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Supercurrent through oscillating quantum dot

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Introduction

It is often said that nanostructures have become the system of choice for studying transport over the past few years. What does this statement mean?

First, consider transport in large, macroscopic system. Quite simply, for the past years, emphasis in studies of transport has been on the Boltzmann transport equation and its application to devices of one sort or another. The assumptions that are usually made for studies are the following: *(i)* scattering processes are local and occur at a single point in space; *(ii)* the scattering is instantaneous (local) in time; *(iii)* the scattering is very weak and the fields are low, such that these two quantities form a separate perturbations on the equilibrium system: *(iv)* the time scale is such that only events that are slow compared to mean free time between collisions are of interest. In short, one is dealing with structures in which the potentials vary slowly on the temporal scale of the scattering processes.

In contrast to the above situation, it has become possible in the last decade or so to make structures in which characteristic dimensions are actually smaller than the free path of interest. This means that transport in a regime in which the Boltzmann equation is clearly invalid become accessible and that new physical processes become important in the transport. These devices have come to be called nanostructures, nanodevices, or mesoscopic devices, depending upon the author.

Granted that the technological momentum is pushing to ever smaller devices, and that the technology is there to prepare really small devices, it become obvious that we must now ask whether our physical understanding of devices and their operation can extrapolated down to very small

space and time scales with out upsetting the basic macroscopic transport physics.

In this atmosphere lays the phenomenon of Coulomb blockade. We deal with two tunnel junctions in which the capacitance of the island is small enough to inhibit the hopping of electrons through it until the charging energy is overcome usually by applying a bias. This results in a stepped current-bias diagram and gives the characteristic Coulomb blockade diamonds in the bias-gate diagram when we apply a gate voltage to the island.

In my work I study at first the transport of electrons in superconducting tunnel junctions with a one level dot. The first calculation is done for single electron transport assuming sequential tunnelling and no coherences. This calculation is carried on using the Orthodox model of single charge tunnelling. This model assumes that the transmission coefficient for the tunnelling Hamiltonian is small enough to use perturbation theory and in particular to calculate the tunnelling rate using the Fermi golden rule. Using a one level dot the calculation can be done analytically and in the plot of bias versus current the steps are visible and the width of the superconducting gap.

The second and main part of my thesis deals with the calculation of the Josephson current through the same system, at first at zero temperature and then at finite temperature. In the Josephson current the coherent tunnelling needs to be taken into account, this leads to a perturbation which is of the fourth order in the tunnelling Hamiltonian. Furthermore we need to take into account that virtually two electrons can be sitting at the same time on the island (this couldn't happen in the previous calculation because we were dealing with the sequential tunnelling limit). This results in an additional Coulomb repulsive term which can't be treated analytically. What we did was at first assume that only one electron at the time could stay on the island, this was done by putting this additional U term to infinity. In this case the calculations can be done almost analytically giving the limit that the superconducting gap is bigger than the thermal energy. Using the equation of motion technique I tried to get a result for the current assuming $U = 0$. Third I did the calculation numerically using Matlab.

The last part of my thesis tries to include oscillations (phonons) in the dot system. This is done using the independent phonons model. The calculation can't be done analytically so they will be done numerically using Matlab.

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Chapter 1

The theory of Coulomb Blockade

1.1 Coulomb Blockade

In so-called single electron transistor we have two electrodes called source(S) and drain(D) separated by an insulating gap.

In the middle of this gap we also have a third metallic electrode called island(Is) because it is surrounded by an insulating sea.

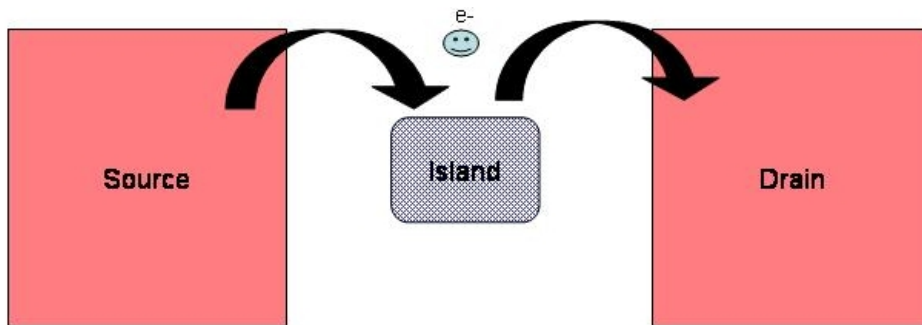


Figure 1.1: The quantum tunnelling of electrons between a source and a drain can be blocked if the electrostatic energy of an excess electron on the island is large compared to the thermal energy fluctuations

To go from the source to the drain one electron needs to travel through the island. We assume that the hopping from the source to the island and from the island to the drain happens by quantum tunnelling. Furthermore, we assume that the hopping is so fast that every electron travels alone from source to drain so that every tunnelling event is uncorrelated to the other.

Does the presence of the island change the amplitude of the electron current between source and drain?

When an electron is transferred from the reservoir into the island, there is a rearrangement of charge on the island resulting in a change in the electrostatic potential. In large systems this change in potential can hardly be seen but in small systems, particularly at low temperature, the potential change can be greater than the thermal energy $k_B T$.

It was found [1, 2] that if the electrostatic energy of the excess electron on the island was much greater than the electron thermal energy the hopping of the electron on the island could be inhibited. In this tunnel junctions systems the transfer of a single charge results in a gap in the energy spectrum at the Fermi energy. This leads to the phenomenon of Coulomb Blockade which arises from the interplay between the single charge of the hopping electron and the other charges in the system. The tunnelling of the electron is inhibited until the charging energy is overcome through an applied bias voltage.

This feedback effect characterizes what is called single charge tunnelling (SCT) phenomena. This phenomena can occur not only between normal metals or semiconductor junction systems where the carriers are electrons or holes but they can occur also in superconducting systems in which the charge carriers are the Cooper pairs.

What is then the recipe to have SCT phenomena?

1. Source island and drain are regions connected only via tunnel barriers.

We want more: we also want the electrons to travel one by one. This is the so called sequential tunnelling regime or weak tunnelling regime. Classically one electron needs an energy of at least $\frac{e^2}{2C}$, where C is the capacitance of the capacitor ($C = C_{S-Is} + C_{Is-D}$), to

overcome the charging barrier. Quantum mechanically the Heisenberg indetermination principle $\Delta E \Delta t \geq \frac{\hbar}{2}$ holds. Using this we can say that if the electron stays on the island at most a time $\tau_Q = \frac{\hbar/2}{e^2/2C}$ then it has an energy uncertainty of at least $\frac{e^2}{2C}$, enough to overcome the charging barrier.

The time to go from source to drain is of the order of $RC + RC$ i.e. the time to charge the capacitor S-Is and discharge the capacitor Is-D. So, if $2RC \ll \tau_Q$ then the electron can travel from source to drain with no feedback on the system because for a time τ_Q it has virtually enough energy. In this case as said we wouldn't have any feedback which means also no Coulomb Blockade. What we want to study is instead the Coulomb Blockade regime so we require that

$$2RC \gg \tau_Q \quad \Rightarrow \quad 2RC \gg \frac{\hbar/2}{e^2/2C} \quad \Rightarrow \quad R_T \gg \frac{\hbar}{2e^2} = R_Q$$

and we call R_T tunnelling resistance and R_Q quantum resistance.

2. $E_C = \frac{e^2}{2C} \gg k_B T$ which means that the energy needed to charge the island is much larger than the thermal fluctuations. Temperature must be low enough and the island small enough: if we consider the example of a conducting sphere above grounded conducting plane we get $C = 10^{-18} F$ for a radius of the sphere of the order of tens of nm assuming $\epsilon = \epsilon_0 = 1$. In real structures $\epsilon > \epsilon_0$ and the charging energy should be several times larger than the thermal energy to see clear single-electron charging effects, this means that at room temperature we need to deal with sub-10-nm structures. That is why most experiments are done at cryogenic temperature $\lesssim 4K$ like in the Park [3] experiment discussed later.

Conditions 1 and 2 assure that the charge transport from source to drain is ruled by the Coulomb charging energy. In general the charging energy of the island can be changed by mean of an external gate voltage, furthermore the island may be reduced to a quantum dot with a discrete energy spectrum.

1.2 The results of Coulomb Blockade

One particular result of the Coulomb blockade phenomenon is the so called Coulomb staircase in the $V_{bias} - I$ characteristic.

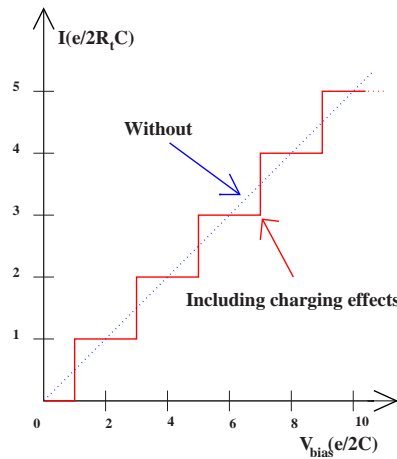


Figure 1.2: Ideal current-voltage characteristic for a double junction system with and without the consideration of the Coulomb charging effects. For this system $C_1 = C_2 = C$. The dotted line represents Ohm's law: $I = V/R_t$

The current rises in jumps giving a stair-case appearance. The subsequent jumps in the $V_{bias} - I$ characteristic correspond to the stable voltage regime in which one or more electron is added to or subtracted from the island. To each plateau correspond a fixed integer number of electrons on the island.

As mentioned before we can relate to each tunnel junction a certain capacitance C and a certain tunnelling resistance R_T so that we can actually introduce a circuit element representing the tunnel junction.

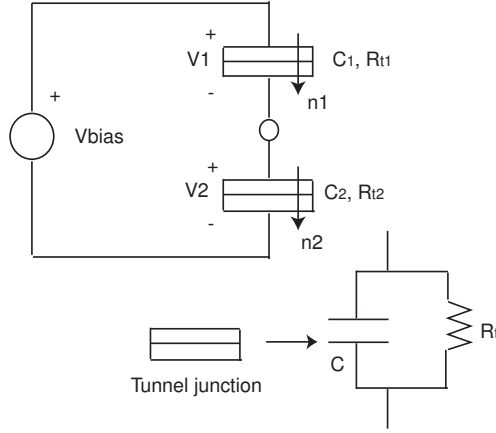


Figure 1.3: Equivalent circuit of an island weakly coupled to a voltage source through two tunnel junctions with capacitance C_1 and C_2 . R_t is the tunnel resistance, n_1 is the number of electrons that have tunnelled into the island through junction 1, and n_2 is the number of electrons that have tunnelled out of the island through junction 2

We assume sequential tunnelling and that electrons that tunnel through the junctions relax immediately so that resonant tunnelling is neglected.

Given the previous circuit, the capacitor charges are given by

$$Q_1 = C_1 V_1 \quad (1.1a)$$

$$Q_2 = C_2 V_2 \quad (1.1b)$$

the capacitance of the island is

$$C_{eq} = C_1 + C_2 \quad (1.2)$$

and the net charge on the island would be the difference $Q = Q_2 - Q_1$. In the absence of tunnelling $Q = 0$, the island would be neutral but tunnelling allows an integer number of electron to accumulate on the island so that

$$Q = Q_2 - Q_1 = -ne \quad \text{where} \quad n = n_2 - n_1 \quad (1.3)$$

n_1 being the number of electron coming on the island from junction 1 and n_2 being the number of electron leaving the island through junction 2.

The sum of the junction voltages is the applied bias voltage, V_{bias} , so that using the previous relations (1.1) and (1.3) we have

$$V_1 = \frac{1}{C_{eq}}(C_2 V_{bias} + ne) \quad (1.4a)$$

$$V_2 = \frac{1}{C_{eq}}(C_1 V_{bias} - ne) \quad (1.4b)$$

The electrostatic energy stored in the system is given by

$$E_s = \frac{Q_1^2}{2C_1} + \frac{Q_2^2}{2C_2}$$

which we can write as

$$E_s = \frac{1}{2C_{eq}}(C_1 C_2 V_{bias}^2 + Q^2)$$

Furthermore we need to consider the work done by the voltage source to transfer electrons through the island

$$W_s = V_{bias} \Delta Q$$

where ΔQ includes both the total charge transferred from the voltage source and the integer number of tunnelling charges.

When an electron tunnels out of the island we have $Q' = Q + e$ and $n' = n - 1$ which means that the voltage across junction 1 changes by an amount of $-e/C_{eq}$ so that the voltage source needs to compensate the loss by a charge $\Delta Q = -eC_1/C_{eq}$. The total work done to tunnel n_2 electron would then be

$$W_s(n_2) = -n_2 e V_{bias} \frac{C_1}{C_{eq}} \quad \text{and similarly} \quad W_s(n_1) = -n_1 e V_{bias} \frac{C_2}{C_{eq}}$$

Now we can find the total energy of the system:

$$E(n_1, n_2) = E_s - W_s = \frac{1}{2C_{eq}}(C_1 C_2 V_{bias}^2 + Q^2) + \frac{e V_{bias}}{C_{eq}}(C_1 n_2 + C_2 n_1) \quad (1.5)$$

At zero temperature a change in the system needs to lead to lower energies, therefore the tunnelling transitions which leads to higher energies are not allowed (at least at zero temperature, thermal fluctuations weakens this condition).

$$\Delta E_2^\pm = E(n_1, n_2) - E(n_1, n_2 \pm 1) = \dots = \frac{e}{C_{eq}} \left[-\frac{e}{2} \pm (en - V_{bias}C_1) \right] \quad (1.6)$$

$$\Delta E_1^\pm = E(n_1, n_2) - E(n_1, \pm 1n_2) = \dots = \frac{e}{C_{eq}} \left[-\frac{e}{2} \mp (en + V_{bias}C_2) \right] \quad (1.7)$$

These are the change in the energy of the system when a particle is tunnelling through the second or the first junction respectively.

As we said only transitions which have $\Delta E_i > 0$ can occur at zero temperature. Considering the island initially neutral $n = 0$ this condition transforms in

$$\Delta E_{1,2}^\pm = -\frac{e^2}{2C_{eq}} \mp \frac{eV_{bias}C_{2,1}}{C_{eq}} > 0 \quad (1.8)$$

For $C_1 = C_2 = C$ the requirement becomes $|V_{bias}| > e/C_{eq}$.

Below this value of V_{bias} tunnelling through the island is prohibited and no current can flow. The effect on the current voltage diagram is a region of very low conductance around zero voltage. For junctions with a large C_{eq} no Coulomb blockade regime is observed since the plateau would be almost insistent.

We can now consider what happens increasing the voltage over the threshold voltage $V_{th} = e/2C$. When we just pass V_{th} one electron jumps on the island so that $n = 1$. The Fermi energy of the dot is raised by e^2/C_{eq} (remember that $C_{eq} = 2C$) and a gap appears that prohibits a second electron to tunnel into the island until we supply energy enough. So that when $V_{bias} > 3e/2C$ a second electron can hop into the island. For $e/2C < V_{bias} < 3e/2C$ we have flow of current only when the $n = 1$ electron hops out so that we are back to the $n = 0$ situation and the process repeats itself giving a non zero current.

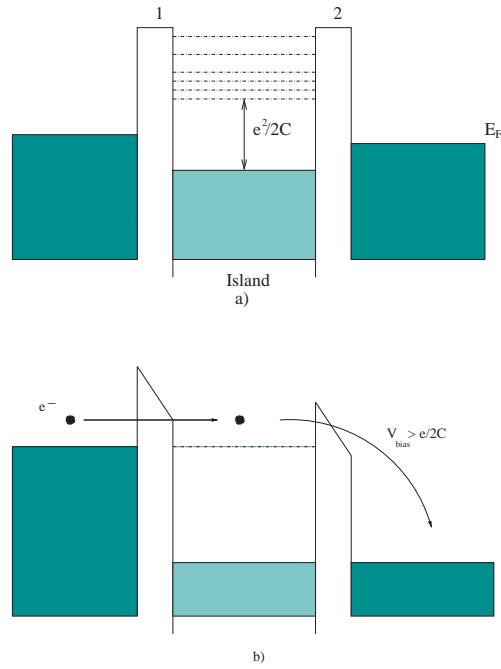


Figure 1.4: Band diagram of a double junction structure (a) in equilibrium and (b) under an applied bias. A gap exists in the density of state of the island system due to the Coulomb charging energy which prohibits tunnelling into and out of the island below the threshold voltage

To increase the complexity of the system we can now couple the island to a separate voltage source V_g .

This additional voltage modifies the charge on the island:

$$Q = Q_2 - Q_1 - Q_g = -ne + Q_P \quad \text{where} \quad Q_g = C_g(V_g - V_2)$$

where Q_P represents random charges trapped near the junctions which explain the asymmetry of the experimental $I - V_{bias}$ characteristic around the origin. Here we won't write this factor anymore for simplicity.

The equivalent capacitance of the island is now

$$C_{eq} = C_1 + C_2 + C_g$$

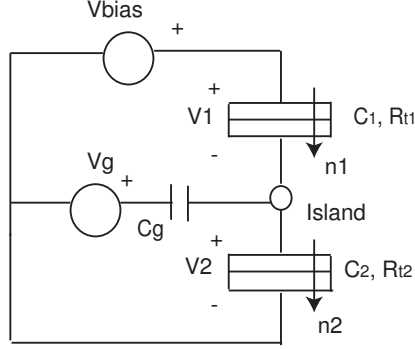


Figure 1.5: Equivalent circuit for a single electron transistor

Carrying on the same calculations as before we find:

$$\begin{aligned}
 \Delta E_1^\pm &= E(n_1, n_2) - E(n_1 \pm 1, n_2) = \dots = \\
 &= \frac{e}{C_{eq}} \left(-\frac{e}{2} \mp (en - V_g C_g + (C_g + C_2)V_{bias}) \right) \\
 \Delta E_2^\pm &= E(n_1, n_2) - E(n_1, n_2 \pm 1) = \dots = \\
 &= \frac{e}{C_{eq}} \left(-\frac{e}{2} \pm (en - V_g C_g - C_1 V_{bias}) \right)
 \end{aligned} \tag{1.9}$$

The gate voltage allows to change the charge on the island and therefore to shift the Coulomb blockade region with V_g .

As before the condition for tunnelling at low temperature is that $\Delta E_{1,2} > 0$ so that the system lowers its energy after the tunnelling.

As before we find four equations for forward or backward tunnelling:

$$-\frac{e}{2} \mp [en - V_g C_g + (C_g + C_2)V_{bias}] > 0 \tag{1.10a}$$

$$-\frac{e}{2} \pm [en - V_g C_g - C_1 V_{bias}] > 0 \tag{1.10b}$$

This equations for each value of n can be used to draw a stability plot in the $V_{bias}V_g$ plane. Corresponding to each value of n we find a diamond-like region in which no solution satisfy (1.10) which means that tunnelling

is not allowed and we can see the effect of the Coulomb blockade phenomenon.

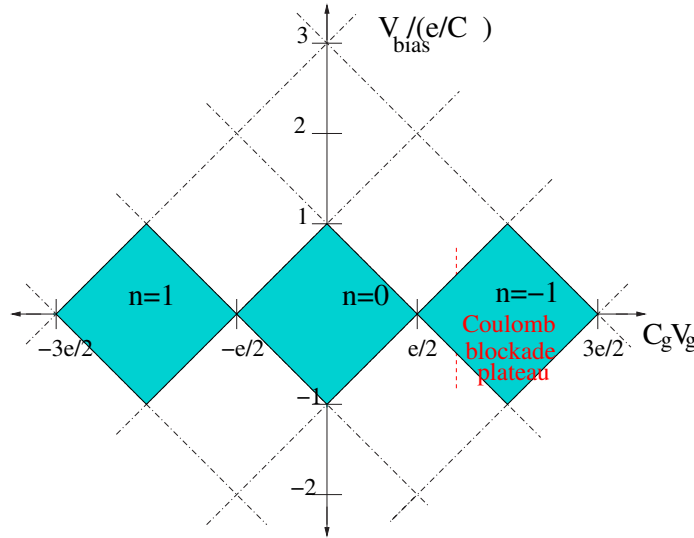


Figure 1.6: A stability diagram for a single electron transistor for the case $C_2 = C_g = C$, $C_1 = 2C$. The colored areas correspond to regions where no tunnelling through either junction may occur, and thus they represent stable regimes of fixed electron number.

Each of this region corresponds to a different stable number of electron on the island which cannot change (at least at low enough temperature where we can neglect thermal fluctuations).

For a given V_g the size of the Coulomb blockade plateau is given by the vertical extent of the non tunnelling region.

It is easy to see that for small source-drain voltage V_{bias} across the junctions a measurement of the current versus gate voltage draws peaks as I gets $\neq 0$. Between this peaks the number of electrons on the dot remains a stable integer value. As long as $eV_{bias} \ll k_B T$ the width of these peaks will be given by the thermal broadening so that we would see really large peaks or no peaks at all when the temperature is greater than the energy scale for the Coulomb blockade regime.

1.3 The Orthodox theory

To deal with this system we use the transfer or tunnelling Hamiltonian approach. In the tunnelling Hamiltonian approach, the tunnelling barrier is treated as a perturbation to the (much larger) system formed by the left and right leads.

The current may be investigated by calculating the rate of transfer of particle from left to right using perturbation theory. As such the perturbation should be sufficiently small, which in this case means that the tunnelling transmission coefficient should be small enough: $t \ll 1$.

The total Hamiltonian is written

$$H = H_L + H_R + H_D + H_T$$

where the Hamiltonians on the left and right and dot presumably are known with eigenvectors and eigenvalues

$$\begin{aligned} H_L \psi_l &= E_l \psi_l \\ H_R \psi_r &= E_r \psi_r \\ H_D \psi_d &= E_d \psi_d \end{aligned}$$

and where we define

$$H_0 = H_L + H_R + H_D = \sum_l E_l c_l^\dagger c_l + \sum_r E_r c_r^\dagger c_r + \sum_d E_d c_d^\dagger c_d \quad (1.11)$$

and

$$H_T = \sum_{l,d} (t_{l,d} c_d^\dagger c_l + \text{H.c.}) + \sum_{r,d} (t_{r,d}^\dagger c_r^\dagger c_r + \text{H.c.}) \quad (1.12)$$

E_d is the on-site energy which also can be controlled by an external gate voltage.

$c_{l,r,d}^\dagger$ and $c_{l,r,d}$ are the fermion creation and annihilation operators of the independent many-body state of the left (Source), right (Drain) and dot system.

In (1.11) the pairs operator represent the occupation or number operators:

$$\begin{aligned} n_l &= c_l^\dagger c_l \\ n_r &= c_r^\dagger c_r \\ n_d &= c_d^\dagger c_d \end{aligned}$$

For finite temperature the expectation value of these operators averaged over the equilibrium ground state gives either the Fermi-Dirac distribution

$$\langle N_{l,r,d} \rangle = n_F(E_{l,r,d}) = \frac{1}{1 + e^{(E_{l,r,d} - \mu)\beta}} \quad (1.13)$$

or the Bose-Einstein distribution

$$\langle N_{l,r,d} \rangle = n_B(E_{l,r,d}) = \frac{1}{e^{(E_{l,r,d} - \mu)\beta} - 1}$$

depending if we are dealing with fermions (f.e. electrons) or bosons (f.e. phonons). Here we define μ as the Fermi energy of the system and $\beta = 1/k_B T$ the thermal energy of the system.

To be more specific we should add to the dot Hamiltonian an interaction part which for example arises from the charging energy of the capacitor:

$$H_{Dint} = E_C \sum_d (n_d)^2$$

This is the so-called constant interaction model or capacitor model. The charging energy of a capacitor is $E = Q^2/2C$ where $Q = -eN = -e \sum_d n_d$.

$E_C = e^2/2C$ is the charging energy for a single electron.

The total dot Hamiltonian will then be

$$H_D = H_{D0} + H_{Dint}$$

where H_{D0} is the free particle Hamiltonian of the dot.

Equation (1.12) is the tunnelling Hamiltonian. Its first term annihilates a particle of wave vector \mathbf{k}_l on the left side and creates it in \mathbf{k}_d on the dot. This process corresponds to tunnelling from left lead to dot, the tunnelling from the dot to the right lead is given by the term in the second part of equation (1.12) which annihilates a particle of wave vector \mathbf{k}_d in the dot and creates it in the right lead with wave vector \mathbf{k}_r . The tunnelling from right to left is given by the other two terms which are the Hermitean conjugates of the previous ones.

At first we restrict the calculation to the leading order, i.e. we calculate the tunnelling rate within the golden rule approximation. We assume that the charge equilibrium is established before a tunnelling event occurs. This allows us to use the defined equilibrium states in the theoretical calculation. This means also that the time between two tunnelling processes should be larger than the charge relaxation time and that the electrodes remain in thermal equilibrium, so that the one-particle distribution functions are still in the form of (1.13). Given this we can treat the island as an isolated system described by the distribution function $P(\nu)$ that gives the probability to find the system in a particular state ν . In equilibrium this would be the Boltzmann distribution function but when we apply a bias across the system we must determine the non-equilibrium distribution function.

As mentioned we will calculate the tunnelling rate by means of the Fermi's golden rule (lets have $\hbar = 1$).

We consider $H_D = H_{D0}$ without taking into account the charging energy of the island. We will find that the current follows Ohm's law and we will define the tunnelling resistance.

$$\Gamma_{i \rightarrow f} = 2\pi | \langle f | H_T | i \rangle |^2 \delta(E_f - E_i)$$

gives the rate for transitions between the initial state $| i \rangle$ and the final state $| f \rangle$.

In our specific case we need to calculate the transition between two states, lets call them $| a \rangle$ and $| b \rangle$ due to tunnelling through the left junctions:

$$\Gamma_{a \rightarrow b}^L = 2\pi \sum_{f_b, i_a} | \langle f_b | H_{TL} | i_a \rangle |^2 \delta(E_{f_b} - E_{i_a})$$

where the sum runs over all configurations of the internal degree of freedom of the initial and final state. Once the transition rates are known we can write the kinetic equation (master equation) for the distribution function $P(a)$:

$$\frac{dP(a)}{dt} = - \sum_b \Gamma_{ab} P(a) + \sum_b \Gamma_{ba} P(b) \quad (1.14)$$

After the equality sign, the first part of the equation gives the rate at which the state a decays: it is the rate of going to a different state b times the probability that the a state is at the beginning occupied, summed over all the possible target states b , with a minus because the process lowers the occupation of the a state; the second part of the equation gives instead the opposite process and takes into account all the decays from other states to the a state.

We assume that on the island there are N electrons and we want to calculate the rate of increasing this number by one: $N + 1$. In this case $i_a = i_N$ and $f_b = f_{N+1}$ where we can write $|f_{N+1}\rangle = c_d^\dagger c_l |i_N\rangle$. We should sum over all the state d of the dot and over all the states l of the left lead to take into account all the possible configurations of the system after the tunnelling event.

$$\begin{aligned} \Gamma_{N \rightarrow N+1}^L &= 2\pi \sum_{d,l} \sum_{i_N} |\langle i_N | c_l^\dagger c_d H_{TL} | i_N \rangle|^2 \delta(\varepsilon_d - \varepsilon_l) \\ &= 2\pi \sum_{d,l} \sum_{i_N} |t_{d,l}|^2 |\langle i_N | c_l^\dagger c_d c_d^\dagger c_l | i_N \rangle|^2 \delta(\varepsilon_d - \varepsilon_l) \end{aligned} \quad (1.15)$$

In the absence of tunnelling Hamiltonian we may write the total state as a product of the dot state and the leads state: the two subsystems are independent and are connected to each other just through the tunnelling Hamiltonian. So we can write:

$$\Gamma_{N \rightarrow N+1}^L = \pi \sum_{d,l} \sum_{i_{N_d}, i_l} |t_{d,l}|^2 |\langle i_l | c_l^\dagger c_l | i_l \rangle \langle i_{N_d} | c_d c_d^\dagger | i_{N_d} \rangle|^2 \delta(\varepsilon_d - \varepsilon_l) \quad (1.16)$$

$\langle i_l | c_l^\dagger c_l | i_l \rangle$ gives the occupation of the states l for the initial state $| i_l \rangle$ and is therefore either zero or one (we can forget about the square). When we sum over all the initial configuration we have the definition of the Fermi-Dirac distribution function:

$$\sum_{i_{N_d}} \langle i_{N_d} | c_d^\dagger c_d | i_{N_d} \rangle = 1 - n_F(\varepsilon_d - \mu_d) \quad \sum_{i_l} \langle i_l | c_l^\dagger c_l | i_l \rangle = n_F(\varepsilon_l - \mu_l)$$

If we are dealing with a metallic island, we can assume that there is a continuous density of electronic states. In this case we can replace the sum over l and d by integrals. This results in:

$$\Gamma_{N \rightarrow N+1}^L = 2\pi \int_{-\infty}^{\infty} d\varepsilon_l d\varepsilon_d \rho(L) \rho(D) |t_{d,l}|^2 n_F(\varepsilon_l - \mu_l) (1 - n_F(\varepsilon_d - \mu_d)) \delta(\varepsilon_d - \varepsilon_l) \quad (1.17)$$

$\rho(L)$ is the density of states in energy of the left lead and $\rho(D)$ is the density of states if the dot.

Since the main contribution from the integral is for a narrow range of energies around the Fermi energies of the lead and the dot, the density of states appearing in the integral may be taken constant: $\rho(L, D) = \rho_0(L, D)$. For the same reason we neglect the variation of the tunnel matrix element with energy and momentum so that we can take it out of the integral.

$$\Gamma_{N \rightarrow N+1}^L = C_{in_L} \int_{-\infty}^{\infty} d\varepsilon_l d\varepsilon_d n_F(\varepsilon_l - \mu_l) (1 - n_F(\varepsilon_d - \mu_d)) \delta(\varepsilon_d - \varepsilon_l) \quad (1.18)$$

where with C_{in_L} we define the combined tunnelling density of states:

$$C_{in_L} = 2\pi \rho_0(L) \rho_0(D) |t_L|^2.$$

The delta function reduces one of the integrations such that

$$\Gamma_{N \rightarrow N+1}^L = C_{in_L} \int_{-\infty}^{\infty} d\varepsilon n_F(\varepsilon - \mu_l) (1 - n_F(\varepsilon - \mu_d)) \quad (1.19)$$

With this useful relations:

$$n_F(\varepsilon_1)[1 - n_F(\varepsilon_2)] = n_B(\varepsilon_1 - \varepsilon_2)[n_F(\varepsilon_2) - n_F(\varepsilon_1)]$$

$$\int_{-\infty}^{\infty} d\varepsilon [n_F(\varepsilon) - n_F(\varepsilon + \omega)] = \omega$$

we arrive at

$$\Gamma_{N \rightarrow N+1}^L = C_{inL} f(\mu_d - \mu_l) \quad (1.20)$$

$$f(\varepsilon) = \frac{\varepsilon}{e^{\beta\varepsilon} - 1}$$

In the same way we find the tunnelling rates out of the island:

$$\Gamma_{N \rightarrow N-1}^L = C_{outL} f(\mu_l - \mu_d) \quad (1.21)$$

$$f(\varepsilon) = \frac{\varepsilon}{e^{\beta\varepsilon} - 1}$$

The total rates are defined as the sum of the left and right contributions:

$$\Gamma_{N \rightarrow N \mp 1} = \Gamma_{N \rightarrow N \mp 1}^L + \Gamma_{N \rightarrow N \mp 1}^R$$

Using the master equation (1.14) gives the recursive relation

$$P(N)\Gamma_{N \rightarrow N-1} = P(N-1)\Gamma_{N \rightarrow N-1}$$

Once $P(N)$ is determined the current through the device can be found as the current through, say, the left junction:

$$I = (-e) \sum_N P(N) (\Gamma_{N \rightarrow N+1}^L - \Gamma_{N \rightarrow N-1}^L) \quad (1.22)$$

Where the first term gives the rate of tunnelling in the island and the second term gives the rate of tunnelling out of the island.

In our calculation Γ doesn't depend on N and by definition $\sum_N P(N) = 1$ so that we find, assuming $C_{inL} = C_{outL}$:

$$I = (-e)(\mu_d - \mu_l)C_L \quad (1.23)$$

if we now call $V = (-e)(\mu_d - \mu_l)$ we find that

$$\frac{1}{C_L} = R_{t_L} = \frac{1}{2\pi\rho_0(L)\rho_0(D) |t_L|^2}$$

Which defines the tunnelling resistance for the left junction R_{t_L} .

Writing in short we find

$$I = \frac{V}{R_{t_L}}$$

This is Ohm's law and we don't see the effect of the Coulomb blockade.

Now we want to consider the modification of the transition rate including the charging energy and the gate voltage:

$$H_{Dint} = E_C \sum_d (n_d)^2 - eV_g N$$

$$H_D = H_{D0} + H_{Dint}$$

We find for the transition rates:

$$\Gamma_{N \rightarrow N+1}^L = \frac{1}{R_{t_L}} f(\mu_d - \mu_l + E(N+1) - E(N)) \quad (1.24a)$$

$$\Gamma_{N \rightarrow N-1}^L = \frac{1}{R_{t_L}} f(\mu_l - \mu_d + E(N-1) - E(N)) \quad (1.24b)$$

and again the current is given by equation (1.22).

The explicit form for the rate transitions is:

$$\Gamma_{N \rightarrow N \pm 1}^L = \frac{1}{R_{t_L}} \frac{\Delta E^\pm}{1 - e^{-\beta \Delta E^\pm}} \quad (1.25)$$

The energetic arguments made in the previous section now may be stated more quantitatively. We see that in the limit that ΔE^\pm is positive and much larger than the thermal energy $k_B T$,

$$\Gamma_{N \rightarrow N \pm 1}^L = \frac{\Delta E^\pm}{R_{t_L}}, \quad \Delta E^\pm \gg k_B T$$

so that the tunnelling is "allowed". On the other and, when ΔE^\pm is large and negative, (1.25) shows that tunnelling is "forbidden":

$$\Gamma_{N \rightarrow N \pm 1}^L \simeq 0, \quad -\Delta E^\pm \gg k_B T. \quad (1.26)$$

Thus the energetic argument leading to the qualitative explanation for Coulomb blockade in the previous section are still valid in the limit that $|\Delta E^\pm| \gg k_B T$.

Considering the system of figure ... as an example, the change in energy associated with forward and backward tunnelling across the junction was given by equation ... as

$$\Delta E_2^\pm = \frac{e}{C_{eq}} \left[-\frac{e}{2} \pm (en - V_{bias} C_1) \right].$$

For zero applied bias and an initially charge-neutral island ($n = 0$), $\Delta E_2^\pm = -e^2/2C_{eq}$.

From (1.26), the tunnelling current is approximately zero as long as $e^2/2C_{eq} \gg k_B T$, which sets the temperature limits for observing coulomb blockade.

Having a look back at the distribution function $P(N)$, we see that Coulomb blockade for metallic island result in an oscillatory dependence as a function of the gate voltage. The optimum number of particles on the island follows form equation ...: $N_{opt} = eV_g/2E_C$. When this is an integer there is an energy gap for adding electrons, when N_{opt} is half integer two charge states are degenerate and current can flow.

1.4 Park's article

An experimental example of Coulomb blockade can be found in a paper from Park [3].

In this paper they perform transport measurement on single molecule (C_{60}) transistor. Basically they measure the current, motion of electrons, through the quantum dot C_{60} . Their results show not only the Coulomb blockade feature given by the diamonds shape in the $V_g - V_{bias}$ characteristic but also that there is some coupling between the center-of-mass motion of the molecule and the single electron hopping from the

lead to C_{60} . This coupling is visible as quantized oscillations of the C_{60} at $1.2THz$.

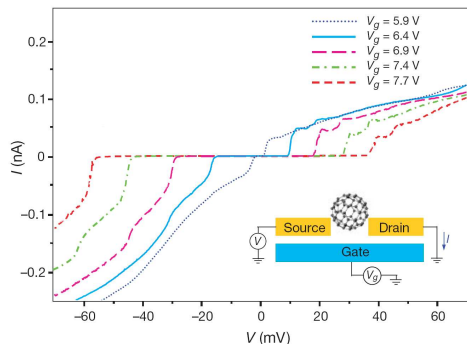


Figure 1.7: Current-voltage $I - V_{bias}$ curves obtained from a single- C_{60} transistor at $T = 1.5K$. Five curves taken at different gate voltage V_g are shown

The results show a stepped $V_{bias} - I$ diagram. Each step is due to the opening of a new electronic gate (a new reachable excited state) in the molecule which allows more electrons to pass through. Also it is clearly seen the conductance gap that changes with V_g . From the Coulomb blockade theory we can say that the conductance gap is a consequence of the finite energy needed to add or remove an electron from the molecule as we have previously explained. The conductance gap changes as a function of V_g and it increases increasing V_g . Finally in the diagrams $V_g - V_{bias}$ we see the gap conductance regions (the diamonds) and the differential conductance $\partial I/\partial V$ peaks in the z direction.

In principle the excitations could arise from different degree of freedom of the SMT (Single Molecule Transistor):

1. the excited electronic states of the system;
2. the internal vibrational modes of the free C_{60}
3. the vibrational excitations of the C_{60} coupled to an electron tunnelling on and off
4. the center of mass oscillation of the C_{60} bounded to the surface.

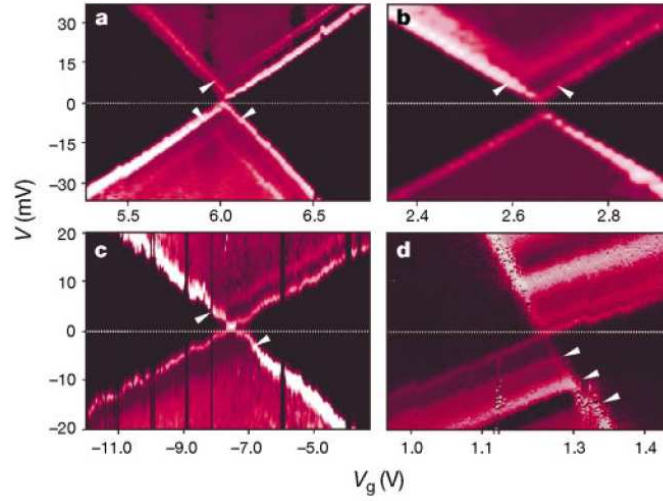


Figure 1.8: Two-dimensional differential conductance $\frac{\partial I}{\partial V}$ plots as a function of the bias voltage V and the gate voltage V_g . Data were obtained from four different devices. The dark triangular regions correspond to the conductance gap, and the bright lines represent the peaks in the differential conductance. The differential conductance values are represented by the color scale, which changes from black ($0nS$) through pink to white ($30nS$)

but

1. here the excitations are the same for both charges and multiple excitations have the same spacing while the excited electronic states have different spacing;
2. the internal vibrational modes of the free C_{60} have been studied and the lowest energy mode (deformation from a sphere to a prolate) has a vibrational quanta of $33meV$ while here the excitation quanta is $5meV$;
3. the coupling between vibrational excitations and electron tunnelling could explain the multiple peaks with same spacing in the differential conductance resulting from an excitation of an integer number of vibrational modes;

4. assuming that the binding potential between C_{60} and the surface is harmonic, calculations using the center of mass of the C_{60} give a vibrational frequency of $1.2THz$ and an energy quanta of $5meV$ which is in perfect agreement with the energy of the excitation quanta found experimentally.

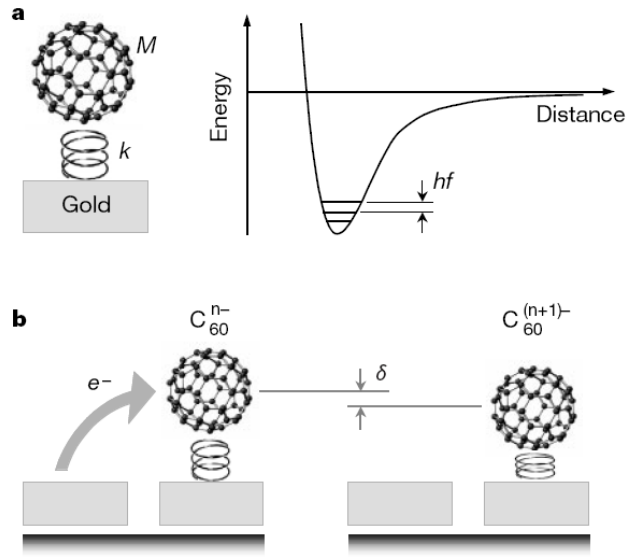


Figure 1.9: Diagram of the center-of-mass oscillation of C_{60} . **a)** A C_{60} molecule is bound to the gold surface by the van der Waals and electrostatic interaction. The interaction potential is shown schematically alongside. The potential near the equilibrium position can be approximated well by a harmonic potential with a force constant k . This harmonic potential gives quantized energy levels with frequency f . Here M represent the mass of the C_{60} and h is the Planck constant. **b)**, When an electron jumps on to C_{60}^{n-} the attractive interaction between the additional electron and its image charge on gold pulls the C_{60} ion closer to the gold surface by the distance δ . This electrostatic interaction results in the mechanical motion of C_{60}

Assuming the model of an harmonic binding potential as in (4), adding an electron to the molecule changes its distance from the surface (image charging) but doesn't significantly change the vibrational frequency ($1.2THz$). The different peaks observed in the differential conductance

are due to electrons that hop on or off the molecule with the system in different vibrational levels. This mechanism is similar to the Franck-Condon process where the vibrational excitation goes together with the electronic motion.

1.5 Franck-Condon on a simple transistor model

In the limits of the Orthodox model we study now a single electron transistor. In particular we want to study the island coupled to a single vibrational mode. In [3] we see an experimental result of this coupling. Here the single phonon mode was associated with the motion of the molecule C_{60} in the confining potential created by the van der Waals interaction with the electrodes.

We begin with the simplest model, i.e. the Franck-Condon model, which is constituted by an electronic system with only two levels for each lattice configuration and a one-dimensional vibrational mode for the lattice.

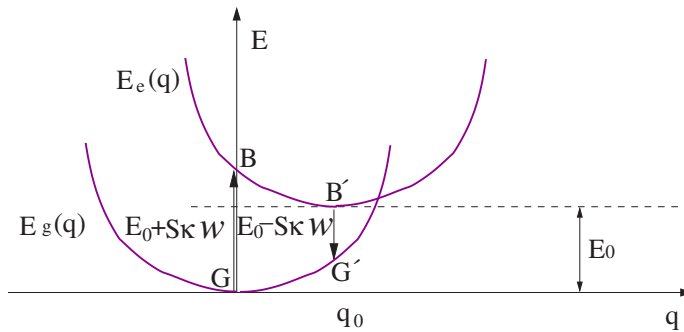


Figure 1.10: Configuration-coordinate diagram for allowed transitions between two non-degenerate electronic states (Franck-Condon model). The adiabatic potential surface for the ground state and the lowest excited state are indicated as a function of a single normal coordinate q .

Consider an electronic system with two (non-degenerate) levels for any given lattice configuration, the ground state ψ_g and the excited state ψ_e . Let us indicate with $E_g(q)$ and $E_e(q)$ the energies of the corresponding

potential, respectively; the normal coordinate q may represent the deviation of the dot distance from its equilibrium value. In the ground state, the equilibrium value of the coordinate q is assumed to be zero. With the choice of axes and origin as in figure, we have

$$\begin{cases} E_g(q) = \frac{1}{2}Cq^2 \\ E_e(q) = E_0 + \frac{1}{2}C(q - q_0)^2 \end{cases} \quad (1.27)$$

Notice that E_0 represents the energy difference between the minima of the ground and the excited potentials, and is called "zero-phonon transition energy"; the elastic constant C is related to the frequency ω of the particle motion, and the mass M by the usual equation $C = M\omega^2$. It is useful to characterize the model by means of the dimensionless parameter S defined as

$$S\hbar\omega \equiv \frac{1}{2}Cq_0^2 = \frac{1}{2}M\omega^2q_0^2 \quad (1.28)$$

or equivalently

$$q_0 = \sqrt{\frac{2\hbar S}{M\omega}} \quad (1.29)$$

We observe that energy difference between lower and upper levels at $q = q_0$ and is given by

$$E_e(0) - E_g(0) = E_0 + S\hbar\omega \quad (1.30)$$

$$E_e(q_0) - E_g(q_0) = E_0 - S\hbar\omega. \quad (1.31)$$

In accordance with an intuitive picture, known as Franck-Condon principle, the particle configuration of a system cannot change during the short time of an electron transition; in other terms, energy transitions are vertical in the configuration diagram, because the dot doesn't move of any significant amount during the electronic transitions.

We can examine more closely the phonon absorption and phonon emission processes. Consider the system initially at the minimum of the ground state (point G in figure). During the transition from G to B the dot position doesn't change, leading to an absorption energy $E_0 + S\hbar\omega$. After the absorption, in the excited curve, the dot is no more in the equilibrium position, and the system moves to the minimum B' at energy E_0 releasing

an energy equal to $S\hbar\omega$. We thus see that the dimensionless parameter S takes the meaning of the average number of phonons accompanying the transition; $S\hbar\omega$ is the energy transferred into vibrational energy (and then into heat). The emission from B' to C' takes place vertically leading to emission energy $E_0 - S\hbar\omega$; the system then relaxes from G' to G releasing the energy $S\hbar\omega$ (transformed into heat).

Quantum treatment of the optical properties of the Franck-Condon vibronic model.

We consider the Franck-Condon model from a quantum mechanical point of view, taking into consideration the motion of the dot; the energy due to this motion is quantized in phonon quanta, which are in general much smaller than the transition electronic energies. We introduce the standard phonon creation and annihilation operators, a^\dagger and a , corresponding to the harmonic oscillator of potential energy $(1/2)M\omega^2q^2$, centred at the origin $q = 0$ of the configurational coordinate q (the oscillator at the origin is also referred as undisplaced oscillator).

We have

$$a = \sqrt{\frac{M\omega}{2\hbar}}q + i\sqrt{\frac{1}{2M\hbar\omega}}p, \quad a^\dagger = \sqrt{\frac{M\omega}{2\hbar}}q - i\sqrt{\frac{1}{2M\hbar\omega}}p \quad (1.32)$$

The state of the undisplaced harmonic oscillator are

$$|\phi_n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|\phi_0\rangle \quad (1.33)$$

the eigenstates and eigenvalues of the vibronic system in the ground state are

$$|\psi_g, \phi_n\rangle \quad \text{and} \quad E_{gn} = E_g(0) + (n + \frac{1}{2})\hbar\omega \quad n = 0, 1, 2, \dots \quad (1.34)$$

For the excited states we can follow a similar treatment, except for a proper account of the displacement at $q = q_0$ of the minimum of the potential energy. We introduce the phonon creation and annihilation operators, \tilde{a}^\dagger and \tilde{a} , corresponding to the harmonic oscillator of potential energy $(1/2)M\omega^2(q - q_0)^2$, centred at the point q_0 of the configuration

coordinate q (displaced oscillator). For the displaced oscillator we have

$$\tilde{a} = \sqrt{\frac{M\omega}{2\hbar}}(q - q_0) + i\sqrt{\frac{1}{2M\hbar\omega}}p \equiv -\sqrt{S} \quad (1.35)$$

$$\tilde{a}^\dagger = \sqrt{\frac{M\omega}{2\hbar}}(q - q_0) - i\sqrt{\frac{1}{2M\hbar\omega}}p \equiv a^\dagger - \sqrt{S} \quad (1.36)$$

The states of the displaced harmonic oscillator are

$$|\tilde{\phi}_n\rangle = \sqrt{\frac{1}{\sqrt{n!}}}(\tilde{a}^\dagger)^n|\tilde{\phi}_0\rangle \quad (1.37)$$

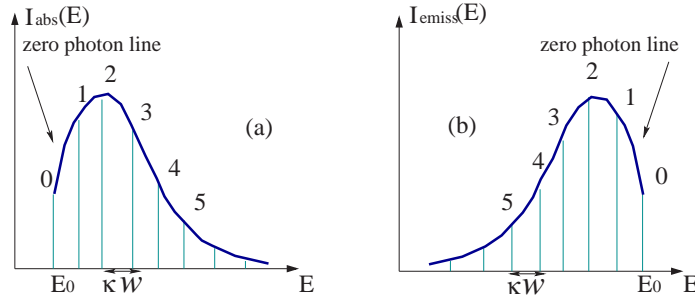


Figure 1.11: (a) Spectrum of absorption for the two-level single-mode model (the system is initially in the ground electronic state and ground vibrational state); the zero-photon line is indicated by an arrow. (b) Spectrum of emission for the two-level single-mode model (the system is initially in the excited electronic state and ground vibrational state); the zero-photon line is indicated by an arrow.

The eigenstates and eigenvalues of the vibronic system in the excited adiabatic surface are

$$|\psi_e, \tilde{\phi}_n\rangle \quad \text{and} \quad E_{en} = E_0 + (n + \frac{1}{2})\hbar\omega \quad n = 0, 1, 2, \dots \quad (1.38)$$

To connect the states of the displaced and undisplaced oscillators, we notice the general property of translation operators

$$f(q + q_0) = f(q) + q_0 f'(q) + \frac{1}{2!} q_0^2 f''(q) + \dots = e^{q_0 \partial / \partial q} f(q) \quad (1.39)$$

From (1.29) and (1.32) we have $\sqrt{S}(a - a^\dagger) = i\sqrt{2S/M\hbar\omega p} = q_0\partial/\partial q$, it follows

$$|\check{\phi}_n\rangle = e^{-q_0\partial/\partial q}|\phi_n\rangle = e^{\sqrt{S}(a^\dagger - a)}|\phi_n\rangle \quad (1.40)$$

We also notice the following matrix elements between displaced and undisplaced harmonic oscillator wavefunctions

$$\begin{aligned} \langle \check{\phi}_n | \phi_0 \rangle &= \langle \phi_n | e^{-\sqrt{S}(a^\dagger - a)} | \phi_0 \rangle = \langle \phi_n | e^{-\sqrt{S}a^\dagger} e^{\sqrt{S}a} | \phi_0 \rangle e^{-[-\sqrt{S}a^\dagger, \sqrt{S}a]/2} \\ &= \langle \phi_n | e^{-\sqrt{S}a^\dagger} | \phi_0 \rangle^{-S/2} = (-1)^n \sqrt{\frac{S^n}{n!}} e^{-S/2} \end{aligned} \quad (1.41)$$

The absorption lineshape at zero temperature (i.e. when the system is initially in the ground electronic state and ground electronic state and ground vibrational state) is obtained via the golden rule

$$I_{abs}(E) = \frac{2\pi}{\hbar} |\langle \psi_e, \check{\phi}_n | T | \psi_g, \phi_0 \rangle|^2 \delta(E_{en} - E_{g0} - E) \quad (1.42)$$

$$= \frac{2\pi}{\hbar} |T_{eg}|^2 |\langle \check{\phi}_n | \phi_0 \rangle|^2 \delta(E_0 + n\hbar\omega - E) \quad (1.43)$$

where T_{eg} is the matrix element between the ground electronic state and the excited electronic state. Using (1.41), the lineshape (1.42) takes the form

$$I_{abs}(E) = \frac{1}{n!} S^n e^{-S} \delta(E_0 + n\hbar\omega - E) \quad (1.44)$$

The absorption spectrum $I_{abs}(E)$ is a diagram of equally spaced lines (at energy E_0 , $E_0 + \hbar\omega$, $E_0 + 2\hbar\omega$...) with intensities varying according to the Poisson distribution, as schematically shown in figure. The factor $\exp(-S)$ gives the fractional intensity of the zero photon line. The maximum of the Poisson distribution occurs for $n \approx S$, and the absorption spectrum is then peaked at energy $E_0 + S\hbar\omega$.

A quite similar analysis can be carried out when the system is initially in the excited electronic state and ground vibrational state. The emission spectrum is given by

$$I_{emiss}(E) = \frac{1}{2!} S^2 e^{-S} \delta(E_0 - n\hbar\omega - E) \quad n = 0, 1, 2, \dots \quad (1.45)$$

The emission spectrum $I_{emiss}(E)$ is a diagram of equally spaced lines at energy E_0 , $E_0 - \hbar\omega$, $E_0 - 2\hbar\omega$, and it is peaked at the energy $E_0 - S\hbar\omega$.

Using this relations we can calculate now as in (??) the current through a single level quantum dot.

The tunnelling Hamiltonian is as usual

$$H_T = \sum_{l\sigma} (t_l d^\dagger c_l + \text{H.c.}) + \sum_{r\sigma} (t_r d^\dagger c_r + \text{H.c.}) \quad (1.46)$$

We look for the tunnelling rate Γ_{01} and Γ_{10} where the first one indicates the tunnelling from empty dot to full dot and the second the inverse process.

We denote

$$|0\rangle_D = |0\rangle_{Del} |0\rangle_{Dph}$$

the empty state of the dot factorized in electronic and phononic part

$$|1\rangle_D = |1\rangle_{Del} T(q_0) |n\rangle_{Dph}$$

the full state of the dot where we inserted the

displacement operator due to the Franck-Condon effect

We need to calculate

$$\langle f | H_{TL} | i \rangle = \dots = t_l \langle n | T(q_0) | 0 \rangle = t_l e^{-S/2} (-)^n \sqrt{\frac{S^n}{N!}}$$

From this, using the Fermi golden rule we have

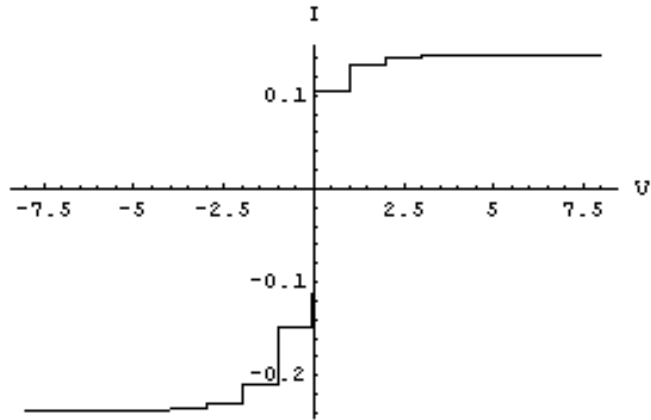
$$\Gamma_{10}^{L,R} = \frac{2\pi}{\hbar} \sum_{k\sigma} |t_k|^2 \sum_n \frac{S^n}{N!} e^{-S} n_F(\varepsilon_0 + n\omega_0\hbar) \quad (1.47)$$

$$\Gamma_{01}^{L,R} = \frac{2\pi}{\hbar} \sum_{k\sigma} |t_k|^2 \sum_n \frac{S^n}{N!} e^{-S} (1 - n_F(\varepsilon_0 - n\omega_0\hbar)) \quad (1.48)$$

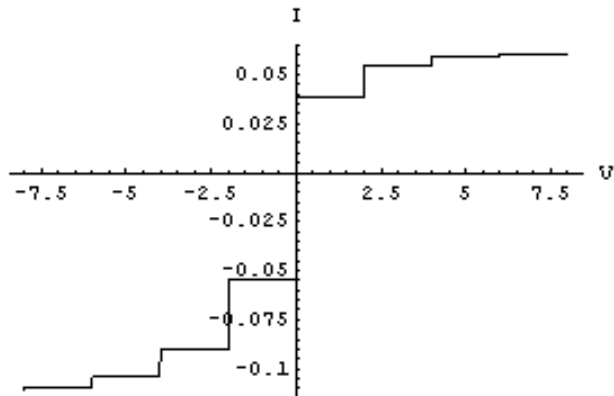
where the sum runs over all the possible n vibrational states, n_F denotes the Fermi distribution function and we assume that in the process energy is conserved.

Using these tunnelling rates we have the following $I - V$ curves.

In both of the plots we clearly see the Coulomb blockade steps. We don't



see the zero current plateau because for simplicity we set the energy of the dot to zero.



Chapter 2

Superconducting leads

From now on we study the same transistor system supposing that the leads are weak superconductors (for weak superconductor we can use the BCS theory). In superconductors the unit particles are no more the electrons but the Cooper pairs. In this chapter we treat the single electron (quasiparticle) current while in the next chapter we will study the Josephson current through the transistor.

2.1 A short review of the BCS theory

2.1.1 The screening interaction

The theory of superconductivity was formulated by Bardeen, Cooper and Schrieffer (BCS) in 1967. It describes the superconducting properties of weak superconductors, such as aluminium, which are weak because of the small strength of the electron-phonon interaction. In this case the theory, which is a mean field theory, works well.

The first hint of the BCS (Cooper 1956) theory is that the ground state of a normal metal is unstable at zero temperature. A normal metal is defined as one which is neither superconducting nor magnetic. The instability is an indication that the metal prefers to be in another state, in this case the superconducting one. The demonstration of the instability doesn't provide a description of the superconducting state but suggests

that the instability is caused by the scattering between pairs of electron where the scattering potential is the exchange of phonons.

If we take the bare Coulomb interaction $V(\mathbf{r}) = e^2/r$ and carry out the computation in the momentum space we find:

$$V(\mathbf{q}) = \frac{4\pi e^2}{q^2}$$

for a unit volume. We see that this interaction potential is always positive so it is repulsive but we need an attractive potential to form Cooper pairs.

We can look insight a little deeper in the theory and take into account also the dielectric function of the medium $\epsilon(\mathbf{q}, \omega)$. In particular we look at the screening effect of the conduction electrons, this introduces the screening length $1/k_s$. We have

$$V(\mathbf{q}) = \frac{4\pi e^2}{q^2 + k_s^2}$$

The electrostatic screening eliminates the divergence at $q = 0$ but still gives a positive potential. No superconductivity would result.

To have negative term we need to consider the motion of the ion cores. The physical idea is that the first electron polarizes the medium by attracting positive ions. This excess of positive charge acts as an attractive potential toward a second electron. The total effect is that two electrons interacts through an attractive potential. If this attractive potential is strong enough to overcome the repulsive Coulomb interaction, we have superconductivity. Since we are dealing with ion motion and deformation of the lattice we can fairly assume that the characteristic vibrational, or phonon, frequencies will play a role. For momentum conservation the phonon must carry a momentum $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ for scattering $\mathbf{k} \rightarrow \mathbf{k}'$ and the characteristic frequency will be $\omega_{\mathbf{q}}$.

It is plausible that the phonons contribution to the screening function would be $1/(\omega^2 - \omega_{\mathbf{q}}^2)^{-1}$. We see that for frequencies $\omega < \omega_{\mathbf{q}}$ we have a negative potential. This means that we have negative potential when the electron energy differences is smaller than $\hbar\omega_{\mathbf{q}}$.

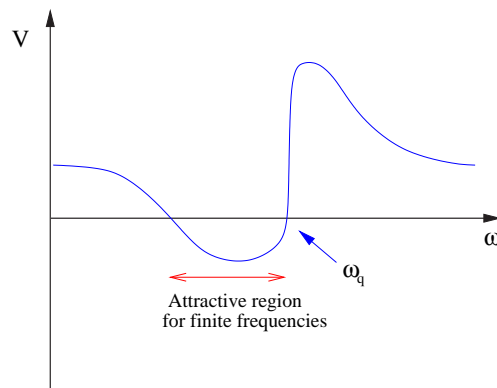


Figure 2.1: This interaction is frequency dependent and has attractive regions for finite frequency. The potential is negative for frequencies to the left of ω_q . Using this part of the interaction potential, it may be possible for two electrons to bind

So it may be possible for two electrons to bind if they can construct a bound state wave function which uses this part of the interaction potential. Not all simple metals are superconductors, so the existence of a small attractive potential is not sufficient.

In the description of the theory we use a model interaction of the form

$$V_s(q, \omega) = \begin{cases} -V_0 & \text{for } |\xi_q| \leq \omega_D \\ 0 & \text{for } |\xi_q| \geq \omega_D \end{cases} \quad (2.1)$$

which is the approximation used by Cooper in 1956.

The potential is constant and attractive ($V_0 > 0$) up to a cutoff energy which is of the order of the Debye energy ω_D of the solid.

2.1.2 The ground state wavefunction

The basic feature of the BCS theory is that pairing occurs between electrons in state with opposite momentum and opposite spins, e.g., between states (\mathbf{k}, \uparrow) and $(-\mathbf{k}, \downarrow)$. The two spins are combined into a spin singlet, with $S = 0$. The singlet was chosen in BCS theory on the basis

that the other choices of spin combination would lead to a triplet state with $S = 1$. The latter choice implies that the superconducting state has magnetic properties, which are in fact absent. Thus the choice $S = 0$ seems most reasonable. Later work by Balian and Werthamer (1963), who solved the BCS equations for $S = 1$, showed that the triplet state had smaller binding energy and was therefore less favored.

Having seen that the Fermi sea is unstable against the formation of bound Cooper pair when the net interaction is attractive, clearly we must then expect the pairs to condensate until an equilibrium point is reached. This will occur when the state of the system is so greatly changed from the Fermi sea (because of the large number of the bound pairs) that the binding energy for an additional pair has gone to zero.

This demanding physical and formal requirements can be adequately described by the following BCS variational form of the ground-state wavefunction for superconductors

$$|\Psi_S\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{-\mathbf{k}}^{\dagger}) |0\rangle \quad (2.2)$$

where $|0\rangle$ is the vacuum state, $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are the real and even function of \mathbf{k} , chosen in such a way to minimize the ground-state energy; $c_{\mathbf{k}}$ and $c_{\mathbf{k}}^{\dagger}$ are the annihilation and creation particle operators which obey the standard anticommutation rules

$$\{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\} = \{c_{\mathbf{k}\sigma}^{\dagger}, c_{\mathbf{k}'\sigma'}^{\dagger}\} = 0, \quad \{c_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}^{\dagger}\} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}. \quad (2.3)$$

For normalization matter $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$.

This form (2.2) of the wavefunction implies that the probability of the pair $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ being occupied is $|v_{\mathbf{k}}|^2$, whereas the probability that it is unoccupied is $|u_{\mathbf{k}}|^2 = 1 - |v_{\mathbf{k}}|^2$. For simplicity we can consider $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ all real, but it will be important to let them differ by a phase factor $e^{i\varphi}$, where φ is independent of k , and will turn out to be the phase of the macroscopic condensate wavefunction.

We can see that in the superconducting ground state described by Ψ_S , electrons are involved only as pairs. To notice is also that the wavefunction (2.2) of the superconductor is reduced to the wavefunction of the normal metal

$$|\Psi_N\rangle = \prod_{\mathbf{k}}^{k < k_F} (c_{\mathbf{k}\uparrow}^\dagger, c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle$$

in the particular case in which $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are given by

$$\begin{cases} u_{\mathbf{k}} = 0 & v_{\mathbf{k}} = 1 & \text{for } k < k_F \\ u_{\mathbf{k}} = 1 & v_{\mathbf{k}} = 1 & \text{for } k > k_F \end{cases} \quad (2.4)$$

An aspect of the wavefunction (2.2) is that the total number of electrons is not well defined.

2.1.3 The variational method

We want to find the appropriate values for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ which minimize the energy of the ground-state wavefunction using the variational method.

We proceed to minimize the expectation value $\langle \Psi_S | H | \Psi_S \rangle$ under the constrains $\langle \Psi_S | N_{op} | \Psi_S \rangle = N$, where

$$N_{op} = \sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$$

is the particle number operator and N is the number of electrons in the actual metal.

The standard method to treat minimization with one or more constraints consist in introducing one or more Lagrange multipliers μ , minimizing without restraint the quantity $\langle \Psi_S | H - \mu N_{op} | \Psi_S \rangle$ and finally determining μ through the condition $\langle \Psi_S | N_{op} | \Psi_S \rangle = N$. It turns out that μ is the Fermi energy, and it is the same for the normal or superconducting state.

In essence we thus arrive to the minimization of the quantity

$$\langle \Psi_S | H_{BCS} | \Psi_S \rangle \quad (2.5)$$

where $H_{BCS} = H - \mu N_{op}$ is the so-called pairing Hamiltonian or reduced Hamiltonian:

$$H_{BCS} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{l}\downarrow} c_{\mathbf{l}\uparrow}. \quad (2.6)$$

Here $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu = \hbar^2 \mathbf{k}^2 / 2m - \mu$ is the single-particle energy relative to the Fermi energy.

The theory presumes that this Hamiltonian includes the terms that are decisive for superconductivity but it omits many other terms which involve electrons not paired as $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$. Such other terms have zero expectation value in the BCS ground-state wavefunction but may be important in other applications.

The expectation value (2.5) can be easily evaluated keeping in mind the practical recipe of anticommutation for fermions (2.3).

We see at once that averaging the first term in (2.6) yields

$$\left\langle \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} n_{\mathbf{k}\sigma} \right\rangle = \langle E_{kinetic} - \mu N \rangle = 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}} |v_{\mathbf{k}}|^2 \quad (2.7)$$

which is exactly what we expect also classically, given that $|v_{\mathbf{k}}|^2$ is the number of particles with momentum \mathbf{k} and taking into account the double spin state.

The interaction term gives

$$\langle V \rangle = \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} u_{\mathbf{k}} v_{\mathbf{k}}^* u_{\mathbf{l}}^* v_{\mathbf{l}} \quad (2.8)$$

Physically this term can be explained noting that $V_{\mathbf{k}\mathbf{l}}$ scatters from a state with $(\mathbf{l} \uparrow, -\mathbf{l} \downarrow)$ to one with $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$. This requires the initial state to have the \mathbf{l} pair occupied and the \mathbf{k} pair empty and viceversa for the final state. The probability amplitude for such an initial state is $u_{\mathbf{k}} v_{\mathbf{l}}$ and for the final state it is $v_{\mathbf{k}}^* u_{\mathbf{l}}^*$, thus leading to the preceding result. We should note that $V_{\mathbf{k}\mathbf{l}}$ contributes nothing to the energy in the normal state. This is obvious at $T = 0$ since the states are either 100 percent occupied or empty, so that the product probability of being full and empty is zero. At $T > 0$, the Fermi distribution doesn't cutoff sharply so one might think that there could be nonzero contribution. However, in the normal state, the appropriate products of probability amplitudes (corresponding to $u_{\mathbf{k}} v_{\mathbf{k}}^* u_{\mathbf{l}}^* v_{\mathbf{l}}$ in the ordered BCS state) average to zero due to random relative phase. Hence, the scattering terms give no contribution to the average energy in the normal state.

Combining the two previous equation and taking $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ reals, the expectation value for the BCS Hamiltonian is

$$\langle H_{BCS} \rangle = 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{l}} v_{\mathbf{l}} \quad (2.9)$$

which we need to minimize under the constrain $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$. This can be done representing $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ in polar form

$$\begin{cases} u_{\mathbf{k}} = \cos \theta_{\mathbf{k}} \\ v_{\mathbf{k}} = \sin \theta_{\mathbf{k}} \end{cases}$$

To solve the set of self-consistent equation we define the energy gap parameter $\Delta_{\mathbf{k}}$

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{l}} V_{\mathbf{k}\mathbf{l}} u_{\mathbf{l}} v_{\mathbf{l}} \quad (2.10)$$

The solution of the minimization problem together with the normalization condition give the results

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left(1 + \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}} \right) \quad \text{and} \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left(1 - \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}} \right). \quad (2.11)$$

The choice of the sign for the sine and cosine (only their relative sign is fixed) has been determined by the requirement that, for vanishing $V_{\mathbf{k}\mathbf{l}}$ interaction and thus for vanishing $\Delta_{\mathbf{k}}$, the standard normal ground-state described by (2.4) is obtained.

We can now substitute (2.11) into the gap equation (2.10) and after some calculation we find a set of self-consistent equations for the gap parameters.

$$\Delta_{\mathbf{k}} = - \frac{1}{2} \sum_{\mathbf{l}} V_{\mathbf{k}\mathbf{l}} \frac{\Delta_{\mathbf{l}}}{\sqrt{\xi_{\mathbf{l}}^2 + \Delta_{\mathbf{l}}^2}} \quad (2.12)$$

A trivial solution to this equation is $\Delta_{\mathbf{k}} = 0$ for every \mathbf{k} , this correspond to the normal metal state with the electrons filling the Fermi sea up to k_F . For $\Delta_{\mathbf{k}} = 0$ we would have $v_{\mathbf{k}} = 1$ for $\xi_{\mathbf{k}} < 0$ and $v_{\mathbf{k}} = 0$ for $\xi_{\mathbf{k}} > 0$ (remember that $\xi = \varepsilon - \mu$). In general equation (2.12) is not easy to be solved. Anyway we expect a nontrivial solution which lowers the energy

of the normal state to the superconducting energy.

We retain the model of $V_{\mathbf{k}\mathbf{l}}$ used by Cooper and by BCS (2.1):

$$V_{\mathbf{k}\mathbf{l}} = \begin{cases} -V & \text{for } |\xi_{\mathbf{k}}|, |\xi_{\mathbf{l}}| \leq \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

with $V > 0$. (Our theoretical discussion of $V_{\mathbf{k}\mathbf{l}}$ actually suggests that the relevant energy is $|\xi_{\mathbf{k}} - \xi_{\mathbf{l}}|$, the energy change of the electron in the scattering process, but to get a simple solution we need to make this stronger restriction).

From the average potential approximation follows that

$$\Delta_{\mathbf{k}} = \begin{cases} \Delta & \text{for } |\xi_{\mathbf{k}}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases} \quad (2.13)$$

We can now simplify equation (2.12) using this approximations. We assume the electron density of state $N(0)$ constant in the small energy shell around the Fermi level and we convert the sum to an integral. We obtain

$$\Delta = \frac{\hbar\omega_D}{\sinh[N(0)V]} \quad (2.14)$$

In the weak coupling limit, when $N(0)V \ll 1$ we obtain

$$\Delta = 2\hbar\omega_D e^{-1/N(0)V} \quad (2.15)$$

For typical conventional superconductors, one has $E_F \approx 1eV$ (measured from the bottom of the conduction band) and $V \approx 0.1 - 0.5eV$; the coupling parameter $N(0)V$ is thus in the range $0.1 - 0.5$. In this range the gap parameter $\Delta \approx 1meV$ is in general a small fraction ($\approx 0.1 - 0.01$) of $\hbar\omega_D$.

Just as a reminder: we have confined our discussion of the BCS theory of superconductivity within the weak coupling limit (i.e. $\Delta \ll \hbar\omega_D$), and s-wave symmetry of the pairing state.

2.1.4 Ground-state energy

The condensation energy of a superconductor is defined as the energy difference between the superconductor ground-state energy, which we

call W_S , and the normal ground-state energy W_N ; its expression is

$$W_S - W_N = 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{l}} v_{\mathbf{l}} - 2 \sum_{\mathbf{k}}^{k < k_F} \xi_{\mathbf{k}}. \quad (2.16)$$

Using the previous relations (2.11) and (2.10) we obtain

$$W_S - W_N = \sum_{\mathbf{k}} [2\xi_{\mathbf{k}} v_{\mathbf{k}}^2 - \Delta_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}] - \sum_{\mathbf{k}}^{k < k_F} \xi_{\mathbf{k}} \quad (2.17)$$

where we also use the fact that the normal state at $T = 0$ correspond to the BCS state with $\Delta = 0$, in which case $\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} = |\xi_{\mathbf{k}}|$

After some calculations, in the average potential approximation, we find

$$W_S - W_N = 2 \sum_{k=|\mathbf{k}| > k_F} \left(\xi_{\mathbf{k}} - \frac{\xi_{\mathbf{k}}^2}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}} \right) - \frac{\Delta^2}{V} \quad (2.18)$$

where the first term describes the change in kinetic energy, whereas the term $-\Delta^2/V$ is the change in potential energy.

Going over to the continuum approximation, carrying out the integration on ξ from 0 to $\hbar\omega_D$ and using the weak-coupling-limit approximation, we find

$$\begin{aligned} W_S - W_N &= \left[\frac{\Delta^2}{V} - \frac{1}{2} N(0) \Delta^2 \right] - \frac{\Delta^2}{V} \\ &= -\frac{1}{2} N(0) \Delta^2 \end{aligned} \quad (2.19)$$

The condensation energy (2.19) of the superconductor can be interpret as originated by the electrons in the energy shell Δ around the Fermi energy which decrease their energy by about Δ because of the pairing mechanism.

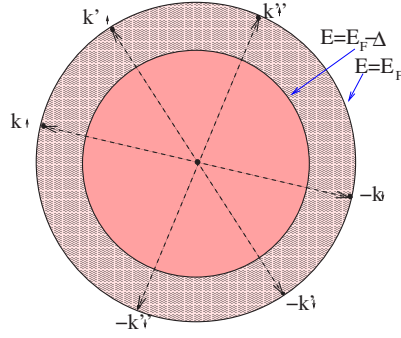


Figure 2.2: Schematic representation of the origin of the condensation energy in the BCS ground-state. The electron pairs ($\mathbf{k} \uparrow, -\mathbf{k} \downarrow$) in the darker region of \mathbf{k} space, within an energy shell Δ around the Fermi level, contribute to the condensation energy of the superconductor (notice that, typically, $\Delta \approx 1\text{meV}$ and $E_F \approx 1\text{eV}$). The lines are a reminder of the binding energy of a Cooper pair.

Momentum distribution and coherence length

The probability of finding an electron in a state with momentum $\hbar\mathbf{k}$ and spin σ in the superconductor is given in terms of the single particle number operator by

$$\langle \Psi_S | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} | \Psi_S \rangle = v_{\mathbf{k}}^2 = \frac{1}{2} \left[1 - \frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}} \right]; \quad (2.20)$$

in the normal gas, the same probability is given by

$$\langle \Psi_N | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} | \Psi_N \rangle = \begin{cases} 1 & \text{for } k < k_F \\ 0 & \text{for } k > k_F \end{cases} \quad (2.21)$$

Notice also that $u_{\mathbf{k}}^2 = 1 - v_{\mathbf{k}}^2$.

We can do a similar analysis for the pair operator $c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger$ (or $c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$). In the superconducting ground state we have

$$\langle \Psi_S | c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger | \Psi_S \rangle = u_{\mathbf{k}} v_{\mathbf{k}} = \frac{1}{2} \frac{\Delta_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}} \quad (2.22)$$

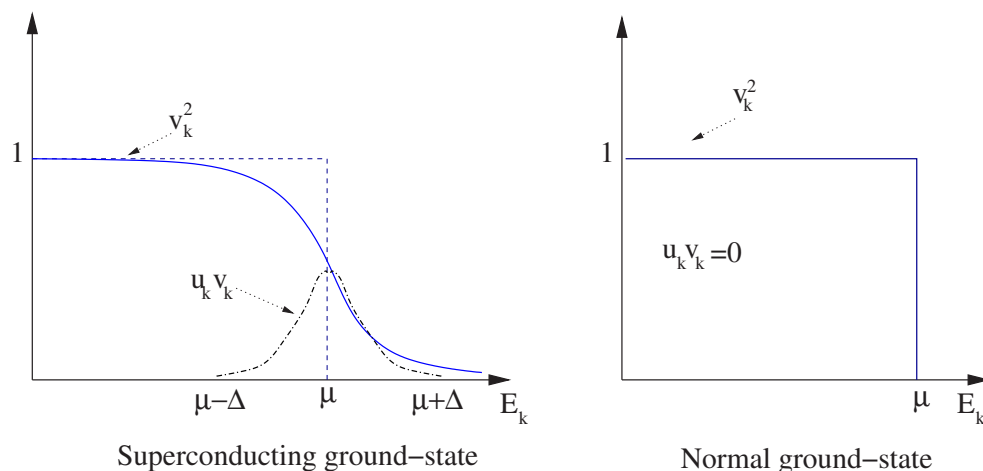


Figure 2.3: Behavior of the quantities v_k^2 and $u_k v_k$ for the superconducting ground state and for the normal ground state. Note that v_k^2 approaches unity well below the Fermi energy and zero well above, rather like the Fermi function that is appropriate to normal metals at finite temperatures.

The above quantity is always zero in the normal state, but it is different from zero in a small shell around k_F in the superconductor state; some of the most typical effects of superconductors (for instance Meissner effect and Josephson tunneling) are related to this fact.

The region in reciprocal space where $u_k v_k$ is different from zero has an energy width Δ around the Fermi energy. From the free-electron dispersion law $E(\mathbf{k}) = \hbar^2 k^2 / 2m$, we have the relation $\delta E = (\hbar^2 k / m) \delta k$ between the width δk in reciprocal space and the energy width δE . With $\delta E = \Delta$ and $k = k_F$, we obtain $\Delta = (\hbar^2 k_F / m) \delta k = \hbar v_F \delta k$. From the uncertainty principle, we have that in real space the spatial extent $\xi_0 \approx 1 / \delta k$ is given by

$$\xi_0 = \frac{1}{\pi} \frac{\hbar v_F}{\Delta} = \frac{1}{\pi} \frac{\hbar^2 k_F}{m \Delta} \quad (2.23)$$

The length ξ_0 is the so-called BCS coherence length, and represents the average distance in real space between the two electrons of the Cooper pair. The pair coherence length is proportional to the Fermi velocity and inversely proportional to the binding energy of the Cooper pair. Typical values of ξ_0 range from thousand \AA in conventional supercon-

ductors, to some tens \AA in high- T_c superconductors. In general there is a large number of Cooper pairs within the spatial coherence length ξ_0 . In fact the density of Cooper pairs is of the order of $\approx n \cdot (\Delta/E_F)$, where $n \equiv 1/[(3/4)\pi r_s^3 a_B^3]$ is the electron density of the metal, and Δ/E_F is the fraction of electrons that condensate in the ground superconducting state with an energy gain of $\approx 2\Delta$; we thus have that the average distance between the centers of mass of the pairs is related to the average distance $r_s a_B$ between electrons by the expression $d \approx r_s a_B (E_F/\Delta)^{1/3}$. For conventional superconductors, $E_F \approx 1\text{eV}$, $\Delta \approx 1\text{meV}$, $d \approx 10r_s a_B \approx 10\text{\AA}$. With ξ_0 of the order of 1000\AA , there are million Cooper pairs within the coherence length; the individual pairs overlap strongly in space and the binding energy 2Δ of any pair depends cooperatively on the presence of all the other pairs.

2.1.5 The Bogoliubov canonical transformation

Until now we have studied the ground-state of a superconductor at zero temperature. We could study the excited states of a superconductor system (still remaining at zero temperature) starting from the ground-state wavefunction (2.2) $|\Psi_S\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger) |0\rangle$, applying to it creation or annihilation operators and elaborating the trial excited state so obtained as done originally by BCS. A more convenient procedure was followed by Bogoliubov and Valantin independently [5, 6] and allows one to obtain in a single stroke the excitation spectrum of the superconductor.

We start with the observation that the characteristic BCS pair-interaction Hamiltonian will lead to a ground-state which is some phase-coherent superposition of many-body states with pairs of Bloch states ($\mathbf{k} \uparrow, -\mathbf{k} \downarrow$) occupied or unoccupied. Because of the coherence, operators such as $c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$ can have nonzero expectation value $b_{\mathbf{k}}$ in such a state, rather than averaging to zero as in the normal metal, where the phases are random. Moreover because of the large number of particles involved, the fluctuation about these expectation values should be small. This suggests that it will be useful to express such a product of operators formally as

$$c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} = b_{\mathbf{k}} + (c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} - b_{\mathbf{k}}) \quad (2.24)$$

where

$$b_{\mathbf{k}} = \langle \Psi_S | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | \Psi_S \rangle \quad (2.25)$$

and subsequently neglect quantities that are linear in the presumably small fluctuation in the parenthesis.

Equation (2.25) defines the expectation value on the ground-state while (2.24) defines the fluctuation operator in the parenthesis. A similar split is performed for the product of two creation operators.

If we follow this procedure we obtain the so-called model Hamiltonian

$$H_{BCS} \simeq H_B = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} (c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger b_{\mathbf{l}} + b_{\mathbf{k}}^* c_{-\mathbf{l}\downarrow} c_{\mathbf{l}\uparrow} - b_{\mathbf{k}}^* b_{\mathbf{l}}) \quad (2.26)$$

where we already neglected terms like $(cc - b)$ or $(c^\dagger c^\dagger - b^*)$.

If we now define

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{l}} V_{\mathbf{k}\mathbf{l}} b_{\mathbf{l}} \quad (2.27)$$

we can write the model Hamiltonian H_B in the form

$$H_B = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \left[c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \right] + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} b_{\mathbf{k}} \quad (2.28)$$

which is a sum of term, each bilinear in the pair of operators corresponding to the partners in a Cooper pair.

The model Hamiltonian can be diagonalized with a suitable canonical transformation. Consider in fact the transformations

$$\begin{aligned} c_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}^\dagger & c_{-\mathbf{k}\downarrow} &= u_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow} - v_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow}^\dagger \\ c_{\mathbf{k}\uparrow}^\dagger &= u_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow}^\dagger + v_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow} & c_{-\mathbf{k}\downarrow}^\dagger &= u_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}^\dagger - v_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} \end{aligned} \quad (2.29)$$

while the inverse transformation are

$$\begin{aligned} \gamma_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger & \gamma_{-\mathbf{k}\downarrow} &= u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger \\ \gamma_{\mathbf{k}\uparrow}^\dagger &= u_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger - v_{\mathbf{k}} c_{-\mathbf{k}\downarrow} & \gamma_{-\mathbf{k}\downarrow}^\dagger &= u_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger + v_{\mathbf{k}} c_{\mathbf{k}\uparrow} \end{aligned} \quad (2.30)$$

The real numerical coefficient $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ satisfy $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$. The linear transformations (2.29) and (2.30) are canonical since the fermion operators $\gamma_{\mathbf{k}\sigma}$ and $\gamma_{\mathbf{k}\sigma}^\dagger$ have the same standard anticommutation rules as those

between $c_{\mathbf{k}\sigma}$ and $c_{\mathbf{k}\sigma}^\dagger$. Note that $\gamma_{\mathbf{k}\uparrow}$ participate in destroying an electron with $\mathbf{k} \uparrow$ or creating one with $-\mathbf{k} \downarrow$; in both cases the net effect is to decrease the system momentum by \mathbf{k} and to reduce S_z by $\hbar/2$. The operator $\gamma_{-\mathbf{k}\downarrow}^\dagger$ has similar properties, so $\gamma_{-\mathbf{k}\downarrow}$ itself decreases the system momentum by $-\mathbf{k}$ and has the net effect of increasing S_z .

We now substitute these new operators in H_B . The model Hamiltonian contains now both diagonal particle number operators of the type $\gamma^\dagger\gamma$, but also undesired terms of the type $\gamma\gamma$ and $\gamma^\dagger\gamma^\dagger$. At this stage we chose $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ so that the coefficient of $\gamma\gamma$ and $\gamma^\dagger\gamma^\dagger$ are zero and the model Hamiltonian becomes diagonal in the particle number operators. For this aim we require

$$2\xi_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} - \Delta_{\mathbf{k}}(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) = 0 \quad (2.31)$$

The solution of this equation, together with the normalization condition $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$, gives for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ the explicit expression already reported in (2.11).

Further comparison of the present procedure with the variational procedure, makes transparent the full equivalence of the variational BCS approach and the Bogoliubov approach based on canonical transformation.

The model Hamiltonian can be written as

$$\begin{aligned} H_B &= \sum_{\mathbf{k}} [\xi_{\mathbf{k}}(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) + 2\Delta_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}] [\gamma_{\mathbf{k}\uparrow}^\dagger\gamma_{\mathbf{k}\uparrow} + \gamma_{-\mathbf{k}\downarrow}^\dagger\gamma_{-\mathbf{k}\downarrow}] + W_S \\ &\text{after some substitution} \\ &= \sum_{\mathbf{k}} \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} [\gamma_{\mathbf{k}\uparrow}^\dagger\gamma_{\mathbf{k}\uparrow} + \gamma_{-\mathbf{k}\downarrow}^\dagger\gamma_{-\mathbf{k}\downarrow}] + W_S \end{aligned} \quad (2.32)$$

where W_S is the ground-state energy of the superconductor and $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ are the energies, above the ground state, of the quasiparticle created by the fermi operators $\gamma_{\mathbf{k}\uparrow}^\dagger$ and $\gamma_{-\mathbf{k}\downarrow}^\dagger$.

In order to clarify the meaning of the Hamiltonian (2.32) we consider the average gap approximation. In this case the energy gap parameters $\Delta_{\mathbf{k}}$ are constant and equal to Δ (in the energy shell $\pm\hbar\omega_D$ around the Fermi energy). The quasiparticle excitation energy in the superconductor becomes

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} \quad (\text{superconductors}) \quad (2.33)$$

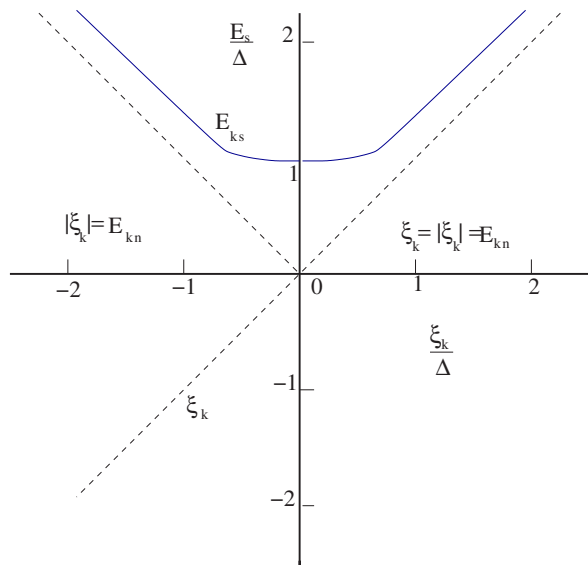


Figure 2.4: Energies of elementary excitations in the normal and superconducting states as functions of ξ_k

In the limiting case of vanishing electron-electron interaction, i.e. for normal metals, we would have $\Delta = 0$ and hence

$$E_{\mathbf{k}} = |\xi_{\mathbf{k}}| \quad (\text{normal metals}) \quad (2.34)$$

The quasiparticle spectrum of the superconductor exhibits thus an energy gap given by Δ . In the superconductor there are no electron-like states with energy in the interval $[E_F, E_F + \Delta]$, and no hole-like states in the energy interval $[E_F - \Delta, E_F]$.

Now that we have seen that the quasi-particle excitations can be described as fermions created by the $\gamma_{\mathbf{k}}^\dagger$, which are in one-to-one correspondence with the $c_{\mathbf{k}}^\dagger$ of the normal metal, we can obtain the superconducting density of states $N_s(E)$ by equating

$$N_s(E)dE = N_n(\xi)d\xi \quad (2.35)$$

Because we are largely interested in energies ξ only a few millielectronvolts from the Fermi energy, we can take $N_n(\xi) = N(0)$, a constant. This

leads directly to the simple result

$$\frac{N_s(E)}{N(0)} = \frac{d\xi}{dE} = \begin{cases} \frac{E}{(E^2 - \Delta^2)^{1/2}} & (E > \Delta) \\ 0 & (E < \Delta) \end{cases} \quad (2.36)$$

We expect a divergent state density just above $E = \Delta$. Of course, the total number of states is conserved because of the one-to-one correspondence between the $\gamma_{\mathbf{k}}$ and the $c_{\mathbf{k}}$.

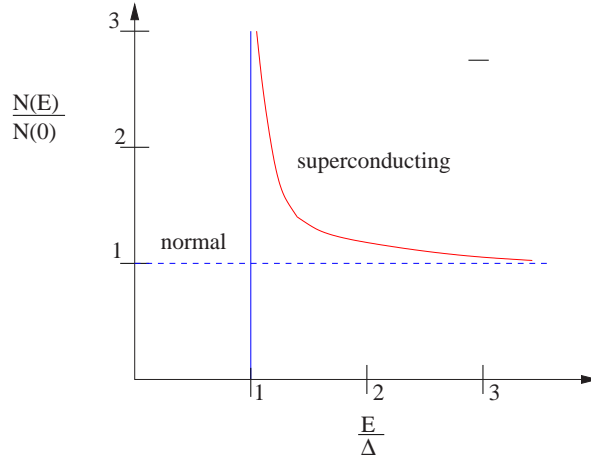


Figure 2.5: Density of states in superconducting compared to normal state. All \mathbf{k} states whose energies fall in the gap in the normal metal are raised in energy above the gap in the superconducting state.

From the above considerations on quasiparticle excitations, we also infer that breaking a pair, giving rise to two quasiparticles, requires at least an energy 2Δ ; the quantity 2Δ can be interpreted as the binding energy of any one pair, due to the cooperative presence of many other pairs (all in the same quantum state of zero total spin and zero momentum) in the superconductor ground state.

2.1.6 Finite temperature

At finite temperature the quasiparticle states of the superconductor are thermally excited and a number of Cooper pairs are broken; this process

is accompanied by a decrease of the energy gap in quasiparticle excitations and eventually leads to the transition to the normal state.

What we want now is an expression temperature dependent for the gap parameter and a way to find the critical temperature T_c at which $\Delta(T) \rightarrow 0$.

Since we have identified $E_{\mathbf{k}}$ as the excitation energy of a fermion quasiparticle, it must be a positive quantity $\geq \Delta$. The probability that a quasiparticle is excited in thermal equilibrium is the usual Fermi function

$$f(E_{\mathbf{k}}) = (e^{\beta E_{\mathbf{k}}} + 1)^{-1} \quad (2.37)$$

where $\beta = 1/k_B T$. We see that $f(E_{\mathbf{k}})$ goes to zero at $T = 0$ for all \mathbf{k} , including $|\mathbf{k}| < k_F$. From equation (2.27) $\Delta_{\mathbf{k}} = -\sum_{\mathbf{l}} V_{\mathbf{kl}} b_{\mathbf{l}}$ using the fact that $\gamma_{\mathbf{k}\uparrow} \gamma_{-\mathbf{k}\downarrow}$ and $\gamma_{\mathbf{k}\uparrow}^\dagger \gamma_{-\mathbf{k}\downarrow}^\dagger$ do not contribute to the average of $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^*$ we write

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{l}} V_{\mathbf{kl}} \langle c_{-\mathbf{l}\downarrow} c_{\mathbf{l}\uparrow} \rangle = -\sum_{\mathbf{l}} V_{\mathbf{kl}} u_{\mathbf{l}}^* v_{\mathbf{l}} \langle 1 - \gamma_{\mathbf{k}\uparrow}^\dagger \gamma_{\mathbf{k}\uparrow} - \gamma_{-\mathbf{k}\downarrow}^\dagger \gamma_{-\mathbf{k}\downarrow} \rangle \quad (2.38)$$

We find that

$$\langle 1 - \gamma_{\mathbf{k}\uparrow}^\dagger \gamma_{\mathbf{k}\uparrow} - \gamma_{-\mathbf{k}\downarrow}^\dagger \gamma_{-\mathbf{k}\downarrow} \rangle = 1 - 2f(E_{\mathbf{k}}) \quad (2.39)$$

so that equation (2.27) becomes

$$\begin{aligned} \Delta_{\mathbf{k}} &= -\sum_{\mathbf{l}} V_{\mathbf{kl}} u_{\mathbf{l}}^* v_{\mathbf{l}} [1 - 2f(E_{\mathbf{k}})] \\ &= -\sum_{\mathbf{l}} V_{\mathbf{kl}} \frac{\Delta_{\mathbf{l}}}{2E_{\mathbf{l}}} \tanh \frac{\beta E_{\mathbf{l}}}{2} \end{aligned} \quad (2.40)$$

This is the desired generalization of equation (2.12) for finite temperature and reduces to it at zero temperature.

In the average potential approximation where $V_{\mathbf{kl}} = V$ and $\Delta_{\mathbf{k}} = \Delta$ the previous self-consistency condition becomes

$$\frac{1}{V} = \frac{1}{2} \sum_{\mathbf{k}} \frac{\tanh \beta E_{\mathbf{k}}/2}{E_{\mathbf{k}}} \quad (2.41)$$

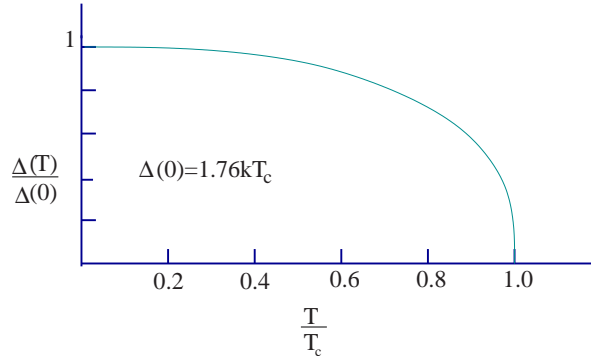


Figure 2.6: Temperature dependence of the energy gap in the BCS theory. Strictly speaking, this universal curve holds only in a weak-coupling limit, but it is a good approximation in most cases.

To find the critical temperature T_c we notice that when $\Delta(T_c) = 0$ then $E_{\mathbf{k}} = |\xi_{\mathbf{k}}|$. Thus T_c is found replacing $E_{\mathbf{k}}$ with $|\xi_{\mathbf{k}}|$ in (2.41) and solving. After changing the sum to an integral, taking advantage of the symmetry of $|\xi_{\mathbf{k}}|$ about the Fermi level and changing to a dimensionless variable of integration, the condition becomes

$$\frac{1}{N(0)V} = \int_0^{\beta_c \hbar \omega_c / 2} \frac{\tanh x}{x} dx \quad (2.42)$$

We find in the weak coupling limit

$$k_B T_c = 1.13 \hbar \omega_c e^{-1/N(0)V} \quad (2.43)$$

Inserting this into equation (2.15) we have

$$\Delta(0) = 1.76 k_B T_c \quad (2.44)$$

so that the gap at $T = 0$ is indeed comparable in energy to $k_B T_c$. The numerical factor 1.76 has been tested in many experiments and found to be reasonable.

The behavior of $\Delta(T)$ as a function of T for $T \rightarrow T_c$ (and $T < T_c$) is found to be

$$\Delta(T) = 3.06 k_B T_c \left(1 - \frac{T}{T_c}\right)^{1/2} \quad (2.45)$$

where the $1/2$ exponent is a characteristic feature of the mean field theories.

2.1.7 Electron tunnelling into superconductors

A central feature in the BCS theory is the presence of an energy gap in the electron density-of-state of superconductors. A most direct evidence of the gap and of the electron structure of the superconductors is provided by the electron tunnelling experiments.

Consider first a junction constituted by two normal metals, separated by a thin insulating film (typically $10 \approx 50\text{\AA}$). It is well known that, if a potential difference is applied across the junction, a current flows because of the capability of electrons to penetrate a thin barrier. For low fields, the tunnelling current is proportional to the applied voltage V . In fact, in quasi equilibrium conditions, the Fermi levels of the two metals are shifted by eV . The density-of-state in the two metals, as well as tunnelling probabilities, are practically independent of energy in the few millielectronvolts around E_F , and this leads to the ohmic behavior of the junction.

Let us now examine the electron tunnelling across a junction formed by normal metal-insulator-superconductor (NIS junction). In the ordinary metal (at zero temperature) all states below the Fermi energy E_F are filled, while all states above E_F are empty, with zero gap between occupied and empty states. In the superconductor the quasiparticle energies differ from the Fermi energy at least by the energy gap Δ . When a bias voltage V is applied to a NIS junction, one-particle states are not available in the superconducting material for accepting or supplying electrons unless the bias exceeds δ/e . When $V > \delta/e$, the $I - V$ characteristic and in particular the differential conductance $G = dI/dV$ is related to the density-of-state of quasiparticle in the superconductor (since the density-of-state in the metal can be taken as constant in the few millielectronvolts of interest). Finally when $V \gg \Delta/e$ the ohmic behavior of the junction is recovered.

Let us now consider the tunnelling between two equal superconductors, of energy gap parameter Δ , separated by a thin insulating barrier (SIS junction). At $T = 0$ we find that there is no quasiparticle tunnelling until the bias voltage V exceeds $2\Delta/e$; in the case the two superconductors are different the threshold voltage is $(\Delta_1 + \Delta_2)/e$.

At the threshold voltage, we expect a discontinuous jump of the current, because of the singularity of the density-of-state of quasiparticle in the

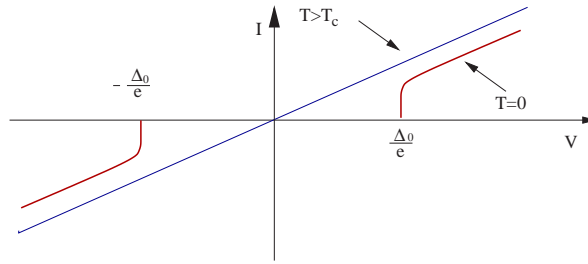


Figure 2.7: Schematic representation of the $I - V$ characteristics of a normal metal-insulator-superconductor junction at zero temperature and above the critical temperature; Δ is the energy gap parameter of the superconductor. At finite temperature $0 < T < T_c$ the presence of thermally excited electrons contribute to smear out and shift the strongly nonlinear $T = 0$ current-voltage characteristic.

two superconductors; eventually for higher bias voltages the ohmic behavior is recovered.

It is important to notice that in the case of SIS junctions, besides the quasiparticle tunnelling current discussed so far, we can have a supercurrent tunnelling due to Cooper pairs transfer between superconductors; this current, called Josephson current, can be observed in SIS junctions with extremely thin insulating layers ($10 - 15 \text{ \AA}$). In this situation the coupling between the two superconductors is sufficiently strong that a definite phase relationship between pairs on opposite sides of the insulating barrier can be maintained. We will treat the Josephson current in the next chapter.

2.2 Single electron tunnelling through transistor *my way*

In this calculation we treat the island as a one level island with infinite Coulomb interaction so that the dot can never be double occupied. We will take into account that a bias voltage V can shift the Fermi sea of the leads. We carry out the calculation at $T = 0$, a generalization to $T > 0$ is straight forward.

As in [4] we derive an expression for the current using the usual kinetic

equation approach.

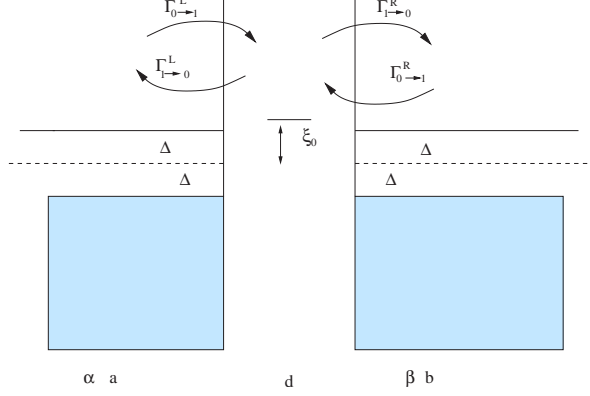


Figure 2.8: Schematic representation of the system studied. We will relate, in this and next chapter, to the leads with the letters a or α and b or β for left and right respectively.

As we said the dot can't be double occupied so it can have only three states: empty, and occupied either with spin up or down. The probabilities for the three states are denoted P_0 , P_\uparrow and P_\downarrow , respectively.

The rate equations in equilibrium are given by:

$$\dot{P}_0 = -2\Gamma_{0\rightarrow 1}P_0 + \Gamma_{1\rightarrow 0}P_\uparrow + \Gamma_{1\rightarrow 0}P_\downarrow = 0 \quad (2.46a)$$

$$\dot{P}_\uparrow = \Gamma_{0\rightarrow 1}P_0 - \Gamma_{1\rightarrow 0}P_\uparrow = 0 \quad (2.46b)$$

$$\dot{P}_\downarrow = \Gamma_{0\rightarrow 1}P_0 - \Gamma_{1\rightarrow 0}P_\downarrow = 0 \quad (2.46c)$$

which combined with the condition $P_0 + P_\uparrow + P_\downarrow = 1$ has the solution

$$P_0 = \frac{\Gamma_{1\rightarrow 0}}{\Gamma_{1\rightarrow 0} + 2\Gamma_{0\rightarrow 1}}, \quad P_\uparrow = P_\downarrow = \frac{\Gamma_{0\rightarrow 1}}{\Gamma_{1\rightarrow 0} + 2\Gamma_{0\rightarrow 1}} \quad (2.47)$$

We denote with $\Gamma_{1\rightarrow 0}$ the tunnelling rate for tunnelling from a singly occupied state to the empty state, and with $\Gamma_{0\rightarrow 1}$ the reverse process. The meaning of (2.46) is clear: the first equation for example gives the rate of change of the empty state \dot{P}_0 . This rate is increased by the probability of the dot being full, with spin up or down, times the rate of leaving the dot (which could only happen if the dot is in fact full) and

is decreased by the probability of the dot being empty times the rate of getting to be occupied, times a factor two which arises because there are two way of occupying the dot, either with spin up or spin down (but there is only one way of leaving it).

Since the electron can tunnel out of both left and right leads, both rates have left and right contributions: $\Gamma_{i \rightarrow j} = \Gamma_{i \rightarrow j}^L + \Gamma_{i \rightarrow j}^R$. The tunnelling rate are calculated using Fermi golden rule which means that we treat H_T (the tunnelling Hamiltonian) as a perturbation.

The current through the dot is given by:

$$I = -e[2P_0\Gamma_{0 \rightarrow 1}^L - (P_\uparrow + P_\downarrow)\Gamma_{1 \rightarrow 0}^L] = 2e \frac{\Gamma_{0 \rightarrow 1}^R \Gamma_{1 \rightarrow 0}^L - \Gamma_{1 \rightarrow 0}^R \Gamma_{0 \rightarrow 1}^L}{\Gamma_{1 \rightarrow 0} + 2\Gamma_{0 \rightarrow 1}} \quad (2.48)$$

We start looking for the expression of $\Gamma_{0 \rightarrow 1}^L$, the expression for $\Gamma_{0 \rightarrow 1}^R$ won't be different but for the different value of the bias applied on the left and right lead.

To find $\Gamma_{0 \rightarrow 1}^L$ we set the initial state as $|i\rangle = |G0G\rangle$ where with $|G\rangle$ we denote the ground state of the superconducting lead right or left and with $|0\rangle$ in the middle we denote the state of the dot. We suppose that the island is initially empty.

The final state for electrons travelling through the left junction would be given by

$$|f\rangle = c_{k'\sigma}^\dagger \alpha_{k\sigma'}^\dagger |i\rangle.$$

This means that we are creating a single quasi particle in the superconducting ground-state breaking a Cooper pair on the left lead and that we are transporting a particle on the dot. α and α^\dagger are the quasiparticle annihilator and creator of the BCS theory. For $T > 0$ a final state could be given also by $|f\rangle = c_{k'\sigma}^\dagger \alpha_{k\sigma'} |i\rangle$ where we annihilate a quasiparticle in the superconducting lead. This could be done because for $T > 0$ the equilibrium state contains thermal excited states. But as we said we work at zero temperature.

The final states are actually four depending on the spins σ and σ' but we will find that only two final states give a non zero contribution to the current.

The four states are:

$$\begin{aligned} |f_1\rangle &= c_{k'\uparrow}^\dagger \alpha_{k\uparrow}^\dagger |i\rangle \\ |f_2\rangle &= c_{k'\uparrow}^\dagger \alpha_{k\downarrow}^\dagger |i\rangle \\ |f_3\rangle &= c_{k'\downarrow}^\dagger \alpha_{k\uparrow}^\dagger |i\rangle \\ |f_4\rangle &= c_{k'\downarrow}^\dagger \alpha_{k\downarrow}^\dagger |i\rangle \end{aligned}$$

The tunnelling Hamiltonian is as usual, we write just the one for the left lead since this is the only one we need in this calculation

$$H_T = \sum_{lm\sigma} t_{lm} [c_{m\sigma}^\dagger a_{l\sigma} + c_{m\sigma} a_{l\sigma}^\dagger]$$

We calculate

$$H_T |f_1\rangle = \sum_{lm\sigma} t_{lm} [c_{m\sigma}^\dagger a_{l\sigma} c_{k'\uparrow}^\dagger \alpha_{k\uparrow}^\dagger + a_{l\sigma}^\dagger c_{m\sigma} c_{k'\uparrow}^\dagger \alpha_{k\uparrow}^\dagger] |i\rangle$$

the first term creates two particles in the dot which is not possible in my model so it is zero, in the second term since the dot is initially empty we need to have $k' = m$ and $\sigma = \uparrow$

$$\begin{aligned} &= \sum_l t_{lk'} c_{k'\uparrow}^\dagger a_{l\uparrow}^\dagger c_{k'\uparrow}^\dagger \alpha_{k\uparrow}^\dagger |i\rangle \\ &= c_{k'\uparrow}^\dagger c_{k'\uparrow}^\dagger |0\rangle \sum_l t_{lk'} [u_l \alpha_{l\uparrow}^\dagger + v_l \alpha_{-l\downarrow}] \alpha_{k\uparrow}^\dagger |G\rangle \end{aligned}$$

where we used the bilinear relation between the quasiparticle operators of the BCS theory and the normal particles operators

In the same way we find:

$$\begin{aligned} H_T|f_2\rangle &= c_{k'\uparrow}c_{k'\uparrow}^\dagger|0\rangle \sum_l t_{lk'}[u_l\alpha_{l\uparrow}^\dagger + v_l\alpha_{-l\downarrow}]\alpha_{k\downarrow}^\dagger|G\rangle \\ &= c_{k'\uparrow}c_{k'\uparrow}^\dagger|0\rangle t_{-kk'}v_k\alpha_{k\downarrow}\alpha_{k\downarrow}^\dagger|G\rangle \end{aligned} \quad (2.49)$$

$$\begin{aligned} H_T|f_3\rangle &= c_{k'\downarrow}c_{k'\downarrow}^\dagger|0\rangle \sum_l t_{lk'}[u_l\alpha_{l\downarrow}^\dagger - v_l\alpha_{-l\uparrow}]\alpha_{l\uparrow}^\dagger|G\rangle \\ &= c_{k'\downarrow}c_{k'\downarrow}^\dagger|0\rangle t_{-kk'}(-v_k)\alpha_{k\uparrow}\alpha_{k\uparrow}^\dagger|G\rangle \end{aligned} \quad (2.50)$$

$$H_T|f_4\rangle = c_{k'\downarrow}c_{k'\downarrow}^\dagger|0\rangle \sum_l t_{lk'}[u_l\alpha_{l\downarrow}^\dagger - v_l\alpha_{-l\uparrow}]\alpha_{k\downarrow}^\dagger|G\rangle \quad (2.51)$$

To use Fermi golden rule we need to find $\langle f|H_T|i\rangle$

It is straight forward to see that for case one and four we have:

$$\begin{aligned} \langle f_1|H_T|i\rangle &= 0 \\ \langle f_3|H_T|i\rangle &= 0 \end{aligned}$$

since we start from the ground state of the superconducting leads which don't contain excited states.

What remains are the second and third terms:

$$H_T|f_2\rangle = +t_{-kk'}c_{k'\uparrow}c_{k'\uparrow}^\dagger|0\rangle v_k\alpha_{k\downarrow}\alpha_{k\downarrow}^\dagger|G\rangle \quad (2.52)$$

$$H_T|f_3\rangle = -t_{-kk'}c_{k'\downarrow}c_{k'\downarrow}^\dagger|0\rangle v_k\alpha_{k\uparrow}\alpha_{k\uparrow}^\dagger|G\rangle \quad (2.53)$$

Remembering that we are dealing with a one level dot we can forget about the k' subscript for the dot operators.

Now we can use Fermi golden rule (as before we set $\hbar = 1$) to find the total rate of tunnelling through the dot. To do so we need to sum over all configuration of the lead. This restores back the sum over k for the lead which we lost in the previous calculation (2.49) (2.50). As we said we apply on the lead a voltage V which shifts its the Fermi energy. We also suppose that the tunnelling is elastic and we apply energy conservation

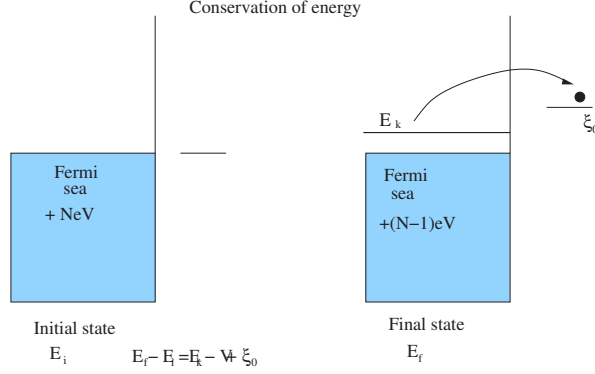


Figure 2.9: Energy conservation for the process of filling the dot. In the initial state the energy of the system is given by the electrons in the Fermi sea which feel the bias voltage applied. The final state is given by the energy of the electron filling the dot, the energy of the excited other pair electron and the energy of the Fermi sea that has lost one electron

to the system.

$$\begin{aligned} \Gamma_{0 \rightarrow 1}^L &= 2\pi \sum_k |\langle f | H_T | i \rangle|^2 \delta(\epsilon_0 + E_k - V) \\ &= 2\pi |t_k|^2 \sum_k v_k^2 (1 - f(E_k)) \delta(\epsilon_0 + E_k - V) \end{aligned}$$

we now change the sum into an integral as it is usually done and write all the constant in one as C

$$\begin{aligned} &= C \int_{\Re} d\xi_k \frac{1}{2} \left(1 - \frac{\xi_k}{E_k}\right) (1 - f(E_k)) \delta(\epsilon_0 + E_k - V) \\ &= \frac{C}{2} \int_{\Re} \frac{d\xi_k}{dE_k} dE_k [(1 - f(E_k)) \delta(\epsilon_0 + E_k - V) - \frac{\xi_k}{E_k} (1 - f(E_k)) \delta(\epsilon_0 + E_k - V)] \end{aligned}$$

using the relation between the density of states of normal-superconducting states

$$\begin{aligned} &= \frac{C}{2} N(0) \int_{\Re} dE_k \frac{E_k}{\sqrt{E_k^2 - \Delta^2}} (1 - f(E_k)) \delta(\epsilon_0 + E_k - V) + \\ &- \frac{C}{2} N(0) \int_{\Re} dE_k \frac{E_k}{|\xi_k|} \frac{\xi_k}{E_k} (1 - f(E_k)) \delta(\epsilon_0 + E_k - V) \end{aligned}$$

the second part of the integral is an odd function so it goes to zero

$$= \frac{C}{2} N(0) \frac{V - \epsilon_0}{\sqrt{(V - \epsilon_0)^2 - \Delta^2}} [1 - f(V - \epsilon_0)] \Theta(V - \epsilon_0 - \Delta) \quad (2.54)$$

Where we need the step function because the excitation energy of the quasi particle is always positive and greater than the gap energy Δ which we took independent from the quasiparticle momentum as in the average potential approximation: $E_k > \Delta > 0$

For a moment we have considered $T \neq 0$. Letting $T = 0$ we see that the terms like $1 - f(V - \varepsilon_0)$ get to be step functions $\Theta(V - \varepsilon_0)$ which are actually contained in the step function due to $E_k > 0$.

Hence

$$\Gamma_{0 \rightarrow 1}^L = \frac{C}{2} N(0) \frac{V - \varepsilon_0}{\sqrt{(V - \varepsilon_0)^2 - \Delta^2}} \Theta(V - \varepsilon_0 - \Delta) \quad (2.55)$$

We now need to carry out the same evaluation for the opposite rate of tunnelling: $\Gamma_{1 \rightarrow 0}^L$.

In this case the initial state is given by $|i\rangle = |G1G\rangle$ and the final states that will contribute with a term different from zero are

$$|f_1\rangle = c_{\uparrow} \alpha_{k\uparrow}^{\dagger} |i\rangle \quad \text{or} \quad |f_2\rangle = c_{\downarrow} \alpha_{k\downarrow}^{\dagger} |i\rangle.$$

We find $H_T = c^{\dagger} c |1\rangle_{t_{kk'}} u_k \alpha \alpha^{\dagger} |G\rangle$ where we omit the subscripts but the meaning is clear.

The calculation for the tunnelling rate is the same as before where instead of

$$v_k^2 = \frac{1}{2} \left(1 - \frac{\xi_k}{E_k} \right) \quad \text{we use} \quad u_k^2 = \frac{1}{2} \left(1 + \frac{\xi_k}{E_k} \right).$$

So we have:

$$\begin{aligned} \Gamma_{1 \rightarrow 0}^L &= 2\pi \sum_k u_k^2 (1 - f(E_k)) \delta(V + E_k - \xi_0) \\ &= C \int_{\mathfrak{R}} d\xi_k u_k^2 [1 - f(E_k)] \delta(V + E_k - \xi_0) \\ &= \dots \\ &= \frac{C}{2} N(0) \frac{\varepsilon_0 - V}{\sqrt{(\varepsilon_0 - V)^2 - \Delta^2}} \Theta(\varepsilon_0 - V - \Delta) \end{aligned}$$

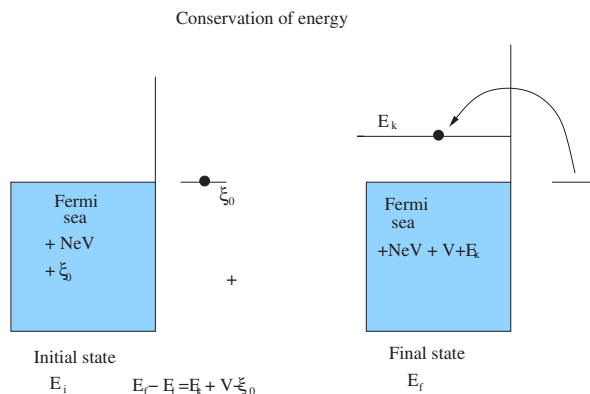


Figure 2.10: Energy conservation for the process of emptying the dot

We set an asymmetric bias voltage to the leads: $+V$ on the left lead and $-V$ on the right lead. The four tunnelling rate in this case are:

$$\Gamma_{0 \rightarrow 1}^L = \frac{\Gamma^L}{2} \frac{V - \varepsilon_0}{\sqrt{(V - \varepsilon_0)^2 - \Delta^2}} \Theta(V - \varepsilon_0 - \Delta) \quad (2.56a)$$

$$\Gamma_{0 \rightarrow 1}^R = \frac{\Gamma^R}{2} \frac{-V - \varepsilon_0}{\sqrt{(-V - \varepsilon_0)^2 - \Delta^2}} \Theta(-V - \varepsilon_0 - \Delta) \quad (2.56b)$$

$$\Gamma_{1 \rightarrow 0}^L = \frac{\Gamma^L}{2} \frac{\varepsilon_0 - V}{\sqrt{(\varepsilon_0 - V)^2 - \Delta^2}} \Theta(\varepsilon_0 - V - \Delta) \quad (2.56c)$$

$$\Gamma_{1 \rightarrow 0}^R = \frac{\Gamma^R}{2} \frac{V + \varepsilon_0}{\sqrt{(V + \varepsilon_0)^2 - \Delta^2}} \Theta(V + \varepsilon_0 - \Delta) \quad (2.56d)$$

where we denoted $\Gamma^{L,R} = 2\pi N_{L,R}(0) |t_{l,r}|^2$.

Now we have everything to find the current as in (2.48).

I used Mathematica 5.1 to carry out the calculations and this are some of voltage-current characteristics assuming that the two superconductors are equal. which means $\Delta_l = \Delta_r$.

What is shown in this plots is just the first step of the Coulomb blockade theory given in chapter one. If we took into account a dot with multiple levels we would have seen more than one step in the plot.

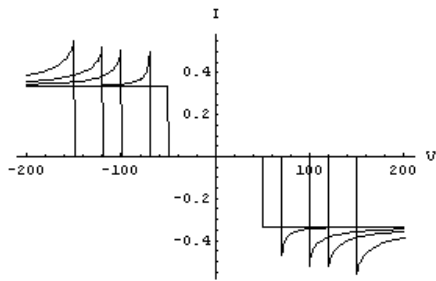


Figure 2.11: $\varepsilon_0 = 50$, $\Delta = 0, 20, 50, 70, 100$. We notice that the zero current plateau is exactly $\varepsilon_0 + \Delta$ in both directions of V . Also we notice that for $\Delta = 0$ the step is sharp. We are back to the Coulomb blockade treated in the previous chapter

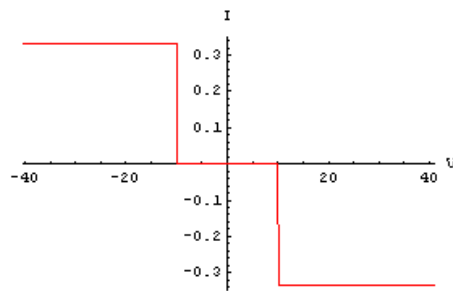


Figure 2.12: $\varepsilon_0 = 10$, $\Delta = 0$. Plot for $\Delta = 0$.

Chapter 3

Josephson current

3.1 Cooper pairs tunnelling

In the pervious section we have considered tunnelling of normal electrons (or quasiparticle) from a superconducting SIS junction, composed by the superconducting films separated by a very thin insulating layer.

For superconducting tunnel junction with extremely thin insulating layers ($10 - 15\text{\AA}$), the electron pair correlations extend through the insulating barrier. In this situation is has been predicted by Josephson that paired electrons can tunnel without dissipation from one superconductor to the other superconductor on the opposite side of the insulating layer. The direct supercurrent of pairs, for currents less than a certain critical value I_J , flows with zero voltage drop across the junction (dc Josephson effect). The width of the insulating barrier of the junction limits the maximum supercurrent that can flow across the junction, but introduces no resistance in the flow. Josephson also predicted that, in the case a constant finite voltage V is established across the junction, an alternating supercurrent $I_J \sin(\omega_J + \phi_0)$ flows with frequency $\omega_J = 2eV/\hbar$ (ac Josephson effect).

We discuss here only the most elementary aspects of this subject, remarkable both for its fundamental aspects and technological applications.

Consider two superconductors separated by a thin insulating barrier of

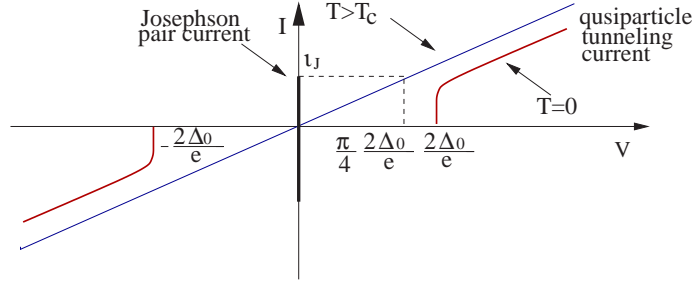


Figure 3.1: Schematic representation of the direct current $I - V$ characteristics (at $T = 0$) of a superconductor-insulator-superconductor junction displaying the Josephson current. For $V = 0$ a direct supercurrent can flow (up to a maximum value I_J). For $0 < V < 2\Delta_0/e$ an alternate supercurrent flows with frequency $\omega = 2eV/\hbar$, and no direct supercurrent is observed. For $V > 2\Delta_0/e$ the quasiparticle tunnelling current is reported.

width b . In the case the insulating barrier is infinitely thick, the superconductor on the left side would be characterized by the order parameter ψ_1 , that can be written as

$$\psi_1 = |\psi_1|e^{i\theta_1} \quad (3.1)$$

with $|\psi_1|$ and θ_1 uniform on the whole volume of superconductor 1. Similarly the superconductor on the right side would be characterized by the order parameter

$$\psi_2 = |\psi_2|e^{i\theta_2} \quad (3.2)$$

with $|\psi_2|$ and θ_2 space independent on the volume of superconductor 2. When the two superconductors are separated by a thin insulating barrier, we can expect that the superconducting order parameters ψ_1 and ψ_2 decay within the insulating region; we can guess that the order parameter $\psi(z)$ within the barrier can be expressed in the form

$$\psi(z) = \psi_1 e^{-\beta z} + \psi_2 e^{+\beta(z-b)}, \quad (3.3)$$

where β characterizes the damping within the barrier.

Using this all in the macroscopic Ginzburg-Landau theory we obtain for the current density

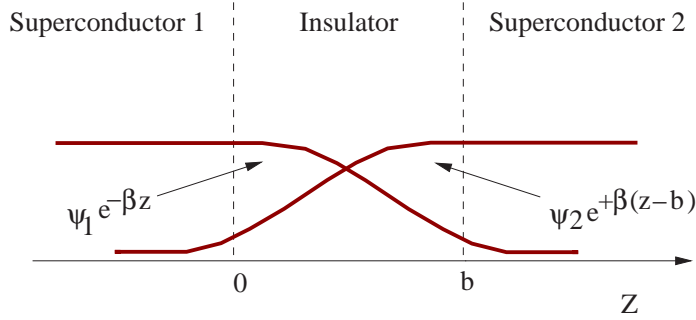


Figure 3.2: Schematic representation of a junction between two superconductor separated by a thin barrier of width b . The behavior of the order parameter wavefunction for the superconductor-insulator-superconductor junction is indicated

$$J_S(z) = \frac{2\hbar e}{2m} \beta e^{-\beta b} |\psi_1| |\psi_2| \sin(\theta_2 - \theta_1) \quad (3.4)$$

We thus see that the Josephson supercurrent, that flows between two superconductors separated by an insulating barrier, is related to the phase difference $\gamma = \theta_2 - \theta_1$ of the order parameters in the two superconductors by the relation

$$I = I_J \sin(\gamma) \quad (3.5)$$

where I_J depends on the geometrical and physical properties of the junction. Equation (3.5) has been derived on the basis of the heuristic approach. At detailed analysis based on the microscopic BCS theory provides not only equation (3.5), but also the maximum current $I = I_J$, which can flow across the junction without dissipation. The critical value I_J of an ideal SIS two tunnel junction is given by the current that would flow applying a voltage equal to $(\pi/4)(2\Delta/e)$ to the normal junction, in the same geometrical conditions. Notice finally that our treatment assumes that the magnetic field flux that threads the junction is negligible; in general, the dependence of I_J on the magnetic field (diffractive pattern) should be appropriately considered.

Consider now a superconducting junction biased with a (constant or time dependent) voltage V . If a potential difference is established between the two superconductors, the relative energy difference between Cooper

pairs belonging to different superconductors is $2eV$. In perfect analogy with the quantum mechanical rate of change of phases of ordinary eigenfunctions (energy divided by \hbar), we expect for the time variation of the relative phase

$$\frac{d\gamma}{dt} = \frac{2eV}{\hbar} \quad (3.6)$$

It is now easy to see that the above equations describe both the dc Josephson effect as well as the ac Josephson effect.

If the potential V across the SIS junction is zero, we see from equation (3.6) that γ is constant; from equation (3.5) we have that any supercurrent with intensity ranging from $-I_J$ to $+I_J$ can flow through the junction (the actual value is determined by the external circuit); this is the origin of the zero resistance spike at $V = 0$ in the $I-V$ characteristics for a Josephson junction.

Suppose that a constant potential V ($0 < V < 2\Delta/e$) is established across the SIS junction (for simplicity we assume that an ideal voltage source maintains a constant voltage V across the SIS junction; this independently from the normal current that could be flowing through the circuit). Integration of equation (3.6) gives

$$\gamma(t) = \frac{2eV}{\hbar}t + \gamma_0 \quad (3.7)$$

The phase difference is the linear function of time and the Josephson current is

$$I = I_J \sin\left(\frac{2eV}{\hbar}t + \gamma_0\right) \quad (3.8)$$

This pair current is oscillatory with angular frequency $\omega_J = 2\pi\nu_J = (2e/\hbar)V$. The frequency ν_J can be expressed as

$$\nu_J = \frac{2e}{\hbar}V = 483.6MHz \cdot \frac{V}{\mu\text{volt}} \quad (3.9)$$

where V is measured in microvolt. So an alternating current of frequency $483.6MHz \cdot \frac{V}{\mu\text{volt}}$ is expected to flow for $V \neq 0$, while for $V = 0$, a steady current is expected, according to (3.5).

3.2 Calculation of the Josephson current trough a single level dot

In this section we will calculate the Josephson current (in the meaning of travelling Cooper pairs) trough the transistor having the island which is a single level dot. This time we will take into account the Coulomb interactions between the electrons travelling trough the dot.

The model Hamiltonian is the same as usual:

$$H = H_0 + H_T \quad (3.10)$$

$$H_0 = H_L + H_R + H_D \quad (3.11)$$

where

$$H_L = \sum_{l\sigma} \xi_l a_{l\sigma}^\dagger a_{l\sigma} - \sum_l \Delta_l a_{l\uparrow}^\dagger a_{-l\downarrow}^\dagger - \sum_l \Delta_l a_{-l\downarrow} a_{l\uparrow} \quad (3.12)$$

$$H_R = \sum_{r\sigma} \xi_r b_{r\sigma}^\dagger b_{r\sigma} - \sum_r \Delta_r b_{r\uparrow}^\dagger b_{-r\downarrow}^\dagger - \sum_r \Delta_r b_{-r\downarrow} b_{r\uparrow} \quad (3.13)$$

$$H_D = \xi_D \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + U n_{\uparrow} n_{\downarrow} \quad (3.14)$$

The left and right lead are superconducting so that we need to use the superconducting Hamiltonians, the dot is single level and we take into account that when is double occupied there is a repulsive energy U that highers the energy state of the island itself.

$$\begin{aligned} H_T &= H_T^+ + H_T^- \\ H_T^+ &= (H_T^-)^\dagger = H_{TL}^+ + H_{TR}^+ \\ H_{TL}^+ &= \sum_{l\sigma} t_l d_{\sigma}^\dagger a_{l\sigma} e^{i\phi/2} \end{aligned}$$

So that the total tunnelling Hamiltonian is

$$H_T = \sum_{l\sigma} [t_l d_{\sigma}^\dagger a_{l\sigma} e^{i\phi/2} + H.c.] + \sum_{r\sigma} [t_r d_{\sigma}^\dagger b_{r\sigma} e^{i\theta/2} + H.c.] \quad (3.15)$$

We absorb the phase dependence of the Hamiltonian in the tunnelling matrix element $t_{l,r}$ so that the tunnelling Hamiltonian becomes

$$H_T = \sum_{l\sigma} [t_l d_{\sigma}^\dagger a_{l\sigma} + H.c.] + \sum_{r\sigma} [t_r d_{\sigma}^\dagger b_{r\sigma} + H.c.] \quad (3.16)$$

where now $t_l = t_l e^{i\phi/2}$ and $t_r = e^{i\theta/2}$

We denote H_T^+ the part of the tunnelling Hamiltonian that tunnels an electron on the dot and H_T^- the one that lowers the number of electrons on the dot.

As in the previous chapter we denote the operators relating to the left lead with a or α (the first one is the normal particle operator and the second one is the quasiparticle operator of the BCS theory), the operators relating to the right lead with b or β and the operators relating to the dot with d . To notice is that we have written explicitly the phase dependence of the operators.

By definition the current is

$$I = i\langle H_{T\alpha}^+ - H_{T\alpha}^- \rangle = -2Im\langle H_{T\alpha}^+ \rangle = 2Im\langle H_{T\alpha}^- \rangle \quad (3.17)$$

where α is either left or right. We work with H_{TL}^+

Using now imaginary time theory we have

$$\langle H_{TL}^+ \rangle = \frac{1}{Z} Tr\{e^{-\beta H} H_{TL}^+\} = \frac{1}{Z} Tr\{e^{-\beta H_0} U(\beta, 0) H_{TL}^+\} = \langle U(\beta, 0) H_{TL}^+ \rangle_0 \quad (3.18)$$

where U is the time evolution operator in the interaction picture and its full form is given by

$$U(\tau, \tau') = \sum_{n=0}^{\infty} \frac{1}{n!} (-1)^n \int_{\tau'}^{\tau} d\tau_1 \cdots \int_{\tau'}^{\tau} d\tau_n T_{\tau}(H_T(\tau_1) \cdots H_T(\tau_n)) \quad (3.19)$$

where all the operators are now in the interaction picture form and where T_{τ} is the time-ordering operator.

We want to find the Josephson current through the dot, this means that we want four particles to pass across the dot. This implies that the first nonzero term for the Josephson current is given by a fourth order perturbation theory. Or also we realize that since we need four steps for the travelling electrons we need to use the tunnelling Hamiltonian four times. We then write

$$\langle H_{TL}^+ \rangle = -\frac{1}{3!} \int_0^{\beta} d\tau_1 \int_0^{\beta} d\tau_2 \int_0^{\beta} d\tau_3 \langle T_{\tau}(H_T(\tau_1) H_T(\tau_2) H_T(\tau_3) H_{TL}^+(0)) \rangle_0 \quad (3.20)$$

As we said we want the electrons to pass trough and the term in the bracket gives three equivalent ways of doing it, either considering

$$H^+H^-H^-H^+ \quad \text{or} \quad H^-H^+H^-H^+ \quad \text{or} \quad H^-H^-H^+H^+.$$

This gives a factor of three to the integral.

We need now to evaluate the bracket and the the integral. We begin with the evaluation of the bracket.

We already said that the terms needed are in the form $H^+H^-H^-H^+$, in particular we look for pairs tunnelling from the left lead to the right lead, this means that what we actually are going to study is the reduced term

$$H_{TL}^+(\tau_1)H_{TR}^-(\tau_2)H_{TR}^-(\tau_3)H_{TL}^+(0) \quad (3.21)$$

where we wrote also the time dependence as appearing in (3.20).

The evaluation of $\langle H_{TL}^+(\tau_1)H_{TR}^-(\tau_2)H_{TR}^-(\tau_3)H_{TL}^+(0) \rangle_0$ is just a matter of simple mathematics and gives the result

$$\begin{aligned} H_{TL}^+(\tau_1)H_{TR}^-(\tau_2)H_{TR}^-(\tau_3)H_{TL}^+(0) = & \\ & \sum_{\substack{l \sigma_1 \\ r \sigma_2 \\ f \sigma_3 \\ p \sigma_0}} t_l t_p t_r^* t_g^* a_{l\sigma_1}(\tau_1) a_{p\sigma_0}(0) \\ & \times b_{r\sigma_2}^\dagger(\tau_2) b_{f\sigma_3}^\dagger(\tau_3) \\ & \times d_{\sigma_1}^\dagger(\tau_1) d_{\sigma_2}(\tau_2) d_{\sigma_3}(\tau_3) d_{\sigma_0}^\dagger(0) \quad (3.22) \end{aligned}$$

where we moved the operators referring to same part of the system all together. This can be done the average we are about to take is in respect of H_0 . H_0 is the Hamiltonian of the non-interacting subsystems. This means that the three Hamiltonian commute and also he operators referring to different subsystem.

Now we need to take the thermal (time ordered) average of this quantity. To do so we already notice that the average is taken in respect of H_0 in which the subsystem's Hamiltonians commute meaning that the three subsystems (left lead, dot and right lead) are independent in that approximation. This allows us to take three different thermal average on the three different subsystem. Furthermore we notice that the thermal

average taken on the superconducting parts leads us to the anomalous Green's functions

$$\begin{aligned}
\left\langle T_\tau \left(c_{-k\downarrow}^\dagger(\tau) c_{k\uparrow}^\dagger \right) \right\rangle &= \left\langle T_\tau \left(c_{k\uparrow}(-\tau) c_{-k\downarrow} \right) \right\rangle^\dagger \\
&= [\mathcal{G}(E_k, \tau) + \mathcal{G}(E_k, -\tau)] \frac{\Delta_k}{2E_k} \\
&= \frac{\Delta_k}{2E_k} [(\theta(\tau) - n_F(E_k))e^{-E_k\tau} + (\theta(-\tau) - n_F(E_k))e^{E_k\tau}] \\
&= \frac{\Delta_k}{2E_k} [e^{-E_k|\tau|} - 2 \cosh(E_k\tau) n_F(E_k)] \\
&\equiv \frac{\Delta_k}{2E_k} f_k(\tau) = (\mathcal{F}_{\uparrow\downarrow}(\tau, k))^\dagger
\end{aligned}$$

This anomalous Green's function have many useful symmetry properties

$$\begin{aligned}
\mathcal{F}_{\downarrow\uparrow}(\tau - \tau', k) &= \langle T_\tau (c_{-k\downarrow}(\tau) c_{k\uparrow}(\tau')) \rangle = - \langle T_\tau (c_{k\uparrow}(\tau) c_{-k\downarrow}(\tau')) \rangle = -\mathcal{F}_{\uparrow\downarrow}(\tau - \tau', k) \\
(\mathcal{F}_{\downarrow\uparrow})^\dagger(\tau - \tau', k) &= \left\langle T_\tau \left(c_{k\uparrow}^\dagger(\tau) c_{-k\downarrow}^\dagger(\tau') \right) \right\rangle \\
\mathcal{F}_{\downarrow\uparrow} &= (\mathcal{F}_{\downarrow\uparrow})^\dagger = -\mathcal{F}_{\uparrow\downarrow} = -(\mathcal{F}_{\uparrow\downarrow})^\dagger
\end{aligned}$$

As we see from the above expression for the anomalous Green's functions, to have nonzero terms in our thermal average we choose

$$\begin{aligned}
p &= -l & \sigma_0 &= \overline{\sigma}_1 \\
f &= -r & \sigma_3 &= \overline{\sigma}_2
\end{aligned}$$

We notice also that for spin symmetry we can choose $\sigma_1 = \downarrow$ and have a factor of 2 for the integral, in the same way we can choose $\sigma_2 = \uparrow$ and have a second factor 2.

Gathering all this information together we have, so far

$$\begin{aligned}
\langle H_{TL}^+ \rangle &= -2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \\
&\quad \times \sum_{\substack{l \downarrow \\ r \uparrow}} t_l t_{-l} t_r^* t_{-r}^* \\
&\quad \times \mathcal{F}_{\downarrow\uparrow}(l, \tau_1) (\mathcal{F}_{\downarrow\uparrow})^\dagger(r, \tau_2 - \tau_3) \\
&\quad \times \left\langle T_\tau \left(d_\downarrow^\dagger(\tau_1) d_\uparrow(\tau_2) d_\downarrow(\tau_3) d_\uparrow^\dagger(0) \right) \right\rangle_0 \quad (3.23)
\end{aligned}$$

We proceed in the evaluation of the (time ordered) thermal average. The evaluation of the thermal average is carried out in the following way

$$\langle \mathcal{O} \rangle_0 = \frac{1}{Z} \sum_{states} \langle \Psi | e^{-\beta H_0} \mathcal{O}(t) | \Psi \rangle$$

where the states $|\Psi\rangle$ form a s.o.n.c. for the Hilbert space we are working in. We also have written the time or imaginary time dependence of the operator ($t = t$ or τ). We remind that through all this calculation we are working with imaginary time and in the interaction picture so that

$$\begin{cases} \text{states:} & |\hat{\psi}(\tau)\rangle & = e^{\tau H_0} |\psi(\tau)\rangle \\ \text{operators:} & \hat{A}(\tau) & = e^{\tau H_0} A e^{-\tau H_0} \end{cases}$$

where H_0 does not depend on time.

We remind also the relations

$$\begin{aligned} |0\rangle &= c_\uparrow c_\downarrow | \downarrow \uparrow \rangle \\ | \downarrow \uparrow \rangle &= c_\downarrow^\dagger c_\uparrow^\dagger |0\rangle \\ | \downarrow \uparrow \rangle &= - | \uparrow \downarrow \rangle \end{aligned}$$

We can easily find the eigenstates and the eigenfunctions of the system we are dealing with:

$$\text{eigenstates} \quad |0\rangle \quad | \uparrow \rangle \quad | \downarrow \rangle \quad | \uparrow \downarrow \rangle \quad (3.24)$$

$$\text{eigenvalue} \quad 0 \quad \varepsilon \quad \varepsilon \quad 2\varepsilon + U \quad (3.25)$$

For the time ordering operator we need to carry out six different thermal averages

$$0 < \tau_3 < \tau_2 < \tau_1 \implies + \left\langle d_\downarrow^\dagger(\tau_1) d_\uparrow(\tau_2) d_\downarrow(\tau_3) d_\uparrow^\dagger \right\rangle_0 \quad (3.26a)$$

$$0 < \tau_2 < \tau_3 < \tau_1 \implies - \left\langle d_\downarrow^\dagger(\tau_1) d_\downarrow(\tau_3) d_\uparrow(\tau_2) d_\uparrow^\dagger \right\rangle_0 \quad (3.26b)$$

$$0 < \tau_3 < \tau_1 < \tau_2 \implies - \left\langle d_\uparrow(\tau_2) d_\downarrow^\dagger(\tau_1) d_\downarrow(\tau_3) d_\uparrow^\dagger \right\rangle_0 \quad (3.26c)$$

$$0 < \tau_1 < \tau_3 < \tau_2 \implies + \left\langle d_\uparrow(\tau_2) d_\downarrow(\tau_3) d_\downarrow(\tau_1)^\dagger d_\uparrow^\dagger \right\rangle_0 \quad (3.26d)$$

$$0 < \tau_2 < \tau_1 < \tau_3 \implies + \left\langle d_\downarrow(\tau_3) d_\downarrow^\dagger(\tau_1) d_\uparrow(\tau_2) d_\uparrow^\dagger \right\rangle_0 \quad (3.26e)$$

$$0 < \tau_1 < \tau_2 < \tau_3 \implies - \left\langle d_\downarrow(\tau_3) d_\uparrow(\tau_2) d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger \right\rangle_0 \quad (3.26f)$$

We find the results

$$0 < \tau_3 < \tau_2 < \tau_1 \implies \langle \dots \rangle = -\frac{1}{Z} e^{\beta\varepsilon} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{-\tau_3 U} \quad (3.27a)$$

$$0 < \tau_2 < \tau_3 < \tau_1 \implies \langle \dots \rangle = -\frac{1}{Z} e^{\beta\varepsilon} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{-\tau_2 U} \quad (3.27b)$$

$$0 < \tau_3 < \tau_1 < \tau_2 \implies \langle \dots \rangle = -\frac{1}{Z} e^{\beta\varepsilon} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{(\tau_1 - \tau_2 - \tau_3)U} \quad (3.27c)$$

$$0 < \tau_2 < \tau_1 < \tau_3 \implies \langle \dots \rangle = \frac{1}{Z} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} \quad (3.27d)$$

$$0 < \tau_1 < \tau_3 < \tau_2 \implies \langle \dots \rangle = \frac{1}{Z} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{(\tau_1 - \tau_3)U} \quad (3.27e)$$

$$0 < \tau_1 < \tau_2 < \tau_3 \implies \langle \dots \rangle = \frac{1}{Z} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{(\tau_1 - \tau_3)U} \quad (3.27f)$$

Where Z is the partition function $Z = \sum_{states} \langle \Psi | e^{-\beta H_0} | \Psi \rangle$ and its value is

$$Z = 1 + 2e^{-\beta\varepsilon} + e^{-\beta(2\varepsilon+U)} \quad (3.28)$$

We can clearly see that (3.27a) and (3.27b) are equal if we exchange τ_2 with τ_3 and also (3.27e) and (3.27f) if again we exchange τ_2 with τ_3 . We label the previous results as follows

$$D_1 = \begin{cases} -e^{\beta\varepsilon} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{-\tau_3 U} \\ -e^{\beta\varepsilon} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{-\tau_2 U} \end{cases}$$

$$D_3 = -e^{\beta\varepsilon} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{(\tau_1 - \tau_2 - \tau_3)U}$$

$$D_5 = e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)}$$

$$D_4 = \begin{cases} e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{(\tau_1 - \tau_3)U} \\ e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} e^{(\tau_1 - \tau_3)U} \end{cases}$$

At this point we need to calculate

$$\begin{aligned} \langle H_{TL}^+ \rangle &= -2 \frac{1}{Z} \sum_i \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 D_i \\ &\quad \times \sum_{\substack{l \downarrow \\ r \uparrow}} t_l t_{-l} t_r^* t_{-r}^* \mathcal{F}_{\downarrow \uparrow}(l, \tau_1) (\mathcal{F}_{\downarrow \uparrow})^\dagger(r, \tau_2 - \tau_3) \end{aligned}$$

We now calculate the sums in the energy space.

$$\begin{aligned}
\sum_{l\downarrow} t_l t_{-l} \mathcal{F}_{\downarrow\uparrow}(l, \tau_1) &\longleftrightarrow (t_l)^2 \rho(E_F) \int_{\Delta_l}^{\infty} dE_l \frac{E_l}{\sqrt{E_l^2 - \Delta_l^2}} \mathcal{F}_{\downarrow\uparrow}(l, \tau_1) \\
&= (t_l)^2 \rho(E_F) (-) \frac{\Delta_l}{2} \int_{\Delta_l}^{\infty} dE_l \frac{1}{\sqrt{E_l^2 - \Delta_l^2}} f_k(\tau) \\
&\text{in the limit } \Delta\beta \gg 1 \\
&\simeq (t_l)^2 \rho(E_F) \frac{\Delta_l}{2} \int_{\Delta_l}^{\infty} dE_l \frac{1}{\sqrt{E_l^2 - \Delta_l^2}} [e^{-E_l(\beta - |\tau_1|)} - e^{-E_l|\tau_1|}] \\
&= (t_l)^2 \rho(E_F) \frac{\Delta_l}{2} [K_0(\Delta_l(\beta - |\tau_1|)) - K_0(\Delta_l|\tau_1|)]
\end{aligned}$$

where K_0 is the modified Bessel function of the second kind.

Concluding we need to calculate

$$\begin{aligned}
\langle H_{TL}^+ \rangle &= -\frac{1}{2Z} \rho_l(E_F) (t_l)^2 \Delta_l \rho_r(E_F) (t_r^*)^2 \Delta_r \sum_i \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 D_i \\
&\quad \times [K_0(\Delta_l(\beta - |\tau_1|)) - K_0(\Delta_l|\tau_1|)] \\
&\quad \times [K_0(\Delta_r(\beta - |\tau_2 - \tau_3|)) - K_0(\Delta_r|\tau_2 - \tau_3|)] \quad (3.29)
\end{aligned}$$

The integration can't be done analytically.

To work analytically we need to make some approximations on the system. Before we remind what we are looking for not to lose the general picture of the calculation.

$$I = -2\text{Im}\langle H_{TL}^+ \rangle \quad (3.30)$$

The first approximation we make is that the dot can't be double occupied. This corresponds to set $U = +\infty$. Given this approximation the only nonzero term in the dot thermal average which survives is the term denoted by $D_5 = e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)}$ and the partition function reduces to $Z = 1 + 2e^{-\beta\varepsilon}$

The calculation to be done is now

$$\begin{aligned} \langle H_{TL}^+ \rangle &= -\frac{2}{Z} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \\ &\quad \times \sum_{\substack{l \downarrow \\ r \uparrow}} t_l t_{-l} t_r^* t_{-r}^* \\ &\quad \times \mathcal{F}_{\downarrow \uparrow}(l, \tau_1) (\mathcal{F}_{\downarrow \uparrow})^\dagger(r, \tau_2 - \tau_3) \\ &\quad \times e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} \end{aligned} \quad (3.31)$$

This gives

$$I_\alpha = 2 \operatorname{Im} \sum_l t_r^* t_{-r}^* t_{-l} t_l \frac{\Delta_l \Delta_r}{4E_l E_r} \mathcal{C} \quad (3.32)$$

where

$$\begin{aligned} \mathcal{C} &= \frac{1}{Z} \int_0^\beta d\tau_3 \int_0^{\tau_3} d\tau_1 \int_0^{\tau_1} d\tau_2 e^{\varepsilon(\tau_1 - \tau_3 - \tau_3)} \\ &\quad \times [(\theta(\tau_1) - n_F(E_l))e^{-E_l \tau_1} + (\theta(-\tau_1) - n_F(E_l))e^{E_l \tau_1}] \\ &\quad \times [(\theta(\tau) - n_F(E_r))e^{-E_r(\tau_2 - \tau_3)} + (\theta(-\tau_2 - \tau_3) - n_F(E_r))e^{E_r(\tau_2 - \tau_3)}]. \end{aligned} \quad (3.33)$$

The time integral can be carried out analytically using the full anomalous Green's functions and gives a long unreadable result. To make the result more friendly we work in the limit $E_{l,r}\beta > \Delta_{l,r} \gg 1$ so that we can set $e^{-\beta E_{l,r}} \rightarrow 0$.

Performing the integrals and letting $e^{-E_{l,r}\beta} \rightarrow 0$, we find

$$\begin{aligned} C &= \frac{2 e^{-\beta \xi}}{1 + 2e^{-\beta \xi}} \frac{\xi(E_p + E_k)(1 + e^{\beta \xi}) + (E_k E_p + \xi^2)(1 - e^{\beta \xi})}{(E_p + E_k)(E_k^2 - \xi^2)(E_p^2 - \xi^2)} \\ &= \frac{2 e^{-\beta \xi}}{1 + 2e^{-\beta \xi}} \left(-\frac{e^{\beta \xi}}{(E_p + E_k)(E_k + \xi)(E_p + \xi)} + \frac{1}{(E_p + E_k)(E_k - \xi)(E_p - \xi)} \right). \end{aligned} \quad (3.34)$$

The current is then

$$I = \frac{\Gamma^L \Gamma^R \Delta_L \Delta_R}{2\pi^2} H(\xi) \sin \varphi, \quad (3.35)$$

where the sin dependence comes from taking the imaginary part of the average. $\varphi = \phi - \theta$ results from the factor $(t_l)^2(t_r^*)^2$. We also assume that the tunnelling matrix depends weakly on the states l or $-l$ so that $t_l = t_{-l}$.

At $T = 0$, this reduces to

$$C = \begin{cases} -\frac{2}{(E_p+E_k)(E_k+\xi)(E_p+\xi)} & \text{for } \xi > 0, \\ \frac{1}{(E_p+E_k)(E_k-\xi)(E_p-\xi)} & \text{for } \xi < 0, \end{cases} \quad (3.36)$$

yielding

$$H(\xi) = \begin{cases} -2h(\xi) & \text{for } \xi > 0, \\ h(-\xi) & \text{for } \xi < 0, \end{cases} \quad (3.37)$$

where

$$h(\xi) = \frac{2\text{ArcSin } \xi \cdot \text{ArcTan} \left(\sqrt{\frac{1-\xi}{1+\xi}} \right)}{\xi(1-\xi^2)} - \frac{1}{4\xi(1-\xi^2)} \left(\pi^2\xi + 2\text{Li}_2(-\xi - i\sqrt{1-\xi^2}) \right. \\ \left. - 2\text{Li}_2(\xi - i\sqrt{1-\xi^2}) + 2\text{Li}_2(-\xi + i\sqrt{1-\xi^2}) - 2\text{Li}_2(\xi + i\sqrt{1-\xi^2}) \right) \quad (3.38)$$

with

$$\text{Li}_2(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^2}. \quad (3.39)$$

For $\beta\Delta \gg 1$ and $\beta\xi \simeq 1$ the integration gives ($h(0) = \pi - \pi^2/4$)

$$H(0) = \frac{2(e^{-\beta\xi} - 1)}{1 + 2e^{-\beta\xi}} \int d\varepsilon d\varepsilon' \frac{1}{(E + E')E^2E'^2} = \frac{2(e^{-\beta\xi} - 1)}{1 + 2e^{-\beta\xi}} \left(\pi - \frac{\pi^2}{4} \right). \quad (3.40)$$

The following is the plot of (3.40). Further results will be given at the end of next chapter where we include the phonon bath.

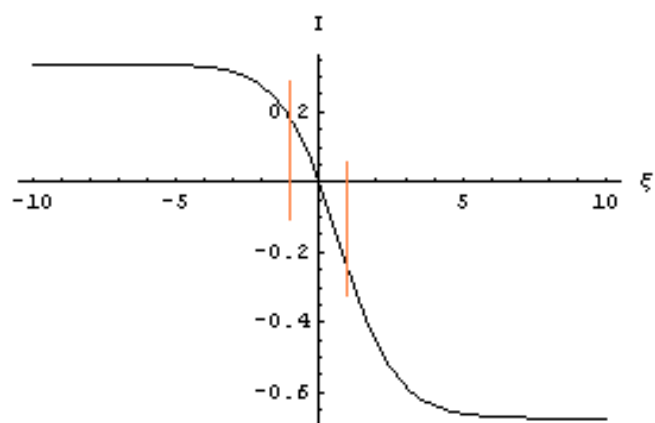


Figure 3.3: The orange lines set the valid limit for this result: $\beta\xi \simeq 1$

Chapter 4

Josephson current through a single level oscillating dot

4.1 Oscillating dot

A step further in the understanding of the system is to let the dot oscillate. This is done adding the coupling to a one-mode phonon bath. The Hamiltonian is then

$$H = H_L + H_R + H_D + H_{DB} + H_B + H_T \quad (4.1)$$

where $H_L + H_R + H_D + H_T$ are as in the previous chapter and

$$H_{DB} = \lambda x_0 (n_\uparrow + n_\downarrow) \quad (4.2)$$

$$H_B = \omega_0 \left(c^\dagger c + \frac{1}{2} \right) \quad (4.3)$$

where H_B is the phonon bath and H_{DB} resembles the force acting on the charged dot (originating for example by image charges). To see it more clearly we can rewrite last term as

$$H_{DB} = \lambda \frac{\ell_0}{\sqrt{2}} (c + c^\dagger) (n_\uparrow + n_\downarrow) \quad \ell_0 = \sqrt{\frac{\hbar}{\omega_0}} \quad (4.4)$$

this means that the force is felt by the dot only when either n_\uparrow or n_\downarrow are different from zero (which means that the dot is charged) and that this

force is associated with the creation or annihilation of a phonon. This is the coupling Hamiltonian between the phonon bath and λ sets the strength of this coupling. We denote as c and c^\dagger the boson annihilation and creation operators.

We eliminated the coupling term H_{DB} of the Hamiltonian by a unitary transformation similar to the one used in the independent phonon model [7], at the cost of introducing displacement operators in the tunnelling term. However, since we are dealing with a somewhat more complicated system due to the coupling to the bosonic bath, the unitary transformation has to be generalized as in [4]. We define the transformation

$$\tilde{H} = e^s H e^{-s} \quad s = -ilp_0 n_d \quad \ell = \frac{\lambda}{m_0 \omega_0^2} \quad n_d = n_\uparrow + n_\downarrow \quad (4.5)$$

We remember the equalities

$$\begin{aligned} \tilde{A} &= e^s A e^{-s} = A + [s, A] + \frac{1}{2!} [s, [s, A]] + \frac{1}{3!} [s, [s, [s, A]]] + \dots \\ [p_0, x_0] &= \frac{\hbar}{i} \quad p_0 = i(a^\dagger - a)/(\ell_0 \sqrt{2}) \quad \text{we set} \quad \hbar = 1 \end{aligned}$$

Given these we calculate

$$\begin{aligned} \tilde{d}_\sigma &= e^s d_\sigma e^{-s} = d_\sigma + [s, d_\sigma] + \frac{1}{2!} [s, [s, d_\sigma]] + \frac{1}{3!} [s, [s, [s, d_\sigma]]] \dots \\ [s, d_\sigma] &= -il[p_0 n_d, d_\sigma] = ilp_0 d_\sigma \\ [s, ilp_0 d_\sigma] &= (il)^2 p_0^2 d_\sigma \\ \Rightarrow \tilde{d}_\sigma &= d_\sigma + ilp_0 d_\sigma + \frac{(ilp_0)^2}{2!} d_\sigma + \frac{(ilp_0)^3}{3!} d_\sigma \dots \end{aligned}$$

then

$$\tilde{d}_\sigma = e^{ilp_0} d_\sigma \quad (4.6)$$

$$\tilde{d}_\sigma^\dagger = e^{-ilp_0} d_\sigma^\dagger \quad (4.7)$$

$$\tilde{x}_0 = e^s x_0 e^{-s} = x_0 + [s, x_0] + \frac{1}{2!} [s, [s, x_0]] + \frac{1}{3!} [s, [s, [s, x_0]]] + \dots \quad (4.8)$$

$$[s, x_0] = -il[p_0 n_d, x_0] = -\ell n_d \quad (4.9)$$

$$[s, -\ell n_d] = -\ell [p_0 n_d, n_d] = 0 \quad (4.10)$$

then

$$\tilde{x}_0 = x_0 - \ell n_d \quad (4.11)$$

analogously we find

$$\tilde{p}_0 = p_0 \quad (4.12)$$

Inserting the new operators in the Hamiltonian we find

$$\tilde{H}_L = H_L \quad \tilde{H}_R = H_R$$

the leads don't feel the phonon-coupling Hamiltonian

$$\tilde{H}_D = H_D = \xi_0(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$$

$$\tilde{H}_T = \sum_{l\sigma} (t_l e^{-ip_0 \ell} d_\sigma^\dagger a_{l\sigma} + H.C) + \sum_{r\sigma} (t_r e^{-ip_0 \ell} d_\sigma^\dagger b_{r\sigma} + H.c.)$$

$$\tilde{H}_{DB} = \lambda(x_0 - \ell n_d) = \lambda x_0 n_d - \ell \lambda n_d^2$$

$$\tilde{H}_B = \frac{p_0^2}{2} + \frac{1}{2} \omega_0^2 (x_0 - \ell n_d)^2 = \frac{p_0^2}{2m_0} + \frac{1}{2} \omega_0^2 m_0 x_0^2 - m_0 \omega_0^2 x_0 \ell n_d + \frac{1}{2} m_0 \omega_0^2 \ell^2 n_d^2.$$

We want to get rid of the Hamiltonian term H_{DB} , for this purpose we see that we need to set

$$\ell = \frac{\lambda}{m_0 \omega_0} \quad (4.13)$$

If we now set

$$\tilde{\xi}_0 = \xi_0 - \frac{\lambda \ell}{2} \quad \tilde{U} = U - \lambda \ell$$

$$\tilde{H}_D = \tilde{\xi}_0 (n_\uparrow + n_\downarrow) + \tilde{U} n_\uparrow n_\downarrow$$

The Hamiltonian is

$$\tilde{H} = H_L + H_R + \tilde{H}_D + \tilde{H}_T + H_B \quad (4.14)$$

We omit the superscript \sim for simplicity and we set

$$H_0 = \begin{cases} H_L & = \sum_{l\sigma} \xi_l a_{l\sigma}^\dagger a_{l\sigma} - \sum_l \Delta_l a_{l\uparrow}^\dagger a_{-l\downarrow}^\dagger - \sum_l \Delta_l a_{-l\downarrow} a_{l\uparrow} \\ H_R & = \sum_{r\sigma} \xi_r b_{r\sigma}^\dagger b_{r\sigma} - \sum_r \Delta_r b_{r\uparrow}^\dagger b_{-r\downarrow}^\dagger - \sum_r \Delta_r b_{-r\downarrow} b_{r\uparrow} \\ H_D & = \xi_0 \sum_\sigma d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow \\ H_B & = \omega_0 (c^\dagger c + \frac{1}{2}) \end{cases} \quad (4.15)$$

$$H_T = \sum_{l\sigma} [t_l e^{-ilp_0} d_\sigma^\dagger a_{l\sigma} + H.c.] + \sum_{r\sigma} [t_r e^{-ilp_0} d_\sigma^\dagger b_{r\sigma} + H.c.] \quad (4.16)$$

where again all the phase factors relay in the tunnelling matrix element. The calculation of the current is the same as in the previous chapter

$$I = i\langle H_{T\alpha}^+ - H_{T\alpha}^- \rangle = -2\text{Im}\langle H_{T\alpha}^+ \rangle = 2\text{Im}\langle H_{T\alpha}^- \rangle \quad (4.17)$$

but with an additional term related to the phonon part.

$$\begin{aligned} \langle H_{TL}^+ \rangle &= -2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \\ &\quad \times \sum_{\substack{l\downarrow \\ r\uparrow}} t_l t_{-l} t_r^* t_{-r}^* \\ &\quad \times \mathcal{F}_{\downarrow\uparrow}(l, \tau_1) (\mathcal{F}_{\downarrow\uparrow})^\dagger(r, \tau_2 - \tau_3) \\ &\quad \times \left\langle T_\tau \left(d_\downarrow^\dagger(\tau_1) d_\uparrow(\tau_2) d_\downarrow(\tau_3) d_\uparrow^\dagger(0) \right) \right\rangle_0 \\ &\quad \times \left\langle T_\tau \left(e^{-ilp_0(\tau_1)} e^{ilp_0(\tau_2)} e^{ilp_0(\tau_3)} e^{-ilp_0} \right) \right\rangle_0 \end{aligned} \quad (4.18)$$

$$G(\tau_1 \tau_2 \tau_3) = \left\langle T_\tau \left(e^{-ilp_0(\tau_1)} e^{ilp_0(\tau_2)} e^{ilp_0(\tau_3)} e^{-ilp_0} \right) \right\rangle_0$$

is evaluated using the Feynmann disentangling model (see for example [7]) and the result gives

$$\begin{aligned} G(\tau_1, \tau_2, \tau_3) &= \\ &\exp(-g(\tau_3 - \tau_2) + g(\tau_3 - \tau_1) + g(\tau_3) + g(\tau_2 - \tau_1) + g(\tau_2) - g(\tau_1)) \end{aligned} \quad (4.19)$$

where

$$\begin{aligned} g(\tau) &= \ell^2 \left(\langle T_\tau(p(\tau)p(0)) \rangle - \langle p^2 \rangle \right) = \\ &g \left(n_B(e^{\omega|\tau|} - 1) + (1 + n_B)(e^{-\omega|\tau|} - 1) \right), \end{aligned} \quad (4.20)$$

and

$$g = \frac{\ell^2}{2\ell_0^2}, \quad n_B = \frac{1}{e^{\beta\omega_0} - 1}. \quad (4.21)$$

We already performed the energy integration for the anomalous Green's functions with the result

$$\begin{aligned}
\sum_p t_{p\alpha}^* t_{-p\alpha}^* \frac{\Delta_{p\alpha}}{2E_{p\alpha}} f_{p\alpha}(\tau) &\approx e^{-i\phi_\alpha} t_\alpha^2 \rho \int d\varepsilon \frac{\Delta_\alpha}{2E} [e^{-E|\tau|} - e^{-E(\beta-|\tau|)}] \\
&= e^{-i\phi_\alpha} t_\alpha^2 \rho \int_{\Delta_\alpha}^{\infty} dE \frac{\Delta_\alpha}{\sqrt{E^2 - \Delta_\alpha^2}} [e^{-E|\tau|} - e^{-E(\beta-|\tau|)}] \\
&= e^{-i\phi_\alpha} \frac{\Gamma_\alpha \Delta_\alpha}{2\pi} [K_0(|\tau|\Delta_\alpha) - K_0((\beta - |\tau|)\Delta_\alpha)] \equiv e^{-i\phi_\alpha} \frac{\Gamma_\alpha \Delta_\alpha}{2\pi} H_\alpha(\tau),
\end{aligned} \tag{4.22}$$

where K_0 is the modified Bessel function of the second kind and α is either left(L) or right(R).

The final expression for the current thus reads

$$I = I_c \sin \varphi, \tag{4.23}$$

where

$$I_c = \frac{\Gamma_L \Gamma_R \Delta_L \Delta_R}{2\pi^2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 H_L(\tau_1) H_R(\tau_2 - \tau_3) B(\tau_1, \tau_2, \tau_3) G(\tau_1, \tau_2, \tau_3). \tag{4.24}$$

where we denoted

$$B(\tau_1, \tau_2, \tau_3) = \left\langle T_\tau \left(d_\downarrow^\dagger(\tau_1) d_\uparrow(\tau_2) d_\downarrow(\tau_3) d_\uparrow^\dagger(0) \right) \right\rangle_0 \tag{4.25}$$

This result generalizes the one found in chapter 3 where no phonon/vibron was present. Currently we are doing numerical integration of this result. We expect that the phonon coupling diminishes the Josephson current, but does not destroy it. This is interesting because it means that the phonon is part of the coherence process. However if the vibron is damped the damping might eventually destroy the coherence. Such an effect can also be calculated within the present formalism.

In figure 4.1 we show some of the $I_c - \xi$ characteristics. For the phonon contribution numerical integration has been done taking again the limit $B(\tau_1, \tau_2, \tau_3) = D_5$ which means that the dot can't be double occupied. We see that adding the phonon part the current amplitude is strongly decreased but still it is not destroyed.

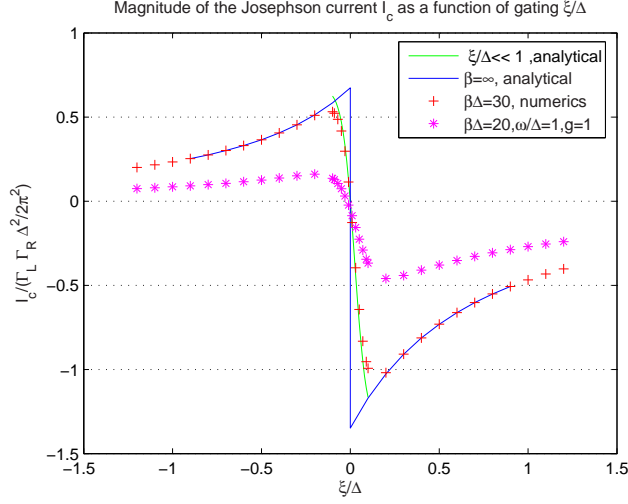


Figure 4.1: $I_c - \xi$ characteristics for the Josephson current with and without the phonon bath. The blue curve shows the analytical result of (3.37) in the previous chapter. The green curve represents (3.40) in its limit of validity as in figure 3.3. The red pluses denote instead the numerical integration of (3.34) which is quite accurate. The pink dotted line is with the contribution of the phonon bath. Courtesy of T. Novotný.

4.2 Independent boson model

The independent boson model is very important in many-body physics. It is an exactly solvable model which describes some relaxation phenomena. It has become very useful for describing a wide variety of effects in solid-state physics. We shall solve it by ordinary operator algebra.

The first Hamiltonian which will be solved is

$$H = c^\dagger c [\varepsilon_c + \sum_q M_q (a_q + a_q^\dagger)] + \sum_q \omega_q a_q^\dagger a_q \quad (4.26)$$

The Hamiltonian describes a fixed particle of energy ε_c interacting with a set of phonons with frequencies ω_q . The interaction occurs only when the state is occupied and $c^\dagger c = 1$. The phonons are independent bosons. By

making a canonical transformation, the Hamiltonian may be rewritten as

$$\bar{H} = c^\dagger c(\varepsilon_c - \Delta) + \sum_q \omega_q a_q^\dagger a_q$$

The solution to this problem is identical with the problem of charge on a harmonic spring in a uniform electric field. The electric field causes a displacement of the charge to a new equilibrium position, about which it vibrates with the same frequency as before.

The present objective is to obtain a better description of the fluctuations about equilibrium. To study relaxation effects, we shall also need to understand the fluctuations. This is obtained from the following Green's function,

$$G(t) = -i\langle T_c(t)c^\dagger(0)\rangle \quad (4.27)$$

where a full description of the time variation is needed. We shall solve this for the real-time Green's function. This is permissible in the present case because the single impurity state $c^\dagger c$ will not alter the photon energies. When we do the thermodynamic averaging over the photon state, the perturbation expansion for the $\exp(-\beta H)$ part. We begin to solve to the Green's function of time at its finite temperature.

4.2.1 Solution by Canonical Transformation

The Hamiltonian is first solved by a canonical transformation. A new Hamiltonian is desired by a transformation of the type

$$\bar{H} = e^s H e^{-s} = c^\dagger c(\varepsilon_c - \Delta) + \sum_q \omega_q a_q^\dagger a_q \quad (4.28)$$

The transformation must be done so that $s^\dagger = -s$. The transformation on any product of operators is done by taking the product of the transformed operators. The last assertion is shown by inserting $1 = e^{-s} e^s$ between each operator.

If we assume that any function of operators may be expressed as a power series, then the transformation on a function of operators is just the

function of the transformed operators:

$$e^s f(A) e^{-s} = e^s \sum_{n=0}^{\infty} a_n A^n e^{-s} = \sum_{n=0}^{\infty} a_n (\bar{A})^n = f(\bar{A}) \quad (4.29)$$

Thus we need to consider only the transformation on each operator separately, and the transformed Hamiltonian is the old one with the new operator. These are evaluated using

$$\begin{aligned} \bar{A} &= e^s A e^{-s} = A + [s, A] + \frac{1}{2!} [s, [s, A]] + \dots \\ s &= c^\dagger c \sum_q \frac{M_q}{\omega_q} (a_q^\dagger - a_q) \end{aligned}$$

which gives

$$\begin{aligned} \bar{c} &= cX \\ \bar{c}^\dagger &= c^\dagger X^\dagger \\ \bar{a} &= a - \frac{M_q}{\omega_q} c^\dagger c \\ \bar{a}^\dagger &= a^\dagger - \frac{M_q}{\omega_q} c^\dagger c \end{aligned}$$

We have introduced the operator

$$X = \exp \left[- \sum_q \frac{M_q}{\omega_q} (a_q^\dagger - a_q) \right] \quad (4.30)$$

Since this commutes with the c operator, then the number operator is the same in the new representation,

$$\bar{c}^\dagger \bar{c} = c^\dagger c X^\dagger X = c^\dagger c$$

since

$$X^\dagger = X^{-1}$$

The transformed Hamiltonian is

$$\begin{aligned} \bar{H} &= \varepsilon_c \bar{c}^\dagger \bar{c} + \sum_q \omega_q \left(a_q^\dagger - \frac{M_q}{\omega_q} c^\dagger c \right) \left(a_q - \frac{M_q}{\omega_q} c^\dagger c \right) \\ &\quad + \sum_q M_q \left(a_q + a_q^\dagger - 2 \frac{M_q}{\omega_q} c^\dagger c \right) c^\dagger c \end{aligned}$$

which is

$$\bar{H} = c^\dagger c(\varepsilon_c - \Delta) + \sum_q \omega_q a_q^\dagger a_q$$

This transformed Hamiltonian is precisely the form which was our objective. This transformation is now applied to the Green's function (4.27). The factor $1 = e^{-s}e^s$ is inserted into the trace, say for $t > 0$:

$$\text{Tr}(e^{-\beta H} e^{iHt} c e^{-itH} c^\dagger e^{-s} e^s)$$

Using the cyclic properties of the trace, we may alter this to

$$\text{Tr}(e^s e^{-\beta H} e^{iHt} c e^{-itH} c^\dagger e^{-s}) = \text{Tr}(e^{-\beta \bar{H}} e^{i\bar{H}t} \bar{c} e^{-it\bar{H}} \bar{c}^\dagger)$$

By using our previous theorems, we see that everything in the trace is now changed to the transformed representation. Thus the Green's function may be written as ($t > 0$)

$$G(t) = -ie^{\beta\Omega} \text{Tr}(e^{-\beta \bar{H}} e^{i\bar{H}t} \bar{c} e^{-i\bar{H}t} \bar{c}^\dagger)$$

It should be emphasized that this $G(t)$ will be exactly equal to the earlier definition. The new equation for $G(t)$ is just another way of evaluating the same thing. At first glance it appears that this evaluation is now trivial, since Hamiltonian is diagonal in the $\bar{c}^\dagger \bar{c}$ operators. But this is untrue and misleading, since \bar{c} and \bar{c}^\dagger do not commute with a or a^\dagger because of the factor X . Thus it is necessary to stick with the c and a representations and to put in X explicitly. The Green's function becomes

$$G(t) = -ie^{\beta\Omega} \text{Tr}(e^{-\beta \bar{H}} e^{i\bar{H}t} c X e^{-i\bar{H}t} c^\dagger X^\dagger)$$

However, it is now possible to achieve a great simplification. Since \bar{H} is diagonal in c and a , it is easy to commute it through cX and obtain the time development of the operators:

$$e^{i\bar{H}t} c X e^{-i\bar{H}t} = e^{it(\varepsilon_c - \Delta)} c X(t)$$

$$X(t) = \exp \left[- \sum_q \frac{M_q}{\omega_q} (a_q^\dagger e^{i\omega_q t} - a_q e^{-i\omega_q t}) \right]$$

The phonon and electron parts of the trace may now be completely separated

$$G(t) = -ie^{\beta\Omega}Tr(e^{-\beta\bar{\varepsilon}_c n}cc^\dagger)Tr[e^{-\beta\Sigma\omega_q n_q}X(t)X^\dagger(0)]$$

$$\bar{\varepsilon}_c = \varepsilon_c - \Delta$$

The result for $G(t)$ has great simplification mentioned above. The particle part is trivial (assuming they are fermions),

$$e^{\beta\Omega_{el}}Tr(e^{-\beta n\varepsilon_c}cc^\dagger) = 1 - n_F(\bar{\varepsilon}_c)$$

so that there remains only the problem of evaluating the photon part of the trace. This evaluation is nontrivial, although it may be done exactly. The method we shall use was introduced by Feynman(1951).

4.2.2 Feynman disentangling of operators

The objective now is to evaluate the trace over the phonon distributions of the operator:

$$F(t) = e^{\beta\Omega_{ph}}Tr[e^{-\Sigma\mathbf{q}\beta n\mathbf{q}\omega\mathbf{q}}X(t)X^\dagger(0)]$$

Each wave vector state q is averaged independently, and the final result is the product over \mathbf{q} states:

$$F(t) = \prod_q F_q(t) \quad (4.31)$$

$$F_q(t) = e^{\beta n_q \Omega_q} Tr \{ e^{-\beta n_q \omega_q} \exp[(-M_q/\omega_q)(a_q^\dagger e^{i\omega_q t} - a_q e^{-i\omega_q t})] e^{(M_q/\omega_q)(a_q^\dagger - a_q)} \} \quad (4.32)$$

For each state q , the trace is merely a summation over all possible integer values of n_q between zero and infinity,

$$e^{\beta\Omega_q}Tr() = (1 - e^{-\beta\omega_q}) \sum_{n_q=0}^{\infty} \langle n_q | () | n_q \rangle$$

where the prefactor is the normalization:

$$e^{\beta\Omega_q} = \left(\sum_{n_q=0}^{\infty} e^{-\beta n_q \omega_q} \right)^{-1} = 1 - e^{-\beta\omega_q}$$

We shall simplify the present notation by first dropping all q subscripts. We shall also use $\lambda = M_q/\omega_q$, so that we need to find

$$F = (1 - e^{-\beta\omega}) \sum_{n=0}^{\infty} \langle n | e^{-\beta n\omega} \exp[-\lambda(a^\dagger e^{i\omega t} - a e^{-i\omega t})] e^{\lambda(a^\dagger - a)} | n \rangle \quad (4.33)$$

The state $|n\rangle$ is the state with n excitations and is given in terms of the operators as

$$|n\rangle = \frac{(a^\dagger)^n}{(n!)^{1/2}} |0\rangle$$

The first step is to separate the operators in the exponential. This step is where we use Feynman's theory on the disentangling of the operators, which is as follow.

Theorem: If the operators A and B have the property that their commutators $C = [A, B]$ commutes with both A and B , then

$$e^{A+B} = e^A e^B e^{-1/2[A, B]} \quad (4.34)$$

this theorem is used to separate the exponents in $X(t)$ and $X^\dagger(0)$. To evaluate $X(t)$, set

$$\begin{aligned} A &= -\lambda a^\dagger e^{i\omega t} \\ B &= \lambda a e^{-i\omega t} \end{aligned}$$

so that

$$[A, B] = \lambda^2$$

and we obtain

$$\begin{aligned} X(t) &= e^{A+B} \\ &= e^{-1/2\lambda^2} \exp(-\lambda a^\dagger e^{i\omega t}) \exp(\lambda a e^{-i\omega t}) \end{aligned}$$

The result for $X^\dagger(0)$ is just the Hermitian conjugate at $t = 0$:

$$\begin{aligned} X^\dagger(0) &= e^{-1/2\lambda^2} e^{\lambda a^\dagger} e^{-\lambda a} \\ X(t)X^\dagger(0) &= e^{-\lambda^2} e^{-\lambda a^\dagger(t)} e^{\lambda a^\dagger} e^{-\lambda a} \end{aligned}$$

The next step is to get all the annihilation operators on the right and the creation operators on the left. Thus we need to exchange the center

two operators. Since they do not commute, this exchange will produce another complex phase factor. These two operators are written as

$$e^{\lambda a^\dagger(t)} e^{\lambda a^\dagger} = e^{\lambda a^\dagger} [e^{-\lambda a^\dagger} e^{\lambda a(t)} e^{\lambda a^\dagger}]$$

The factor in brackets has exactly the form derived earlier. Thus if we evaluate

$$\begin{aligned} e^{-\lambda a^\dagger} a e^{-i\omega t} e^{\lambda a^\dagger} &= e^{-i\omega t} \left(a - \lambda [a^\dagger, a] + \frac{\lambda^2}{2} [a^\dagger [a^\dagger, a]] \dots \right) \\ &= e^{-i\omega t} (a + \lambda) \end{aligned}$$

then

$$e^{-\lambda a^\dagger} e^{\lambda a(t)} e^{\lambda a^\dagger} = \exp[\lambda e^{-i\omega t} (a + \lambda)] = \exp(\lambda^2 e^{-i\omega t}) e^{\lambda a(t)} \quad (4.35)$$

$$e^{\lambda a(t)} e^{\lambda a^\dagger} = \exp(\lambda^2 e^{-i\omega t}) e^{\lambda a^\dagger} e^{\lambda a(t)} \quad (4.36)$$

so the desired form is

$$F(t) = (1 - e^{-\beta\omega}) \exp[-\lambda^2(1 - e^{-i\omega t})] \quad (4.37)$$

$$\times \sum_{n=0}^{\infty} \langle n | e^{-\beta n\omega} \exp[\lambda a^\dagger(i - e^{-i\omega t})] \exp[-\lambda a(i - e^{-i\omega t})] | n \rangle \quad (4.38)$$

All the terms with a can be collected together in exponential since all these terms commute - and likewise for all the terms with a^\dagger . Next we wish to prove that

$$(1 - e^{-\beta\omega}) \sum_{n=0}^{\infty} e^{-\beta n\omega} \langle n | e^{u^* a^\dagger} e^{-ua} | n \rangle = e^{-|u|^2 N} \quad (4.39)$$

$$N = \frac{1}{e^{\beta\omega} - 1} \quad (4.40)$$

where, for our case, $u = \lambda(1 - e^{-i\omega t})$. The previous equation is proved by expanding the exponent in powers series:

$$e^{-ua} | n \rangle = \sum_{l=0}^{\infty} \frac{(-u)^l}{l!} a^l | n \rangle$$

Recalling the properties of the destruction operator acting on a state and that $a^l|n\rangle = 0$ for $l > n$ we have:

$$e^{-ua}|n\rangle = \sum_{l=0}^{\infty} \frac{(-u)^l}{l!} \left[\frac{n!}{(n-l)!} \right]^{1/2} |n\rangle$$

That is way the destruction operators were arranged on the right. The other operator may be taken to operate on the left and produces the Hermitian conjugate of the above result.

This two results must be multiplied together. Using the basic orthogonality of states we have the compact result

$$\langle n|e^{u^*a^\dagger}e^{-ua}|n\rangle = \sum_{l=0}^{\infty} \frac{(-|u|^2)^l}{(l!)^2} \frac{n!}{(n-l)!}$$

This power series is the Laguerre polynomial of order n . The final step is to sum the series over n . We get

$$(1-z)^{-1}e^{|u|^2z/(z-1)} = \sum_{n=0}^{\infty} L_n(|u|^2)z^n$$

In our case we identify

$$z = e^{-\beta\omega}$$

$$\frac{z}{z-1} = -N$$

When these factors are collected, this proves our thesis. The result for $F(t)$ is then

$$F(t) = e^{-\phi(t)}$$

$$\phi(t) = \lambda^2[(1 - e^{-i\omega t}) + N|1 - e^{i\omega t}|^2]$$

We return to (4.31) and reintroduce the product over all q states. The function $F(t)$ contains a summation of the exponential factor:

$$F(t) = \prod_q F_q(t) = \exp \left[- \sum_q \phi_q(t) \right] = \exp[-\Phi(t)]$$

$$\Phi(t) = \sum_q \left(\frac{M_q}{\omega_q} \right) [N_q(1 - e^{i\omega_q t}) + (N_q + 1)(1 - e^{-i\omega_q t})]$$

$$N_q = (e^{\beta\omega_q} - 1)^{-1}$$

The final result for the particle Green's function for $t > 0$ is

$$G(t) = -ie^{-it(\varepsilon_c - \Delta)} e^{-\Phi(t)} (1 - n_F). \quad (4.41)$$

This is the exact result.

Chapter 5

Unpublished paper

The results presented in this thesis will be written in a paper by, K. Flensberg, K. Flensberg and myself. In this chapter, I'll give some of the details to be included in the paper, which will also contain the numerical result.

We consider Josephson through a single level in a molecular or mesoscopic single-electron transistor. The junction becomes a π -junction when the level energy is below the chemical potential.

5.1 The model

$$H = H_0 + H_T, \quad (5.1)$$

$$H_0 = H_L + H_R + H_M, \quad (5.2)$$

and

$$H_T = \sum_{\alpha} (H_{T\alpha}^+ + H_{T\alpha}^-), \quad H_{T\alpha}^+ = (H_{T\alpha}^-)^{\dagger}, \quad H_{T\alpha}^- = \sum_{\sigma=\uparrow,\downarrow} H_{T\alpha\sigma}^-, \quad H_{T\alpha\sigma}^- = \sum_k t_{k\alpha} c_{k\alpha\sigma}^{\dagger} d_{\sigma} \quad (5.3)$$

5.2 The Josephson current

By definition:

$$\begin{aligned} I_\alpha &= i \langle H_{T\alpha}^+ - H_{T\alpha}^- \rangle \\ &= 2 \operatorname{Im} \langle H_{T\alpha}^- \rangle. \end{aligned}$$

To the fourth order in H_T :

$$I_\alpha = 2 \operatorname{Im} \frac{1}{4!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \langle T_\tau (H_T(\tau_1) H_T(\tau_2) H_T(\tau_3) H_{T\alpha}^-) \rangle_0.$$

The Josephson current must involve two H_T^+ and two H_T^- , which can be chosen in 3! ways, and hence

$$I_\alpha = 2 \operatorname{Im} \frac{1}{4} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \langle T_\tau (H_{T\bar{\alpha}}^+(\tau_1) H_{T\bar{\alpha}}^+(\tau_2) H_{T\alpha}^-(\tau_3) H_{T\alpha}^-) \rangle_0, \quad (5.4)$$

where we also used that in order to have Cooper pair tunneling, the H_T^+ must be on the left of the junction. Here $\bar{\alpha}$ means the lead opposite to α . Because of spin symmetry we can choose the spin in last factor to up, and thus

$$\begin{aligned} I_\alpha &= 2 \operatorname{Im} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \langle T_\tau (H_{T\bar{\alpha}\downarrow}^+(\tau_1) H_{T\bar{\alpha}\uparrow}^+(\tau_2) H_{T\alpha\downarrow}^-(\tau_3) H_{T\alpha\uparrow}^-) \rangle_0 \\ &= \sum_k \sum_p t_{p\bar{\alpha}}^* t_{-p\bar{\alpha}}^* \langle T_\tau (c_{p\bar{\alpha}\uparrow}(\tau_1) c_{-p\bar{\alpha}\downarrow}(\tau_2)) \rangle_0 t_{-k\alpha} t_{k\alpha} \langle T_\tau (c_{-k\alpha\downarrow}^\dagger(\tau_3) c_{k\alpha\uparrow}^\dagger) \rangle_0 \\ &\quad \times \langle T_\tau (d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger(\tau_2) d_\downarrow(\tau_3) d_\uparrow(0)) \rangle_0. \end{aligned} \quad (5.5)$$

The anomalous Green's functions are

$$\begin{aligned} \langle T_\tau (c_{-k\alpha\downarrow}^\dagger(\tau) c_{k\alpha\uparrow}^\dagger) \rangle &= \langle T_\tau (c_{k\alpha\uparrow}(-\tau) c_{-k\alpha\downarrow}) \rangle^* \\ &= [\mathcal{G}(E_{k\alpha}, \tau) + \mathcal{G}(E_{k\alpha}, -\tau)] \frac{\Delta_{k\alpha}}{2E_{k\alpha}} \\ &= \frac{\Delta_{k\alpha}}{2E_{k\alpha}} [(\theta(\tau) - n_F(E_{k\alpha})) e^{-E_{k\alpha}\tau} + (\theta(-\tau) - n_F(E_{k\alpha})) e^{E_{k\alpha}\tau}] \\ &= \frac{\Delta_{k\alpha}}{2E_{k\alpha}} [e^{-E_{k\alpha}|\tau|} - 2 \cosh(E_{k\alpha}\tau) n_F(E_{k\alpha})] \\ &\equiv \frac{\Delta_{k\alpha}}{2E_{k\alpha}} f_{k\alpha}(\tau). \end{aligned}$$

Assuming low temperatures $\Delta\beta \gg 1$, we approximate

$$f_{k\alpha}(\tau) \approx e^{-E_{k\alpha}|\tau|} - e^{-E_{k\alpha}(\beta-|\tau|)}. \quad (5.6)$$

Inserting this into (5.5), we have

$$I_\alpha = 2 \operatorname{Im} \sum_k \sum_p t_{p\bar{\alpha}}^* t_{-p\bar{\alpha}}^* \frac{\Delta_{p\bar{\alpha}}^*}{2E_{p\bar{\alpha}}} t_{-k\alpha} t_{k\alpha} \frac{\Delta_{k\alpha}}{2E_{k\alpha}} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 f_{p\bar{\alpha}}(\tau_1 - \tau_2) f_{k\alpha}(\tau_3) B(\tau_1, \tau_2, \tau_3). \quad (5.7)$$

where

$$B(\tau_1, \tau_2, \tau_3) = \left\langle T_\tau \left(d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger(\tau_2) d_\downarrow(\tau_3) d_\uparrow(0) \right) \right\rangle_0 \quad (5.8)$$

For a system with interactions, we cannot use Wick's theorem, and hence we must evaluate this directly. There are four many-body states, $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$. In (5.8) only $|\uparrow\rangle$ and $|\uparrow\downarrow\rangle$ contributes to the trace, i.e.

$$B = B_1 + B_U, \quad (5.9)$$

where

$$B_1 = P_\uparrow \left\langle \uparrow \left| T_\tau \left(d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger(\tau_2) d_\downarrow(\tau_3) d_\uparrow(0) \right) \right| \uparrow \right\rangle, \quad (5.10)$$

$$B_U = P_{\uparrow\downarrow} \left\langle \uparrow\downarrow \left| T_\tau \left(d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger(\tau_2) d_\downarrow(\tau_3) d_\uparrow(0) \right) \right| \uparrow\downarrow \right\rangle. \quad (5.11)$$

For B_1 only three orderings of the operators give a non-zero result, and we find

$$\begin{aligned} B_1 &= P_\uparrow \left\langle \uparrow \left| T_\tau \left(d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger(\tau_2) d_\downarrow(\tau_3) \right) \right| 0 \right\rangle \\ &= P_\uparrow \left[\left\langle \uparrow \left| d_\downarrow^\dagger(\tau_2) d_\downarrow(\tau_3) d_\uparrow^\dagger(\tau_1) \right| 0 \right\rangle \theta(\tau_2 - \tau_3) \theta(\tau_3 - \tau_1) \right. \\ &\quad - \left\langle \uparrow \left| d_\downarrow(\tau_3) d_\uparrow^\dagger(\tau_2) d_\downarrow^\dagger(\tau_1) \right| 0 \right\rangle \theta(\tau_3 - \tau_2) \theta(\tau_2 - \tau_1) \\ &\quad \left. + \left\langle \uparrow \left| d_\downarrow(\tau_3) d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger(\tau_2) \right| 0 \right\rangle \theta(\tau_3 - \tau_1) \theta(\tau_1 - \tau_2) \right]. \quad (5.12) \end{aligned}$$

This becomes

$$B_1 = P_\uparrow \left\{ e^{\xi(\tau_1 - \tau_3 + \tau_2)} \theta(\tau_2 - \tau_3) \theta(\tau_3 - \tau_1) + e^{E_2(\tau_2 - \tau_3)} e^{\xi(\tau_1 - \tau_2 + \tau_3)} \theta(\tau_3 - \tau_2) \theta(\tau_2 - \tau_1) \right. \\ \left. + e^{E_2(\tau_1 - \tau_3)} e^{\xi(\tau_2 - \tau_1 + \tau_3)} \theta(\tau_3 - \tau_1) \theta(\tau_1 - \tau_2) \right\}. \quad (5.13)$$

Likewise, for B_U we find

$$\begin{aligned} B_U &= P_{\uparrow\downarrow} \left\langle \uparrow\downarrow \left| T_\tau \left(d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger(\tau_2) d_\downarrow(\tau_3) \right) \right| \downarrow \right\rangle \\ &= P_{\uparrow\downarrow} \left[\left\langle \uparrow\downarrow \left| d_\downarrow^\dagger(\tau_1) d_\uparrow^\dagger(\tau_2) d_\downarrow(\tau_3) \right| \downarrow \right\rangle \theta(\tau_1 - \tau_2) \theta(\tau_2 - \tau_3) \right. \\ &\quad \left. - \left\langle \uparrow\downarrow \left| d_\downarrow^\dagger(\tau_1) d_\downarrow(\tau_3) d_\uparrow^\dagger(\tau_2) \right| \downarrow \right\rangle \theta(\tau_1 - \tau_3) \theta(\tau_3 - \tau_2) \right], \end{aligned} \quad (5.14)$$

and thus

$$B_U = P_{\uparrow\downarrow} \left[e^{\xi(\tau_2 - \tau_3)} e^{E_2 \tau_1} \theta(\tau_1 - \tau_2) \theta(\tau_2 - \tau_3) + e^{\xi(\tau_3 - \tau_1 - \tau_2)} e^{E_2(\tau_1 + \tau_2 - \tau_3)} \theta(\tau_1 - \tau_3) \theta(\tau_3 - \tau_2) \right], \quad (5.15)$$

5.3 $E_2 \gg 0$

Let $E_2 \gg 0$ such that the double occupied state is taken out. Hence

$$B_1 = P_1 e^{\xi(\tau_1 - \tau_3 + \tau_2)} \theta(\tau_2 - \tau_3) \theta(\tau_3 - \tau_1), \quad (5.16)$$

and when inserted into the current formula

$$I_\alpha = 2 \operatorname{Im} \sum_{kp} t_{p\bar{\alpha}}^* t_{-p\bar{\alpha}}^* t_{-k\alpha} t_{k\alpha} \frac{\Delta_{p\alpha}^* \Delta_{k\alpha}}{4E_{p\alpha} E_{k\alpha}} C, \quad (5.17)$$

where

$$C = P_1 \int_0^\beta d\tau_2 \int_0^{\tau_2} d\tau_3 \int_0^{\tau_3} d\tau_1 \left(e^{-E_p(\tau_2 - \tau_1)} - e^{E_p(\tau_2 - \tau_1 - \beta)} \right) \left(e^{-E_k \tau_3} - e^{E_k(\tau_3 - \beta)} \right) P_1 e^{\xi(\tau_1 - \tau_3 + \tau_2)} \quad (5.18)$$

Performing the integrals and letting $e^{-E_{p,k}\beta} \rightarrow 0$, we find

$$\begin{aligned} C &= \frac{2 e^{-\beta\xi}}{1 + 2e^{-\beta\xi}} \frac{\xi(E_p + E_k)(1 + e^{\beta\xi}) + (E_k E_p + \xi^2)(1 - e^{\beta\xi})}{(E_p + E_k)(E_k^2 - \xi^2)(E_p^2 - \xi^2)} \\ &= \frac{2 e^{-\beta\xi}}{1 + 2e^{-\beta\xi}} \left(-\frac{e^{\beta\xi}}{(E_p + E_k)(E_k + \xi)(E_p + \xi)} + \frac{1}{(E_p + E_k)(E_k - \xi)(E_p - \xi)} \right). \end{aligned} \quad (5.19)$$

At $T = 0$, this reduces to

$$C = \begin{cases} -\frac{2}{(E_p+E_k)(E_k+\xi)(E_p+\xi)} & \text{for } \xi > 0, \\ \frac{2}{(E_p+E_k)(E_k-\xi)(E_p-\xi)} & \text{for } \xi < 0. \end{cases} \quad (5.20)$$

Hence

$$I = \frac{\Gamma^L \Gamma^R \Delta_L \Delta_R}{2\pi^2} \sin \phi H(\xi), \quad (5.21)$$

where

$$H(\xi) = \int dE dE' \frac{1}{\sqrt{E^2 - \Delta_L^2}} \frac{1}{\sqrt{E'^2 - \Delta_R^2}} C \quad (5.22)$$

For $\xi \ll \Delta$, we can perform the integrations and we get

$$H(0) = \frac{e^{-\beta\xi} - 1}{1 + 2e^{-\beta\xi}} \int d\varepsilon d\varepsilon' \frac{1}{(E + E')E^2 E'^2} = \frac{2(e^{-\beta\xi} - 1)}{1 + 2e^{-\beta\xi}} \left(\pi - \frac{\pi^2}{4} \right). \quad (5.23)$$

5.4 Josephson current with coupling to a localized phonon

In the following we consider a single level between two superconductors as above but now with an additional coupling to a bosonic mode. We thus have two new terms in the Hamiltonian: $H_B + H_{eB}$, where

$$H_B = \omega_0 \left(a^\dagger a + \frac{1}{2} \right), \quad (5.24)$$

$$H_{eB} = \frac{\lambda \ell_0}{\sqrt{2}} (a + a^\dagger) \sum_{\sigma} n_{\sigma}. \quad (5.25)$$

We remove the last term using the usual canonical transformation, which renormalizes ξ and U and transform the d -operator into

$$d \rightarrow d e^{-ip\ell}, \quad \ell = \frac{\lambda}{m\omega_0^2}, \quad (5.26)$$

where $p = i(a^\dagger - a)/(\ell_0\sqrt{2})$.

Now everything carries through as above with d replaced as in (5.26). Thus the function B in (5.8) acquires an additional factor, namely

$$F(\tau_1, \tau_2, \tau_3) = \langle T_\tau (e^{ip(\tau_1)\ell} e^{ip(\tau_2)\ell} e^{-ip(\tau_3)\ell} e^{-ip\ell}) \rangle_0. \quad (5.27)$$

This is evaluated as

$$F(\tau_1, \tau_2, \tau_3) = \exp(-g(\tau_1 - \tau_2) + g(\tau_1 - \tau_3) + g(\tau_1) + g(\tau_2 - \tau_3) + g(\tau_2) - g(\tau_3)) \quad (5.28)$$

where

$$g(\tau) = \ell^2 (\langle T_\tau (p(\tau)p(0)) \rangle - \langle p^2 \rangle) = g (n_B (e^{\omega|\tau|} - 1) + (1 + n_B)(e^{-\omega|\tau|} - 1)), \quad (5.29)$$

where

$$g = \frac{\ell^2}{2\ell_0^2}, \quad n_B = \frac{1}{e^{\beta\omega_0} - 1}. \quad (5.30)$$

In order to study how the coupling to the vibration changes the Josephson current, we will perform a numerical integration of the three imaginary time integrals. For this purpose we first find:

$$\begin{aligned} \sum_p t_{p\alpha}^* t_{-p\alpha}^* \frac{\Delta_{p\alpha}^*}{2E_{p\alpha}} f_{p\alpha}(\tau) &\approx e^{-i\phi_\alpha} t_{\alpha\rho}^2 \int d\varepsilon \frac{\Delta_\alpha}{2E} [e^{-E|\tau|} - e^{-E(\beta-|\tau|)}] \\ &= e^{-i\phi_\alpha} t_{\alpha\rho}^2 \int_{\Delta_\alpha}^{\infty} dE \frac{\Delta_\alpha}{\sqrt{E^2 - \Delta_\alpha^2}} [e^{-E|\tau|} - e^{-E(\beta-|\tau|)}] \\ &= e^{-i\phi_\alpha} \frac{\Gamma_\alpha \Delta_\alpha}{2\pi} [K_0(|\tau|\Delta_\alpha) - K_0((\beta - |\tau|)\Delta_\alpha)] \equiv e^{-i\phi_\alpha} \frac{\Gamma_\alpha \Delta_\alpha}{2\pi} H_\alpha(\tau), \end{aligned} \quad (5.31)$$

where K_0 is the modified Bessel function of the second kind.

The final expression for the current thus reads

$$I_\alpha = I_c \sin \phi, \quad (5.32)$$

where

$$I_c = \frac{\Gamma_L \Gamma_R \Delta_L \Delta_R}{2\pi^2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 H_L(\tau_1 - \tau_2) H_R(\tau_3) B(\tau_1, \tau_2, \tau_3) F(\tau_1, \tau_2, \tau_3). \quad (5.33)$$

5.4.1 Vibron and $E_2 \gg 0$

Again study the case, where double occupied state is "out", then we have $B = B_1$, where B_1 is given in Eq.(5.16), and hence

$$I_c = \frac{\Gamma_L \Gamma_R \Delta_L \Delta_R}{2\pi^2} \frac{e^{-\beta\xi}}{1 + 2e^{-\beta\xi}} \int_0^\beta d\tau_2 \int_0^{\tau_2} d\tau_3 \int_0^{\tau_3} d\tau_1 e^{\xi(\tau_1 - \tau_3 + \tau_2)} H_L(\tau_2 - \tau_1) H_R(\tau_3) F(\tau_1, \tau_2, \tau_3). \quad (5.34)$$

In the numerical calculation the following symmetry is useful

$$\begin{aligned} g(\xi) &= \int_0^{\beta/2} d\tau_2 \int_0^{\tau_2} d\tau_3 \int_0^{\tau_3} d\tau_1 e^{\xi(\tau_1 - \tau_3 + \tau_2)} H_L(\tau_2 - \tau_1) H_R(\tau_3) F(\tau_1, \tau_2, \tau_3) \\ &= \int_{\beta/2}^1 d\tau'_2 \int_0^{\tau'_2 - \beta/2} d\tau_3 \int_0^{\tau_3} d\tau_1 e^{\xi(\tau_1 - \tau_3 + \tau'_2 - \beta/2)} H_L(\tau_2 - \tau_1 - \beta/2) H_R(\tau_3) F(\tau_1, \tau_2 - \beta/2, \tau_3) \\ &= - \int_{\beta/2}^1 d\tau'_2 \int_0^{\tau'_2 - \beta/2} d\tau_3 \int_0^{\tau_3} d\tau_1 e^{\xi(\tau_1 - \tau_3 + \tau'_2 - \beta/2)} H_L(\tau_2 - \tau_1 + \beta/2) H_R(\tau_3) F(\tau_1, \tau_2 - \beta/2, \tau_3) \\ &= - \int_{\beta/2}^1 d\tau'_2 \int_0^{\tau'_2} d\tau'_3 \int_0^{\tau_3} d\tau_1 e^{\xi(\tau_1 - \tau_3 + \tau'_2 - \beta/2)} H_L(\tau_2 - \tau_1 + \beta/2) H_R(\tau_3) F(\tau_1, \tau_2 - \beta/2, \tau_3) \end{aligned}$$

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