

CHAPTER 1. INTRODUCTION TO SUPERCONDUCTIVITY

1.1 Introductory elements of superconductivity

This lecture will be based on references [1], [2], [3], [4].

0 Introduction

Building a new technology requires two basic sets of elements: the raw materials which will form the basis of the technology, and the techniques by which this technology will be operated. In the case of superconducting qubits, this is on one hand the role played by superconductivity, and on the other hand quantum optics and microwave engineering.

Superconductors are essential to the operation of superconducting qubits, particularly given the absence of dissipation to the flow of electrical currents and the Josephson effect, which is a consequence of quantum phase coherence in the superconductor, in other words, a purely quantum mechanical effect. Therefore, it is imperative to learn at a basic level what are superconductors and why are they necessary. Superconductors offer the possibility to generate low energy excitations that do propagate and behave like photons and artificial atoms and do not lose their energy. In order to generate these low energy excitations one needs a quantum system with unevenly spaced energy levels such that they can be individually addressed. This is provided by another intrinsic effect associated to superconductivity: the Josephson effect

Quantum optics is a broad subject, dealing with few-level quantum systems (also known as atoms) and electromagnetic fields following quantization rules and obeying commutation relations. The blindness of quantum optics to the systems it is treating makes it an extremely versatile tool that can be translated to many physical platforms. In particular, superconducting quantum circuits turned out to be an ideal paradigm on which to implement all textbook quantum optics physics, and even explore new regimes unattainable before, such as ultrastrong light-matter interactions. Therefore, before going to the precise physics of superconducting qubits interacting with microwave photons, it is necessary to learn the basic elements in quantum optics that later will reappear dressed in the right form.

Microwave engineering has become a necessity to build superconducting quantum circuits, as they operate in the gigahertz range of frequencies. Therefore, one needs to know how to propagate microwave fields without loss or dispersion, how to avoid

spurious resonant modes that may interfere with qubits, suppress crosstalk between different qubits, etc.

Together, quantum optics and microwave engineering one learns how it is possible to connect atom-like excitations with those propagating, photon-like, allowing the coupling of resonant qubit circuits to transmission line waveguides and in this way scale up the system size to build a full-fledged quantum computer.

Theoretically, this is all that is needed. Experimentally there are a few more layers. For example, how do we place the circuit in such a low temperature so as to prepare it to its quantum ground state? how do we process the signals to excite and read out qubit states? the answer to the first question is cryogenics, and in particular dilution refrigeration. The answer to the second question is signal processing, as it is precisely done in radio transmission. Other advanced technological tools are being incorporated to the control of superconducting quantum systems such as FPGAs (field programmable gate arrays), ultralow noise amplifiers, etc. Even though these components existed before, they are now being adapted to put to work a new technology with new demands that is shaping these existing tools and permitting the appearance of new ones, such as quantum-limited amplifiers, broadband cryogenic circulators, infrared filters, etc.

1 Basic phenomenology

1.1 Phenomenology and evolution of superconductivity

There are few technologies that raise much interest and expectations as superconductivity does. The effects of superconductivity are as spectacular as counter-intuitive, and the exploration for an explanation of its existence has drawn in many physicists, mainly because it is so robust and because at the same time there are so many ways to destroy it. Superconductivity is truly a macroscopic quantum effect with observable (and usable) consequences. Nowadays, applications to superconducting materials other than quantum technology are varied:

- Power cables for sea windmills (coaxial tube with YBaCuO material with LN2)
- Electromagnets of NbTi, such as those used at CERN and at any MRI scanner, current densities of $\sim 10^{10}$ A/m², vs $\sim 10^7$ A/m² in copper, and with minor input energy.
- SFQ logic, GHz-speed classical computer processors
- Resonator pixels for cameras to explore Cosmic Microwave Background
- SQUIDs, such as MRI scanners, detect Φ 10^{-15} Wb·m.
- Using the Josephson effect, definition of the voltage standard.

All superconducting materials (including high- T_c ones) require extremely low temperatures. Many materials do not exhibit superconductivity until near absolute zero. So the field had to wait until cryogenic technology was developed.

Early days scientists were motivated to liquefy gases. The last element left was helium, only achieved by Kammerlingh Onnes in 1908, 10 years after hydrogen liquefaction. Using LHe, other experiments may be realized, such as electrical resistance of materials. Onnes tried mercury, and saw a sudden drop in resistance. Onnes coined the term ‘superconductor’ from its experiments with mercury. He defined a ‘critical temperature’ T_c above which superconductivity disappears. Onnes also defined a critical current density J_c , as function of temperature, above

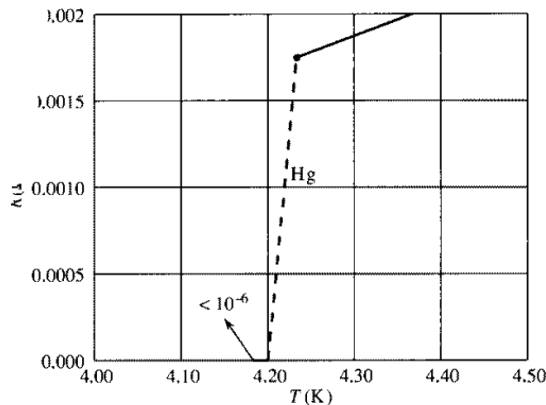


Figure 1: Original measurements of Kammerlingh Onnes using mercury. Source: Orlando

which superconductivity was destroyed, increasing as T was lowered. He found a critical field H_c , above which superconductivity was destroyed to fit empirically $H_c(T) \approx H_{co}(1 - (T/T_c)^2)$.

In 1933, Walther Meissner and Robert Ochsenfeld found that superconductors expel flux, contrary to perfect conductors. The flux density (below the critical field) was found to be zero inside a large piece of superconductor. This is the behaviour of a diamagnetic material, and maintaining $B = 0$ in its inside is what a perfect diamagnet does. This is known as the Meissner effect and shows that superconductors are more than perfect conductors, as they possess both particular magnetic and electric properties.

Search for higher T_c materials began early-on. First, with metallic elements. Surprisingly, it is not a rare phenomenon, and very few materials do not become superconducting at low enough T . Interestingly, the best conductors (Cu, Ag, Au, Pt) do not become superconductors. Highest T_c material is Nb (see table).

Attention was next placed to compounds, with a strong drive by W. J. de Haas and Meissner in the 1920s and 1930s. Non-superconducting materials superconduct (CuS $T_c = 1.6$ K). Alloys do exist, such as NbTi, the most popular one as electromagnets are made out of it (CERN). In the 1950s, another class of materials A15 (crystal structure) V_3Ga , Nb_3Sn , Nb_3Ge , with T_c of 16K, 18K, 23K. In 1970s, Chevrel materials, such as $PbMo_6S_8$ have very high critical field, 60T for T_c of 15K.

By early 1980s, there were little perspectives of getting higher T_c materials. Suddenly, K. Alex Müller and J. Georg Bednorz found $La_{1.85}Ba_{0.85}CuO_4$ superconducted at 30K. High excitement was generated, which led to awarding them the Nobel prize

Material	T_c (K)	H_{co} (mT)	Type
W	0.015	0.12	I
Ti	0.39	10.0	I
Al	1.18	10.5	I
In	3.41	23.0	I
Sn	3.72	30.5	I
Hg	4.15	40.0	I
Pb	7.20	80.0	I
Nb	9.25	195	II

Table 1: Superconducting properties of pure metallic elements, all except niobium being type I. Source: Orlando/Hyperphysics.

Material	T_c (K)	H_{co} (T)	Type
NbTi	10	15	II
PbMoS	14.4	6.0	II
V ₃ Ga	14.8	2.1	II
NbN	15.7	1.5	II
Nb ₃ Sn	18.0	24.5	II
Nb ₃ Ge	23.2	38	II

Table 2: Superconducting properties of alloys, all of them Type II. Source: Hyperphysics/Wikipedia.

in 1988. In 1987, Paul C. W. Chu (U. Huston) and Maw-Kuen Wu (U Tokyo) found YBa₂Cu₃O₇ had a critical temperature of 95K, higher than liquid nitrogen.

Material	T_c (K)	H_{co} (T)	Type
La _{2-x} Ba _x CuO ₄	30	-	High- T_c
La _{2-x} Sr _x CuO ₄	38	-	High- T_c
La _{2-x} Sr _x CaCuO ₄	60	-	High- T_c
YBa ₂ Cu ₃ O ₇	92	> 100	High- T_c
Bi ₂ Sr ₂ Ca ₂ Cu ₃ O ₁₀	110	-	High- T_c

Table 3: Superconducting properties high- T_c superconductors. Source: Hyperphysics.

Since then, different types of High- T_c superconductors were found, some including iron (known as iron picnities) and more recently hydrides, leading to the first room temperature superconductor (non-metallic and under huge pressures, ~ 2700 atm). The chart below shows the evolution of the field.

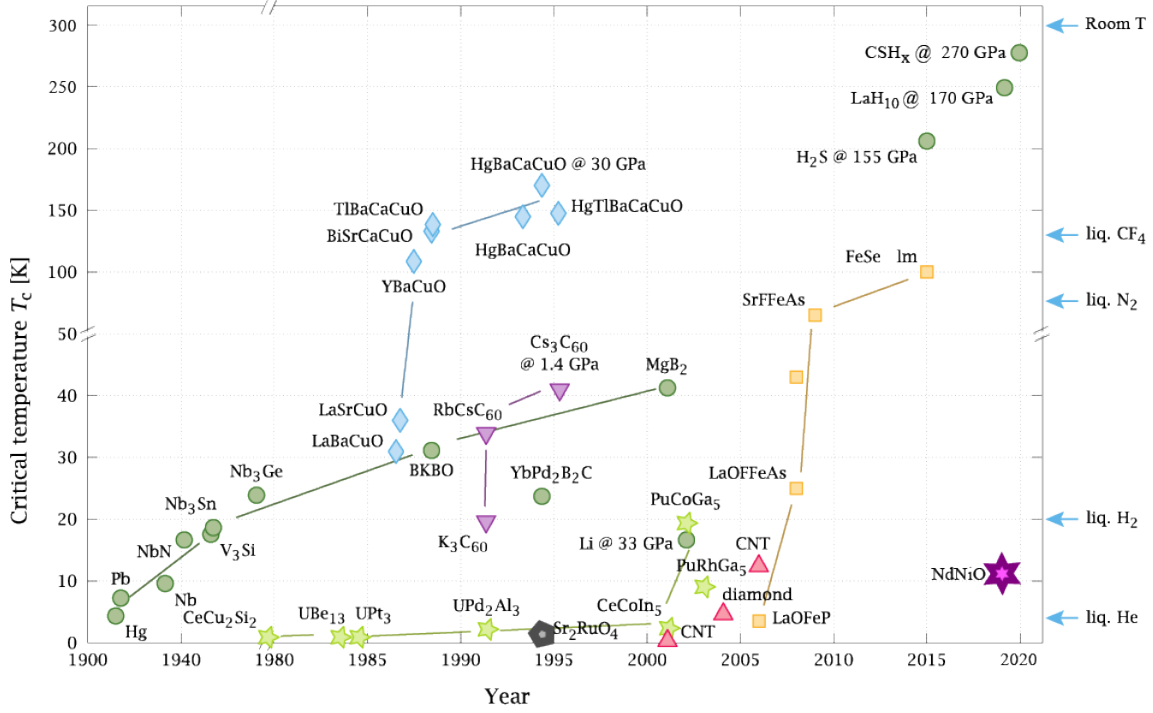


Figure 2: Chart of evolution of high-temperature superconductors over time. Source: Wikipedia.

1.1.1 Models of superconductivity

Simplest model of superconductivity is the *classical model*: zero resistance and perfect diamagnetism in London equations. Superconductivity was first modeled in 1935 by Fritz and Heinz London [5], using an empirical modification of Maxwell's equations that lead to perfect conductivity and the Meissner effect. These equations (London equations) describe the macroscopic properties of superconductors remarkably well, but tell no information about its origin. Analogous to Ohm's law.

Later in 1948, Fritz London [6], who had the intuition that superconductivity was an intrinsic quantum effect, showed that the London equations can be derived from a simplified form of the superconducting wave function, known as the macroscopic model. Again, giving no clue about its microscopic origin, but now encompassing many other effects that the classical model could not capture, such as flux quantization, type-II superconductors, and the Josephson effect.

Later in 1950, Vitali Ginzburg and Lev Landau produced a new quantum mechanical model that not only provided the correct electromagnetic response, but also the thermodynamics of superconductors. Still, it was a phenomenological model, albeit a quite accurate one.

It wasn't until 1957 when John Bardeen, Leon Cooper, and Robert Schrieffer that established a truly microscopic quantum mechanical description of superconductivity, in what is known today as the BCS theory [7]. Within this theory, electrons are bound by elastic phonon-electron interactions and form pairs of total spin 0 and anti-parallel momentum. The BCS theory correctly predicts the properties of the pure materials, including a superconducting gap that protects the superconducting

state from thermal excitations. Effects that involve energies below the gap can be captured by phenomenological models, as those energies cannot be absorbed by the superconductor. For higher energies than the gap, only the BCS model correctly predicts the behavior of the material.

In 1959, L. P. Gorkov showed that near T_c , the BCS theory and the Ginzburg-Landau theory are equivalent, validating the latter, much simpler to use than the former. BCS still does not describe High- T_c superconductors, where despite more than 3 decades of exploration, no true quantum mechanical description has been arrived at although the Cooper pairing is still happening in these materials, with different electronic orbital angular momenta. Still, phenomenological models work pretty well.

It is important to understand the basics of superconductivity to the particular use case of Josephson junctions, together with circuit quantization, which later leads to defining superconducting qubits.

This course is not on superconductivity. Therefore, only a very superficial introduction to BCS will be given, putting a stronger focus on the Macroscopic quantum model and the London equations.

1.2 The classical model of superconductivity

In a normal metal, valence electrons from the host material form a sea of charge that has certain mobility. When an external potential is applied, the electrons accelerate towards areas of lower potential creating an electrical current. Due to collisions with the lattice of positively charged ions forming the material, the electrons experience friction, as each collision results in a random change of velocity and direction of motion. This is the usual microscopic description of the model for Ohm's law. Macroscopically, the friction experienced by the electrons leads to the electrical resistance R , which connects the applied voltage with the induced electrical current:

$$V = IR. \quad (1)$$

R is an extensive quantity that depends on the geometry of the material and on its intrinsic properties, combined in an intensive quantity known as the resistivity ρ . In normal metals, the resistivity follow a temperature dependence

$$\rho(T) \sim \rho_0(1 + \alpha \max(T - T_0, 0)), \quad (2)$$

with ρ_0 being an intrinsic plateau that is material and sample dependent.

As a reminder that will be useful to compare to the case of superconductors, microscopically, Ohm's law takes the form:

$$\mathbf{J}(\omega) = \sigma(\omega)\mathbf{E}. \quad (3)$$

The conductivity parameter $\sigma(\omega) = \rho^{-1}(\omega)$ contains all the microscopic physics and is therefore material dependent, as well as frequency and temperature dependent.

By contrast, superconductors exhibit a macroscopic phenomenology very different from normal metals, even perfect metals with perfect conductance. The main

signatures are reviewed in the following subsections: absence of dissipation and persistent currents, and the Meissner effect and levitation. Another set of macroscopic consequences of superconductivity, suppressed heat capacity and flux quantization, require a quantum description and are therefore introduced in the following section.

1.2.1 Perfect conductivity. First London equation.

The first striking phenomenon associated to superconductors is the absence of energy dissipation when an electrical current flows through them. One could consider that a superconductor is related to a “perfect” conductor, which is theoretically defined as a medium which displays a conductivity as $\sigma \rightarrow \infty$. This is not correct, and we will not pose all arguments here. Interested readers should examine [1].

Need to find ways to calculate field distribution for a truly lossless perfect conductor. No easy way to move from perfect conductor. Plus, $\sigma \rightarrow \infty$ not correct. Need new constitutive law.

Before moving on, a strong assumption is made to obtain simple expressions, which is that time variations are slow. If the medium conducts well with a high σ_0 , then it behaves like a wire that will store magnetic energy and the system will become a magnetoquasistatic (MQS) system. Now, $\nabla \times \mathbf{H} \approx \mathbf{J}$, then $\nabla \cdot \mathbf{J} \approx 0$, current is conserved (no charges accumulate). Finally, diffusion equation is obtained $(\mu\sigma_0\partial/\partial t - \nabla^2)\mathbf{H} = 0$. Diffusion time is $\tau_m \equiv \mu\sigma_0 l^2$, l being a dimension of the system over which the magnetic field is changing.

Superconductors carry current easily, problems will be just MQS. $\nabla \cdot \mathbf{J} \approx 0$ implies that currents form closed loops. Electric fields are calculated from magnetic induction (Faraday) but only after magnetic field is found first.

Follow Drude’s model of ohmic conductivity: electron carriers are in equilibrium similar to perfect gas. Total response is sum of individual electrons, no interactions added. Motion of single electron:

$$m \frac{dv}{dt} = f_{em} + f_{drag} = qE - \frac{m}{\tau_{tr}}v \quad (4)$$

B field no role, as it does not point in direction of motion. τ_{tr} scattering time, mean time between collisions, obtained from experiment. For sinusoidal field:

$$v = \left(\frac{q\tau_{tr}}{m} \right) \frac{1}{1 + j\omega\tau_{tr}} E \quad (5)$$

Summing for all carriers, get J :

$$J = nqv = \sigma_0 \frac{1}{1 + j\omega\tau_{tr}} E \quad (6)$$

More generally,

$$\mathbf{E} = \frac{1}{\sigma_0} \left(1 + \tau_{tr} \frac{\partial}{\partial t} \right) \mathbf{J} \quad (7)$$

$\sigma(\omega) = \sigma_0(1/1 + j\omega\tau_{tr})$. For copper, $\tau_{tr} \approx 2.4 \times 10^{-14}$ s. σ no frequency dependence up to 1 THz, as $\omega\tau_{tr} \ll 1$. For $\omega\tau_{tr} \gg 1$, σ is complex, power not dissipated. Notice that in this case, $\vec{E} = j\omega\tau_{tr}/\sigma_0 \vec{J}$.

Electrons act as magnetic dipoles moving back and forth due to their inertia (since they don't scatter), contributing to μ (like an additional inductance) and allowing em waves to propagate with negligible loss. Model equivalent to voltage-driven RL network, as

$$Y(\omega) = \left(\frac{1}{R}\right) \frac{1}{1 + i\omega\tau_{RL}} \quad (8)$$

leading to $L = \tau_{tr}/\sigma_0 = m/nq^2$ and $R = 1/\sigma_0 = m/(nq^2\tau_{rt})$. Here, high frequencies will find a voltage drop across the inductor and little in the resistor, consistent with electron's motion (no scattering, just oscillating). How come ohmic systems do not dissipate? Key now is to consider that medium is dispersive (frequency-dependent). In normal systems of small enough dimensions the material appears lossless because $\tau_{tr} > \tau_{em}$, and electrons do not scatter within a period of the wave.

Now, it seen in experiment that perfect conductors under steady-state. What constitutive law do they follow to be perfect conductors? We need to postulate the existence of a new carrier: superelectrons. Need to solve Drude's model for $\tau_{tr} \rightarrow \infty$, as the inequalities for being quasistatic and lossless need to be true at $\omega = 0$. Now R vanishes. What about L ? it's still there! Transport of superelectrons is that of an inductance of value

$$L_s = \frac{m^*}{n^*(q^*)^2} \quad (9)$$

where the star is for superelectrons, ie Cooper pairs.

Now a new law can be postulated:

$$\boxed{\mathbf{E} = \frac{\partial}{\partial t}(\Lambda \mathbf{J})}, \quad (10)$$

with

$$\Lambda \equiv \frac{m^*}{n^*(q^*)^2} \quad (11)$$

With this equation we recover that $E \propto J$. This is the first London equation [5]. This type of equation is also called an "acceleration" equation, as the electric field provides a means for superelectrons to accelerate without loss. This means perfect conductors will develop a voltage across them when driven by ac currents. This voltage is coming from the inertia of superelectrons, motion of carriers out of phase with drive develops a voltage.

Now, the equation of motion for the magnetic field becomes

$$\left(\frac{\mu_0}{\Lambda} - \nabla^2\right) \frac{\partial}{\partial t} \mathbf{H} = 0 \quad (12)$$

No characteristic time constant but length, $\sqrt{\Lambda/\mu_0}$.

Slab problem, sinusoidal field, leads to defining the penetration depth $\lambda \equiv \sqrt{\Lambda/\mu_0}$. Equivalent to skin depth, but frequency-independent. Material-dependent. Bulk approximation when screening currents are superficial, $\lambda/\text{thickness} \ll 1$. Compared to ohmic material, field inside material is complex, thus phase changes with depth (it gets damped). In a perfect conductor phase is constant, as wavenumber is real, leading to evanescent or nonwavelike fields. Consistent with material

being reactive, it stores energy and returns it, losslessly. Remember that the average energy dissipated in a normal conductor is $P_{\text{diss}} = (1/T) \int_0^T \mathbf{J} \cdot \mathbf{E} dt$. For a perfect conductor, $\mathbf{E} \sim i\mathbf{J}$ so that \mathbf{E} and \mathbf{J} are out of phase and the power dissipated is null.

What about fields before the application of an external field? in an ohmic material, no matter how perfect, eventually they are dissipated. But not in a perfect conductor. A constant external field results in no time dependence inside the perfect conductor, as London eq. is identically satisfied $\partial H / \partial t = 0$. Therefore, no way to couple to the steady-state field. Fields are found from initial conditions. Example of slab:

$$H(y, t) = [H(a, t) - H(a, 0)] \frac{\cosh(y/\lambda)}{\cosh(a/\lambda)} + H(y, 0), \quad (13)$$

with $H(a, t) = H(a, 0)$ for static external field. Therefore, initial conditions must be explicitly defined. This example shows that the Meissner effect is not included. If the material was normal with an external field, that field inside the material will remain after transitioning to the superconducting state. Superconductors are flux expelling media, contrary to flux-preserving perfect conductors. Thus the “wrong” thing here is the time dependence. We need another constitutive relation to obtain a fully classical model of superconductivity.

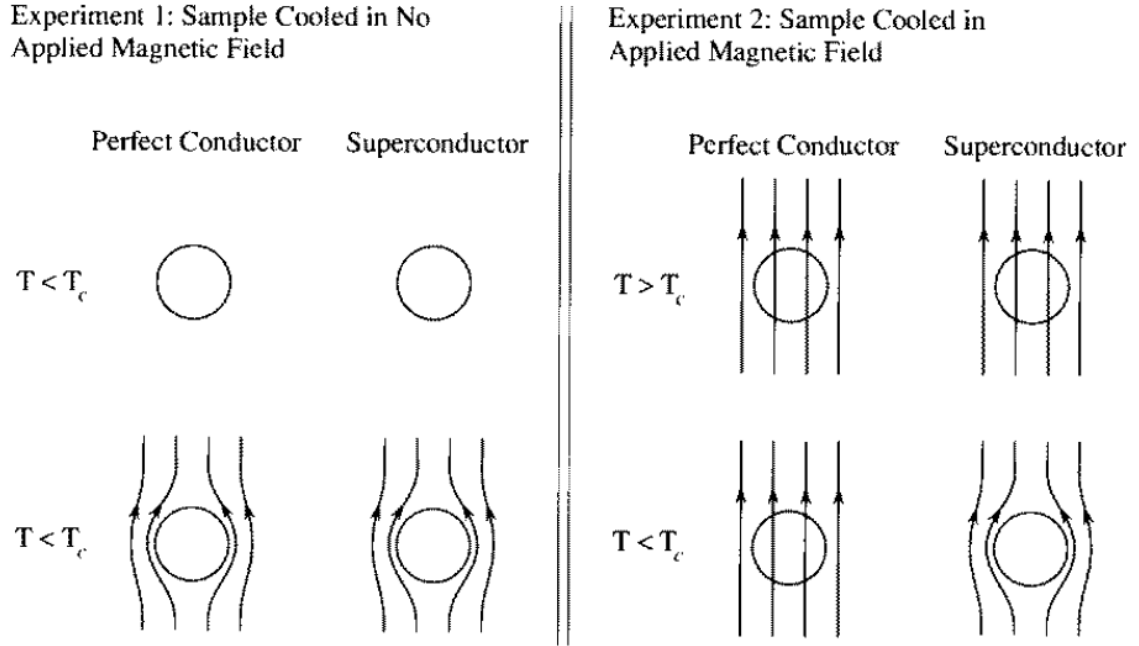


Figure 3: Scenarios with applied fields and cooling down for a perfect conductor, showing how it is a flux-preserving medium. Source: Orlando book.

1.2.2 The Meissner effect. Second London equation

What about $B = \mu M$, and $\mu \rightarrow 0$? wouldn't work as field wouldn't be continuous.

Key observation: λ is independent of frequency. Therefore, if external field is increasingly slower, the field distribution will not change. This means the field distribution will be the same as in the *static* case.

Take Farady's law with the first London equation:

$$\nabla \times \frac{\partial}{\partial t}(\Lambda \mathbf{J}) = -\frac{\partial \mathbf{B}}{\partial t} \quad (14)$$

integrate it with respect to time, and *postulate* that the constant of integration is identically 0! Then, the resulting constitutive equation is

$$\nabla \times (\Lambda \mathbf{J}) = -\mathbf{B} \quad (15)$$

This is the second London equation. Using some identities we arrive at the field equation:

$$(\lambda^{-2} - \nabla^2)\mathbf{B} = 0 \quad (16)$$

This is the same as the first London equation but without the time dependence, because we have postulated that this relationship holds for all frequencies. Thus, the 2nd London equation is consistent with the Meissner effect of flux exclusion in steady state, and is independent of the previously obtained field relations. In practice, the 2nd London equation is only used implicitly. It “just” guarantees that magnetic flux is expelled from superconductors.

Take the example of a hollow superconducting cylinder. All fields inside the superconductor are 0, like $\mathbf{E} = 0$. Integrating the field along a contour, using Faraday's law:

$$\oint_C \mathbf{E} \cdot d\mathbf{l} = -\frac{d}{dt} \int_S \mathbf{B} \cdot d\mathbf{s} = 0 \quad (17)$$

Therefore, the magnetic flux must be constant in time inside the hole.

Example 1: hollow cylinder with no background field. External surface currents cancel any applied fields in the cylinder.

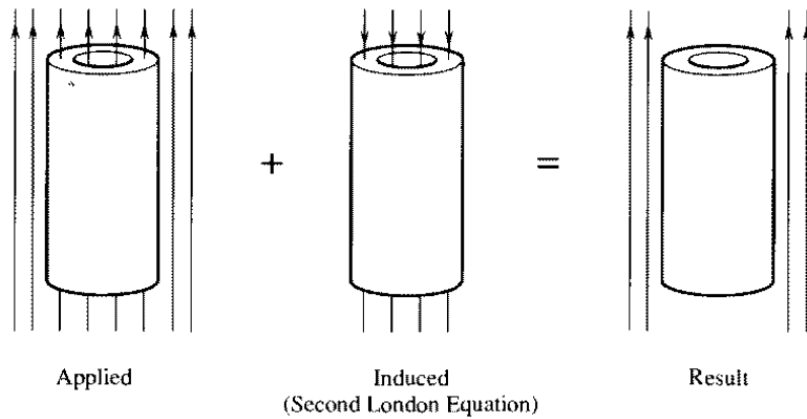


Figure 4: Superconducting cylinder when a field is applied after entering the superconducting state. Source: Orlando book.

Example 2: Start with hollow cylinder above T_c . Apply magnetic field and wait for induced currents to relax away, so field penetrates material. Now lower $T < T_c$.

Material is superconducting, but outer current would cancel total flux, violating flux conservation. Therefore a new current, equal but in the opposite direction, flows in the inner surface to keep flux constant! Now, remove the external field. Because flux has to stay constant, this traps or “freezes” the flux in the cylinder, to never decay away due to the persistent current.

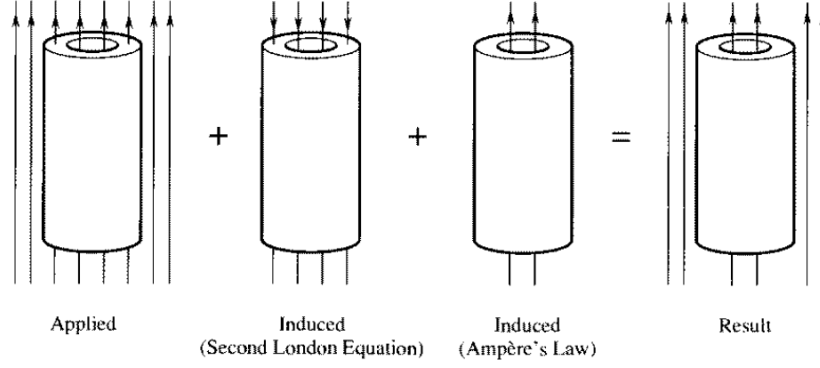


Figure 5: Superconducting cylinder when a field is applied before entering the superconducting state. Source: Orlando book.

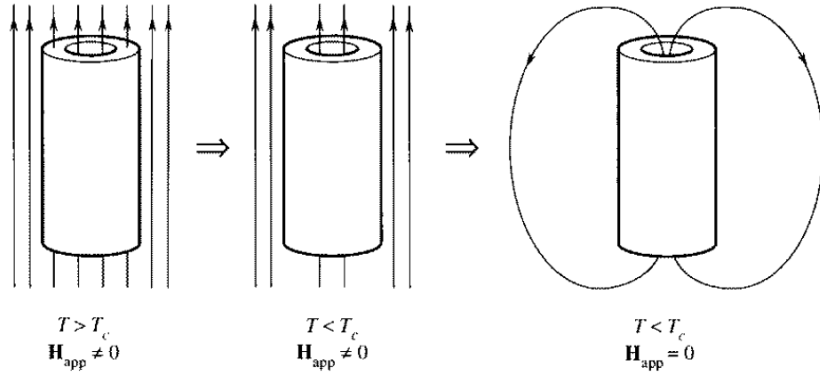


Figure 6: Superconducting cylinder trapping flux when a field is applied before entering the superconducting state. Source: Orlando book.

1.2.3 Two-fluid model

Superconductivity is a thermodynamic phenomenon, the superconducting state is a change of thermodynamic state, it requires transitioning through a certain temperature.

We can now wonder, where do electrons go below T_c ? and where do superelectrons go above T_c ? To answer these questions, we need to look at the penetration depth. Experimentally, it is found that

$$\lambda(T) = \frac{\lambda_0}{\sqrt{1 - (T/T_c)^4}} \quad (18)$$

$\lambda_0 = \lambda(0)$. It's a smooth curve, contrary to the resistance. Since $\lambda(T) = \sqrt{m^*/n^*(T)(q^*)^2}$, as the other quantities don't change. Then,

$$n^*(T) = n_0^* \left(1 - \left(\frac{T}{T_c} \right)^4 \right), \text{ for } T \leq T_c \quad (19)$$

$n_0^* \equiv m^*/(\lambda_0^2(q^*)^2\mu_0)$. Superelectron number increases monotonically. Since super-electrons are Cooper pairs, $n_0^* = n_{tot}/2$ at $T = 0$. n_{tot} is not a function of T . Then,

$$n_{tot} = n(T) + 2n^*(T), \forall T \quad (20)$$

from where

$$n(T) = n_{tot} \left(\frac{T}{T_c} \right)^4 \text{ for } T \leq T_c \quad (21)$$

For intermediate temperatures, both carriers coexist simultaneously, $\mathbf{J} = \mathbf{J}_n + \mathbf{J}_s$. The proper lumped element model is a parallel $R - L_n$ with L_s . This is the two-fluid model proposed in 1934 by C. Gorter and H. B. G. Casimir. A conclusion of this model is that for ac excitations, the superconductor will exhibit loss at finite temperature. The current equation is thus

$$\mathbf{J} = \left(\frac{\tilde{\sigma}_0(T)}{1 + j\omega\tau_{tr}} + \frac{1}{j\omega\mu_0\lambda(T)^2} \right) \mathbf{E} \quad (22)$$

where $\tilde{\sigma}_0(T) = (n_{tot}e^2\tau_{tr}/m)(T/T_c)^4$ for $T \leq T_c$. For completeness, the total magnetic field becomes

$$\left(1 - \lambda^2(T)\nabla^2 + (\mu_0\tilde{\sigma}_0(T)\lambda^2(T) - \tau_{tr}\lambda^2(T)\nabla^2 + \tau_{tr})\frac{\partial}{\partial t} \right) \mathbf{B} = 0 \quad (23)$$

All these expressions are only valid if $\omega < \omega_{pair}$, with ω_{pair} being the pairing energy of Cooper pairs.

The expressions found for calculating the electric and magnetic fields in superconductors already allow solving many interesting problems in engineering.

2 Quantum mechanics of superconductors

So far, we obtained a rather good description of the macroscopic effects of superconductivity, more than enough to start producing real world applications such as levitation, power transmission, coils, etc. but we remain as clueless about the origin of superconductivity as we were in the beginning of the previous chapter. The true explanation of the physics behind superconductivity evaded physicists for decades, until 1956-1957 where the theory put together by John Bardeen, Leon Cooper and John Robert Schrieffer (known as the BCS theory) accomplished the extraordinary feat of explaining all observations related to low-temperature superconductors (type I-II), so-called “s”-wave superconductors for reasons that will be clear later. The theory does not explain high-temperature superconductivity (which actually relates to “d”-wave superconductivity), but it has been extended to describe other exotic types of superconductors such as “p”-wave superconductors.

It is not strictly necessary to apply the BCS theory as a whole to describe and understand superconducting circuits, as the energies involved in qubits are far below the superconducting gap. The BCS-related superconducting effects are there as a sort of ‘scenario’ for the qubit physics to take place. Nevertheless, it is important to have well-understood concepts from BCS to understand the physics of the Josephson effect, as will be seen in the next lecture. Therefore, it is relevant to have a basic understanding of BCS theory to understand the motivations that define superconducting qubits later on. Besides, some decoherence effects found in superconducting qubits that will be studied in lecture 9 have their origin in superconductivity physics. So it is worth taking a look at it.

2.1 A glimpse of BCS theory

2.1.1 The Cooper problem

The key aspect of the BCS theory is the existence of a bound state of electrons below the Fermi level of the material. Understanding how such a state can exist was first proposed by Leon Cooper [8] prior to the establishment of the formal BSC theory.

In a normal metal the ground state can be visualized as a free-electron gas where all one-electron states with energy $\hbar^2 k^2/2m$ are filled up to an energy $E_F = \hbar^2 k_F^2/2m$ known as the Fermi energy of the material, with wave vector modulus k_F . With any kind of interaction, no matter how small, this ground state becomes unstable. To understand this, let us take the case of two electrons with coordinates \mathbf{r}_1 and \mathbf{r}_2 , with the rest of the electrons still a free electron gas. By the exclusion principle, the two electrons only interact with each other as they cannot occupy states with $k < k_F$. The orbital wavefunction of the two-electron state is $\psi_o(\mathbf{r}_1, \mathbf{r}_2)$. Following a theorem by Bloch about the ground state in a metal, let’s consider the state with the center of gravity at rest, therefore total momentum $\mathbf{k}_1 + \mathbf{k}_2 = 0$, and only the relative position $\mathbf{r}_1 - \mathbf{r}_2$ matters. Expanding ψ_o in plane waves¹,

$$\psi_o(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)}, \quad (24)$$

$g_{\mathbf{k}}$ are the weighting coefficients. Remember that for electrons we need total antisymmetric wavefunctions, including orbital and spin parts. We take a total wavefunction being the product of orbital ψ_o and spin parts χ

$$\psi(\mathbf{r}, \sigma) = \psi_o(\mathbf{r})\chi(\sigma_1, \sigma_2). \quad (25)$$

Here, $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$. Anticipating an attractive interaction, the (antisymmetric) singlet state, $\chi = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, will have lower energy as the (symmetric) orbital part $\psi_o(\mathbf{r}) \sim \cos(\mathbf{r})$ will lead to a maximum when $\mathbf{r}_1 - \mathbf{r}_2$ is small, implying the electrons being close to each other. For ease of the math, let’s keep the complete form from Eq. (24).

¹Remember that electrons in a crystal travel as plane waves with periodic boundary conditions following Bloch’s theorem [9].

The Schrödinger equation for the two electrons is

$$-\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) \psi(\mathbf{r}_1 - \mathbf{r}_2) + V(\mathbf{r}_1 - \mathbf{r}_2) \psi(\mathbf{r}_1 - \mathbf{r}_2) = E \psi(\mathbf{r}_1 - \mathbf{r}_2) \quad (26)$$

Defining the plane-wave energy $\epsilon_k \equiv \hbar^2 k^2 / 2m$, multiplying by $\frac{1}{\sqrt{V}} e^{-i\mathbf{k} \cdot \mathbf{r}}$ and integrating over the volume V , we find an equation for the coefficients $g_{\mathbf{k}}$

$$\sum_{|\mathbf{k}'| > k_F} g_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} = (E - 2\epsilon_k) g_{\mathbf{k}}, \quad (27)$$

where

$$V_{\mathbf{k}\mathbf{k}'} \equiv \frac{1}{\sqrt{V}} \int V(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}} d\mathbf{r}, \quad (28)$$

is the matrix element of the interaction with electronic states $(\mathbf{k}, -\mathbf{k})$ and $(\mathbf{k}', -\mathbf{k}')$. If a set of $g_{\mathbf{k}}$ exists with energy $E < 2E_F$, a bound pair exists.

In order to complete the problem, Cooper introduced a simplification to the form of the potential, considering it constant $V_{\mathbf{k}\mathbf{k}'} = -\bar{V}$ up to some energy $\hbar\omega_c$ away from E_F and $V_{\mathbf{k}\mathbf{k}'} = 0$ for higher energies than $\hbar\omega_c$. Then, the left-hand-side of Eq. (27) is a constant independent of \mathbf{k} , and we have

$$g_{\mathbf{k}} = \bar{V} \frac{\sum_{\mathbf{k}'} g_{\mathbf{k}'}}{E - 2\epsilon_k}. \quad (29)$$

Summing both sides over \mathbf{k} , we have

$$\frac{1}{\bar{V}} = \sum_{|\mathbf{k}| > k_F} \frac{1}{2\epsilon_k - E}. \quad (30)$$

The sum can be turned into an integration for a large volume system, with $N(0)$ denoting the density of states at the Fermi level. Then

$$\frac{1}{\bar{V}} = N(0) \int_{E_F}^{E_F + \hbar\omega_c} \frac{d\epsilon}{2\epsilon - E} = \frac{1}{2} N(0) \ln \frac{2E_F - E + 2\hbar\omega_c}{2E_F - E}. \quad (31)$$

Re-arranging terms,

$$E = 2E_F + \frac{2\hbar\omega_c}{1 - e^{2/N(0)\bar{V}}} \simeq 2E_F - 2\hbar\omega_c e^{-2/N(0)\bar{V}}, \quad (32)$$

where it was used that for typical superconductors $N(0)V \ll 1$, the so-called weak coupling approximation.

Therefore, an attracting potential, regardless of its magnitude, produces a bound state with negative energy with respect to the Fermi level made up of electrons with $k > k_F$, i.e., with kinetic energy in excess of E_F . The binding energy from the potential term compensates this excess kinetic energy. In a gas of free electrons, whenever a negative interaction is turned on, all electrons will eventually bind in pairs.

From Eq. (29), we see that the wave function coefficients only depend on the modulus of \mathbf{k} , not its direction. Therefore this is a spherically symmetric state, corresponding to an S-wave type wavefunction. Also, this coefficient has a maximum

for electrons with $\epsilon_k = E_F$ at the Fermi energy, which will be those most strongly involved in forming the bound state. Since the excess energies from E_F are much smaller than $\hbar\omega_c$ in practice, the shape of the potential at those energies will have little effect on the result, justifying the crude approximation made on the potential. Finally, it can be shown that the average Cooper pair size ρ is of order ξ , the coherence length of the system, which turns out to be much larger than the inter-particle size, implying that the pairs in a superconductor highly overlap. For example, aluminum has a conduction band electronic density of 18.1×10^{10} electrons/ μm^3 , while $\xi_{\text{Al}} \sim 1.6 \mu\text{m}$.

The origin of the negative interaction can only be explained when one introduces the motion of the (positive) ion cores. The idea is that the first electron polarizes the medium by attracting positive ions, which in its turn attracts a second electron. If this net attraction between electrons outweighs the Coulomb repulsion, superconductivity results. The ionic lattice vibrates at certain phononic frequencies, which must be connected with the interaction. Therefore, electrons exchange phonons in order to attract each other. It is shown by De Gennes [4] that the interaction calculated becomes

$$V = U_q + \frac{2|W_q|^2}{\hbar} \frac{\omega_q}{\omega^2 - \omega_q^2}, \quad (33)$$

where ω_q is the phonon created in the interaction, W_q is the electron-phonon matrix element, and U_q is the Coulomb interaction. Therefore, for energies $\omega < \omega_q$ the second term may exceed the Coulomb interaction, depending on each material, leading to the effective electron-electron attraction needed for achieving a superconducting state.

2.1.2 The BCS ansatz

Previously we found a wave function $\psi(\mathbf{r}_1 - \mathbf{r}_2)$ for a pair of bound electrons in a normal metal. A natural generalization for the condensed state of a superconductor is to treat all electrons equally, by a wave function of the form

$$\psi_N(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \psi(\mathbf{r}_1 - \mathbf{r}_2)\psi(\mathbf{r}_3 - \mathbf{r}_4) \cdots \psi(\mathbf{r}_{N-1} - \mathbf{r}_N). \quad (34)$$

This state describes all electrons bound in pairs. At this point it is very convenient to change notation and use the second quantization, in which the occupied states (including spin) are specified by creation operators $a_{\mathbf{k}\uparrow}^\dagger$, which creates an electron of momentum \mathbf{k} and spin up. The annihilation operators $a_{\mathbf{k}\uparrow}$ empty the corresponding state. The singlet wave function of two electrons found earlier becomes

$$|\psi\rangle = \sum_{k > k_F} g_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger |F\rangle, \quad (35)$$

where $|F\rangle$ represents the Fermi sea with all states filled up to k_F . The creation and annihilation operators obey anticommutation relations characteristic of fermion operators

$$[a_{\mathbf{k}\sigma}, a_{\mathbf{k}'\sigma'}^\dagger] \equiv a_{\mathbf{k}\sigma} a_{\mathbf{k}'\sigma'}^\dagger + a_{\mathbf{k}'\sigma'}^\dagger a_{\mathbf{k}\sigma} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}, \quad (36)$$

$$[a_{\mathbf{k}\sigma}^\dagger, a_{\mathbf{k}'\sigma'}^\dagger]_+ = [a_{\mathbf{k}\sigma}, a_{\mathbf{k}'\sigma'}]_+ = 0. \quad (37)$$

The particle number operator is defined as $n_{\mathbf{k}\sigma} = a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}$.

Now we can express the BCS wave function in the most general case for N electrons with all prescriptions of Cooper pairing introduced above as

$$|\psi_N\rangle = \sum g(\mathbf{k}_1, \dots, \mathbf{k}_l) a_{\mathbf{k}_1\uparrow}^\dagger a_{-\mathbf{k}_1\downarrow}^\dagger \cdots a_{\mathbf{k}_l\uparrow}^\dagger a_{-\mathbf{k}_l\downarrow}^\dagger |vac\rangle. \quad (38)$$

Each term in the sum is characterized by the set of occupied states $\mathbf{k}_1, \dots, \mathbf{k}_l$. $|vac\rangle$ represents a vacuum state with no electrons. The sum runs on all values of \mathbf{k} in the band, implying many g 's to determine. This form of the wave function is very difficult to work with. Here comes the discovery of BCS. They proposed a new state to describe the ground state

$$|\psi_G\rangle = \prod_{\mathbf{k}=\mathbf{k}_1, \dots, \mathbf{k}_M} (u_{\mathbf{k}} + v_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger) |vac\rangle, \quad (39)$$

with $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$. The probability of a pair with $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ to be occupied is $|v_{\mathbf{k}}|^2$ and the probability to be unoccupied is $|u_{\mathbf{k}}|^2 = 1 - |v_{\mathbf{k}}|^2$. It can be shown (see [4]) that this state displays the same expectation values of simple operators as the general wavefunction $|\psi_N\rangle$. In fact, $|\psi_N\rangle$ is the part of $|\psi_G\rangle$ that has N creation operators acting upon $|vac\rangle$, i.e., the component of $|\psi_G\rangle$ that describes an N -particle state. This approximation to the ground state by BCS is known as a mean-field approach.

The calculation of the energy is performed using the so-called pairing Hamiltonian which assumes it contains superconductivity, as it omits other terms not paired as $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$,

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger a_{-\mathbf{l}\downarrow} a_{\mathbf{l}\uparrow}. \quad (40)$$

Here we defined the number operator $n_{\mathbf{k}\sigma} \equiv a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}$. The first term corresponds to the kinetic energy of pairs of electrons. The second term scatters a pair from $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$ to $(\mathbf{l} \uparrow, -\mathbf{l} \downarrow)$, representing the virtual exchange of a phonon between two electrons that pairs them.

2.1.3 Variational method

The following step is to minimize the energy of the system in the state $|\psi_G\rangle$, $\langle\psi_G|\mathcal{H}|\psi_G\rangle$, by minimizing the coefficients $u_{\mathbf{k}}, v_{\mathbf{k}}$. The state $|\psi_G\rangle$ does not fix the number of particles, and therefore the quantity that needs to be minimized is

$$\langle\psi_G|\mathcal{H}|\psi_G\rangle - E_F \langle\psi_G|N|\psi_G\rangle, \quad (41)$$

with $N \equiv \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma}$. The inclusion of the second term is equivalent to offsetting the kinetic energy to be that with respect to the Fermi energy, $\xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - E_F$. That is, the minimization is performed over the following operators

$$\delta\langle\psi_G| \left(\sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{l}} V_{\mathbf{k}\mathbf{l}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger a_{-\mathbf{l}\downarrow} a_{\mathbf{l}\uparrow} \right) |\psi_G\rangle = 0. \quad (42)$$

Using the form in Eq. (39), it can be shown [2, 4] that Eq. (41) becomes

$$\langle \psi_G | (\mathcal{H} - E_F N) | \psi_G \rangle = 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum_{\mathbf{kl}} V_{\mathbf{kl}} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{l}} v_{\mathbf{l}}. \quad (43)$$

Here, $u_{\mathbf{k}}, v_{\mathbf{k}}$ were taken as real without loss of generality. Since we must satisfy $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$, by making the replacement

$$u_{\mathbf{k}} = \sin \theta_{\mathbf{k}}, \quad v_{\mathbf{k}} = \cos \theta_{\mathbf{k}}, \quad (44)$$

the function to be minimized with respect to $\theta_{\mathbf{k}}$ is

$$\langle \psi_G | \mathcal{H} - E_F N | \psi_G \rangle = \sum_{\mathbf{k}} (1 + \cos 2\theta_{\mathbf{k}}) + \frac{1}{4} \sum_{\mathbf{kl}} V_{\mathbf{kl}} \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{l}}, \quad (45)$$

The minimization leads to

$$\tan 2\theta_{\mathbf{k}} = \frac{\sum_{\mathbf{l}} \sin 2\theta_{\mathbf{l}}}{2\xi_{\mathbf{k}}}. \quad (46)$$

Now let's define

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{l}} V_{\mathbf{kl}} \sin 2\theta_{\mathbf{l}}, \quad (47)$$

$$E_{\mathbf{k}} = (\Delta_{\mathbf{k}}^2 + \xi_{\mathbf{k}}^2)^{1/2} \quad (48)$$

Now,

$$\tan 2\theta_{\mathbf{k}} = -\frac{\Delta_{\mathbf{k}}}{\xi_{\mathbf{k}}}, \quad \sin 2\theta_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}}, \quad \cos 2\theta_{\mathbf{k}} = -\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}, \quad (49)$$

the choice of signs in the last two expressions is such that for $\xi_{\mathbf{k}} \rightarrow \infty$, $v_{\mathbf{k}}^2 \rightarrow 0$, so no probability to pair two electrons if their kinetic energy far exceeds the Fermi level.

Going back to Eq. (46),

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{l}} \frac{\Delta_{\mathbf{l}}}{\sqrt{\Delta_{\mathbf{l}}^2 + \xi_{\mathbf{l}}^2}} V_{\mathbf{kl}}. \quad (50)$$

A trivial solution exists with $\Delta_{\mathbf{k}} = 0$, so that $v_{\mathbf{k}} = 1$ for $\xi_{\mathbf{k}} < 0$ and $v_{\mathbf{k}} = 0$ for $\xi_{\mathbf{k}} > 0$. This state contains all \mathbf{k} states occupied until $\mathbf{k}_{\mathbf{F}}$, the normal Fermi sea at $T = 0$. But we look for a nontrivial solution for negative $V_{\mathbf{kl}}$. Following from Cooper's derivation,

$$V_{\mathbf{kl}} = \begin{cases} -V & \text{if } |\xi_{\mathbf{k}}| \text{ and } |\xi_{\mathbf{l}}| \leq \hbar\omega_c \\ 0 & \text{otherwise} \end{cases} \quad (51)$$

Within this approximation, $\Delta_{\mathbf{k}}$ is a constant Δ if $|\xi_{\mathbf{k}}|, |\xi_{\mathbf{l}}| < \hbar\omega_c$. The equation we want to solve now is

$$\Delta = \frac{1}{2} \sum_{\mathbf{k}} \frac{\Delta}{\sqrt{\Delta^2 + \xi_{\mathbf{k}}^2}} V \quad (52)$$

We replace the sum by an integral that will contain the density of states per unit energy in the normal state $N(\xi_{\mathbf{k}})$ for a given spin direction. Since the energy interval

we are interested has width $\hbar\omega_c \ll E_F$, we can replace $N(\xi_{\mathbf{k}})$ by its value at the Fermi level $N(0)$,

$$\Delta = \frac{N(0)V}{2} \int_{-\hbar\omega_c}^{\hbar\omega_c} \Delta \frac{\xi}{\sqrt{\Delta^2 + \xi^2}}, \quad (53)$$

which leads to the solution

$$\Delta = \frac{\hbar\omega_c}{\sinh \frac{1}{N(0)V}}, \quad (54)$$

which in the limit $N(0)V \ll 1$ (typical for many pure metal superconductors) reduces to

$$\Delta = 2\hbar\omega_c e^{-1/N(0)V}. \quad (55)$$

Finally we can determine the values of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ to find the BCS wavefunction that minimizes the energy. They are

$$v_{\mathbf{k}}^2 = \frac{1}{2} \left[1 - \frac{\xi_{\mathbf{k}}}{\sqrt{\Delta^2 + \xi_{\mathbf{k}}^2}} \right], \quad (56)$$

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left[1 + \frac{\xi_{\mathbf{k}}}{\sqrt{\Delta^2 + \xi_{\mathbf{k}}^2}} \right] = 1 - v_{\mathbf{k}}^2. \quad (57)$$

There is a striking resemblance between the occupation probability $v_{\mathbf{k}}^2$ at $T = 0$ and a Fermi distribution at $T = T_c$. This means that the superconducting state does not imply a change in occupation in \mathbf{k} -space, no gap opens up. In the normal state, there is no phase relation between occupied states, phases are random. Now, below T_c , there is a *single* quantum state with approximately the same set of many-body states with various one-electron states occupied but having a *fixed* phase relation.

Now let's evaluate the ground state energy of the BCS Hamiltonian, using the relations found above for $\theta_{\mathbf{k}}$ in Eq. (45)

$$\langle \psi_G | (\mathcal{H} - E_F N) | \psi_G \rangle = \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} - \frac{\xi_{\mathbf{k}}^2}{E_{\mathbf{k}}} \right) - \frac{\Delta^2}{V} \quad (58)$$

We will consider the contribution to the Hamiltonian from the normal-state, the terms that survive by setting $\Delta = 0$, $E_{\mathbf{k}} = |\xi_{\mathbf{k}}|$:

$$\langle E_n \rangle \equiv \langle \psi_G | (\mathcal{H} - E_F N) | \psi_G \rangle_{\Delta=0} = \sum_{|\mathbf{k}| < k_F} 2\xi_{\mathbf{k}}, \quad (59)$$

the terms with $|\mathbf{k}| > k_F$ giving zero. Using the symmetry of the Fermi function around the Fermi energy, we can compute the energy difference:

$$\langle E_s \rangle - \langle E_n \rangle = 2 \sum_{|\mathbf{k}| > k_F} \left(\xi_{\mathbf{k}} - \frac{\xi_{\mathbf{k}}^2}{E_{\mathbf{k}}} \right) - \frac{\Delta^2}{V} \quad (60)$$

Going from discrete to continuum integral, this energy difference becomes

$$\langle E_s \rangle - \langle E_n \rangle = -\frac{1}{2} N(0) \Delta(0)^2, \quad (61)$$

which is known as the condensation energy, and it is negative, so the system releases energy when condensing. $T = 0$ has been specified for the function Δ . This energy is rather small, on the order $\Delta^2/E_F \sim 0.01\text{K}$.

2.1.4 BCS excitations and finite temperature

Without going through the derivation, excited states of the BCS ground state can be calculated. These have an energy [2, 4]

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}. \quad (62)$$

Clearly, $\Delta_{\mathbf{k}}$ has the role of an energy gap or minimum excitation. Note that breaking a Cooper pair requires a minimum energy of $2\Delta_{\mathbf{k}}$. $E_{\mathbf{k}} \leq \Delta$ represents a fermionic excitation of momentum $\hbar\mathbf{k}$ we name as *quasiparticle*, as it is not a simple electron but a dressed particle with phonons and other electrons. The probability to find this state excited in thermal equilibrium will be given by a Fermi distribution of quasiparticles

$$f(E_{\mathbf{k}}) = \frac{1}{e^{\beta E_{\mathbf{k}}} + 1}, \quad (63)$$

where $\beta = 1/k_B T$. At $T = 0$, $f(E_{\mathbf{k}}) = 0$ for all \mathbf{k} . Quasiparticles will become an important topic when considering decoherence channels for superconducting qubits, as even though thermal equilibrium dictates that there shouldn't be nearly any at conventional operating temperatures the experiments observe orders of magnitude larger densities, indicating a mechanism of generation of those quasi particles. Recent findings indicate that this could be related to ionizing radiation, including cosmic rays.

At this finite temperature, the gap equation becomes (see [2] for a derivation)

$$\frac{1}{V} = \frac{1}{2} \sum_{\mathbf{k}} \frac{\tanh(\beta E_{\mathbf{k}}/2)}{E_{\mathbf{k}}}. \quad (64)$$

This equation can be solved to find the critical temperature T_c of the superconductor, by considering that at T_c , $\Delta \rightarrow 0$, then $E_{\mathbf{k}} \rightarrow |\xi_{\mathbf{k}}|$. Using this in the previous equation and integrating as done before

$$\frac{1}{N(0)V} = \ln \left(\frac{2e^{\gamma} \hbar \omega_c}{\pi k_B T_c} \right), \quad (65)$$

where $2e^{\gamma}/\pi \approx 1.13$, $\gamma = 0.577...$ being the Euler constant. Therefore,

$$k_B T_c = 1.13 \hbar \omega_c e^{-1/N(0)V}. \quad (66)$$

Using Eq. (55), finally

$$\Delta(0) = 1.764 k_B T_c. \quad (67)$$

This is a very important equation to relate gap energy with transition temperature in low- T_c superconductors and is the final result from BCS theory we will use in this course, as it will become important to understand energy scales in the superconductors used to build quantum circuits.

It is important to highlight at this point that the BCS theory captures the phenomenology from many superconducting materials, particularly those consisting of a single material, but it does not include the higher T_c ones, nor the hydride ones that need extremely high pressures.

2.1.5 Two kinds of superconductors

To derive London equation, $v(r)$ was assumed to vary slowly. In the condensed state, two electron velocities are correlated if their distance is $R_{12} < \xi_0$, ξ_0 being some correlation length. The London equation is valid if the velocity variation $v(r)$ within ξ_0 is negligible. The important domain in momentum space is

$$E_F - \Delta < p^2/2m < E_F + \Delta$$

. This is the energy range relevant electrons (the ones that may be excited in the superconductor) occupy within the superconductor. Assuming $\Delta \ll E_F$ (momentum δp constant over 2Δ), this is a layer of $\delta p \simeq 2\Delta/v_F$, $v_F = p_F/m$ is the Fermi velocity. Finally, $\xi_0 = \hbar v_F/\pi\Delta$.

In London materials, $h(r)$, $j(r)$, or $v(r)$ vary with λ_L . Then, **Type I superconductors exhibiting $\lambda_L \ll \xi_0$ do not follow London's equation. They still exhibit the Meissner effect but the penetration length has a more complicated form developed by A. B. Pippard [10].** In Type II superconductors (usually compounds) $\lambda_L \gg \xi_0$, and they may be called London superconductors. In the case of alloys, the addition of impurities has effects on the mean free path and ξ_0 may be reduced, turning a Pippard superconductor into a London superconductor.

Type-II superconductors let field penetrate in discrete tubes that contain a quantized amount of flux, the flux quantum Φ_0 . The core of the vortex is the size of the coherence length ξ and is in the normal state. This allows defining critical fields H_{c1} for the first vortex to enter, and H_{c2} for complete destruction of superconductivity. The reason superconductivity is destroyed at these fields is due to the enhanced kinetic energy of Cooper pairs near the vortex core. When this energy approaches the binding energy 2Δ , the Cooper pairs de-pair, leading to a maximum depairing current J_d .

2.2 The macroscopic quantum model

Up to here, we have obtained a quantum description of superconductors using the BCS theory. The solution is satisfactory to explain the phenomena observed from BCS-type superconductors but it is really not ideal to start building a quantum technology out of it. We need to be more pragmatic, more like engineers. This means finding a model that reproduces the quantum properties without invoking the complexity of BCS theory. This calls for a new model, that following Ref. [1] we will name the Macroscopic Quantum Model (MQM).

2.2.1 Macroscopic Quantum Currents

A single quantum particle in a general potential $V(\mathbf{r}, t)$ with kinematic (canonical) momentum $\mathbf{p} = m\mathbf{v}$ has an associated wave function which obeys the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{r}, t)\psi. \quad (68)$$

The probability density of to find a particle at location \mathbf{r} and time t in state ψ is given by $\mathcal{P} \equiv \psi^\dagger \psi$. If we calculate the time evolution of the probability, we are led

to

$$i\hbar \frac{\partial}{\partial t}(\psi\psi^*) = -\frac{\hbar^2}{2m}[\nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)], \quad (69)$$

which can be rewritten as

$$\frac{\partial \mathcal{P}}{\partial t} = -\nabla \cdot \mathbf{J}_{\mathcal{P}}, \quad (70)$$

where

$$\mathbf{J}_{\mathcal{P}} \equiv \frac{\hbar}{2im}(\psi^* \nabla \psi - \psi \nabla \psi^*) = \text{Re} \left\{ \psi^* \frac{\hbar}{im} \nabla \psi \right\}, \quad (71)$$

is the probability current. This equation is a local constraint to the probability of a quantum particle at a certain point, which cannot change instantaneously. That is, if the particle is moving, there is a flow of the probability in the form of a current. For a single particle, $\mathbf{J}_{\mathcal{P}}$ cannot be measured.

When the particle is charged, the interaction with external electromagnetic fields needs to be taken into account. The most convenient procedure is by invoking the vector potential \mathbf{A} which relates to the electric and magnetic fields, $\mathbf{B} = \nabla \times \mathbf{A}$, $\mathbf{E} = -\partial \mathbf{A} / \partial t - \nabla \phi$. In this case the canonical momentum gets replaced by

$$\mathbf{p} = m\mathbf{v} + q\mathbf{A}. \quad (72)$$

It can be shown (left as exercise) that the Schrödinger equation now becomes

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m} \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right)^2 \psi + q\phi\psi. \quad (73)$$

The probability current is also modified in the following form

$$\mathbf{J}_{\mathcal{P}} = \text{Re} \left\{ \psi^* \left(\frac{\hbar}{im} \nabla - \frac{q}{m} \mathbf{A} \right) \psi \right\}. \quad (74)$$

This form will be important in the quantum description of superconductivity.

Analogously to the Schrödinger equation describing the stable microscopic currents of electrons orbiting around the atomic nucleus, Fritz London [6] hypothesized that supercurrents, which had a clear quantum origin, may be similarly examined, leading to the macroscopic quantum model (MQM) of superconductivity, prior to BCS theory.

The MQM provides no explanation to the microscopic evidence of superconductivity. It is however a much more convenient method to analyze certain engineering problems, providing a good quantum as well as classical explanation for macroscopic quantum phenomena related to superconductivity.

The central hypothesis is the following: *There exists a macroscopic wavefunction, $\Psi(\mathbf{r}, t)$, that describes the behavior of the entire ensemble of superelectrons in the superconductor.*

This assumption takes into account the fact that superconductivity is a coherent phenomenon between all superelectrons. Now Ψ will be sufficient to describe the macroscopic supercurrent \mathbf{J}_s analogously to ψ for a single particle. Also, by analogy, we can define the density of superelectrons $n^*(\mathbf{r}, t)$ as

$$\Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t) \equiv n^*(\mathbf{r}, t), \quad (75)$$

This formulation presents analogies to fluid mechanics, where the number of particles is assumed large enough to yield a continuous fluid density. We are then dealing with a charged superfluid. But a high density implies that the particles must be close to each other and in the same state, which is precisely what bosons do. Fermions, on the contrary, like to avoid each other and electrons are fermions. But since in a superconductor they pair up, a Cooper pair behaves like a boson and the formulation of the MQM results appropriate since bosons like to bunch up. In fact, Cooper pairs are actual bosons since exchange of the two electrons leads to the same wavefunction. The probability to break a Cooper pair at low T is given by Eq. (63) $\sim e^{-E_k/k_B T} \ll 1$, therefore electrons prefer to pair up as bosons and accumulate in the superconducting state. In fact, bosons experience the bunching effect that for a state ψ with n bosons, the probability for another boson to occupy the same state is related to n . That is in fact why the superconductor exhibits no resistance, all electrons collectively occupy the same state, there is no degradation in the phase of the wave function.

The analogy with a single particle leads now to the conservation of flow of particles, and therefore it represents a physical current! Let's call this the macroscopic quantum current density, or simply supercurrent density. In the presence of an e.m. field:

$$\mathbf{J}_s = q^* \text{Re} \left\{ \Psi^* \left(\frac{\hbar}{im^*} \nabla - \frac{q^*}{m^*} \mathbf{A} \right) \Psi \right\}. \quad (76)$$

The factor q^* is to obtain an electrical current density. The macroscopic wavefunction will obey a Schrödinger-like equation for the electron ensemble:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - q^* \mathbf{A} \right)^2 \Psi(\mathbf{r}, t) + q^* \phi(\mathbf{r}, t) \Psi(\mathbf{r}, t). \quad (77)$$

This means Ψ will be of the form

$$\Psi(\mathbf{r}, t) = \sqrt{n^*(\mathbf{r}, t)} e^{i\theta(\mathbf{r}, t)}, \quad (78)$$

with $\theta(\mathbf{r}, t)$ a real number. This form will guarantee that the modulus of the wavefunction yields the superelectron density. Plugging this function in the supercurrent equation, we find

$$\mathbf{J}_s = q^* n^* \left(\frac{\hbar}{m^*} \nabla \theta(\mathbf{r}, t) - \frac{q^*}{m^*} \mathbf{A}(\mathbf{r}, t) \right). \quad (79)$$

The quantity in parentheses can be identified as the superfluid velocity, \mathbf{v}_s . This relation is peculiar, as it depends on the phase of the macroscopic wavefunction and the vector potential, neither of which is a measurable quantity! It turns out these two quantities are not arbitrary but are related. Particularly \mathbf{A} can have many possible values, what is known as gauges. We would like the supercurrent equation to be gauge invariant. Let's define the vector potential \mathbf{A}'

$$\mathbf{A}' = \mathbf{A} + \nabla \chi. \quad (80)$$

From the definition of the electric field $\mathbf{E} = -\partial \mathbf{A}' / \partial t - \nabla \phi'$, the scalar potential in the new gauge takes the form $\phi' = \phi - \partial \chi / \partial t$. From the invariance of the Schrödinger equation, the macroscopic wavefunction has the form

$$\Psi'(\mathbf{r}, t) = \sqrt{n^*(\mathbf{r}, t)} e^{i\theta'(\mathbf{r}, t)}, \quad (81)$$

since the modulus has to yield the same observable superelectron density n^* . In the new variables, the supercurrent equation results in

$$\boxed{\mathbf{J}_s = q^* n^* \left(\frac{\hbar}{m^*} \nabla \theta' - \frac{q^*}{m^*} \mathbf{A}' \right)}. \quad (82)$$

The gauge invariance of this observable is only possible if $\theta' = \theta + (q^*/m^*)\chi$, so that χ changes both θ and \mathbf{A} in order to yield a uniquely defined \mathbf{J}_s , while \mathbf{A}' and θ' remain unobservable. Their combination *is* observable.

Inserting the complex form of Ψ in the Schrödinger equation, the imaginary part yields the charge conservation:

$$\nabla \cdot \mathbf{J}_s = -\frac{\partial}{\partial t}(q^* n^*) = -\frac{\partial}{\partial t} \rho_s. \quad (83)$$

This expression results from considering a constant superelectron density $n^*(\mathbf{r}, t) \simeq n^*$, which is consistent with small-scale fluctuations of the density. In this limit, taking the curl of the supercurrent equation yields the second London equation:

$$\nabla \times (\Lambda \mathbf{J}_s) = -\nabla \times \mathbf{A} = -\mathbf{B}. \quad (84)$$

If instead we take the partial time derivative of the supercurrent equation, we find

$$\frac{\partial}{\partial t}(\Lambda \mathbf{J}_s) = -\left[\frac{\partial \mathbf{A}}{\partial t} - \frac{\hbar}{q^*} \nabla \left(\frac{\partial \theta}{\partial t} \right) \right]. \quad (85)$$

From the real part of the Schrödinger equation with the complex wavefunction form, one obtains

$$-\hbar \frac{\partial \theta}{\partial t} = \left(\frac{\Lambda}{2m^*} \right) \mathbf{J}_s^2 + q^* \phi. \quad (86)$$

This is known as the energy-phase relationship. Together, the last two expressions become

$$\frac{\partial}{\partial t}(\Lambda \mathbf{J}_s) = \mathbf{E} - \frac{1}{n^* q^*} \nabla \left(\frac{1}{2} \Lambda \mathbf{J}_s^2 \right). \quad (87)$$

This expression is the first London equation with the magnetic field term from Faraday's law included. It is not a quantum mechanical correction (no \hbar), but for many relevant semiclassical problems from engineering, it is negligible.

We have therefore attained an important success. The classical formulation of superconductors results from a MQM, therefore consistent with experimental observations which at the end of the day are the ones dictating the veracity of physical theories.

2.2.2 Flux quantization

The MQM reproduces the results obtained from a classical formulation of superconductivity by modification of Maxwell's equation. We will show now that it also reproduces intrinsically quantum phenomena.

Let's recall the supercurrent equation (clearly the cornerstone of the MQM):

$$\mathbf{J}_s = q^* n^* \left(\frac{\hbar}{m^*} \nabla \theta(\mathbf{r}, t) - \frac{q^*}{m^*} \mathbf{A}(\mathbf{r}, t) \right). \quad (88)$$

Now we integrate this expression in a closed countour C . From Stoke's theorem,

$$\oint_C \mathbf{A} \cdot d\mathbf{l} = \int_S (\nabla \times \mathbf{A}) \cdot d\mathbf{s} = \int_S \mathbf{B} \cdot d\mathbf{s}, \quad (89)$$

s being the surface defined by contour C . The θ -term yields

$$\int_{r_a}^{r_b} \nabla \theta \cdot d\mathbf{l} = \theta(r_a, t) - \theta(r_b, t). \quad (90)$$

For a closed contour $r_a \rightarrow r_b$ this integral would be 0, but turns out that the phase is not well defined. It has an infinite number of possible values as the wavefunction is invariant if an additional phase of $2\pi N$ is added, N being an integer. Then, $\theta(\mathbf{r}, t) = \theta_p(\mathbf{r}, t) + 2\pi N$, where θ_p is the principal value, restricted to the range $[-\pi, \pi]$. The integral then yields,

$$\oint_C (\Lambda \mathbf{J}_s) \cdot d\mathbf{l} + \int_S \mathbf{B} \cdot d\mathbf{s} = N \Phi_0, \quad (91)$$

where we defined the flux quantum

$$\Phi_0 \equiv \frac{h}{|q^*|} \simeq 2.07 \times 10^{-15} \text{Wb}, \quad (92)$$

since remember that the superconductor will have $|q^*| = 2|e|$. In fact, this became one important demonstration that the effective charge of the superelectrons is twice the electron's charge [11, 12]. The left hand side of the previous equation is known as a fluxoid. Therefore, the equation describes fluxoid quantization. This equation implies that the *total* amount of fluxoids is quantized, not the externally applied or the screening one generated by the material. This is a purely quantum mechanical effect, and it is macroscopic because it can be measured! The first evidence of this effect was reported by Deaver and Fairbank [11] and Doll and Nábauer [12], as seen in the figure below.

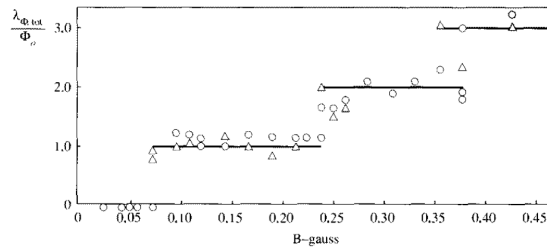


Figure 7: Original measurements of Deaver and Fairbank [11]. Source: Orlando

In a thick superconducting cylinder, we can take the contour integral deep where $\mathbf{J}_s = 0$ and the fluxoid quantization becomes flux quantization equation:

$$\int_s \mathbf{B} \cdot d\mathbf{s} = N\Phi_0. \quad (93)$$

If the superconducting material is cooled from above T_c to a temperature below T_c under an external magnetic field, the total flux will become quantized, even when we remove the externally applied field.

In order to understand even further the consequence of this quantization condition, let's consider a bulk cylinder where currents only flow near the surface, and let's assume the loop has inductance L . When the system is cooled below T_c , the cylinder will generate extra current Δi to lead to a total quantized flux with N quanta trapped. The extra current needed to be generated by the material to yield a quantized total flux is

$$\Delta i = \frac{N\Phi_0 - \Phi_{\text{ext}}}{L}, \quad (94)$$

where Φ_{ext} is the externally applied flux. Therefore, there are infinitely possible values of Δi . Which one gets picked? the one that minimizes the energy of the system, and therefore the amount of current flowing. The extra current is bound to a maximum of $\Delta i|_{\text{max}} = \Phi_0/2L$, corresponding to an extra $\Phi_0/2$. The minimum external flux required to trap N flux quanta is then

$$\Phi_{\text{ext}}|_{\text{min}} = (2N - 1)\frac{\Phi_0}{2}, \quad (95)$$

as it is the point in which the applied current is maximum. Note that once the system is superconducting, the amount of fluxoids is frozen in. It cannot be changed. Flux is indeed trapped! We will see that when we add weak links in the superconductor a very different phenomena takes place.

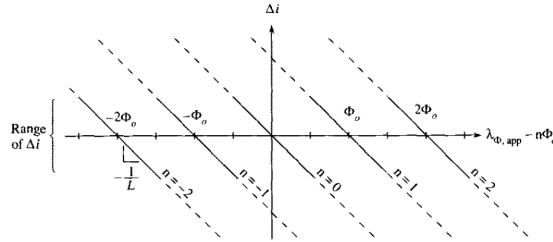


Figure 8: Current flow in a superconducting ring with different trapped fluxoids. Source: Orlando

Let's take the opportunity here to look back at the first term of Eq. (91). This is a term that depends on the current flowing in the loop and its net effect is to add flux to the quantization condition. Note that this term does not generate an actual magnetic field. All magnetic field contributions (external plus the screening one) are inside the second term. Let's examine the first term closer by considering a homogeneous current density for a loop of cross section σ with a total length l . The term is rewritten as

$$\oint \Lambda \mathbf{J}_s \cdot d\mathbf{l} = \left(\mu_0 \lambda^2 \frac{l}{\sigma} \right) I. \quad (96)$$

Here we used the definition of $\Lambda = \mu_0 \lambda^2$, λ being the London penetration length. Since this term adds a fraction of a fluxoid in the quantization condition, it needs to have units of flux. Therefore, the prefactor in parentheses must have units of inductance. We then define the **kinetic inductance** of a superconductor by

$$L_k \equiv \mu_0 \lambda^2 \frac{l}{\sigma}, \quad (97)$$

since its origin can be connected to the kinetic energy of Cooper pairs having a certain inertia to change their velocity whenever a change of the external electric field accelerating the electrons takes place.

Often, the kinetic inductance will be merged together with the self geometric inductance of the loop L_G . Take Eq. (91) for a thin film of constant cross section σ and total length L and total kinetic inductance L_k as defined above,

$$L_k I + \int_s (\mathbf{B}_{\text{ext}} + \mathbf{B}_{\text{loop}}) \cdot d\mathbf{s} = N\Phi_0. \quad (98)$$

The term $\mathbf{B}_{\text{loop}} \cdot d\mathbf{s}$ is nothing but the flux generated by the loop itself to screen the external flux. Therefore it equals $L_G I$, with L_G the self inductance of the loop. The fluxoid quantization equation can be recast as

$$(L_k + L_G)I + \Phi_{\text{ext}} = N\Phi_0, \quad (99)$$

where we defined the external flux as $\int_s \mathbf{B}_{\text{ext}} \cdot d\mathbf{s} \equiv \Phi_{\text{ext}}$.

With the MQM it is now possible to examine in a simple way the case when we connect two superconductors by a weak link, which will be the subject of next lecture.

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