in their classic paper on normal-superconductor (N-S) junctions (see Ref. [3.1]). For simple N-S junctions the difference was purely philosophical - the (1-f) factors canceled out making no difference to the final result. But the difference can be significant in a practical sense for multi-terminal structures.

We will now describe how one can apply this viewpoint to mesoscopic structures that include superconductors. We will focus on the theoretical framework, mentioning experiments only incidentally. A recent review of the experimental developments can be found in Ref. [1.10]. A good collection of recent papers by leading researchers in this field can be found in Ref.[1.11].

2. BdG-based scattering theory

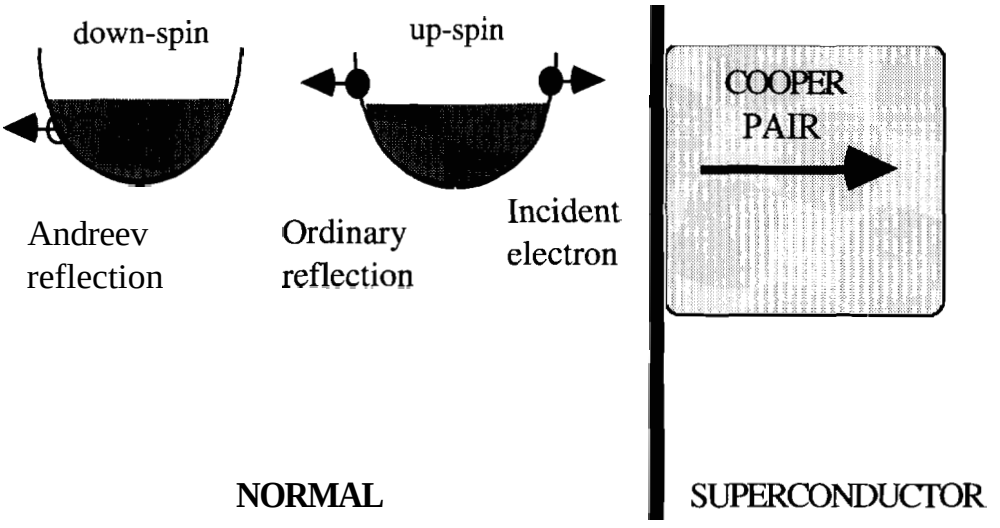
As we have seen, the basic strategy in the scattering theory of transport is to construct scattering states and fill them up according to their reservoir of origin. For normal conductors, the scattering states are based on the Schrodinger equation. In the presence of superconductors, we need to use the Bogoliubov-de Gennes (BdG) equation to construct the scattering states, as we will describe in this section. A formal derivation of the BdG equation starting from the BCS Hamiltonian is provided in appendix A. Here we will adopt a more heuristic approach and try to concentrate on results and physical explanations.

We proceed as follows. (1) First we will try to motivate the BdG equation by showing that it follows almost inevitably if we accept the phenomenon of Andreev reflection at normal-superconductor interfaces as an experimental fact. However, the BdG equation describes not only normal-superconductor interfaces, but also bulk superconductors, homogeneous and inhomogeneous. Indeed, (2) we will show that the BdG equation can be viewed as a one-particle wave equation whose states can be filled up systematically to describe the superconducting state, in much the same way that we fill up the states of the Schrodinger equation to describe the normal state. This justifies the use of the BdG equation to construct a scattering theory in the same way that the Schrodinger equation is used for normal systems. (3) We will then obtain an expression for the expectation value of any quantity of interest in terms of the occupation factors of the different eigenstates (cf. Eqs.(1.5) and (1.6)). (4) Finally we will discuss how we can assign different occupation factors to different scattering states depending on their reservoir of origin, pointing out the different issues that can arise in different types of structures.

Andreev reflection

The basic phenomenon that distinguishes superconductive mesoscopic systems from normal ones is that of Andreev reflection [2.1]. In normal reflection, an up-spin electron incident with energy E is reflected back as an up-spin electron with the same energy. In Andreev reflection, on the other hand, an incident up-spin electron with energy E "drags" a down-spin electron with energy 2Ef - E along with it into the superconductor. This leaves behind an empty state in the down-spin band that flows away from the interface (see Fig.2.1a). How can we write down a one-particle wave equation that will describe this process ?

(a)



(b)

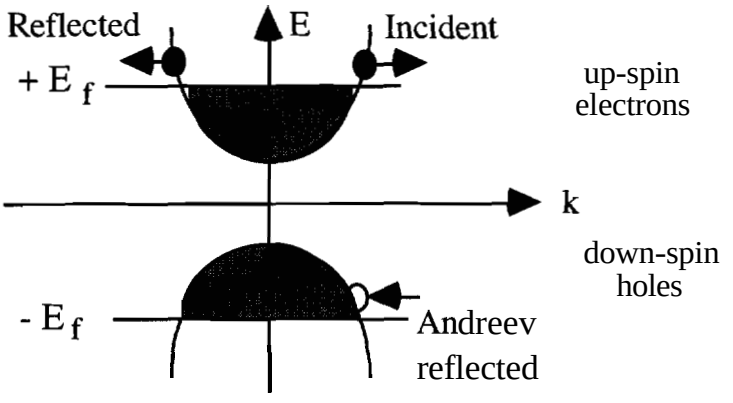


Fig.2.1. Andreev reflection : (a) An incident up-spin electron with energy E **"drags"** a down-spin electron with energy 2Ef - E along with it into the superconductor. This leaves behind an empty down-spin state that flows away from the interface. (b) Same process shown with the down-spin band flipped in energy about E = 0 and k=O to correspond to holes.

Let us first write down two separate wave equations for up-spin electrons and down-spin holes. If H is the standard one-electron Hamiltonian (V : scalar potential, A : vector potential)

$$H = \frac{(\vec{p} - e\vec{A})^2}{2m} + eV \qquad (2.1)$$

then the wave equation for electrons is simply the standard Schrodinger equation $i\hbar(\partial\Psi / at) = HY$. The wave equation for holes is the complex conjugate of the corresponding equation for electrons : $i\hbar(\partial\Psi_h / at) = -H^*\Psi_h$, because the hole wave function is the complex conjugate of the corresponding electron wave function. This can be justified heuristically by noting that in the second quantized formalism the creation operator for holes (ψ) is the Hermitian conjugate of that for electrons (ψ^+). We can thus write

Up-spin electrons	***Down-spin holes***
$H u' = i\hbar\frac{\partial u'}{\partial t}$	$-H^* v' = i\hbar\frac{\partial v'}{\partial t}$

The reason for using the primes on u' and v' will be clear shortly. From these wave equations, it follows easily that the energy band for holes is the mirror image (about E = 0 and k = 0) of that for electrons as shown in Fig.2.1b.

To describe Andreev reflection, we need to couple an up-spin electron with energy E to a down-spin hole with energy - ($2E_f$ - E). This is accomplished by the following equation :

$$\begin{bmatrix} H & \Delta\, e^{-i2E_f t/\hbar} \\ \Delta^* e^{+i2E_f t/\hbar} & -H^* \end{bmatrix} \begin{Bmatrix} u' \\ v' \end{Bmatrix} = i\hbar\frac{\partial}{\partial t} \begin{Bmatrix} u' \\ v' \end{Bmatrix} \qquad (2.2)$$

The pairing potential $\Delta\, e^{-i2E_f t/\hbar}$ provides the coupling necessary for Andreev reflection. If Δ is equal to zero, we recover the uncoupled equations for the up-spin electron and the down-spin hole.

The time-dependence $e^{-i2E_f t/\hbar}$ is needed to cause the change in energy from E to $E-2E_f$. It is common to suppress this time-dependence through a gauge transformation defined by

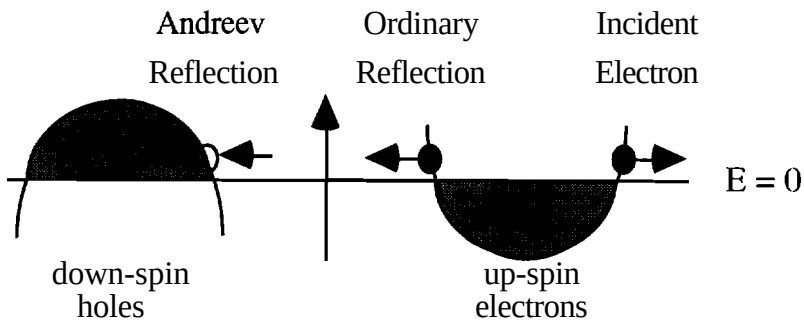


Fig.2.3. The gauge transformation in **Eq.(2.3)** shifts the electron band down in energy by E_f and shifts the hole band up in energy by the same amount, making the process of Andreev reflection look "elastic".

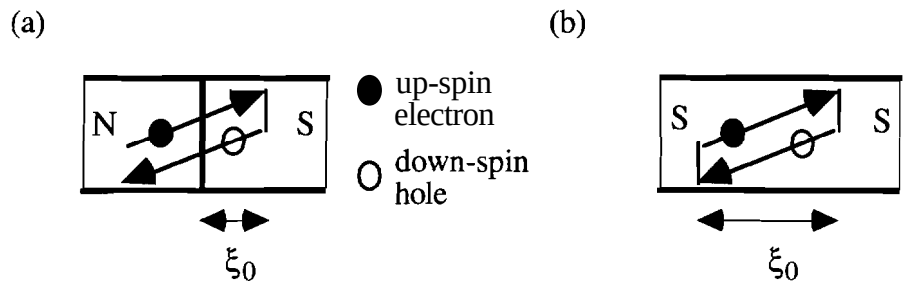


Fig.2.3. Andreev reflection processes occurring in (a) a clean **normal**-superconductor (N-S) interface, and (b) a clean bulk superconductor. The **coherence** length ξ_0 ($=\hbar v_f / \Delta$, v_f : Fermi velocity) is the distance that an electron travels in a time $\sim \hbar / \Delta$, which is the time that it **takes** for an **up**-spin electron to be converted into a down-spin hole. Adapted **from** Ref.2.4.

$$u = u'\, e^{+iE_f t/\hbar} \qquad \text{and} \qquad v = v'\, e^{-iE_f t/\hbar} \tag{2.3}$$

This transforms Eq.(2.2) into the standard form of the **equilibrium** BdG equation [2.2]:

$$\begin{bmatrix} H - E_f & \Delta \\ \Delta^* & -(H^* - E_f) \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = i\hbar \frac{\partial}{\partial t} \begin{Bmatrix} u \\ v \end{Bmatrix} \tag{2.4}$$

The gauge transformation effectively shifts the electron band down in energy by E_f and shifts the hole band up in energy by the same amount, making the process of Andreev reflection look "elastic" (see Fig.2.2).

It is important to note, however, that if there are two or more superconductors with different electrochemical potentials, then the time-dependence cannot be completely transformed away. The **non-equilibrium** BdG equation has the form [2.3]

$$\begin{bmatrix} (H - E_f) & \Delta\, e^{-i2\mu(r)t/\hbar} \\ \Delta^* e^{+i2\mu(r)t/\hbar} & -(H^* - E_f) \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = i\hbar \frac{\partial}{\partial t} \begin{Bmatrix} u \\ v \end{Bmatrix} \tag{2.5}$$

where the local electrochemical potential is given by $(E_f + \mu(r))$. We can choose the reference energy E_f such that $\mu(r)$ is zero in one of the superconductors and the pairing potential in that superconductor will not vary with time. But the pairing potential(s) in the other superconductor(s) will still be time-varying. This leads to the well-knovvn Josephson-type effects. Note that Eq.(2.5) **cannot** be transformed into

$$\begin{bmatrix} H - E_f - \mu(r) & \Delta \\ \Delta^* & -(H^* - E_f - \mu(r)) \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = i\hbar \frac{\partial}{\partial t} \begin{Bmatrix} u \\ v \end{Bmatrix} \qquad \text{('WRONG)}$$

We have tried to show above that if we accept Andreev reflection at normal-superconductor (N-S) interfaces as an experimental fact then we are led inevitably to the BdG equation. The pairing potential **A** leads to Andreev reflection, in much the same way that a change in the ordinary potential (denoted 'eV' in Eq.(2.1)) leads to ordinary reflection. However, this phenomenon is not limited to N-S interfaces. Inside a bulk superconductor repeated Andreev reflection leads to a modification of the energy eigenstates, just as repeated ordinary reflections inside a solid lead to the formation of Bloch states and energy bands (see Fig.2.3).

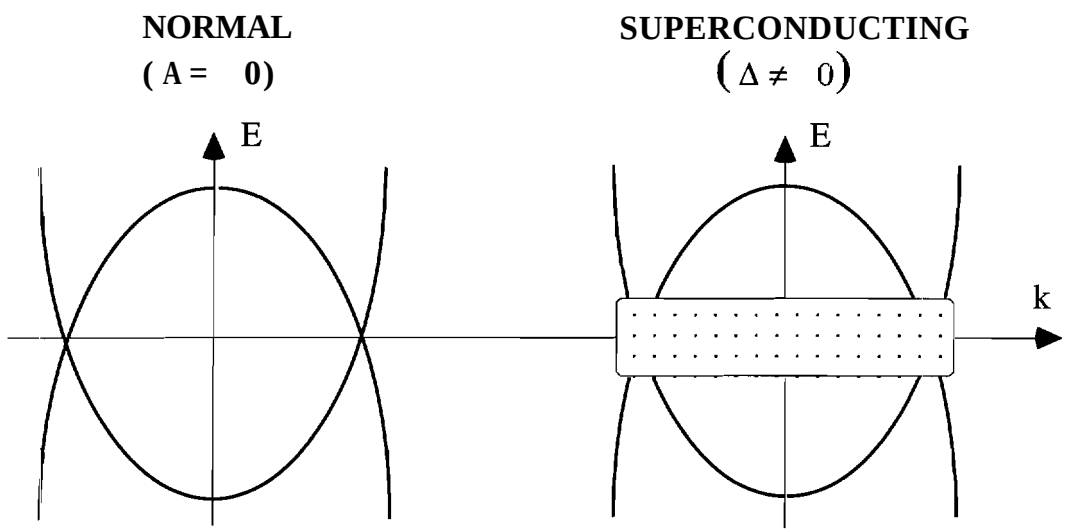


Fig.2.41. Eigenstates of the BdG equation for a normal conductor (A = 0) and a superconductor (Δ ≠ 0). A gap of 2A opens up symmetrically around E = 0.

We will now discuss the nature of the eigenstates in a bulk superconductor. This will be useful in understanding the connection between the BdG equation and the BCS ground state.

Eigenstates of the BdG equation

Let us assume for simplicity that the pairing potential Δ is spatially constant. We can then write each eigenstate 'M' of the BdG equation (see Eq.(2.4)) in terms of a single eigenstate 'm' of H :

$$|M\rangle \equiv \begin{pmatrix} u_M(R) \\ v_M(R) \end{pmatrix} = U_M \begin{pmatrix} \varphi_m(R) \\ 0 \end{pmatrix} + V_M \begin{pmatrix} 0 \\ \varphi_m^*(R) \end{pmatrix} \tag{2.6}$$

where $H\,\varphi_m = \varepsilon_m \varphi_m$ and $H^*\,\varphi_m^* = \varepsilon_m \varphi_m^*$ (2.7)

and the coefficients U_M and V_M are obtained by solving the (2x2) matrix eigenvalue problem

$$\begin{pmatrix} \varepsilon_m - E_f & \Delta \\ \Delta^* & -(\varepsilon_m - E_f) \end{pmatrix} \begin{Bmatrix} U_M \\ V_M \end{Bmatrix} = E_M \begin{Bmatrix} U_M \\ V_M \end{Bmatrix} \tag{2.8}$$

This yields two eigenvalues symmetrically around E = 0:

$$E_M = \pm \sqrt{(\varepsilon_m - E_f)^2 + |\Delta|^2} \tag{2.9}$$

For a clean homogeneous superconductor, the eigenstates of H are plane waves that can be labeled by the wavenumber 'k' with $\varepsilon_k = \mathbf{h}^2\mathbf{k}^2 / 2m$. We then obtain the dispersion curves shown in Fig.2.4.

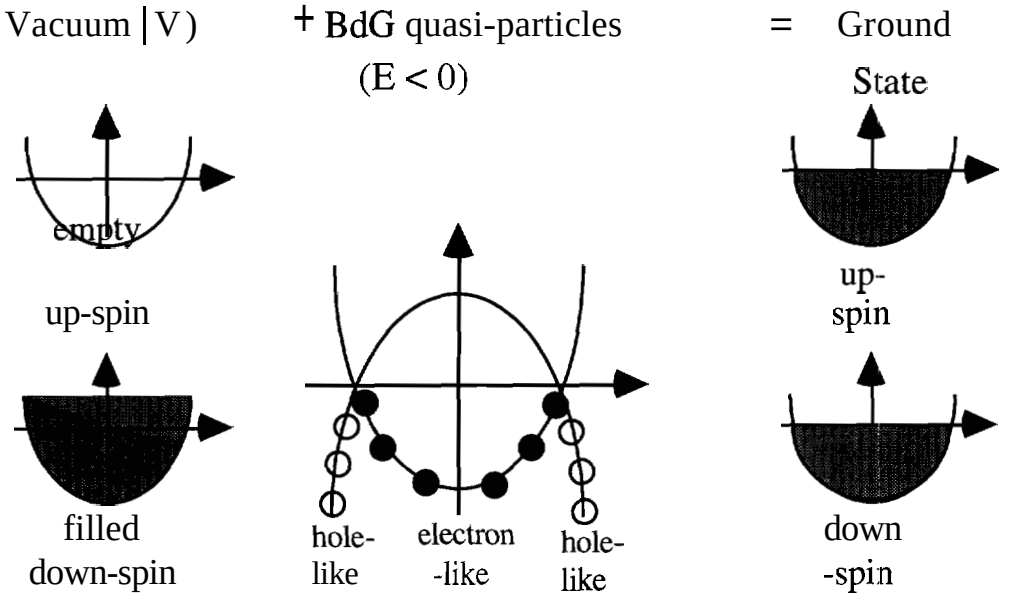


Fig.2.5. For a normal conductor the ground state can be obtained by filling all the! negative energy states of the **BdG** equation ($A = 0$) starting from the special vacuum $|V\rangle$ consisting of a full band of down-spin electrons. The electron-like quasi-particles fill up the empty up-spin band while the hole-like quasi-particles extending to negative infinity empty out the filled down-spin band, giving the standard ground state with both bands filled **upto** $E = 0$.

Ground state (T = 0)

We know that for normal systems the many-body ground state is obtained by filling up all the eigenstates of the Schrodinger equation having energies less than the Fermi energy. In second quantized notation we can write

$$|G\rangle = \prod_{E_m < E_f} c_m^+ |0\rangle$$

where $|0\rangle$ is the empty vacuum and the operator c_m^+ creates an electron in the eigenstate 'm' of the Schrodinger equation. Can we construct the superconducting ground state $|G)$ in the same way by filling up all the eigenstates of the BdG equation having energy less than zero ? The answer is yes provided we start from a special vacuum $|V)$ consisting of a full band of down-spin electrons. This is easy to see pictorially for the special case of a normal conductor having $A = 0$ (see Fig.(2.5)).

For a superconductor ($A \neq 0$), too, we can show that we indeed obtain the standard BCS ground state if we start from the special vacuum $|V)$ consisting of a full band of down-spin electrons

$$|V\rangle = \prod_m c_{m,\downarrow}^+ |0\rangle \tag{2.10}$$

and fill up the negative energy states:

$$|G\rangle = \prod_{E_M < 0} \gamma_M^+ |V\rangle \tag{2.11}$$

where the operator γ_M^+ creates a particle in eigenstate 'M' of the BdG equation. Since an eigenstate 'M' of the BdG equation represents a mixture of an up-spin electron and a down-spin hole in an eigenstate 'm' of the normal Hamiltonian H (see Eq.(2.6)), we can write

$$\gamma_M^+ = U_M c_{m,\uparrow}^+ + V_M c_{m,\downarrow} \tag{2.12}$$

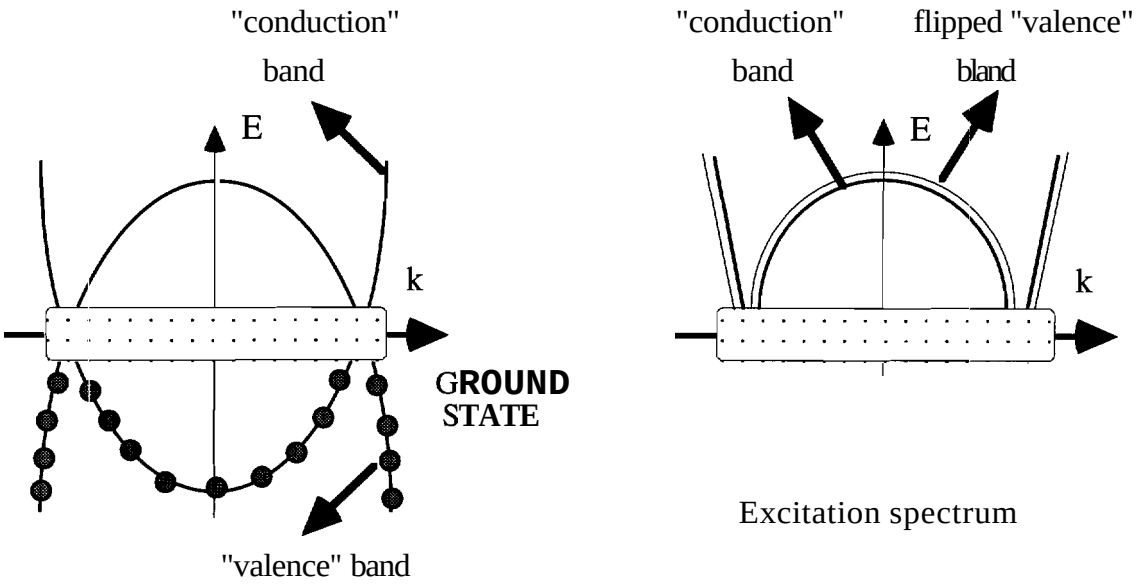


Fig.2.6. (a) The ground state is equivalent to the state obtained by filling all the, negative energy states of the **BdG** equation. Excitations are created by **taking** a particle out of these states or by inserting one in the positive energy states. (b) The excitation spectrum is obtained by leaving the **"conduction"** band intact and flipping the "valence" band about $E = 0$.

Combining Eqs.(2.10) - (2.12) we obtain

$$|G\rangle = \prod_{E_M<0} \left(U_M\, c^{+}_{m,\uparrow} + V_M\, c_{m,\downarrow} \right) c^{+}_{m,\downarrow}|0\rangle$$

$$= \prod_{E_M<0} \left(U_M\, c^{+}_{m,\uparrow} c^{+}_{m,\downarrow} + V_M \right)|0\rangle$$

which is just the standard BCS wavefunction obtained by pairing time-reversed eigenstates of 'H' [2.5].

If the pairing potential varies spatially, then an eigenstate of the BdG equation cannot be expressed in terms of a single eigenstate of 'H' as we have done above. Filling up the negative energy states of the BdG equation then yields a ground state that can have a lower energy than the BCS state obtained by pairing time-reversed eigenstates of 'H' [2.2].

Excitations ($T \neq 0$)

We have seen above that the state obtained by filling all the negative energy states of the BdG equation represents the ground state (see Fig.2.6). The situation is thus much like a semiconductor with a gap of 2Δ. The negative energy states form the "valence band" while the positive energy states form the "conduction band". Excitations are created by adding a particle to the conduction band or by taking one out of the valence band. The **excitation spectrum** can be obtained from the eigenstates of the BdG equation by leaving the "conduction" band intact and flipping the valence band about $E = 0$ as shown in Fig.2.6b. Due to the electron-hole symmetry (which we will discuss further shortly), the "conduction" and "valence" bands are always precise mirror images of each other, so that the flipped "valence" band looks identical to the "conduction" band. Consequiently one can simply assume a doubly degenerate "conduction band" as is commonly done in the literature.

The important point to note is that the BdG equation not only describes the excitations, but also describes the ground state (that is, the "condensate"). Several authors have noted that the negative energy solutions of the BdG equation describe the ground state, but we are not aware of a clear demonstration that one could indeed construct the ground state by filling up these states starting from a suitable vacuum. Indeed we are not aware of any other work that refers to the special vacuum $|V\rangle$.

In appendix A we provide a formal justification for this viewpoint by showing that using a mean field approximation the BCS Hamiltonian can be written in the form ('mf stands for mean field, see Eq.(A.18))

$$H_{mf} = H_{VAC} + \sum_M E_M \gamma_M^+ \gamma_M$$

H_{VAC} is the energy of the "vacuum" $|V\rangle$ consisting of a completely full band of down-spin electrons. On top of this vacuum, the operator γ_M^+ creates particles in eigenstates of the BdG equation as we have discussed. Thus the BdG equation can be viewed as a ***one-particle wave equation*** whose eigenstates can be filled up systematically to describe the superconducting state. This justifies the use of the BdG equation to construct a scattering theory in the same way that Schrodinger equation is used for normal systems.

The excitation picture (see Fig.2.6b) on the other hand, can be justified by defining ('c' and 'v' denote conduction and valence band respectively)

$$\gamma_{M\uparrow}^+ = \gamma_{M,c}^+ \quad \text{and} \quad \gamma_{M\downarrow}^+ = \gamma_{M,v}$$

and rewriting H_{mf} as (see Eq.(A.20))

$$H_{mf} = H_G + \sum_{E_M>0} E_M \left[\gamma_{M\uparrow}^+ \gamma_{M\uparrow} + \gamma_{M\downarrow}^+ \gamma_{M\downarrow} \right]$$

Expectation values

To proceed further we need an expression for the expectation value of any quantity of interest in terms of the occupation factors of the different eigenstates (cf. Eqs.(1.5) and (1.6)). It is shown in appendix B that the expectation value of any quantity 'A' is given by

$$A = \sum_M f_M \langle u_M | A_{op} | u_M \rangle + \sum_M (1 - f_M) \langle v_M | A_{op}^* | v_M \rangle \qquad (2.13)$$

where A_{op} is the corresponding one-particle operator. For example, if 'A' represents the electron density $n(r)$, then $A_{op} = \delta(r - R)$ so that from Eq.(2.13)

$$n(r) = \sum_M f_M |u_M(r)|^2 + \sum_M (1 - f_M) |v_M(r)|^2$$

To "understand" the meaning of the expression in Eq.(2.13), let us rewrite it in the form

$$A = \underbrace{\sum_M f_M \left\langle u_M \quad v_M \right| \begin{bmatrix} A_{op} & 0 \\ 0 & -A_{op}^* \end{bmatrix} \left| \begin{matrix} u_M \\ v_M \end{matrix} \right\rangle}_{f_M A_{MM}} + \underbrace{\sum_M \left\langle v_M \right| A_{op}^* \left| v_M \right\rangle}_{A_{VAC}} \qquad (2.14)$$

The first term is proportional to f_M and can be interpreted as the contribution due to the filled eigenstates of the BdG equation. The second term on the other hand is independent of f_M. It can be interpreted as the "vacuum expectation value" arising from the full band of down-spin electrons that comprises $|V\rangle$ (see Eq.(2.10), Fig.2.5). To verify this we first write the vacuum expectation value as

$$A_{VAC} = \sum_m \left\langle \varphi_m \right| A_{op} \left| \varphi_m \right\rangle = \sum_m \left\langle \varphi_m^* \right| A_{op}^* \left| \varphi_m^* \right\rangle$$

where φ_m represents any complete set of basis functions spanning the one-particle, one-spin Hilbert space. We could rewrite this in the form

$$A_{VAC} = Tr \begin{bmatrix} 0 & 0 \\ 0 & A_{op}^* \end{bmatrix}$$

noting that the Hilbert space of the BdG Harniltonian is spanned by the basis kets $|\varphi_m \quad 0\rangle$ and $|\ 0 \quad \varphi_m^*\rangle$. We could just as well evaluate the trace using the eigenkets of the BdG Hamiltonian to write

$$A_{VAC} = \sum_M \left\langle u_M \quad v_M \right| \begin{bmatrix} 0 & 0 \\ 0 & A_{op}^* \end{bmatrix} \left| \begin{matrix} u_M \\ v_M \end{matrix} \right\rangle = \sum_M \left\langle v_M \right| A_{op}^* \left| v_M \right\rangle$$

thus proving that we are indeed justified in identifying the second term in Eq.(2.14) as the vacuum.expectation value.

Electron-hole symmetry

The eigenstates of the BdG equation occur in pairs, one of which has an energy greater than zero while the other has an energy less than zero. To every state in the "conduction" band there is a counterpart in the "valence" band whose wavefunctions and energies are related as follows :

$$E_{m,v} = - E_{m,c} \qquad u_{m,v} = - v_{m,c}^{*} \qquad v_{m,v} = u_{m,c}^{*} \tag{2.15a}$$

$$f_{m,v} = 1 - f_{m,c} \tag{2.15b}$$

Due to this symmetry, the "conduction" and "valence" bands are always precise mirror images of each other [2.6]. Eq.(2.15b) relating the occupation factors for the "conduction" and "valence" band states is obviously true at equilibrium, since $E_{m,v} = - E_{m,c}$. But the point to note is that it is true even away from equilibrium.

We can make use of this symmetry to write the expectation value from Eq.(2.13) solely in terms of the "conduction" band states :

$$A = 2 \left[\sum_{E_M > 0} f_M \langle u_M | A_{op} | u_M \rangle + \sum_{E_M > 0} (1 - f_M) \langle v_M | A_{op}^{*} | v_M \rangle \right] \tag{2.16a}$$

This is the approach commonly used in the literature. Indeed most authors work with the excitation spectrum (see Fig.2.5b) and do not even mention the "valence" band explicitly. Alternatively, we could retain the summation over both bands and use the electron-hole symmetry to get rid of the second term :

$$A = 2 \sum_{M} f_M \langle u_M | A_{op} | u_M \rangle \tag{2.16b}$$

This is the approach used in Ref.[3.1]. Either Eq.(2.16a) or (2.16b) may be more convenient depending on the problem in hand.

Electrochemical potential

Once we have obtained the scattering states $|M)$ from the BdG equation, we can use Eq.(2.13) (or Eq.(2.16)) to evaluate any quantity of interest if we know the occupation factors f_M for the different states. At equilibrium the factor f_M is equal to $f_0(E_M)$, where f_0 is the Fermi function defined in Eq.(1.4). Under non-equilibrium conditions, each scattering state is associated with a Fermi factor f_M determined by its reservoir of origin. This raises a few questions which we will now discuss.

An incident wave from reservoir 'i' having an electrochemical potential μ_i can be written in the form

$$|M\rangle = \begin{pmatrix} u_M\, e^{-i(E_M+\mu_i)t/\hbar} \\ v_M\, e^{-i(E_M-\mu_i)t/\hbar} \end{pmatrix} \tag{2.17}$$

Note that the electron component and the hole component have different energies (that is, time variations) and they are coupled together by the time-varying pair potential $A\, e^{-i2\mu_i t/\hbar}$. What Fermi factor f_M should we associate with such a state ? The answer is obtained by noting that this state can be locally gauge transformed into the form

$$\begin{pmatrix} u_M\, e^{-iE_M t/\hbar} \\ v_M\, e^{-iE_M t/\hbar} \end{pmatrix}$$

which should clearly have a Fermi factor of $f_0(E_M)$ (f_0 is defined in Eq.((1.4)). Hence we can write

$$f_M = f_0(E_M) \tag{2.18a}$$

$$= f_0(E_{M,e} - \mu_i) = f_0(E_{M,h} + \mu_i) \tag{2.18b}$$

where $E_{M,e}$ is the energy associated with the electron component of the incident wave, $E_{M,h}$ is the energy associated with the hole component of the incident wave and E_M is the average of the two energies.

Eq.(2.18a) for the Fermi factor f_M suggests that we should always use an electrochemical potential of zero (that is, equal to the reference energy E_f) for all scattering states emerging from any reservoir. However, we have to remember that the energy E_M of

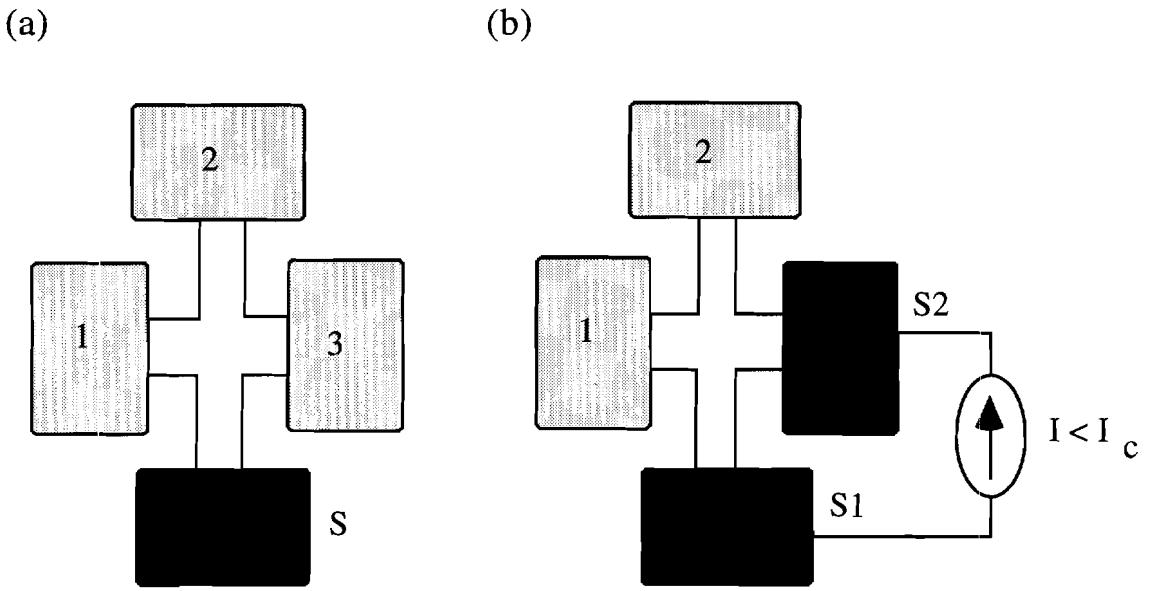


Fig.2.7. Examples of two mesoscopic structures where the BdG equation becomes time-independent and its solutions consist of a single-energy component. (a) A structure with only one superconducting contact. (b) A structure with two superconducting contacts having the same electrochemical potential (I < critical current, I,).

a scattering state is the average of the energies associated with the electron and hole components of the incident wave. While this is a reasonable way to do the book-keeping for scattering states emerging from a superconducting terminal, it seems somewhat silly for scattering states emerging from a normal terminal. The reason is that at a normal terminal the electron and hole components are decoupled - either u_M or v_M in Eq.(2.17) is equal to zero. Thus we have two types of scattering states, one for which the incident wave is purely electron-like (labeled 'e') and another for which it is purely hole-like (labeled 'h'):

$$|M,e\rangle = \begin{pmatrix} u_M\, e^{-iE_{M,e}\,t/\hbar} \\ 0 \end{pmatrix} \quad \text{and} \quad |M,h\rangle = \begin{pmatrix} 0 \\ v_M\, e^{-iE_{M,h}\,t/\hbar} \end{pmatrix} \qquad (2.19)$$

It seems more natural to view $E_{M,e}$ and $E_{M,h}$ as the energies of these states. Eq.(2.18b) then tells us that the corresponding electrochemical potentials are $+\mu_i$ and $-\mu_i$ respectively and not zero.

Even at a superconducting terminal we can distiguish between an electron-like state and a hole-like state and label their energies in terms of $E_{M,e}$ and $E_{M,h}$ respectively, instead of E_M. The corresponding electrochemical potentials are then given by $+\mu_i$ and $-\mu_i$, just like the normal terminals. On the other hand, if we were to treat $(E_{M,e} + E_{M,h}) / 2$ as the energy, the electrochemical potential is zero. We could follow either scheme in doing our energy book-keeping. However, we need to deal with superconducting contacts with non-zero electrochemical potentials only if a structure has multiple superconducting contacts with different electrochemical potentials. In this case, we can choose the reference energy E_f so that the pairing potential is time-independent in one of the superconducting contacts, but not in the others. Consequently the solutions to the BdG equation contain multiple energy components, similar to normal conductors with an applied **ac** potential [2.7].

If a structure has only one superconducting contact (Fig.2.7a), then we can choose the reference energy E_f so that the pairing potential (see Eq.(2.5)) is time-independent in the superconducting contact (at the normal terminals it is zero anyway). The BdG equation then becomes time-independent and its solutions consist of a single-energy component just like normal conductors. The same is true of structures like the one shown in Fig.2.7b having multiple superconducting contacts but with the same electrochemical potential. It is fairly straightforward to extend the standard results of normal mesoscopic physics to such structures. ***We just have to replace each physical lead 'i' with two leads - an electron lead 'ie' and a hole lead 'ih'.***

Self-consistency of the pairing potential

An important point to note is that the pairing potential can be written as $\Delta\, e^{-i2\mu(r)t/\hbar}$ only inside a large superconducting contact that can be assumed to remain close to local equilibrium with a well-defined electrochemical potential. But this is not correct near any interface in a region with dimensions of the order of a coherence length. The correct pairing potential has to be calculated self-consistently just as we calculate the Hartree potential self-consistently in normal conductors. The self-consistency relation (g : electron-phonon coupling constant)

$$\Delta(r,t) = -\, g(r) \sum_{M} u_M(r,t)\, v_M^*(r,t)\, f_M \tag{2.20}$$

can be obtained from Eq.(2.14) if we associate the following one-particle operator

$$\Delta_{op}(r) \;\rightarrow\; \begin{bmatrix} 0 & 0 \\ -g(r)\delta(R-r) & 0 \end{bmatrix}$$

with the pairing potential and note that the vacuum contribution is zero. A derivation of Eq.(2.20) using the second quantized formalism is provided in appendix B.

Eq.(2.20) is actually not quite right. It assumes that the electron-electron attraction is instantaneous in space and time having a strength characterized by 'g' that can vary slowly from one point to another. More accurate expressions can be derived using the Eliashberg - Migdal theory [2.8] that take into account the temporal and spatial non-locality of the electron-phonon interaction. We will not discuss these refinements further in this article. However, even in a zero-order theory it is necessary to modify Eq.(2.20) in order to obtain sensible results, since the summation over 'M' diverges. The simplest way to get around this difficulty is to cut off the summation in Eq.(2.20) for energies exceeding $\hbar\omega_D$, ω_D being the highest phonon frequency in the material :

$$\Delta(r,t) = -\, g(r) \sum_{|E_M| < \hbar\omega_D} u_M(r,t)\, v_M^*(r,t)\, f_M \tag{2.21a}$$

$$= g(r) \sum_{0 < E_M < \hbar\omega_D} u_M(r,t)\, v_M^*(r,t) \left[1 - 2f_M\right] \tag{2.21b}$$

This is justified by noting that a detailed theory of the electron-phonon interaction shows that the effective interaction between two electrons is attractive only if their energies lie approximately within $\hbar\omega_D$ of the Fermi energy.

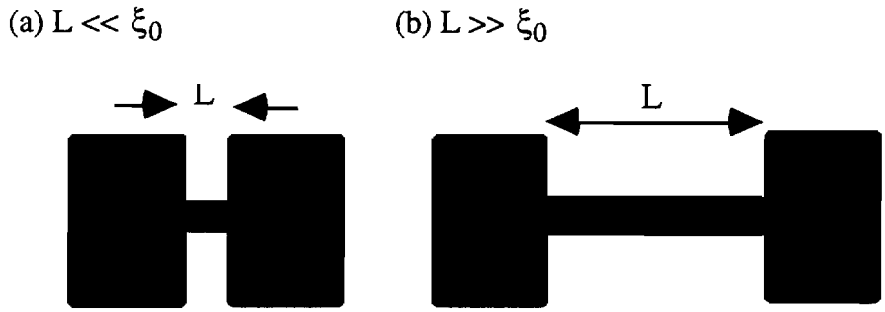
Note that the self-consistency relation (Eq.(2.21)) contains all the microscopic physics producing superconductivity. Eq.(2.21) would be different if we were to consider a different pairing mechanism, or work out a more accurate theory for the same mechanism. By contrast the BdG equation should remain unchanged as long as we are describing a microscopic state consisting of singlet Cooper pairs, regardless of how they are formed.

In much of the work on mesoscopic superconductivity a fixed pairing potential is assumed, that changes abruptly from zero inside the normal material to the appropriate bulk value inside a superconductor. The self-consistency equation is ignored, just as the Poisson equation is ignored in most of the work on normal mesoscopic systems. The general belief is that the results should be qualitatively correct, though the quantitative details may change. However, a few caveats are in order.

Firstly, during an Andreev reflection process, an incident electron drags another electron along with it into the superconductor, leaving behind the reflected hole (see Fig.2.1). This causes the pairing potential to deform and acquire a phase gradient of the form Δe^{i2qx}. It can be shown that in the presence of such a pairing potential a non-zero current is carried by a filled 'valence' band (see Fig.2.6)! The resulting current is often called a "supercurrent" to distinguish it from the "quasi-particle" current carried by filled states in the 'conduction' band or empty states in the 'valence' band. The point to note is that any theory which neglects the deformation of the pairing potential will not predict the current in the superconducting regions correctly. Indeed, starting from the BdG equation (see Eq.(2.4)), it can be shown that the continuity equation for the electrical charge has a source term

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}.\vec{J} = \frac{4e}{\hbar} \sum_{M} \mathrm{Im}\left[\Delta(r)\, u_M^*(r) v_M(r)\, f_M\right] \qquad (2.22)$$

indicating that the electrical current is conserved only if the quantity on the right is zero. It is easy to see that this quantity is zero if we use Eq.(2.20) for the pairing potential, proving that the conservation of electrical current can be ensured only if Δ is determined self-consistently [3.1, 2.10-2.12]. For this reason, in non self-consistent theories the current is evaluated only in the normal regions (where current is conserved since $\Delta = 0$) and the current in the superconducting regions is inferred indirectly (see Fig.4.4).



(a) Dashed ····· (b) Solid _____

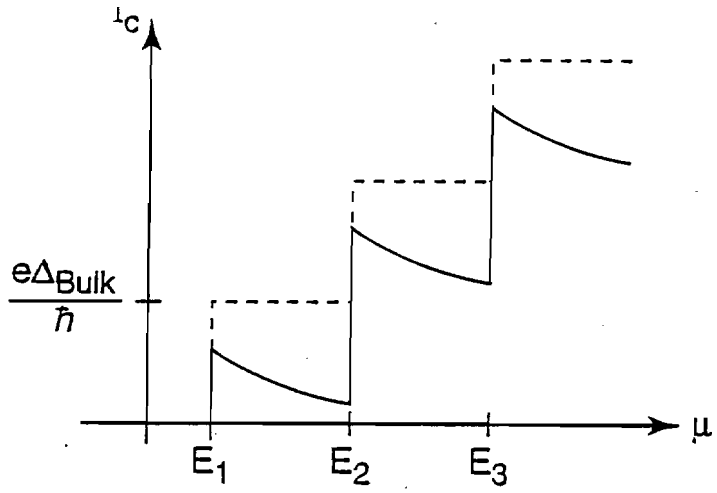


Fig.2.9. A superconductor with a constriction. In (a) the constriction is much shorter than the coherence length and has essentially the same pairing potential Δ_{bulk} as the bulk material. The critical current **has** then been shown to increase in steps as the number of modes in the narrow region is increased. But in (b) the constriction is much longer than **the** coherence length and has a different pairing potential Δ_{wire} that follows the density of states in the superconducting "wire". The critical current **should** also follow the density of states instead of increasing in steps. **Adapted** from **Chang,** Chaudhuri and **Bagwell** [2.13].

Secondly, if the superconductor forms part of the mesoscopic region then it may be driven away from local equilibrium by relatively small values of current. Even at equilibrium, a small superconducting region may have a pairing potential that is different from the bulk value. Consider for example a superconductor with a constriction. If the constriction is much shorter than the coherence length (Fig.2.8a) then it should have essentially the same pairing potential A_{bulk} as the bulk material. The critical current has then been shown to increase in steps as the number of modes in the narrow region is increased [2.9]. But if the constriction is much longer than the coherence length (Fig.2.8b) then it will have a different pairing potential A_{wire} that follows the density of states of the superconducting "wire" rather than that of the bulk superconductor. The critical current in this case should also follow the density of states of the wire instead of increasing in steps as shown in the figure.

Now that we have laid out the basic principles underlying the scattering theory for mesoscopic superconductivity, let us look at a few examples of how it is applied. We will not go into the details of how the scattering parameters can be calculated from the BdG equation since this is very similar to the standard procedures used in normal mesoscopic physics (see for example, chapter 3 of Ref.[1.2]).

3. Normal (N) - superconductor (S) junctions

In any mesoscopic structure, if the superconducting contacts are all at the same potential then the scattering states constructed from Eq.(2.5) consist of a single energy component as in normal conductors. We can then proceed as we do in normal conductors to derive expressions for the terminal current. Since such expressions have already been derived in the literature [3.1 - 3.3] we will not repeat it here. Instead we will show how these results can be obtained from the standard results of normal mesoscopic theory simply by using the following prescription:

- **Every physical lead 'i' splits into an electron-like lead 'ie' and a hole-like lead 'ih', whose potentials are related to the potential μ_i at contact 'i' by the relation**

$$\mu_{ie} = +\mu_i \qquad \text{and} \qquad \mu_{ih} = -\mu_i \tag{3.1}$$

This prescription is motivated by Eq.(2.18b) which states that the correct Fermi factor to associate with a state emerging from reservoir 'i' is given by

$$f_M = f_0(E_{M,e} - \mu_i) = f_0(E_{M,h} + \mu_i)$$

where $E_{M,e}$ is the energy associated with the electron component of the incident wave, $E_{M,h}$ is the energy associated with the hole component of the incident wave. In this section we will apply this principle to N-S junctions. In section 5 we will apply it to multiterminal structures and in section *6* we will use it to obtain an expression for the current fluctuations.

Linear response

(Considera normal(N) - superconductor (S) junction (Fig.3.1a). According to the prescription in Eq.(3.1), the N and the S terminal each splits into an electron-like and a hole-like terminal as shown in Fig.3.1. It is well-known that the linear response current in a multiterminal normal mesoscopic systems is given by [1.8]

$$I_i = \frac{e}{h} \sum_j \left[M_i \delta_{ij} - T_{ij} \right] \mu_j \tag{3.2}$$

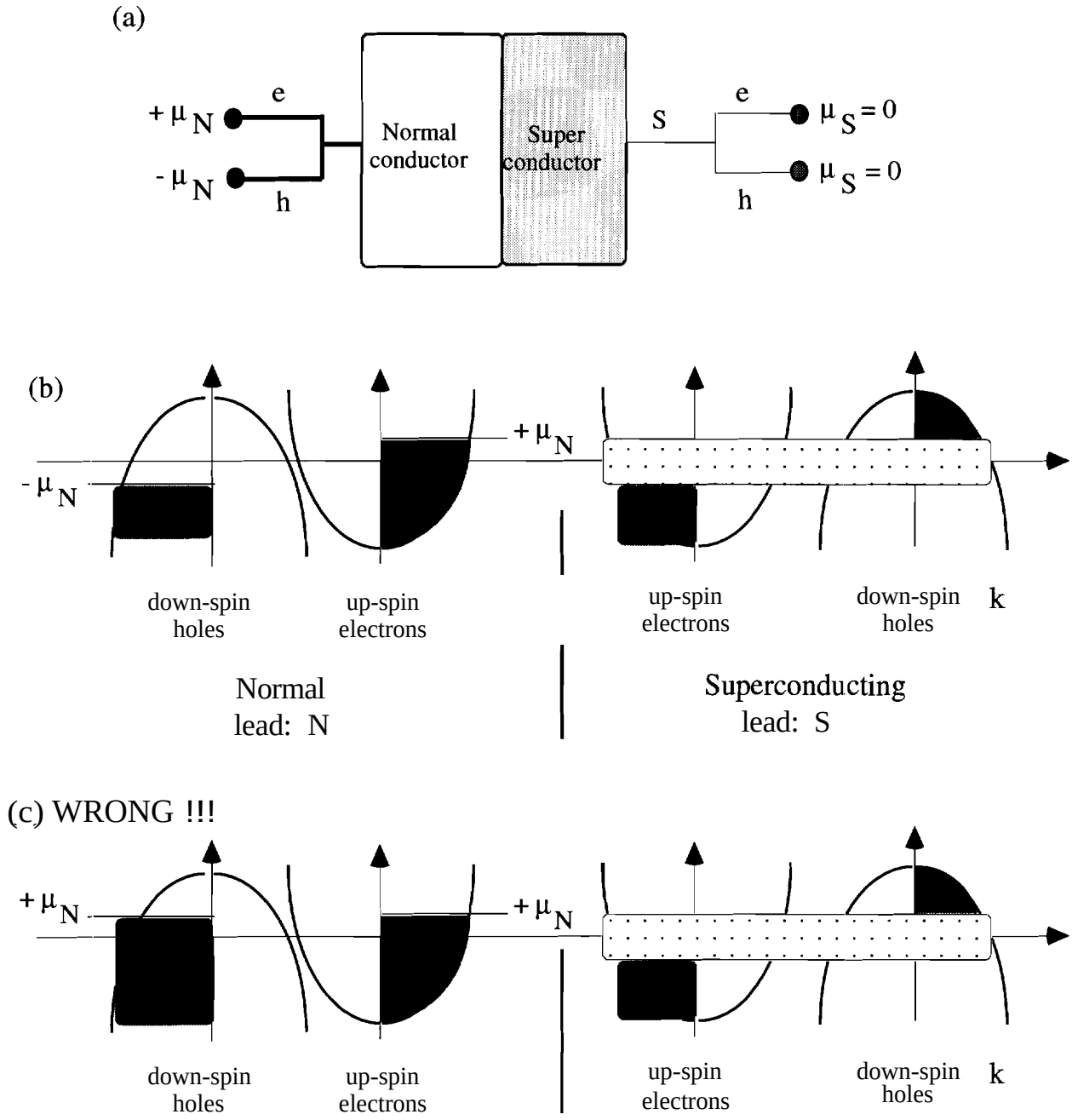


Fig.3.1. (a) A mesoscopic structure with a normal lead (N) and a superconducting lead (S). Each physical lead conceptually splits into an up-spin electron lead (e) and a down-spin hole lead (h). (b) Dispersion relations and electrochemical potentials in the leads. (c) A plausible but WRONG alternative to (b).

where M_i is the number of modes in lead 'i' and T_{ij} is the total transmission from lead 'j' to lead 'i' summed over all modes [1.1, 1.21. Applying Eq.(3.2) to the structure in Fig.3.1 we obtain

$$I_{Ne} = \frac{e}{h}\left[(M - T_{Ne,Ne})\,\mu_N + (-T_{Ne,Nh})\,(-\mu_N)\right]$$

$$I_{Nh} = \frac{-e}{h}\left[(-T_{Nh,Ne})\,\mu_N + (M - T_{Nh,Nh})\,(-\mu_N)\right]$$

It can be shown that due to electron-hole symmetry, the current at the electron lead is exactly equal to the current at the hole lead (we will discuss this in more detail shortly). So we can obtain the total current simply by multiplying either component by 2 :

$$I_N = 2I_{Ne} = 2I_{Nh} = \frac{2e}{h} M\left[(1 - R + R_a)\,\mu_N\right] \qquad (3.3)$$

where R is the normal reflection coefficient ($MR = T_{Ne,Ne} = T_{Nh,Nh}$) and R_a is the Andreev reflection coefficient ($MR_a = T_{Ne,Nh} = T_{Nh,Ne}$). Hence the conductance is given by

$$G = \frac{I}{\mu_N / e} = \frac{2e^2}{h} M\left[1 - R + R_a\right] \qquad (3.4)$$

The conductance is enhanced by the Andreev reflection R_a, leading to the well-known "excess conductance" at low bias discussed in Ref.3.1.

Current at the superconducting leads

'Note that this approach can only be used to calculate the current at the normal terminals. It cannot be used to calculate the current at the superconducting terminals. Indeed if we use Eq.(3.2) to calculate the current at the superconducting terminal 'Se', we obtain

$$I_{Se} = \frac{2e}{h}\left[-T_{Se;Ne}(E)\,\mu_N + T_{Se;Nh}(E)\,(-\mu_N)\right] = 0 \qquad !!!$$

since no particles are transmitted into the superconductor, as long as the bias and temperature are much less than the superconducting energy gap. But this cannot be right.

Since we have only two leads, the current in the superconductor must be equal to that in the normal lead, which we have seen is non-zero (see Eq.(3.3)). Why is Eq.(3.2) not applicable to superconducting leads ? As we discussed in the last section, the "supercurrent" is not described by the simple version of the scattering theory which assumes a fixed pairing potential A ; one has to take the deformation of the pairing potential into account.

Beyond linear response

To understand the nature of the current flow at an N-S junction it is useful to go beyond the linear response formula and look at the full energy spectrum of the current. For normal mesoscopic systems the general current-voltage relation is given by

$$I_i = \frac{e}{h}\int dE \sum_j \left[M_i\delta_{ij} - T_{ij}\right] f_0(E-\mu_j) \qquad (3.5)$$

Applying this relation to the "four-terminal" structure in Fig.3.1a, we obtain

$$I_{Ne} = \frac{e}{h}\int dE \left\{ \begin{array}{r} \left[M_{Ne} - T_{Ne,Ne}\right] f_0(E-\mu_N) \;+\; \left[-T_{Ne,Nh}\right] f_0\left(E+\mu_N\right) \\ +\; \left[-T_{Ne,Se}\right] f_0(E) \;+\; \left[-T_{Ne,Sh}\right] f_0(E) \end{array} \right\}$$

Making use of the "sum rule" (see appendix C)

$$M_{Ne} = T_{Ne,Ne} + T_{Ne,Nh} + T_{Ne,Se} + T_{Ne,Sh}$$

we rewrite this in the form

$$I_{Ne} = \frac{e}{h}\int dE \left\{ \begin{array}{r} \left[M_{Ne} - T_{Ne,Ne}\right]\left[f_0(E-\mu_N) - f_0(E)\right] \\ +\; \left[-T_{Ne,Nh}\right]\left[f_0(E+\mu_N) - f_0(E)\right] \end{array} \right\} \qquad (3.6a)$$

Similarly the current at the 'Nh' terminal is given by

$$I_{Nh} = \frac{-e}{h}\int dE \left\{ \begin{array}{r} \left[-T_{Nh,Ne}\right]\left[f_0(E-\mu_N) - f_0(E)\right] \\ +\; \left[M_{Nh} - T_{Nh,Nh}\right]\left[f_0(E+\mu_N) - f_0(E)\right] \end{array} \right\} \qquad (3.6b)$$

The two terms in Eq.(3.6a) represent the currents at 'Ne' due to injection from 'Ne' and 'Nh' respectively. Similarly the two terms in Eq.(3.6b) represent the currents at 'Nh' due to injection from 'Ne' and 'Nh' respectively :

$$I_{Ne} = I_{Ne\leftarrow Ne} + I_{Ne\leftarrow Nh} \quad \text{and} \quad I_{Nh} = I_{Nh\leftarrow Ne} + I_{Nh\leftarrow Nh} \tag{3.7}$$

The symmetry properties of the transmission functions (see appendix C) ensure that

$$I_{Ne\leftarrow Ne}(+E) = I_{Nh\leftarrow Nh}(-E) \quad \text{and} \quad I_{Ne\leftarrow Nh}(+E) = I_{Nh\leftarrow Ne}(-E)$$

This relation together with the property that $f_0(+E) = 1\text{-}f_0(-E)$ allows us to rewrite Eq.(3.6a,b) as

$$I_N = \frac{2e}{h}\int dE \left[1 - T_{Ne,Ne} + T_{Nh,Ne}\right]\left[f_0(E-\mu_N) - f_0(E)\right] \tag{3.8}$$

This is the well-known Blonder-Tinkham-Klapwijk(BTK) formula [3.1].

4. Contact resistance

As we mentioned in the introduction, a very important lesson in mesoscopic physics is the realization that a ballistic conductor connected between two large contacts exhibits a non-zero resistance arising from the interface resistance between the conductor and the contacts. How is this interface resistance modified for a superconducting contact ?

N-N-N structure

Consider a perfect ballistic conductor with M modes connected between two normal contacts (Fig.4.1a). Let us assume that there is no normal or Andreev reflection at either contact as in normal mesoscopic point contacts. We can calculate the current in this structure by noting that in a ballistic conductor, the +k states are populated solely by electrons coming out of the left contact, while the -k states are populated solely by electrons from the right contact..Consequently, inside the conductor, the electrochemical potential fo the +k states is equal to μ_1, while that for the -k states is equal to 0 (Fig.4.2b). This means that at zero temperature the current is entirely due to the occupied +k states between μ_1 and 0. Since the current carried per unit energy per mode is (2e/h), we can write

$$I = \frac{2eM}{h}\mu_1 \qquad \rightarrow \qquad R_C = \frac{\mu_1}{eI} = \frac{h}{2e^2M} \tag{4.1}$$

This is exactly what we get from Eq.(3.4) if we set both R and R_a equal to zero corresponding to perfect transmission.

Where does this resistance R_C (which was experimentally observed in 1988 [1.7]) come from ? After all, a ballistic conductor should not have any resistance. This question led to much argument and controversy in the early 1980's. But it is now understood that this is basically a contact resistance arising at the two interfaces between the conductor and the contacts, as pointed out by Imry. This interpretation can be justified by noting that the average electrochemical potential inside the conductor is given by

$$\mu = \frac{\mu(+k) + \mu(-k)}{2} = \frac{\mu_1}{2}$$

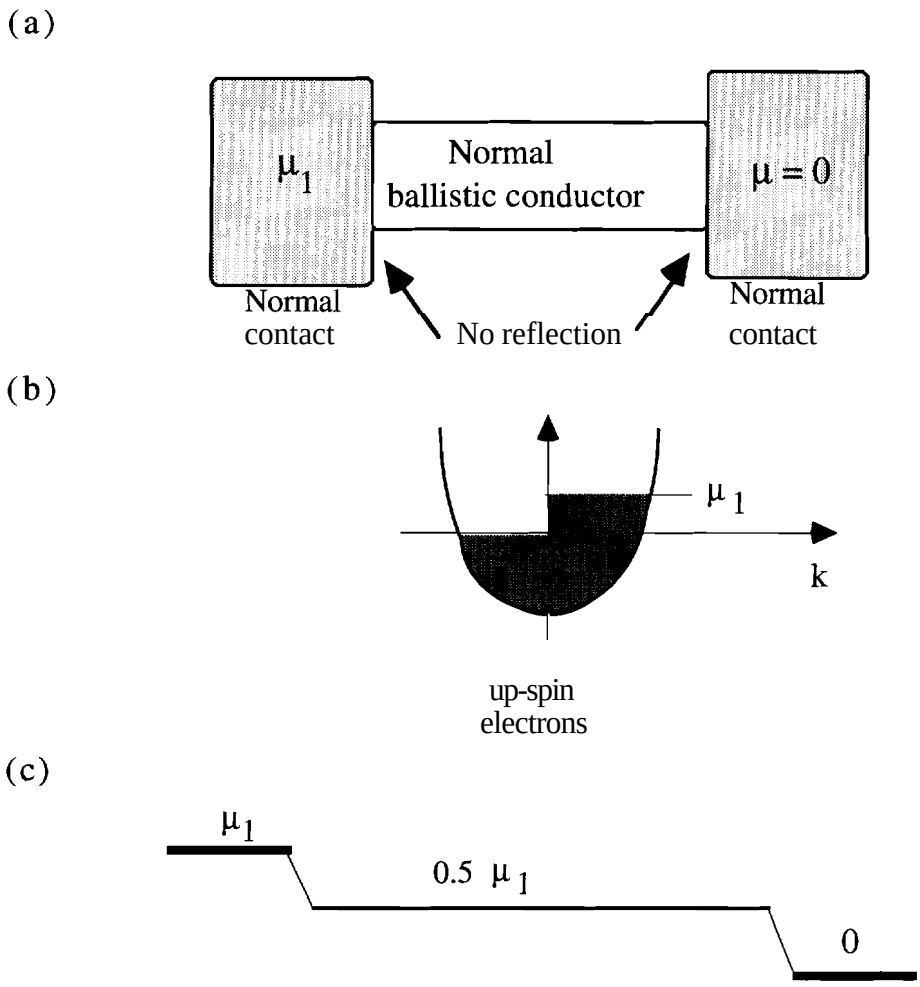


Fig.4.1. (a) A normal ballistic conductor connected to two wide contacts such tlhat there is no normal or Andreev reflection. (b) The electrochemical potential of +k states in the conductor follows the left contact, vvhile that of -k states follows the right contact. (c) Average electrochemical potential profile across the structure.

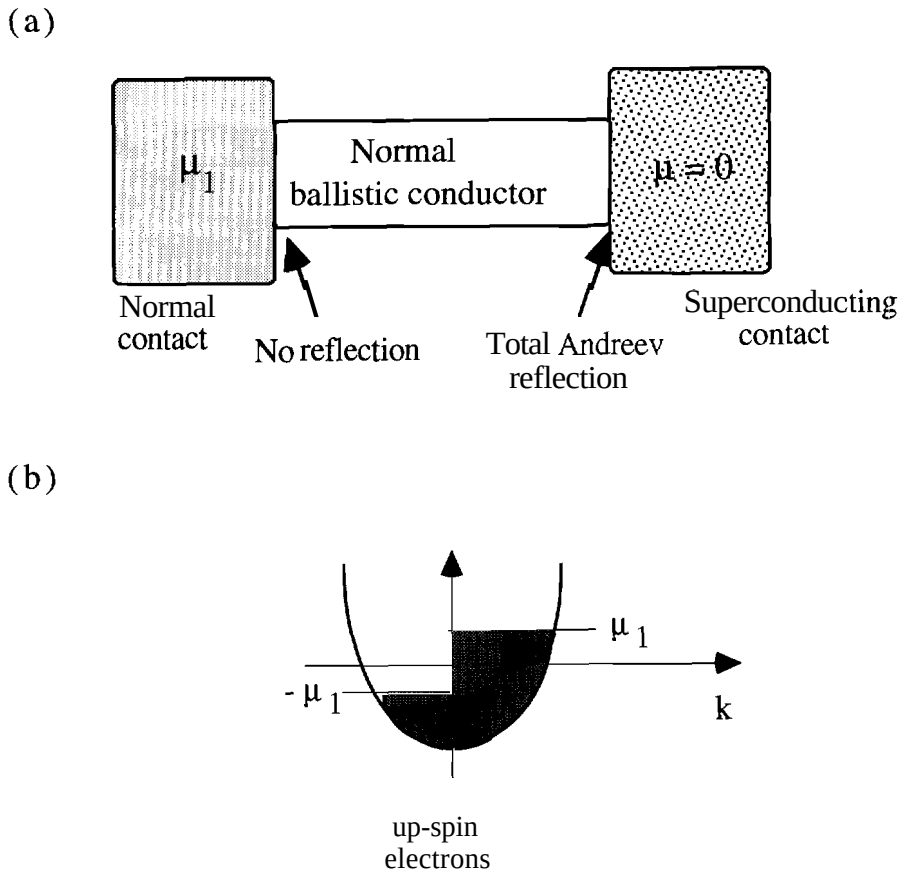


Fig.4.2. (a) A normal ballistic conductor connected between two contacts such **that** there is complete Andreev reflection at the right contact. (b) The electrochemical potential of +k states in the conductor follows that of electrons in the left contact, while that of -k states follows that of holes in the **left** contact. (c) Electrochemical potential profile across the structure.

leading to a potential profile across the structure as shown in Fig.4.1c. There are step changes in the potential at the two interfaces, thus justifying the interpretation of R_C as a contact or interface resistance.

N-N-S structure

Consider now what happens if there is complete Andreev reflection at the right contact as we would expect if it were superconducting (Fig.4.2a). We now expect the potential for +k states to be μ_1 as before since these are populated by electrons from the left contact. But the -k states in the conductor are now populated by electrons that arise from the Andreev reflection of holes incident from the left contact. Consequently the electrochemical potential for these states equals that of holes in the left contact :

$$\mu(+k) = \mu_1 \qquad \text{and} \qquad \mu(-k) = -\mu_1$$

The current is now twice the previous case since it is carried by all the electrons with energies in the range $-\mu_1$ to $+\mu_1$ (instead of 0 to $+\mu_1$) :

$$I = \frac{4eM}{h}\mu_1 \qquad \rightarrow \qquad R_C = \frac{\mu_1}{eI} = \frac{h}{4e^2M} \qquad (4.2)$$

This is exactly what we get from Eq.(3.4) if we set R equal to zero and R_a equal to one. Thus the contact resistance should be

$$h/4e^2M \qquad \text{instead of} \qquad h/2e^2M$$

if we make one contact superconducting.This is exactly what we get from Eq.(3.4) if we set R equal to zero and R_a equal to one corresponding to complete Andreev reflection.

The average electrochemical potential inside the conductor is given by

$$\mu = \frac{\mu(+k) + \mu(-k)}{2} = 0$$

leading to a potential profile across the structure as shown in Fig.4.2c. There is a step change in the potential at the left interface as before, but there is no drop at the right interface. One could say that the contact resistance is only half the previous case because the superconducting contact has no contact resistance.

N-I-N-S structure

For normal contacts, if the conductor is not ballistic, the overall resistance R can be written as

$$R = \frac{h}{2e^2MT} = \frac{h}{2e^2M} + \frac{h}{2e^2M}\left(\frac{1-T}{T}\right)$$

and interpreted as the contact resistance ($R_C = h/2e^2M$) in series with the actual resistance of the conductor. With a superconducting contact we might naively write down the resistance as

$$R = \frac{h}{4e^2M} + \frac{h}{2e^2M}\left(\frac{1-T}{T}\right) = \frac{h}{4e^2M}\left(\frac{2-T}{T}\right) \qquad (4.3)$$

assuming that the contact resistance has been halved while the conductor resistance remains the same. But with a superconducting contact we cannot simply treat the resistances as additive since the Andreev reflection gives rise to multiple reflection paths that interfere (Fig.4.3). We would obtain the result in Eq.(4.3) if we were to calculate the total Andreev reflection probability by summing the probabilities for all the multiple paths. But this is not appropriate unless there are strong phase-breaking processes inside the conductor. For a phase-coherent conductor, we should sum the probability amplitudes and not the probabilities. We then have interference among the multiple paths and the differential resistance shows oscillatory behavior, known as the McMillan-Rowell oscillations [4.1]. The zero-bias resistance has been shown to be [4.2]

$$R = \frac{h}{4e^2M}\left(\frac{2-T}{T}\right)^2 \qquad (4.4)$$

which can be much larger than the phase-incoherent result (Eq.(4.3)) if $T << 1$.

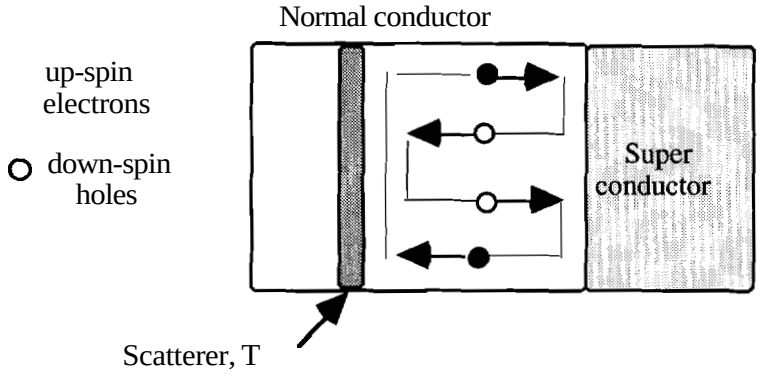


Fig.4.3. A normal conductor containing a scatterer is connected between two contacts such that there is complete Andreev reflection at the right contact. There is interference between the multiple reflection paths between the superconductor and the scatterer.

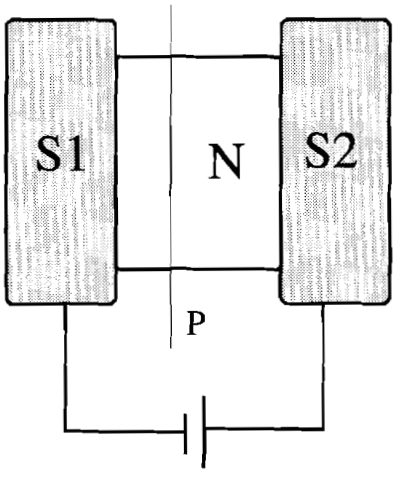


Fig.4.4. To calculate the current in an Sl-N-S2 structure, we evaluate it at a plane 'P' inside the normal region.

S-N-S structures

What would happen if both contacts were superconducting (Fig.4.4)? Naively one might expect that the contact resistance should disappear entirely and the resistance should simply be proportional to (I-T) / T. With a ballistic normal region (T = 1), this means that the low bias conductance should approach infinity. The actual picture is more complicated due to the multiple paths involving Andreev reflections at the two interfaces [4.3].

In applying scattering theory to this problem, we run into a complication. Since the leads are all superconducting, where do we evaluate the current ? As we discussed in section 2, the current in the superconducting regions cannot be evaluated correctly without taking the deformation of the pairing potential self-consistently into account. We can get around this problem by evaluating the current inside the normal material at a plane 'P' (Fig.4.4). Note that although we usually calculate the terminal currents, we could in principle use scattering theory to evaluate any quantity like the charge density or the current density at an interior point. From Eq.(2.16b) we could write

$$I = \sum_M I_M f_M \tag{4.5}$$

where I_M is the current carried by eigenstate 'M' at the plane 'P'

$$I_M = 2\langle u_M | I_{op} | u_M \rangle = -\frac{ie\hbar}{m}\left(u_M^* \frac{\partial u_M}{\partial z} - u_M \frac{\partial u_M^*}{\partial z} \right) \tag{4.6}$$

and f_M is the occupation factor for that state. Unlike the previous structures, the scattering states :now involve multiple energy components, since the two superconductors are at different potentials. But we can still assign a Fermi factor f_M as we discussed earlier (see Eq.(2.18)).

Numerical calculations based on this approach [4.4] on an Sl-N-S2 structure do show a significant increase in the low bias conductance (see Fig.4.5) as the pairing potential A_1 in S1 is increased systematically from zero to A_2 (the pairing potential in S2 is fixed at Δ_2). With $A_1 = 0$, we have an N-N-S structure with a low bias conductance equal to $4e^2/h$ as we have discussed. But with Δ_1 = A2, we have an SNS structure, and the low bias conductance appears to increase indefinitely due to multiple Andreev reflections.

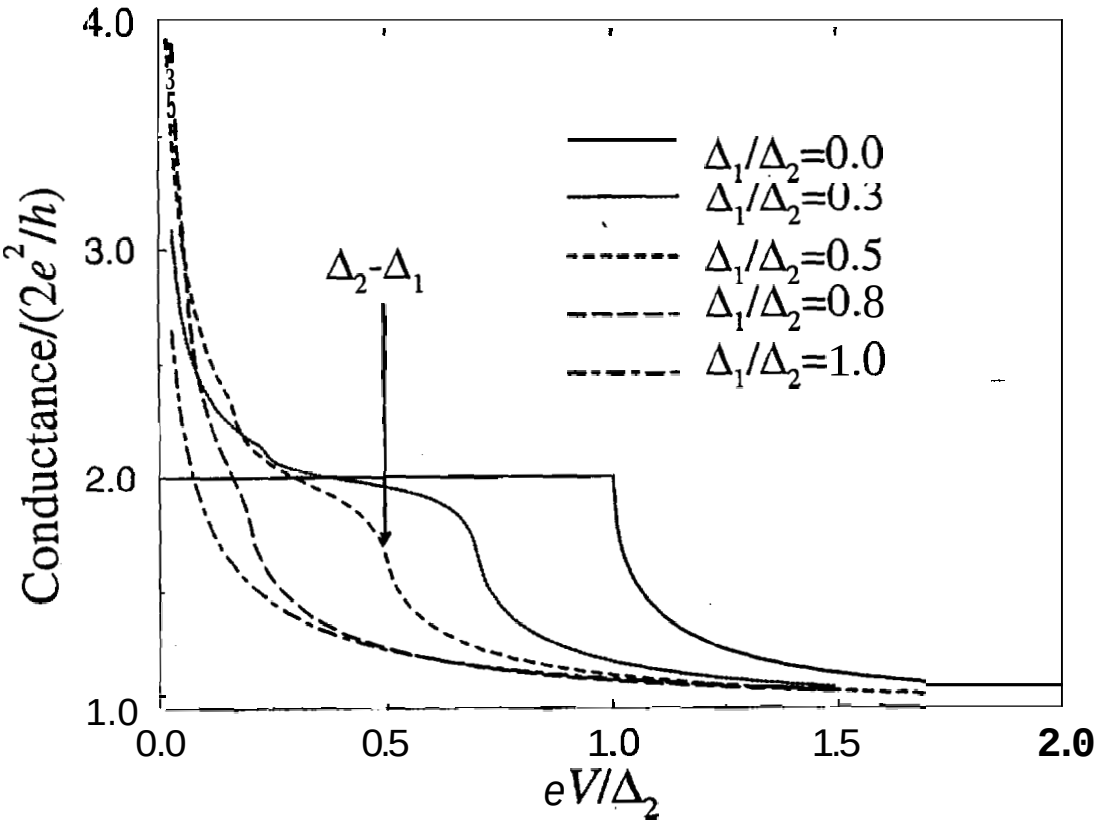


Fig.4.5. Differential conductance dI/dV calculated for an S1-N-S2 structure as the pairing potential Δ_1 in S1 is increased systematically from zero to Δ_2 (the pairing potential in S2 is fixed at Δ_2). Reproduced from Hurd, Datta and Bagwell [4.4].

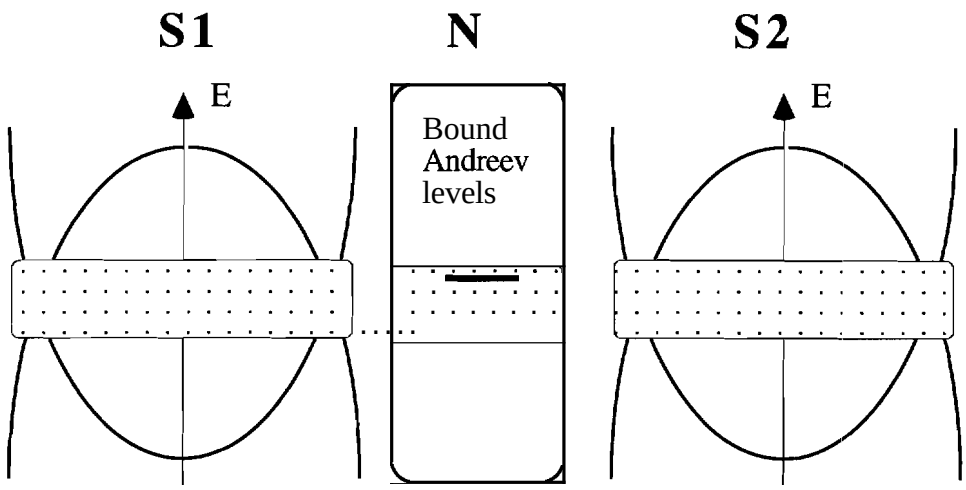


Fig.4.6. At zero-bias, multiple Andreev reflections lead to the formation of bound states in the normal regions.

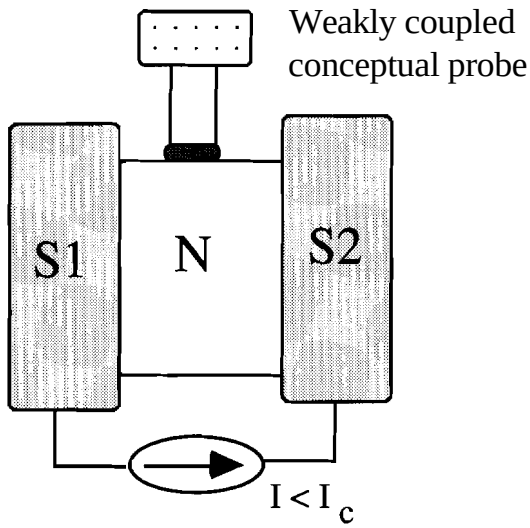


Fig.4.7. One or more conceptual probes can be weakly coupled to the normal regions to convert the bound states into scattering states [4.7].

Zero-bias current in S-N-S structures

At zero-bias the multiple Andreev reflections lead to the formation of bound states (see Fig.4.6) that can carry a net Josephson current, I_J. No voltage develops between S1 and S2, as long as the current is less than the critical current I_c. The magnitude of the current is related to the phase difference $\delta = \theta_1 - \theta_2$ between the pairing potentials at the two interfaces (we are assuming their magnitudes to be identical).

Calculating this Josephson current, is basically an ***equilibrium*** problem with all eigenstates occupied according to the equilibrium Fermi factor. We could modify Eq.(4.5) to write

$$I_J(\theta) = \sum_M I_M(\theta)\, f_0(E_M) \qquad (4.7)$$

In applying Eq.(4.7), it is important to note that in an S-N-S structure, in addition to the scattering eigenstates, we also have bound states with discrete energies lying inside the superconducting gap ($-\Delta < E < +\Delta$) as shown in Fig.4.6. We should include these discrete states in the summation in Eq.(4.7) [4.5, 4.6]. Alternatively, following Ref.[4.7], we could conceptually attach one or more weakly coupled probes to the structure that convert the bound levels into scattering states (see Fig.4.7). This eliminates the need to worry about bound states and their proper normalization.

It may be possible to use conceptual probes of the type shown in Fig.4.7 to introduce the effect of phase-breaking processes, following the work of Buttiker on normal systems [4.8]. Interestingly a lot of recent experimental work involves structures like that shown in Fig.4.7, with real probes (rather than conceptual ones) used to measure the resistance in the normal region [5.1, 5.2]. We will discuss such measurements in the next section.

5. Reciprocity

Suppose we perform a four-terminal resistance measurement as shown in Fig.5.1, using a pair of terminals 'i' and 'j' to drive the current and a pair 'k' and 'l' to measure the voltage. How do we calculate the resistance ? For simplicity we will just consider the linear response regime. We know that the linear response current in multiterminal normal mesoscopic systems is given by

$$I_i = \frac{e}{h} \sum_j \left[M_i \delta_{ij} - T_{ij} \right] \mu_j \qquad \text{(same as (3.2))}$$

In the presence of the superconductor, we simply split each physical lead 'i' into an electron lead with potential $+\mu_i$ and a hole lead with potential $-\mu_i$, to obtain

$$I_{ie} = \frac{e}{h} \sum_j \left[M_i \delta_{ij} - T_{ie,je} \right] \mu_j + \left[-T_{ie,jh} \right] \left(-\mu_j \right)$$

We could write down I_{ih} as well, but it is equal to I_{ie} due to electron-hole symmetry as we discussed in section 3. The total current I_i is simply equal to two times I_{ie} :

$$I_i = \frac{2e}{h} \sum_j g_{ij} \mu_j \quad \text{where} \quad g_{ij} \equiv M_i \delta_{ij} - T_{ie;je} + T_{ie;jh} \qquad (5.1)$$

This relation was derived independently by Lambert [3.2] and by Takane and Ebisawa [3.3] and has since been applied to many different structures [5.1]. As we have discussed before, the current in the superconducting leads cannot be calculated by this approach. One way to calculate the current in the superconductor is to evaluate the current inside the normal material right at the interface with each of the superconducting leads and equate it to the current at the corresponding superconducting terminal (see Fig.4.4).

To calculate the four-terminal resistance from Eq.(5.1), we invert it to write ($eV = \mu$)

$$V_i = \frac{h}{2e^2} \sum_j r_{ij} I_j \qquad \text{where} \qquad [r] = [g]^{-1} \qquad (5.2)$$

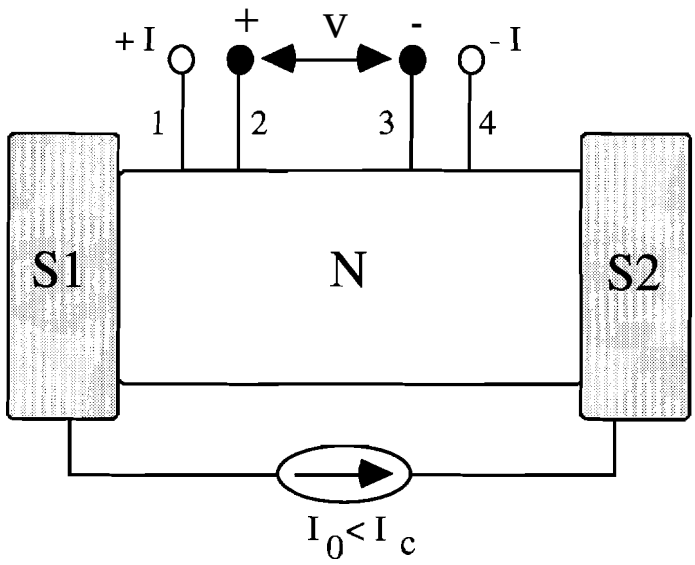


Fig.5.11. Andreev interferometer : The four-terminal resistance measured at the **normal** terminals 1-4 oscillates as the phase difference θ $(=\theta_1 - \theta_2)$ **between** the pairing potentials in **S1** and S2 is changed by changing the current $\mathbf{I_0}$. In practice, a series of Josephson junctions is used to get a large **change** in the phase with a smaller current **[5.2 -** 5.41.

If we connect a source directly across leads 'i' and 'j' then I_i must equal - Ij. .Assuming that all other leads are left floating we can write the resistance obtained by measuring the voltage drop across leads 'k' and 'l' as

$$R_{i,j;k,l} = \left[\frac{V_k - V_l}{I_i}\right]_{\substack{I_i=-I_j \\ \text{all other } I's=0}} = \frac{\pi}{2e^2}\left[r_{ki} - r_{kj} - r_{li} + r_{lj}\right] \qquad (5.3)$$

Reciprocity

Buttiker showed that for normal systems the four-terminal resistance obeys the reciprocity relation [1.81,

$$R_{i,j;k,l}(+B) = R_{k,l;i,j}(-B) \qquad (5.4a)$$

Here $R_{i,j;k,l}$ is the resistance measured using i,j as the current terminals and k,l as the voltage: terminals. Does this result hold in the presence of the superconductor ? Making use of the symmetry properties of the conductance matrix g_{ij} (see appendix C).,we can show that

$$R_{i,j;k,l}(+B,\Delta) = R_{k,l;i,j}(-B,\Delta^*) \qquad (5.4b)$$

In normal systems the effect of reversing the magnetic field is to transform H into H* in the Schrodinger equation $H\Psi = E\Psi$. Reversing the magnetic field ***and*** complex conjugating the pair potential has a similar effect on the BdG equation. From this point of view Eq.(5.4b) seems like a reasonable generalization of Eq.(5.4a) to include the effect of A for mesoscopic circuits containing superconducting elements. However, this has not been discussed theoretically or demonstrated experimentally to our knowledge.

If a structure has a single superconducting boundary with a constant pairing potential, then the measured resistance is insensitive to the phase of A. We would then expect the four-terminal resistance to obey Eq.(5.4a) (as well as Eq.(5.4b)). But a new class of wave interference effects have recently been observed that are sensitive to the variation of the phase of A along the boundaries, which can be tuned by changing the magnetic field or by changing the current through a series of Josephson junctions [5.2 - 5.71. These structures are suitable for checking the validity of Eq.(5.4b). Consider for example, the Andreev interferometer shown in Fig.5.1. Periodic oscillations of the measured conductance

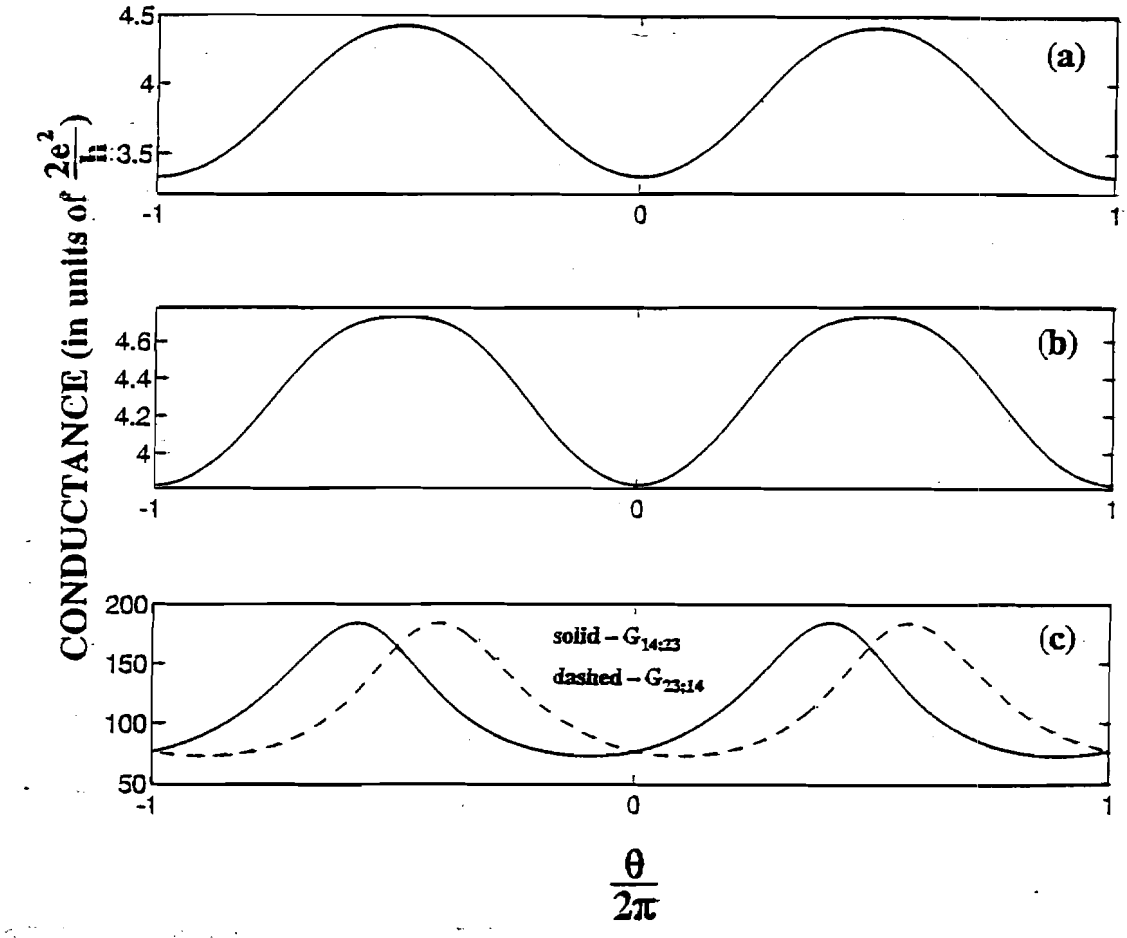


Fig.5.2. Plot of conductance as a function of $\theta(=\theta_1-\theta_2)$ **for** a ballistic **sample** of the type shown in Fig.5.1 having 10 transverse modes: (a) 1,4 used as current as well as voltage terminals, (b) 2,3 used as **current** as well as voltage terminals, (c) 1,4 used as current terminals and 2,3 used as voltage terminals and vice versa. Note that $\mathbf{G_{i,j;k,l}} = (1/\mathbf{R_{i,j;k,l}})$ normalized to $(2e^2/h)$.

have been reported as a function of $(\theta_1 - \theta_2)$, where θ_1 and θ_2 are the phases of the pairing potentials at the two superconducting boundaries.

Fig.5.2 shows the predicted modulation in the conductance for different combinations of current and voltage terminals. The two-terminal conductances (that is, the conductances measured using the same terminals to drive the current and to measure the voltage) are symmetric with respect to the phase difference θ (see Figs.5.2a,b). The four-terminal conductance (Fig.5.2c) is not symmetric but it obeys the reciprocity relation stated in Eq.(5.4b). Note that while the two-terminal conductance modulation is approximately $-e^2/h$, the four-terminal conductance can be much larger.

The conductance modulation shown in Fig.5.2 is much larger than that reported in [5.2] but comparable to that reported in [5.3]. However, it should be noted that the calculations shown in Fig.5.2 do not include scattering (coherent or incoherent), which is expected to be significant in the experimental structures investigated so far. The actual number of modes is also much larger than the number used in the calculations. As such the calculations correspond more closely to ballistic interferometers that couldl be fabricated using semiconductor samples with long mean free paths of the order of microns [5.8].

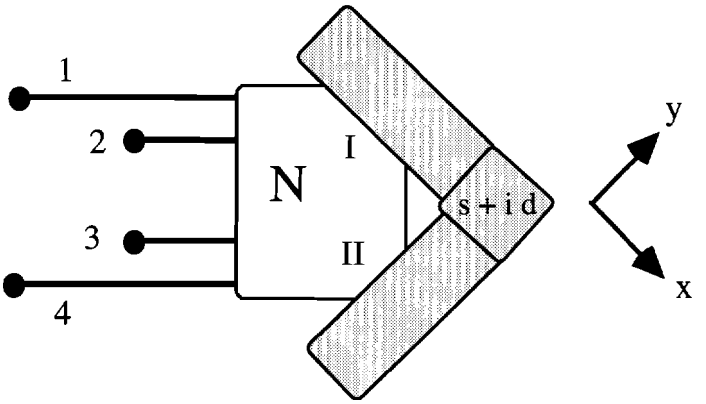


Fig.5.3. An Andreev interferometer constructed with a superconductor that breaks time-reversal symmetry. There is a phase difference between the two normal-superconductor interfaces I and II, even without any external current.

Exotic superconductors

It is interesting to note that the reciprocity relation could be used to test if the pairing potential breaks time-reversal symmetry. This effect could not be used to distinguish between s-wave and d-wave superconductors, neither of which break time-reversal symmetry. But it could be used to check for (s+id)-type symmetry [5.9]. Consider for example, the structure shown in Fig.5.3. The pairing potential in an (s+id) superconductor can be written as [5.10]

$$\Delta(\vec{k}) = \Delta_0 \left\{ \varepsilon + i(1-\varepsilon)\left[\cos(k_x a) - \cos(k_y a)\right] \right\}$$

where E is a constant less than one. Since the two interfaces I and II correspond to $k_x = 0$ and $k_y = 0$ respectively we can write

$$\Delta_I = \Delta_0 \left[\varepsilon - i(1-\varepsilon)\right] \qquad \text{and} \qquad \Delta_{II} = \Delta_0 \left[\varepsilon + i(1-\varepsilon)\right]$$

Hence there is a phase difference between the two interfaces given by $\theta = 2\tan^{-1}[(1-\varepsilon)\,I\,E]$. .

Note that this phase difference exists ***automatically*** without any external current and cannot be easily reversed. A four-terminal measurement of the type shown in Fig.5.3 without a magnetic field should thus yield non-reciprocal results for (s+id)-wave superconductors. But the results should be reciprocal for s-wave ($\Delta_I = \Delta_{II}$) or d-wave ($A_I = - A_{II}$) superconductors since in either case $A^* = A$. Thus we can expect that at zero magnetic field

$$R_{i,j;k,l} \neq R_{k,l;i,j} \qquad R_{i,j;k,l} = R_{k,l;i,j}$$

(s+id-wave) **(s-** or d-wave)

6. Noise

The scattering theory has also been applied to calculate the current fluctuations in normal mesoscopic systems [6.1, 1.91. The central result is summarized by the following expression for the correlation between the current fluctuations at terminal 'i' and terminal 'j' (B: measurement bandwidth):

$$\langle \delta I_i \delta I_j \rangle = 2B(e^2/h) \int dE \sum_{k,l} \{ f_k(1-f_l)\, I_i(k,l) I_j(l,k) \}_E \qquad (6.1)$$

where $I_i(k,l) \equiv \delta_{ik}\delta_{il} - s^*_{ik} s_{il}$ (6.2)

Here [s] represents the scattering matrix, each lead being assumed to be single-moded. For a detailed derivation of Eq.(6.1), we refer the reader to the original literature. Here we will simply outline the derivation in order to make the result plausible. In second quantized notation, we could write the operator for the current at terminal 'i' as

$$I \equiv \sum_k \sum_l I_i(k,l)\, a^+_k a_l \quad \text{where} \quad I_i(k,l) \equiv \langle k | I_{i,op} | l \rangle \qquad (6.3)$$

Here k,l are the scattering eigenstates, $I_i(k,l)$ represents the matrix elements of the one-particle current operator and a+, a are the creation and annihilation operators. Since the scattering states are linear combinations of plane waves running in both directions, the off-diagonal matrix elements with $k \neq l$ are in general non-zero. However, if we calculate the expectation value of the current, only the diagonal elements contribute because the density matrix is diagonal. Specifically,

$$\langle I_i \rangle \equiv \sum_k I_i(k,k)\, f_k \qquad (6.4)$$

since $\langle a^+_k a_l \rangle = f_k \delta_{kl}$ (6.5)

Eq.(6.4) is easily understood physically. A state 'k', if occupied, contributes a current equal to $I_i(k,k)$ and f_k is the probability that the state is occupied. We really do not need second quantized operators to derive this. But it is difficult to discuss quantities like current fluctuations in purely physical terms because they depend on the off-diagonal elements even

when the density matrix is diagonal. For example, the noise arising from the correlations between the currents at terminals 'i' and 'j' is defined as

$$\left\langle \delta I_i \, \delta I_j \right\rangle \equiv \left\langle I_i \, I_j \right\rangle - \left\langle I_i \right\rangle \left\langle I_j \right\rangle \tag{6.6}$$

From Eqs.(6.3) and (6.6)

$$\left\langle \delta I_i \, \delta I_j \right\rangle = \sum_k \sum_1 \sum_{k'} \sum_{1'} I_i(k,1)\, I_j(k',1') \left[\left(a_1 a_{k'}^{+} a_{1'} \right) - \left\langle a_k^{+} a_1 \right\rangle \left\langle a_{k'}^{+} a_{,,} \right\rangle \right]$$

$$= \sum_k \sum_1 \sum_{k'} \sum_{1'} I_i(k,1)\, I_j(k',1') \left\langle a_k^{+} a_{1'} \right\rangle \left\langle a_1 a_{k'}^{+} \right\rangle$$

$$= \sum_k \sum_1 I_i(k,1)\, I_j(1,k)\, f_k \left[1 - f_1 \right]$$

making use of Eq.(6.6). This is basically the result we stated earlier (Eq.(6.1)) apart from the multiplicative constants. The point to note is that the off-diagonal elements of the current operators appear in this result and it is difficult to rationalize it from purely physical reasoning (see, however, Ref.6.1).

Superconductive Structures

It is shown in Ref.[6.2] that the correct expression for the current fluctuations in the presence of Andreev scattering can be obtained from Eq.(6.1) simply by replacing each terminal 'j' with 'j,a' where the index a takes on one of two values 'e' or 'h':

$$\left\langle \delta I_i \delta I_j \right\rangle = B(e^2/h) \int dE \sum_{k,1} \sum_{\alpha,\beta} \operatorname{sgn}(\alpha)\operatorname{sgn}(\beta) \sum_{\gamma,\delta} \left\{ f_{k\gamma}(1 - f_{1\delta})\, I_{i\beta}(k\gamma;1\delta) I_{j\alpha}(1\delta;k\gamma) \right\}_E \tag{6.7}$$

where $$I_{i\beta}(k\gamma;1\delta) \equiv \left[\delta_{ik}\delta_{\beta\gamma}\delta_{il}\delta_{\beta\delta} - s^{*}_{i\beta;k\gamma}\, s_{i\beta;1\delta} \right] \tag{6.8}$$

The 'sgn' function is defined as +1 for 'e' terminals and as -1 for 'h' terminals. It accounts for the fact that the electrical charge associated with the electron and hole terminals is +e and -e respectively.

Fluctuations in the pairing potential

It should be noted that in deriving Eq. (6.7) we are treating the pairing potential as a rigid unchanging quantity. It is relatively difficult to account for the fluctuations in the pairing potential. Indeed even for normal conductors, it is not yet clear how one can handle the analogous problem involving the effect of fluctuations in the Hartree-Fock potential on the noise. Ref.[6.2] describes an approximate approach that could be used to account for the fluctuations in the pairing potential. However, in this article we will neglect such effects and only discuss some physical consequences based on Eq.(6.7).

Equilibrium Current Fluctuations

It is a general principle of statistical mechanics [6.3] that the equilibrium current fluctuations should be related to the linear response conductance by the Johnson-Nyquist relation :

$$\left\langle \delta I_i \delta I_j \right\rangle_{eq} = 2 k_B T B \, (g_{ij} + g_{ji}) \qquad (6.10)$$

where g_{ij} are the elements of the conductance matrix [1.9] appearing in Eq.(5.1). We can show that this relation is indeed satisfied, starting from our general expression for noise (see Eq.(6.7)) and noting that at equilibrium the occupation factors for all states are identical.

Sign of Current Correlations

Ref.[1.9] showed that the low frequency correlation between the current at two different leads of a purely normal device is always negative. An interesting difference in the presence of Andreev scattering is that the current correlation between two different leads can be positive. To see this we write the total current as the sum of the electron and hole components, $I = I_{i,e} + I_{i,h}$, so that, from Eq. (6.6),

$$\langle \delta I_i \, \delta I_j \rangle \equiv \langle (I_{i,e} + I_{i,h})(I_{j,e} + I_{j,h}) \rangle - \langle (I_{i,e} + I_{i,h}) \rangle \langle (I_{j,e} + I_{j,h}) \rangle$$

$$= \langle \delta I_{i,e} \, \delta I_{j,e} \rangle + \langle \delta I_{i,h} \, \delta I_{j,h} \rangle + \langle \delta I_{i,e} \, \delta I_{j,h} \rangle + \langle \delta I_{i,h} \, \delta I_{j,e} \rangle \qquad (6.11)$$

In normal systems, the last two terms do not contribute to the current fluctuations because the electron and hole channels are independent. However, in the presence of Andreev scattering, the up-spin electron and down-spin hole channels mix, so that the last two terms of Eq. (6.7) also contribute to the current correlation. Interestingly, they always contribute with a positive sign while the first two terms contribute with a negative sign (the difference is because of the factor $\mathrm{sgn}(\alpha)\,\mathrm{sgn}(\beta)$ in Eq.(6.7)). If the mixing of electron and hole channels is strong enough, the last two terms could dominate, thereby changing the net sign of the correlation, which should be experimentally observable.

At equilibrium, it is quite easy to see the conditions under which the correlation becomes positive. The equilibrium correlation obeys the Johnson-Nyquist relation (see Eq.(6.10)) and will be positive if g_{ij} is positive. From Eq.(5.1) it is evident that this will happen (note that $i \neq j$) if $T_{ie;jh} > T_{ie;je}$, that is if the Andreev transmission exceeds the normal transmission between the two leads.

Shot noise at zero temperature

Consider for simplicity a single-moded two-terminal ***normal*** device at zero temperature. The electrochemical potentials are assumed to be μ_1 and zero at its terminals, labeled. 1 and 2. For normal systems we can start from Eq.(6.1) to obtain

$$\langle \delta I_1 \delta I_1 \rangle = 2B(e^2/h) \int_0^{\mu_1} dE \, \{ I_1(1,2) I_1(2,1) \}_E$$

$$= 2B(e^2/h) \int_0^{\mu_1} dE \, T_{11} \, T_{12}$$

Since $T_{11} + T_{12} = 1$, we find that the shot noise in a two-terminal device is proportional to T (1 - T) where T is the transmission from one terminal to the other (that is, T_{12}). Since the current is proportional to T, this means that the noise to current ratio is proportional to (I-T) and is strongly suppressed in the ballistic limit when T is close to one. There is experimental evidence that this is true.

Consider next what happens if the second terminal is superconducting (Fig.6.1). We now have a device with four terminals : (1,e), (1,h), (2,e) and (2,h). The algebra is more complicated but we can show from Eq.(6.7) that [6.2]

$$\langle \delta I_1 \delta I_1 \rangle = B\frac{4e^2}{h}\int_0^{\mu_1} dE \left\{ T_{1e;1e}(1-T_{1e;1e}) + T_{1h;1e}(1-T_{1h;1e}) + 2T_{1e;1e}T_{1h;1e} \right\}_E \quad (6.12)$$

Eq.(6.12) can be used to study the noise in N-S junctions for different bias values from the clean limit to the dirty limit by changing the transmission T through the scatterer (see Fig.6.1) from one to a value much less than one.

Let us now specialize to a clean N-S junction (T=0) and see how the noise changes as the bias is increased. In this limit, $T_{1e;1e} = T_{1h;1h} = 0$ so that Eq.(6.12) simplifies to

$$\langle \delta I_1 \delta I_1 \rangle = B\frac{4e^2}{h}\int_0^{\mu_N} dE\, T_{1h;1e}(1-T_{1h;1e}) \quad (6.13)$$

Fig.6.2a shows how the noise changes as the bias is increased. The overall behavior can be understood as follows. For electrons with energies E < A, every incident electron is reflected as a hole ($T_{1h;1e} = 1$) and there is no noise. For electrons with energies E > A, there are two competing processes, Andreev reflection and quasi-particle transmission, so that $T_{1h;1e} \neq 1$ or 0 and the current is noisy. For electrons with E >> A, every electron incident from the normal region is transmitted as an electron like quasi-particle and there is no reflection, ordinary or Andreev. Since $T_{1h;1e} = 0$, again there is no noise. The shot noise is thus zero if the bias is less than A, increases as the bias is increased above A and finally saturates for large bias. The current on the other hand continues to increase with bias since we are adding more and more channels (Fig.6.2b). This is easily :seen from the expression we derived earlier (see Eq.(3.8)); with $T_{1e;1e} = 0$ we have

$$I_1 = \frac{2e^2}{h}\int_0^{\mu_1} dE\,(1+T_{1h;1e}) \quad (6.14)$$

Thus for a ballistic NS junction the shot noise to current ratio should increase at first when the bias is increased above A, but should decrease as the bias is increased further (Fig.6.2c). This was first predicted by Khlus using the non equilibrium Green's function formalism [6.4].

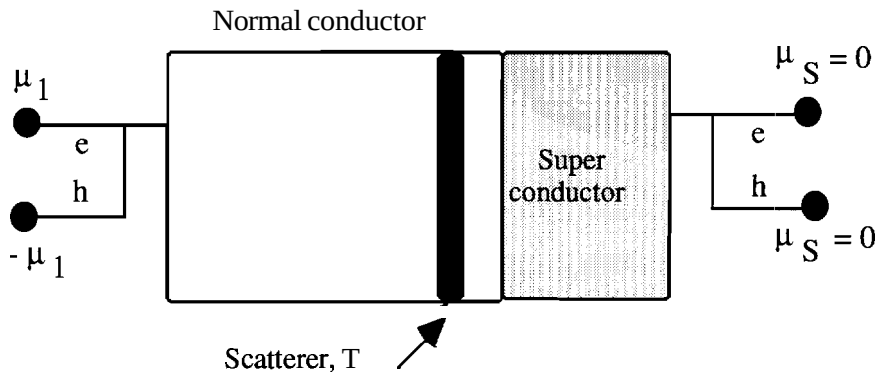


Fig.6.1. A single-moded N-S junction with a normal scatterer near the interface having a transmission T less than or equal to one. A clean junction can be modeled by setting T = 1, while in the dirty limit T << 1.

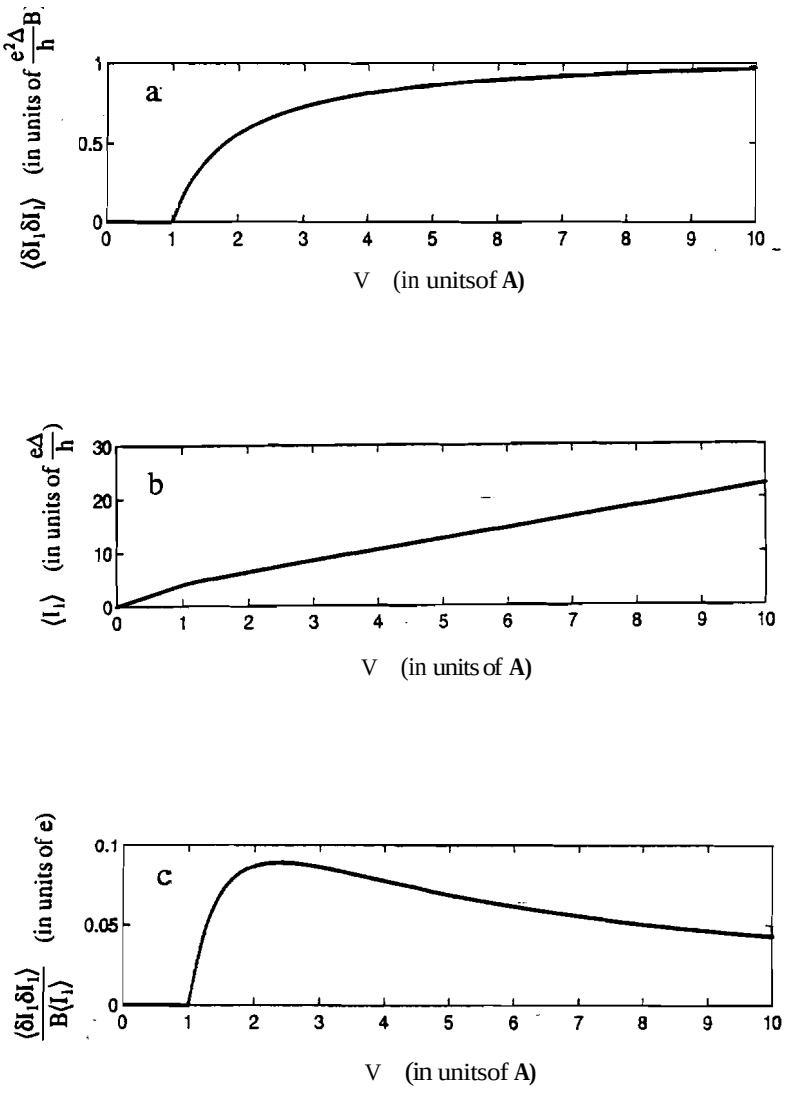


Fig.6.2. Shot noise and current flow at a clean N-S junction as a function of the: bias (V/e). (a) Shot noise, (b) current and (c) shot noise to current ratio.

7. Relation to the Green's function fornialisni

In this section we will show that for systems in equilibrium the results of scattering theory are identical to those derived from the ***equilibrium*** Green's function formalism [7.1, 7.21. As we mentioned in the introduction, scattering theory is really a simple extension of the equilibrium theory to non-equilibrium problems, based on the observation that as long as there are no inelastic processes, each scattering state remains in equilibrium with a particular reservoir. To account for inelastic processes one needs the non-equilibrium Green's function formalism, which we will not be discussing in this article [7.3].

The centerpiece of the scattering theory is the BdG equation (see Eq.(2.5)) :

$$\begin{bmatrix} H - E_f & \Delta \\ \Delta^* & -(H^* - E_f) \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = i\hbar \frac{\partial}{\partial t} \begin{Bmatrix} u \\ v \end{Bmatrix} \tag{7.1}$$

We will assume equilibrium conditions such that the electrochemical potential is constant everywhere, and E_f is chosen such that the pairing potential is time-independent. Corresponding to this wave equation one can define a Green's function as follows :

$$\begin{bmatrix} \omega - (H - E_f) & -\Delta \\ -\Delta^* & \omega + (H^* - E_f) \end{bmatrix} \begin{Bmatrix} G(x,x';\omega) \\ -F^+(x,x';\omega) \end{Bmatrix} = \begin{Bmatrix} \delta(x - x') \\ 0 \end{Bmatrix} \tag{7.2}$$

Here ω represents the energy variable defined over the entire complex plane. We will be using the thermodynamic Green's function defined along the ***imaginary*** axis. We have used - F^+ to denote the lower component so as to correspond to the standard notation in the literature (see for example, Eq.(34.30) of Ref.[7.1]).

The results of scattering theory are formulated in terms of the eigenfunctions of the BdG equation

$$\begin{bmatrix} H - E_f & \Delta \\ \Delta^* & -(H^* - E_f) \end{bmatrix} \begin{Bmatrix} u_M \\ v_M \end{Bmatrix} = E_M \begin{Bmatrix} u_M \\ v_M \end{Bmatrix} \tag{7.3}$$

while in the Green's function formalism they are formulated in terms the Green's functions G and F^+ . The equivalence of the two formulations can be proved by making use of the standard expression for the Green's function in terms of the eigenfunctions :

$$G(r,r';\omega) = \sum_M \frac{u_M(r)\, u_M^*(r')}{\omega - E_M} \tag{7.4a}$$

and

$$-F^+(r,r';\omega) = \sum_M \frac{u_M(r)\, v_M^*(r')}{\omega - E_M} \tag{7.4b}$$

together with the expansion for the Fermi function as a summation over its poles in the complex energy plane [7.2]

$$f_0(E_M) = \frac{1}{e^{E_M/k_BT}+1} = \frac{1}{2} + \sum_{n=-\infty}^{n=+\infty} \frac{k_BT}{i\omega_n - E_M} \tag{7.5}$$

where ω_n are the Matsubara frequencies defined as

$$\omega_n = (2n+1)\,\pi k_B T \tag{7.6}$$

We will now illustrate the equivalence of the two formulations by considering two equilibrium quantities that are often calculated, namely, the pairing potential and the Josephson current.

Pairing potential

In the scattering theory formalism, the equilibrium pairing potential is given by (see Eq.(2.20a))

$$\Delta(r) = -g(r) \sum_M u_M(r) v_M^*(r) f_0(E_M) \tag{7.7}$$

Substituting for the Fermi function from Eq.(7.6) we obtain

$$\Delta(r) = -g(r) \sum_M u_M(r) v_M^*(r) \left[\frac{1}{2} + \sum_{n=-\infty}^{n=+\infty} \frac{k_BT}{i\omega_n - E_M} \right]$$

The summation over 'M' corresponding to the the term (112) is zero because of the electron-hole symmetry relations (see Eq.(2.15)). Hence,

$$\Delta(r) = -g(r)\, k_B T \sum_{n=-\infty}^{n=+\infty} \sum_{M} \frac{u_M(r) v_M^*(r)}{i\omega_n - E_M}$$

Making use of Eq.(7.4b),

$$\Delta(r) = g(r)\, k_B T \sum_{n} F^+(r,r; i\omega_n) \tag{7.8}$$

which is the standard result in the Green's function formalism [7.1].

Josephson current

Another example is the equilibrium current density, which is often useful in evaluating the Josephson current. Using the standard form for the current operator we can write from Eq.(2.16b)

$$\vec{J}(r) = \frac{e\hbar}{2im} \sum_{M} f_0(E_M) \left[u_M^*(r) \vec{\nabla} u_M(r) - u_M(r) \vec{\nabla} u_M^*(r) \right] \tag{7.7}$$

which can be rewritten as

$$\vec{J}(r) = \frac{e\hbar}{2im} \sum_{M} f_0(E_M) \left[(\vec{\nabla} - \vec{\nabla}')\, u_M(r) u_M^*(r') \right]_{r'=r}$$

As before we substiute for the Fermi function from Eq.(7.6) to obtain

$$\vec{J}(r) = \frac{e\hbar k_B T}{2im} \sum_{n=-\infty}^{n=+\infty} \left[(\vec{\nabla} - \vec{\nabla}') \sum_{M} \frac{u_M(r) u_M^*(r')}{i\omega_n - E_M} \right]_{r'=r}$$

Making use of Eq.(7.5a), we obtain the standard expression in the Green's function formalism

$$\vec{J}(r) = \frac{e\hbar k_B T}{2im} \sum_{n=-\infty}^{n=+\infty} \left[(\vec{\nabla} - \vec{\nabla}')\, G(r,r'; i\omega_n) \right]_{r'=r} \tag{7.8}$$

Summary

(1) Scattering theory provides a rigorous framework for the discussion of transport phenomena, as long as dissipative effects are unimportant. Under these conditions each scattering state remains in equilibrium with a particular contact, and one can use a simple extension of equilibrium statistical mechanics to evaluate any quantity of interest.

(2) The BdG equation

$$\begin{bmatrix} (H - E_f) & \Delta(r,t) \\ A^*(r,t) & -(H^* - E_f) \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = i\hbar \frac{\partial}{\partial t} \begin{Bmatrix} u \\ v \end{Bmatrix} \qquad (2.5)$$

can be used to construct scattering states in much the same way that the Schrodinger equation is used in normal mesoscopic systems. H is the standard one-electron Hamiltonian describing the normal state (see Eq.(2.1). E_f is any convenient reference energy. A is the "pairing potential" which is non-zero only in the superconducting regions. Inside a large superconducting region that is close to equilibrium, the pairing potential can be written as

$$\Delta(r,t) = \Delta_0 \, e^{-i2\mu(r)t/\hbar}$$

where Δ_0 is the pairing potential in the bulk superconductor and the electrochemical potential $\mu(r)$ is measured with respect to the reference energy E_f. In general, one should calculate the pairing potential self-consistently from Eq.(2.21), but this is often ignored just as one often ignores the Poisson equation in normal mesoscopic calculations.

(3) Each scattering state of the non-equilibrium BdG equation is associated with a Fermi factor f_M given by

$$f_M = f_0(E_{M,e} - \mu_i) = f_0(E_{M,h} + \mu_i) = f_0(E_M) \qquad (2.18)$$

where μ_i is the electrochemical potential in the contact from which the scattering state is incident, $E_{M,e}$ is the energy associated with the electron component of the incident wave, $E_{M,h}$ is the energy associated with the hole component of the incident wave and E_M is the average of the two.

(4) If there is more than one superconducting segment with differing electrochemical potentials then the problem is analogous to a normal mesoscopic system with an applied alternating field of frequency $(\mu_1 - \mu_2)/A$ But for structures in which the superconducting segments are at the same potential, we can adapt the results for normal systems to superconducting systems simply by replacing each normal lead N with an electron lead Ne and a hole lead Nh, with

$$\mu_{Ne} = +\mu_N \qquad \text{and} \qquad \mu_{Nh} = -\mu_N$$

We have tried to illustrate this principle with different examples in sections 3 - 6.

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$$i\hbar\frac{\partial}{\partial t}\begin{Bmatrix} u \\ v \end{Bmatrix} = \begin{pmatrix} H + U + \mu_B B_z & \Delta \\ \Delta^* & -(H^* + U - \mu_B B_z) \end{pmatrix}\begin{Bmatrix} u \\ v \end{Bmatrix}$$

Since the [22] element is no longer just the negative complex conjugate of the [11] element, Eq.(2.17a) would not hold (this is easy to see in the special case when **A** is zero). Even if the [22] element is equal to the negative complex conjugate of the [11] element and Eq.(2.17a) holds, their occupation factors may not obey Eq.(2.17b), if we have a contact that injects spin-polarized electrons, like a ferromagnetic contact (see for example, H.L. Zhao and S. Hershfield, Phys. Rev. B52, 3632 (1995)). **A** general treatment of such problems with arbitrarily directed magnetic fields requires one to go beyond a simple (2x2) BdG equation (see for example Chapter 9 of Ref.2.2) and is outside the scope of this review. In this review we will assume spin-independent interactions.

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APPENDIX A : BdG equation from the BCS Hamiltonian

It is well-known that the BCS Hamiltonian ($s = \uparrow,\downarrow$)

$$H_{BCS} = \int dr \sum_s \Psi_s^+(r,t)\, H\, \Psi_s(r,t) - \int dr\, g(r)\, \Psi_\uparrow^+(r,t)\, \Psi_\downarrow^+(r,t)\, \Psi_\downarrow(r,t)\, \Psi_\uparrow(r,t) \qquad (A.1)$$

can be approximated as $H_{BCS} \approx H_I + H_{mf}$ where

$$H_I = \int dr \left[U_\uparrow(r,t) U_\downarrow(r,t) / g(r)\right] + \int dr \left[|\Delta(r,t)|^2 / g(r)\right] \qquad (A.2)$$

and

$$H_{mf} = \int dr \sum_s \Psi_s^+(r,t) \left[H + U_s\right] \Psi_s(r,t) + \int dr \left[\Delta(r,t)\, \Psi_\uparrow^+(r,t)\, \Psi_\downarrow^+(r,t) + \Delta^*(r,t)\, \Psi_\downarrow(r,t)\, \Psi_\uparrow(r,t)\right] \qquad (A.3)$$

where the self-consistent fields U_S and A are defined as

$$U\uparrow(r,t) \equiv -g(r) \left\langle \Psi_\downarrow^\dagger(r,t)\, \Psi_\downarrow(r,t) \right\rangle = U_\uparrow^*(r,t) \qquad (A.4a)$$

$$U_\downarrow(r,t) \equiv -g(r) \left\langle \Psi_\uparrow^+(r,t)\, \Psi_\uparrow(r,t) \right\rangle = U_\downarrow^*(r,t) \qquad (A.4b)$$

and

$$\Delta(r,t) \equiv -g(r) \left\langle \Psi_\downarrow(r,t)\, \Psi_\uparrow(r,t) \right\rangle \qquad (A.5)$$

We are neglecting expectation values of the form $\left\langle \Psi_\uparrow^+(r) \Psi_\downarrow(r) \right\rangle$, assuming that there are no magnetic impurities or paramagnetic effects.

H_{mf} is the mean-field Harniltonian and H_I is the negative of the interaction energy which has to be added because the self-consistent field method double-counts the interaction energy. It is a constant that plays no role in the dynamics and we will ignore it in the following discussion. Note that we are using the Heisenberg representation with time-dependent operators.

The difficulty with H_{mf} is the second term in Eq.(A.3) which involves the product of creation operators ($\psi^+\psi^+$) or annihilation operators ($\psi\,\psi$). "Normal" Hamiltonians involve creation and annihilation operators in pairs like $\psi^+\psi$ or $\psi\,\psi^+$. To make H_{mf} look like a "normal" Hamiltonian we use a "particle-hole" transformation for the down-spin operators, leaving the up-spin operators intact :

$$\Phi^+_{\uparrow}(r,t) \equiv \psi^+_{\uparrow}(r,t) \quad \text{and} \quad \Phi^+_{1}(r,t) \equiv \psi_{1}(r,t) \tag{A.6}$$

We will show that this transforms H_{mf} into $(H_{VAC} + H_{BdG})$ where H_{VAC} represents an inert "vacuum" consisting of a full down-spin band, while

$$H_{BdG} = \int dr\, \Phi^+_{\uparrow}(r,t)\left[H + U_{\uparrow}\right]\Phi_{\uparrow}(r,t) - \int dr\, \Phi^+_{\downarrow}(r,t)\left[H^* + U_{\downarrow}\right]\Phi_{\downarrow}(r,t)$$

$$+ \int dr\left[\Delta(r,t)\,\Phi^+_{\uparrow}(r,t)\Phi_{\downarrow}(r,t) + \Delta^*(r,t)\,\Phi^+_{\downarrow}(r,t)\Phi_{\uparrow}(r,t)\right] \tag{A.7}$$

which has the same form as the second quantized Hamiltonian ***for a set of non-interacting particles obeying the one-particle wave equation***

$$i\hbar\frac{\partial}{\partial t}\begin{Bmatrix} u \\ v \end{Bmatrix} = \begin{pmatrix} H + U_{\uparrow} & \Delta \\ \Delta^* & -(H^* + U_{\downarrow}) \end{pmatrix}\begin{Bmatrix} u \\ v \end{Bmatrix} \tag{A.8}$$

This is slightly different from the usual BdG equation (see Eq.(2.5)) since the fields $U_{\uparrow}$ and U_{1} need not be equal in general under non-equilibrium conditions. However, in our subsequent discussion we will assume spin-independent systems such that $U_{\uparrow} = U_{1} = U$ and assume that 'U' is included as part of H [2.6].

Since H_{BdG} looks like a "normal" Hamiltonian we can use all the standard techniques to diagonalize it, calculate expectation values etc. But let us first show that the particle-hole transformation (Eq.(A.6)) transforms H_{mf} (Eq.(A.3)) into $(H_{VAC} + H_{BdG})$.

From Eq.(A.3) to Eq.(A.7)

It is convenient to transform from the position representation to a discrete basis using any complete basis set $\phi_{\mu}(r)$ that spans the one-particle, one-spin Hilbert space.

$$\Psi_{\uparrow}(r,t) = \sum_{\mu} c_{\mu,\uparrow}(t)\,\phi_{\mu}(r) \quad \text{and} \quad \Psi_{\downarrow}(r,t) = \sum_{\mu} c_{\mu,\downarrow}(t)\,\phi^{*}_{\mu}(r) \tag{A.9}$$

The mean-field Hamiltonian then takes the form

$$H_{mf} = \sum_{\mu,\nu} \left[H + U_{\uparrow}\right]_{\mu\nu} c^{+}_{\mu,\uparrow}\, c_{\nu,\uparrow} + \sum_{\mu,\nu} \left[H^{*} + U_{\downarrow}\right]_{\mu\nu} c^{+}_{\nu,\downarrow}\, c_{\mu,\downarrow}$$

$$+ \sum_{\mu,\nu} \left[\Delta_{\mu\nu}\, c^{+}_{\mu,\uparrow} c^{+}_{\nu,\downarrow} + \left(\Delta^{*}\right)_{\nu\mu}\, c_{\nu,\downarrow} c_{\mu,\uparrow}\right] \tag{A.10}$$

where $$\left[H + U_s\right]_{\mu\nu} \equiv \int dr\, \phi^{*}_{\mu}(r) \left(\left[H + U_s\right]\phi_{\nu}(r) \right) \tag{A.11}$$

and $$[\Delta]_{\mu\nu} \equiv \int dr\, \phi^{*}_{\mu}(r)\,\Delta(r,t)\,\phi_{\nu}(r) \tag{A.12}$$

Note that (see Eq.(A.9)) we are expanding the up-spin field $\Psi_{\uparrow}$ operator using the set $\{\phi_{\mu}\}$ and the down-spin field operator $\Psi_{\downarrow}$ using the ***'time-reversed set'*** $\{\phi^{*}_{\mu}\}$. As a result we obtain the "normal" matrix elements $A_{\mu\nu}$ (see Eq.(A.12)). If instead we were to use the same set $\{\phi_{\mu}\}$ to expand both $\Psi_{\uparrow}$ and Ψ_{1} we would obtain "abnormal" quantities of the form $\int dr\, \phi^{*}_{\mu}(r)\Delta(r,t)\phi^{*}_{\nu}(r)$.

In terms of the discrete basis set the particle-hole transformation in Eq.(A.6) corresponds to

$$d^{+}_{\mu,\uparrow} \equiv c^{+}_{\mu,\uparrow}, \quad d^{+}_{\mu,\downarrow} \equiv c_{\mu,\downarrow} \tag{A.13}$$

Making use of the anti-commutation property $c^{+}_{\nu,\downarrow} c_{\mu,\downarrow} + c_{\mu,\downarrow} c^{+}_{\nu,\downarrow} = \delta_{\mu\nu}$, we can write H_{mf} as $(H_{BdG} + H_{VAC})$ where

$$H_{BdG} = \sum_{\mu,\nu} \left[H + U_{\uparrow}\right]_{\mu\nu} d^{+}_{\mu,\uparrow}\, d_{\nu,\uparrow} - \sum_{\mu,\nu} \left[H^{*} + U_{\downarrow}\right]_{\mu\nu} d^{+}_{\mu,\downarrow}\, d_{\nu,\downarrow}$$

$$+ \sum_{\mu,\nu} \left[\Delta_{\mu\nu}\, d^{+}_{\mu,\uparrow} d_{\nu,\downarrow} + \left(\Delta^{*}\right)_{\nu\mu}\, d^{+}_{\nu,\downarrow} d_{\mu,\uparrow}\right] \tag{A.14}$$

and $$H_{VAC} = \sum_{\mu} [H^* + U_{\downarrow}]_{\mu\mu} \qquad (A.15)$$

Noting that from Eqs.(A.6), (A.9) and (A.13) :

$$\Phi_s(r,t) = \sum_{\mu} d_{\mu,s}(t)\, \phi_{\mu}(r) \qquad (A.16)$$

we can transform Eq.(A.14) back to the position representation to obtain the expression for H_{BdG} stated earlier in Eq.(A.7).

Bogoliubov transformation

Since H_{BdG} looks just like the second quantized Hamiltonian for a set of non-interacting particles obeying the BdG equation, it can be diagonalized simply by defining a new operator γ_M^+ as follows :

$$\gamma_M^+ = \int dr \left[u_M(r,t)\Phi_{\uparrow}^+(r,t) + v_M(r,t)\Phi_{\downarrow}^+(r,t) \right]$$

$$= \int dr \left[u_M(r,t)\Psi_{\uparrow}^+(r,t) + v_M(r,t)\Psi_{\downarrow}(r,t) \right] \qquad (A.17)$$

Here u_M and v_M are the eigenfunctions that diagonalize the BdG equation:

$$E_M \begin{Bmatrix} u_M \\ v_M \end{Bmatrix} = \begin{pmatrix} H & \Delta \\ \Delta^* & -H^* \end{pmatrix} \begin{Bmatrix} u_M \\ v_M \end{Bmatrix}$$

Note that we are using the Heisenberg representation with time-dependent operators, and E_M could in general be time-dependent. However, for a region close to equillibrium $\Delta(r,t) = \Delta_0\, e^{-i2E_f t/\hbar}$ and E_M is time-independent.

In terms of this new quasi-particle operator the mean-field Hamiltonian H_{mf} takes the form

$$H_{mf} = H_{VAC} + \sum_{M} E_M\, \gamma_M^+ \gamma_M \qquad (A.18)$$

H_{VAC} is the energy of the "vacuum" consisting of a completely full band of down-spin electrons. On top of this vacuum we create particles in eigenstates of the BdG equation with energies E_M. A BdG quasi-particle represents a superposition of an up-spin electron and a down-spin hole, as evident from Eq.(A.17). Eq.(A.18) provides a formal justification for the one-particle interpretation of the BdG equation (Fig.2.5a).

Excitation picture

The ground state is obtained by filling up all the negative energy states. In the literature it is common to treat this ground state as the reference :

$$H_{mf} = H_{VAC} + \sum_{E_M<0} E_M - \sum_{E_M<0} E_M (1-\gamma_M^+\gamma_M) + \sum_{E_M>0} E_M \gamma_M^+\gamma_M$$

Making use of the anticommutation property of the creation and annihilation operators ($\gamma_M^+\gamma_M + \gamma_M\gamma_M^+=1$) we can write

$$H_{mf} = \underbrace{H_{VAC} + \sum_{E_M<0} E_M}_{H_G} - \sum_{E_M<0} E_M \gamma_M\gamma_M^+ + \sum_{E_M>0} E_M \gamma_M^+\gamma_M$$

The first two terms represent the energy H_G of the ground state while the last two terms give the energy of the two types of excitations that can be created by taking a particle out of the "valence" band ($E_M < 0$) or by adding a particle to the "conduction" ($E_M > 0$) band. Defining ('c' and 'v' denote conduction and valence band respectively)

$$\gamma_{M\uparrow}^+ = \gamma_{M,c}^+ \quad \text{and} \quad \gamma_{M\downarrow}^+ = \gamma_{M,v} \tag{A.19}$$

we have $$H_{mf} = H_G + \sum_{E_M>0} E_M \left[\gamma_{M\uparrow}^+\gamma_{M\uparrow} + \gamma_{M\downarrow}^+\gamma_{M\downarrow}\right] \tag{A.20}$$

Eq.(A.20) is the basis for the excitation picture shown in Fig.2.5b commonly used in the literature.

APPENDIX B : Expectation values

In this appendix we will derive Eq.(2.13) which gives the expectation value of an arbitrary one-particle operator and Eq.(2.20) which gives the pair potential. For converdence, we will not write the 't' dependence explicitly.

Inverse transformation

Eq.(A.17) defines a unitary transformation in a Hilbert space spanned by (r,s) that is double the usual size. We can rewrite Eq.(A.17) compactly as

$$\gamma_M^+ = \sum_s \int dr\, w_M(r,s)\, \Phi_s^+(r) \tag{B.1}$$

where $w_M(r,\uparrow) \equiv u_M(r)$ and $w_M(r,\downarrow) \equiv v_M(r)$ (B.2)

The functions $w_M(r,s)$, being eigenvectors of a Hermitian operator, obey the orthogonality and completeness relations :

$$\sum_s \int dr\, w^*_{M'}(r,s)\, w_M(r,s) = \delta_{M',M} \tag{B.3}$$

and $$\sum_M w^*_M(r',s')\, w_M(r,s) = \delta(r'-r)\, \delta_{s',s} \tag{B.4}$$

Using these properties it is straightforward to invert Eq.(B.1)

$$\Phi_s^+(r) = \sum_M w^*_M(r,s)\, \gamma_M^+ \tag{B.5}$$

that is, using Eqs.(A.6) and (B.2),

$$\psi^+_\uparrow(r) = \sum_M u^*_M(r)\, \gamma_M^+ \quad \text{and} \quad \psi_\downarrow(r) = \sum_M v^*_M(r)\, \gamma_M^+ \tag{B.6}$$

Expectation value of a one-particle operator

Consider any one particle operator A(r,r') corresponding to some quantity 'A'. The expectation value is given by

$$A = \left\langle \int dr \int dr' \left[\Psi^{+}_{\uparrow}(r) A(r,r') \Psi_{\uparrow}(r') + \Psi^{+}_{\downarrow}(r) A(r,r') \Psi_{\downarrow}(r') \right] \right\rangle$$

Using Eq.(B.6) we can write this as

$$A = \sum_{M,M'} \int dr \int dr' \; u^{*}_{M}(r) A(r,r') u_{M'}(r') \left\langle \gamma^{+}_{M} \gamma_{M'} \right\rangle$$

$$+ \sum_{M,M'} \int dr \int dr' \; v_{M}(r) A(r,r') v^{*}_{M'}(r') \left\langle \gamma_{M} \gamma^{+}_{M'} \right\rangle \qquad \text{(B.7)}$$

For a general non-equilibrium state, the quasi-particle states can be occupied arbitrarily, which will be reflected in arbitrary values of the quantity $\left\langle \gamma^{+}_{M} \gamma_{M'} \right\rangle$. If the density matrix is assumed to be diagonal as we have done, that is, if

$$\left\langle \gamma^{+}_{M} \gamma_{M'} \right\rangle = f_{M} \, \delta_{M,M'} \qquad \text{and} \qquad \left\langle \gamma_{M} \gamma^{+}_{M'} \right\rangle = (1 - f_{M}) \, \delta_{M,M'} \qquad \text{(B.8)}$$

where f_M denotes the occupation factor for the eigenstate 'M'. From Eqs.(B.7) and (B.8) we obtain

$$A = \sum_{M} f_{M} \int dr \int dr' \; u^{*}_{M}(r) A(r,r') u_{M}(r')$$

$$+ \sum_{M} (1 - f_{M}) \int dr \int dr' \; v_{M}(r) A(r,r') v^{*}_{M}(r')$$

which is the same as Eq.(2.13).

Pairing potential

In appendix A we defined the pairing potential in terms of second quantized operators (see Eq.(A.5)). Using Eq.(B.6) we can rewrite the pairing potential as

$$\Delta(r) = g(r) \sum_{N} \sum_{M} u_{M}(r) \, v^{*}_{N}(r) \left\langle \gamma^{+}_{N} \gamma_{M} \right\rangle$$

Assuming the density matrix to be diagonal (see Eq.(B.8)) we obtain Eq.(2.20).

C. Useful properties

In this appendix we will derive a few useful properties starting from the BdG equation .

Sum rule

$$\sum_j T_{ie;je}(E) + \sum_j T_{ie;jh}(E) = M_{ie}(E) \qquad \text{(C.1a)}$$

$$\sum_j T_{ih;je}(E) + \sum_j T_{ih;jh}(E) = M_{ih}(E) \qquad \text{(C.1b)}$$

$$\sum_j T_{je;ie}(E) + \sum_j T_{jh;ie}(E) = M_{ie}(E) \qquad \text{(C.1c)}$$

$$\sum_j T_{je;ih}(E) + \sum_j T_{jh;ih}(E) = M_{ih}(E) \qquad \text{(C.1d)}$$

Proof : Since the BdG Hamiltonian is Hermitian (see Eq.(2.5)), it conserves the number of "particles". Thus the S-matrix relating the particle currents is unitary and consequently the transmission coefficients (given by the squared magnitude of the corresponding S-matrix elements) must obey the sum rules stated above (see p.122, Ref.[1.2])

Symmetry of "conduction" and "valence" bands

The eigenstates of the BdG equation occur in pairs symmetrically about the zero of energy. Labeling the positive energy states as 'c' states and the negative energy states as 'v' states,

$$E_{mv} = -E_{mc}\,, \qquad u_{mv} = -v_{mc}^{*}\,, \qquad v_{mv} = u_{mc}^{*} \qquad \text{(C.2)}$$

Proof : Suppose we have a solution that satisfies the BdG equation

$$E_{mc}\begin{Bmatrix} u_{mc} \\ v_{mc} \end{Bmatrix} = \begin{pmatrix} H+U & \Delta \\ \Delta^{*} & -(H^{*}+U) \end{pmatrix}\begin{Bmatrix} u_{mc} \\ v_{mc} \end{Bmatrix} \qquad \text{(C.3)}$$

with $E_{mc} > 0$. A little straightforward algebra shows that

$$-E_{mc}\begin{Bmatrix} -v^{*}_{mc} \\ u^{*}_{mc} \end{Bmatrix} = \begin{pmatrix} H+U & \Delta \\ \Delta^{*} & -(H^{*}+U) \end{pmatrix}\begin{Bmatrix} -v^{*}_{mc} \\ u^{*}_{mc} \end{Bmatrix} \qquad \text{(C.4)}$$

But $$E_{mv}\begin{Bmatrix} u_{mv} \\ v_{mv} \end{Bmatrix} = \begin{pmatrix} H+U & A \\ A^{*} & -(H^{*}+U) \end{pmatrix}\begin{Bmatrix} u_{mv} \\ v_{mv} \end{Bmatrix} \qquad \text{(C.5)}$$

by definition. Comparing Eqs.(C.4) and (C.5) we obtain Eq.(C.2).

Electron-hole symmetry

$$\left[s^{ee}_{ij}(E)\right] = \left[s^{hh}_{ij}(-E)\right]^{*} \quad \text{and} \quad \left[s^{eh}_{ij}(E)\right] = \left[-s^{he}_{ij}(-E)\right]^{*} \qquad \text{(C.6)}$$

Proof : Suppose we have a solution at energy E consisting of a set of incorning waves of the form $\begin{pmatrix} a_i \exp[+ik_e x] \\ b_i \exp[-ik_h x] \end{pmatrix}$ and a set of outgoing waves of the form $\begin{pmatrix} a, \exp[-ik_e x] \\ b, \exp[+ik_h x] \end{pmatrix}$. The amplitudes of the incoming and outgoing waves are related by the S-matrix at energy E :

$$\begin{pmatrix} s^{ee} & s^{eh} \\ s^{he} & s^{hh} \end{pmatrix}_{E}\begin{Bmatrix} a_i \\ b_i \end{Bmatrix} = \begin{Bmatrix} a_o \\ b_o \end{Bmatrix} \qquad \text{(C.7a)}$$

But we have seen that if (u v) is a solution of the BdG equation at energy E then $(-v^{*}\ \ u^{*})$ is a solution at energy - E. Hence the solution at energy - E must be given by a set of incoming waves $\begin{matrix} -b_i \exp[+ik_h x] \\ {}_{*}a_i \exp[-ik_e x] \end{matrix}$ and a set of outgoing waves $\begin{pmatrix} -b^{*}_o \exp[+ik_h x] \\ a^{*}_o \exp[-ik_e x] \end{pmatrix}$. These must be related by the S-matrix at energy - E :

$$\begin{pmatrix} s^{ee} & s^{eh} \\ s^{he} & s^{hh} \end{pmatrix}_{-E}\begin{Bmatrix} -b^{*}_i \\ a^{*}_i \end{Bmatrix} = \begin{Bmatrix} -b^{*}_o \\ a^{*}_o \end{Bmatrix}$$

We can rewrite this in the form

$$\begin{pmatrix} s^{hh} & -s^{he} \\ -s^{eh} & s^{ee} \end{pmatrix}_{-E} \begin{Bmatrix} a_i^* \\ b_i^* \end{Bmatrix} = \begin{Bmatrix} a_o^* \\ b_o^* \end{Bmatrix} \tag{C.7b}$$

Comparing Eqs.(C.7a,b) we obtain the results stated earlier in Eq.(C.6).

Reciprocity of the S-matrix

$$\left[s_{ij}^{ee}(E)\right]_{-B,\Delta^*} = \left[s_{ji}^{ee}(E)\right]_{B,\Delta} \tag{C.8a}$$

$$\left[s_{ij}^{hh}(E)\right]_{-B,\Delta^*} = \left[s_{ji}^{hh}(E)\right]_{B,\Delta} \tag{C.8b}$$

$$\left[s_{ij}^{eh}(E)\right]_{-B,\Delta^*} = \left[s_{ji}^{he}(E)\right]_{B,\Delta} \tag{C.8c}$$

Proof: Suppose (u v) represents a solution to the BdG equation at an energy E such that

$$\begin{pmatrix} E - H_{op} & -\Delta \\ -\Delta^* & E + H_{op}^* \end{pmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \tag{C.9a}$$

while (u' v') represents a solution at the same energy E, but with the magnetic field B reversed (that is, H_{op} replaced by H_{op}^*) and the pair potential **A** replaced by $\mathbf{A}^*$.

$$\begin{pmatrix} E - H_{op}^* & -\Delta^* \\ -\Delta & E + H_{op} \end{pmatrix} \begin{Bmatrix} u' \\ v' \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}$$

We can rewrite this in the form

$$\begin{pmatrix} E - H_{op} & -\Delta \\ -\Delta^* & E + H_{op}^* \end{pmatrix} \begin{Bmatrix} u'^* \\ v'^* \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \tag{C.9b}$$

Comparing Eqs.(C.9a,b) we see that u'* = u and v'* = v. This means that if (u v) is a solution of the BdG equation with a magnetic field B and pair potential A then (u* v*) is a solution with a magnetic field -B and pair potential A^* (all at the same energy E, which we will not mention explicitly any more).

Now suppose we have a solution at (B, A) consisting of a set of incoming waves of the form $\begin{pmatrix} a_i \exp[+ik_e x] \\ b_i \exp[-ik_h x] \end{pmatrix}$ and a set of outgoing waves of the form $\begin{pmatrix} a, \exp[-ik_e x] \\ b_o \exp[+ik_h x] \end{pmatrix}$. The amplitudes of the incoming and outgoing waves are related by the S-matrix at energy

$$\begin{pmatrix} s^{ee} & s^{eh} \\ s^{he} & s^{hh} \end{pmatrix}_{+B,\Delta} \begin{Bmatrix} a_i \\ b_i \end{Bmatrix} = \begin{Bmatrix} a_o \\ b_o \end{Bmatrix} \qquad \text{(C.1Oa)}$$

But we have just seen that the solution at (-B, A*) must be given by a set of incoming waves $\begin{pmatrix} a_o^* \exp[+ik_e x] \\ b_o^* \exp[-ik_h x] \end{pmatrix}$ and a set of outgoing waves $\begin{pmatrix} a_i \exp[-ik_e x] \\ b_i \exp[+ik_h x] \end{pmatrix}$ (note that the incoming and outgoing sets have been interchanged due to the complex conjugation). These must be related by the S-matrix at (-B, A*) :

$$\begin{pmatrix} s^{ee} & s^{eh} \\ s^{he} & s^{hh} \end{pmatrix}_{-B,\Delta^*} \begin{Bmatrix} a_o^* \\ b_o^* \end{Bmatrix} = \begin{Bmatrix} a_i^* \\ b_i^* \end{Bmatrix}$$

We can rewrite this in the form (noting that the S-matrix is unitary, so that its inverse is equal to its conjugate transpose)

$$\begin{pmatrix} [s^{ee}]^t & [s^{he}]^t \\ [s^{eh}]^t & [s^{hh}]^t \end{pmatrix}_{-B,\Delta^*} \begin{Bmatrix} a_i \\ b_i \end{Bmatrix} = \begin{Bmatrix} a_o \\ b_o \end{Bmatrix} \qquad \text{(C.10b)}$$

Comparing Eqs.(C.10a,b) we obtain the results stated earlier in Eqs.(C.9).

Symmetry of the linear response coefficients

$$T_{ie;je}(B,\Delta) = T_{ih;jh}(B,\Delta) \tag{C.11a}$$

$$T_{ie;jh}(B,\Delta) = T_{ih;je}(B,\Delta) \tag{C.11b}$$

$$T_{ie;je}(B,\Delta) = T_{je;ie}(-B,A^*) \tag{C.12a}$$

$$T_{ih;jh}(B,\Delta) = T_{jh;ih}(-B,\Delta^*) \tag{C.12b}$$

$$T_{ie;jh}(B,\Delta) = T_{jh;ie}(-B,A^*) \tag{C.12c}$$

$$M_{ie}(B,A) = M_{ie}(-B,A^*) = M_{ih}(B,A) = M_{ih}(-B,A^*) \tag{C.13}$$

$$g_{ij}(+B,\Delta) = g_{ij}(-B,\Delta^*) \tag{C.14}$$

Proof : The ***linear response*** transmission functions are related to the corresponding energy dependent transmission functions by the relation

$$T_{ij} = \int dE \left(-\frac{\partial f_0(E)}{\partial E} T_{ij}(E) \right)$$

$$= \int dE \left(\frac{f_0(E)\left[1-f_0(E)\right]}{k_B T} T_{ij}(E) \right) \tag{C.15}$$

Noting that the energy-dependent transmission coefficients are just the squured magnitudes of the corresponding S-matrix elements and that $f_0(E) = 1\text{-}f_0(\text{-}E)$, we can prove Eqs.(C.11a,b) from Eq.(C.6) and Eqs.(C.12a,b,c) from Eqs.(C.8a,b,c). Eq.(C.13) for the (thermally averaged) number of modes then follows on using the sum rule.

To prove Eq.(C.14) we start from the definition of the conductance matrix (see Eq.(5.1)), and make use of Eqs.(C.11) - (C.13):

$$
\begin{aligned}
g_{ij}(-B,\Delta^*) &= M_i(-B,\Delta^*)\delta_{ij} - T_{ie;je}(-B,\Delta^*) + T_{ih;je}(-B,\Delta^*) \\
&= M_i(+B,\Delta)\delta_{ij} - T_{je;ie}(+B,\Delta) + T_{je;ih}(+B,\Delta) \\
&= M_j(+B,\Delta)\delta_{ij} - T_{je;ie}(+B,\Delta) + T_{jh;ie}(+B,\Delta) \\
&= g_{ji}(+B,\Delta)
\end{aligned}
$$

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