Superconductivity, Josephson effect and applications

Alexander Shnirman

Institute TKM, Karlsruhe Institute of Technology, Karlsruhe, Germany

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Contents

I. LITERATURE

1) A.A. Abrikosov, Fundamentals of the theory of metals.

2) J.R. Schrieffer, Theory of Superconductivity.

3) M. Tinkham, Introduction to Superconductivity.

4) P. G. De Gennes, Superconductivity Of Metals And Alloys.

II. SHORT HISTORY

1911 - discovery by Dutch physicist Heike Kamerlingh Onnes in mercury. Observed disappearance of resistance at $T \approx 4.2$K. Nobel prize in 1913.

1913 - led is superconducting at $T \approx 7$K, 1930's - niobium at $T \approx 10$K.

1933 - Walther Meissner and Robert Ochsenfeld discover that superconductors expel magnetic field - Meissner effect.

1935 - London equations (Fritz London and Heinz London).

1950 - Ginzburg–Landau theory of superconductivity (Lev Landau and Vitaly Ginzburg).

1957 - Abrikosov vortices in type II superconductors (Alexei Abrikosov). Nobel Prize for Ginzburg, Abrikosov and A. Leggett in 2003.

1957 - BCS theory by John Bardeen, Leon N. Cooper, and Robert Schrieffer. Microscopic theory. Nobel Prize in Physics in 1972.

1962 - Josephson effect (Brian Josephson). Nobel Prize in Physics in 1973. First observed experimentally by P. W. Anderson and J. M. Rowell in 1963. In 1964 first SQUID (Superconducting QUantum Interference Device). P.W. Anderson - one of the greatest theoretical physicists. Numerous contributions to understanding superconductivity (Andersson-Higgs mechanism). Nobel Prize in 1977 (not for superconductivity).

1986 - Beginning of the era of High Temperature Superconductors (HTS). Georg Bednorz and Alex Müller discovered superconductivity in $La_{2-x}Ba_xCuO_4$ at $T \approx 35$K. Nobel Prize in Physics, 1987. Soon YBCO with $T \approx 92$K. No full theory up today.

III. IMPORTANT APPLICATIONS

1) Superconducting Magnets. E.g. in Magnetic Resonance Imaging (MRI), at Large Hadron Collider (LHC), Trains.

2) Superconducting wires in the electricity grid (only very recently, with HTS materials).

3) All possible Josephson devices as sensors (SQUID), metrological standards (Volt standard). SQUIDS are used for magnetometry in brain, geology, search for dark matter etc.

4) Quantum Bits.

IV. PHENOMENOLOGY

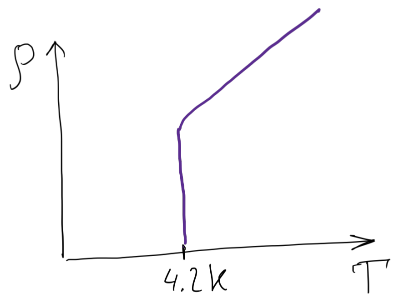

FIG. 1: Illustration: Disappearance of resistivity ρ of Hg below critical temperature $T_c \approx 4.2$K. H. Kamerlingh Onnes 1911.

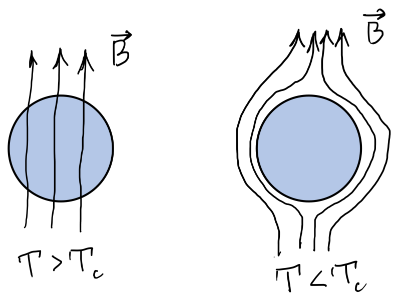

FIG. 2: Illustration: Meissner effect. Magnetic field is expelled from the superconductor.

V. LONDON EQUATIONS

The zero resistivity and the Meissner effect are closely related. Assume the electrons are accelerated without resistance (the electron charge is equal to $-e$):

$$m\frac{d}{dt}\vec{v} = -e\vec{E} \ . \tag{1}$$

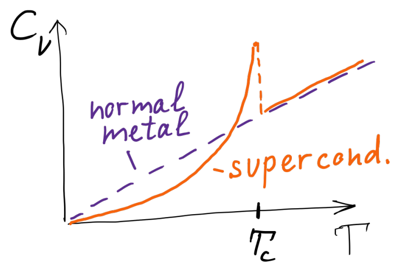

FIG. 3: Illustration: Specific heat capacity as a function of temperature. Indicated a second order phase transition.

With the current density given by $\vec{j} = -ne\vec{v}$, where n is the density of electrons, we obtain

$$\frac{\partial}{\partial t}\vec{j} = \frac{ne^2}{m}\vec{E} \ , \tag{2}$$

The Maxwell equation reads:

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c}\frac{\partial}{\partial t}\vec{B} \tag{3}$$

Thus we obtain

$$\frac{\partial}{\partial t}\left(\vec{\nabla} \times \vec{j} + \frac{ne^2}{mc}\vec{B}\right) = 0 \tag{4}$$

But deep inside the superconductor both $\vec{B} = 0$ and $\vec{j} = 0$ (Meissner effect). Thus F. London and H. London postulated that everywhere inside the superconductor:

$$\vec{\nabla} \times \vec{j} + \frac{ne^2}{mc}\vec{B} = 0 \tag{5}$$

1. *Time-independent situation*

An external magnetic field is applied. We consider magnetization currents explicitly, thus we use microscopic Maxwell equation:

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c}\vec{j} \tag{6}$$

This gives

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{B}) = \vec{\nabla} \cdot (\vec{\nabla} \cdot \vec{B}) - (\vec{\nabla}^2)\vec{B} = -(\vec{\nabla}^2)\vec{B} = \frac{4\pi}{c}\vec{\nabla} \times \vec{j} \tag{7}$$

From the London equation (5) we obtain

$$\frac{4\pi}{c}\vec{\nabla} \times \vec{j} = -\frac{4\pi ne^2}{mc^2}\vec{B} \ . \tag{8}$$

Substituting the London equation we obtain

$$(\vec{\nabla}^2)\vec{B} = \frac{4\pi ne^2}{mc^2}\vec{B} = \frac{1}{\lambda_L^2}\vec{B}\ , \tag{9}$$

Where we have introduced the London penetration depth $\lambda_L = \sqrt{\frac{mc^2}{4\pi ne^2}}$.

The London penetration depth does not change if we transform to (Cooper) pairs, i.e., $e \to 2e$, $m \to 2m$, $n \to n/2$.

A. Another form of London equations

$$\vec{B} = \vec{\nabla} \times \vec{A} \tag{10}$$

With this the London equation

$$\vec{\nabla} \times \vec{j} + \frac{ne^2}{mc}\vec{B} = 0 \tag{11}$$

reads

$$\vec{\nabla} \times \vec{j} + \frac{ne^2}{mc}\vec{\nabla} \times \vec{A} = 0 \tag{12}$$

If both $\vec{\nabla} \cdot \vec{j} = 0$ (continuity equation in static (time-independent) case) and $\vec{\nabla} \cdot \vec{A} = 0$ (Coulomb gauge) this gives

$$\vec{j} = -\frac{ne^2}{mc}\vec{A} = -\frac{c}{4\pi\lambda_L^2}\vec{A}\ . \tag{13}$$

In this form the London equation is convenient to connect to the microscopic theory.

VI. GINZBURG-LANDAU THEORY

Theory works for $T \approx T_c$. One postulates that electron liquid consists of two parts: superconducting (superfluid) with density $n_s(T)$ and normal with density $n_n(T)$. Dropping the historical perspective we understand that the density of Cooper pairs is equal to $n_s/2$.

One introduces the order parameter

$$\Psi = \sqrt{\frac{n_s}{2}}\, e^{i\phi} \tag{14}$$

1. *Landau Theory*

One postulates for the free energy

$$\mathcal{F} = \int dV\, F = \int dV\, \left\{ F_n + a|\Psi|^2 + \frac{b}{2}|\Psi|^4 \right\} \tag{15}$$

In order to describe the phase transition one postulates $a = \alpha\tau$, where

$$\tau = \frac{T - T_c}{T_c} \tag{16}$$

and $\alpha > 0$, $b > 0$.

By varying (over $|\Psi|$) we obtain:

$$2a|\Psi| + 2b|\Psi|^3 = 0\ . \tag{17}$$

For $\tau < 0$ this gives

$$|\Psi|^2 = -\frac{\alpha\tau}{b} = \frac{\alpha}{b}\frac{T_c - T}{T_c} \tag{18}$$

For $\tau > 0$ we have $|\Psi|^2 = 0$. Phase transition.

We define

$$\Psi_0^2 \equiv -\frac{a}{b}\ . \tag{19}$$

2. *Ginsburg-Landau Theory, equations*

Theory for inhomogeneous situations, currents and magnetic fields. One postulates for the free energy

$$\mathcal{F} = \int dV\, F = \int dV\, \left\{ F_n + a|\Psi|^2 + \frac{b}{2}|\Psi|^4 + \frac{1}{4m}\left|\left(-i\hbar\vec{\nabla} + \frac{2e}{c}\vec{A}\right)\Psi\right|^2 + \frac{\vec{B}^2}{8\pi} \right\}\ . \tag{20}$$

Here, for a while, we consider the superconductor on its own. Thus $\vec{B}$ is the field induced by the currents in the superconductor itself. Below we will include the external field.

It is important to note that the GL free energy is gauge invariant. A general time-independent gauge transformation reads

$$\vec{A}' = \vec{A} + \vec{\nabla}\chi \quad , \quad \Psi' = \Psi \exp\left[-\frac{2ie}{\hbar c}\chi\right]\ . \tag{21}$$

Here we have to vary with respect to Ψ regarding Ψ^* as independent. This gives

$$\frac{1}{4m}\left(-i\hbar\vec{\nabla} + \frac{2e}{\hbar c}\vec{A}\right)^2 \Psi + a\Psi + b|\Psi|^2\Psi = 0 \tag{22}$$

Next we vary with respect to $\vec{A}$. The variation of the magnetic energy goes as follows:

$$\delta \int dV \, \frac{\vec{B}^2}{8\pi} = \int dV \, \frac{\vec{B} \cdot \delta \vec{B}}{4\pi} = \int dV \, \frac{\vec{B} \cdot (\vec{\nabla} \times \delta \vec{A})}{4\pi} \tag{23}$$

Next we perform integration by parts (dropping as usual the boundary terms):

$$\vec{B} \cdot (\vec{\nabla} \times \delta \vec{A}) = B_i \epsilon_{ikp} (\nabla_k \delta A_p) \underset{\text{int. by parts}}{\rightarrow} -\delta A_p \epsilon_{ikp} (\nabla_k B_i) = \delta A_p \epsilon_{pki} (\nabla_k B_i) = \delta \vec{A} \cdot (\vec{\nabla} \times B) \ . \tag{24}$$

Performing the variation we obtain

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c} \vec{j} \tag{25}$$

with

$$\vec{j} = \frac{2ie\hbar}{4m} \left(\Psi^* \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^* \right) - \frac{(2e)^2}{2mc} |\Psi|^2 \vec{A} \tag{26}$$

For $\Psi = \Psi_0 e^{i\phi(\vec{r})}$ we obtain again the London equation.

$$\vec{j}_s = -\frac{4e^2}{2mc} \Psi_0^2 \left(\vec{A} + \frac{\hbar c}{2e} \vec{\nabla} \phi \right) = -\frac{e^2 n_s}{mc} \left(\vec{A} + \frac{\hbar c}{2e} \vec{\nabla} \phi \right) \tag{27}$$

This is the gauge invariant form of the original London equation. It also allows to introduce the so called superconducting velocity $\vec{v}_s$. Namely, from the general relation $\vec{j} = -e n_s \vec{v}_s$ we obtain

$$\vec{v}_s = \frac{\hbar}{2m} \left(\vec{\nabla} \phi + \frac{2e}{c} \vec{A} \right) \ . \tag{28}$$

In the literature one frequently has a different sign, i.e., $\vec{v}_s = \frac{\hbar}{2m} \left(\vec{\nabla} \phi - \frac{2e}{c} \vec{A} \right)$. This has to do with the negative sign of the electron charge and creates some confusion. For example Tinkham (Ch. 4) first has $\vec{v}_s = \frac{\hbar}{m^*} \left(\vec{\nabla} \phi - \frac{e^*}{c} \vec{A} \right)$, where m^* is the mass of the relevant charge carrier and e^* its charge. Then a substitution is made $m^* = 2m$ and $e^* = 2e$, meaning probably that $e < 0$. Later, however, Tinkham uses e^* in the definition of the flux quantum $\Phi_0 = \frac{2\pi\hbar c}{e^*} = \frac{2\pi\hbar c}{2e}$. This would mean that $\Phi_0 < 0$. Here I use the substitution $e^* = -2e$, so that $e > 0$. Also $\Phi_0 = \frac{2\pi\hbar c}{2e} > 0$.

Introducing again the London penetration depth

$$\lambda_{\mathrm{L}} = \sqrt{\frac{c^2 m}{4\pi n_s e^2}} = \sqrt{\frac{c^2 m}{8\pi \Psi_0^2 e^2}} \ . \tag{29}$$

we can rewrite the London equation as

$$\vec{j}_s = -\frac{c}{4\pi \lambda_L^2} \left(\vec{A} + \frac{\hbar c}{2e} \vec{\nabla} \phi \right) \ . \tag{30}$$

3. Coherence length

Coherence length is obtained by considering small fluctuations of the amplitude of Ψ. So we assume $\vec{A} = 0$, and $\Psi = \Psi_0 + \delta\Psi$ (both real), and $\Psi_0^2 = -a/b$. Then we obtain

$$-\frac{\hbar^2}{4m}\nabla^2\delta\Psi + \delta\Psi(a + 3b\Psi_0^2) = 0 \ . \tag{31}$$

In the normal state $\Psi_0 = 0$ and $a > 0$ we obtain solutions of the type $e^{\pm x/\xi}$, where

$$\xi = \frac{\hbar}{\sqrt{4ma}} \tag{32}$$

In the superconducting state $\Psi_0^2 = -a/b$, $a < 0$

$$-\frac{\hbar^2}{4m}\nabla^2\delta\Psi + \delta\Psi(a + 3b\Psi_0^2) = -\frac{\hbar^2}{4m}\nabla^2\delta\Psi - 2a\delta\Psi = 0 \ . \tag{33}$$

We still define the coherence length as in the normal case

$$\xi = \frac{\hbar}{\sqrt{4m|a|}} \ . \tag{34}$$

However the solutions look like $e^{\pm\sqrt{2}x/\xi}$.

A. Flux quantization

In the bulk of a superconductor, where $\vec{j}_s = 0$, we obtain

$$\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi = 0 \tag{35}$$

$$\oint \vec{A}d\vec{l} = -\frac{\hbar c}{2e}\oint \vec{\nabla}\phi d\vec{l} = \frac{\hbar c}{2e}2\pi n = \frac{2\pi\hbar c}{2e}n = n\Phi_0 \ , \tag{36}$$

Where $\Phi_0 \equiv \frac{2\pi\hbar c}{2e}$ is the superconducting flux quantum.

This quantization is very important for, e.g., a ring geometry. If the ring is thick enough (thicker than λ_L) the total magnetic flux threading the ring is quantized.

B. Anderson-Higgs mechanism

We consider again the GL free energy density (action):

$$\begin{aligned} F &= a|\Psi|^2 + \frac{b}{2}|\Psi|^4 + \frac{1}{4m}\left|\left(-i\hbar\vec{\nabla} + \frac{2e}{c}\vec{A}\right)\Psi\right|^2 + \frac{\vec{B}^2}{8\pi} \\ &= a|\Psi|^2 + \frac{b}{2}|\Psi|^4 + \frac{1}{4m}\left[\left(-i\hbar\vec{\nabla} + \frac{2e}{c}\vec{A}\right)\Psi\right]\left[\left(i\hbar\vec{\nabla} + \frac{2e}{c}\vec{A}\right)\Psi^*\right] + \frac{(\vec{\nabla}\times\vec{A})^2}{8\pi} \ . \end{aligned} \tag{37}$$

Consider small fluctuations around the real solution $\Psi_0 = \sqrt{-a/b}$.

$$\Psi(\vec{r}) = \Psi_0 + \phi_1(\vec{r}) + i\phi_2(\vec{r}) \ , \tag{38}$$

where ϕ_1 and ϕ_2 are real. Considering also $\vec{A}(\vec{r})$ to be small we expand the action to second order in ϕ_1, ϕ_2 and $\vec{A}$:

$$\begin{aligned}\delta F^{(2)} &= \frac{1}{4m}\left[\left(\frac{2e}{c}\right)^2 \Psi_0^2 \left(\vec{A}\right)^2 + \hbar^2 \left(\vec{\nabla}\phi_1\right)^2 + \hbar^2 \left(\vec{\nabla}\phi_2\right)^2 + 2\hbar\left(\frac{2e}{c}\right)\Psi_0\left(\vec{A}\vec{\nabla}\phi_2\right)\right] \\ &- \ 2a\phi_1^2 + \frac{(\vec{\nabla}\times\vec{A})^2}{8\pi} + \text{higher orders} \ .\end{aligned} \tag{39}$$

We still have the gauge freedom:

$$\vec{A}' = \vec{A} + \vec{\nabla}\chi \quad , \quad \Psi' = \Psi \exp\left[-\frac{2ie}{\hbar c}\chi\right] \ . \tag{40}$$

To keep $\vec{A}'$ small we perform an infinitesimal gauge transformation, which then reduces to $\Psi' \approx \Psi(1 - i\tilde{\chi}) = (\Psi_0 + \phi_1 + i\phi_2)(1 - i\tilde{\chi})$, where $\tilde{\chi} \equiv \frac{2e}{\hbar c}\chi$. In terms of the deviations we obtain

$$\phi_1' = \phi_1 + \phi_2\tilde{\chi} \quad , \quad \phi_2' = \phi_2 - \phi_1\tilde{\chi} - \Psi_0\tilde{\chi} \ . \tag{41}$$

We can always find a gauge transformation such that $\phi_2' = 0$. In our expansion this is achieved with $\tilde{\chi} \approx \phi_2/\Psi_0$. Thus $\tilde{\chi}$ is of the first order in fluctuations and the terms $-\phi_1\tilde{\chi}$ and $\phi_2\tilde{\chi}$ are of the second order and can be dropped. Dropping the primes we obtain

$$\begin{aligned}\delta F^{(2)} &= \frac{\hbar^2}{4m}\left(\vec{\nabla}\phi_1\right)^2 - 2a\phi_1^2 \\ &+ \frac{(\vec{\nabla}\times\vec{A})^2}{8\pi} + \frac{1}{4m}\left(\frac{2e}{c}\right)^2 \Psi_0^2 \left(\vec{A}\right)^2 + \text{higher orders} \\ &= \frac{\hbar^2}{4m}\left[\left(\vec{\nabla}\phi_1\right)^2 + 2\xi^{-2}\phi_1^2\right] + \frac{1}{8\pi}\left[(\vec{\nabla}\times\vec{A})^2 + \lambda_L^{-2}\left(\vec{A}\right)^2\right] + \text{higher orders}\end{aligned} \tag{42}$$

Thus we obtain two modes. The first mode, ϕ_1, called also Higgs mode, has a characteristic length, which coincides with the coherence length ξ (we have defined $\xi = \frac{\hbar}{\sqrt{4m|a|}}$, this explains factor 2). The second mode is described by field $\vec{A}$. The transversal components of $\vec{A}$ are characterized by the London penetration depth (cf. Eq. (29)), i.e.,

$$\lambda_L^{-2} = \frac{8\pi}{4m}\left(\frac{2e}{c}\right)^2 \Psi_0^2 = \frac{4\pi e^2 n_s}{mc^2} \ . \tag{43}$$

This can also be seen as the photon mass. Our theory has no time-dependence, but is otherwise complete with respect to the transversal components of the field $\vec{A}$. This means, in the relativistic dispersion relation $E^2 = \mu^2 c^4 + c^2 p^2$ we should take $E = \hbar\omega = 0$. Then $p^2 = -\mu^2 c^2$. Since $p^2 < 0$, we obtain spatial decay, i.e., penetration depth. Identifying $p^2 = -\hbar^2 \lambda_L^{-2}$, we obtain the photon mass

$$(\mu c^2)^2 = \hbar^2 \frac{4\pi e^2 n_s}{m} = (\hbar\omega_{ps})^2 \ . \tag{44}$$

Here

$$\omega_{ps}^2 = \frac{4\pi e^2 n_s}{m} \tag{45}$$

is the plasma frequency of the superconducting electronic liquid. At $T = 0$ ($n_s = n$) it coincides with the usual plasma frequency.

The variation of (42) with respect to the longitudinal component of $\vec{A}$ results simply in $\vec{A}_{\|} = 0$. Thus, unlike in full Higgs case, no longitudinal photon appears at $\omega = 0$. In order to treat the longitudinal modes (plasmons) properly we have to introduce time-dependence and the scalar potential. This is beyond the scope of this text.

C. Comparison with Higgs mechanism in quantum field theory

$$\mathcal{L} = -\frac{1}{16\pi} F_{\mu\nu} F^{\mu\nu} + (D_\mu \Psi)^\dagger (D^\mu \Psi) - V(\Psi) \ , \tag{46}$$

where $D_\mu = \partial_\mu + ieA_\mu$ and $V(\Psi) = -\mu^2 |\Psi|^2 + \lambda |\Psi|^4$.

D. External field

If a superconductor is placed in an external magnetic field $\vec{H}_0$ the proper free energy reads

$$\mathcal{F}_H = \int dV \, F_H = \int dV \, F - \frac{1}{4\pi} \vec{H}_0 \int dV \, \vec{B} \ . \tag{47}$$

Here $\vec{B}$ is the total magnetic field, $\vec{B} = \vec{H}_0 + \vec{B}_i$. Here $\vec{B}_i$ is the field induced by currents in the superconductor. Thus

$$\mathcal{F}_H = \int dV \left\{ F_n + a|\Psi|^2 + \frac{b}{2}|\Psi|^4 + \frac{1}{4m} \left| \left(-i\hbar\vec{\nabla} + \frac{2e}{c}\vec{A} \right) \Psi \right|^2 + \frac{\vec{B}^2}{8\pi} - \frac{\vec{H}_0 \cdot \vec{B}}{4\pi} \right\} \ . \tag{48}$$

Note, that this gives the same Ginsburg-Landau equations. Indeed $B^2/(8\pi) - BH_0/(4\pi) = B_i^2/8\pi + const.$ and we vary, actually, the field B_i.

In the normal state we have $B = H_0$ and $F_H = F_n - H_0^2/(8\pi)$. Deep in the superconductor $B = 0$ and $F_H = F_n + a|\Psi|^2 + \frac{b}{2}|\Psi|^4 = F_n - \frac{a^2}{2b} = F_n - \frac{(\alpha\tau)^2}{2b}$. Thus we obtain the critical field H_c, i.e., the value of H_0 above which the normal state has a lower free energy. We obtain $H_c^2/(8\pi) = \frac{(\alpha\tau)^2}{2b}$ and

$$H_c = \sqrt{\frac{4\pi a^2}{b}} = |\tau|\sqrt{\frac{4\pi\alpha^2}{b}} \ . \tag{49}$$

1. *Reduced Ginsburg-Landau equations*

We define

$$\begin{aligned} &\Psi' = \Psi/\Psi_0 \quad , \quad r' = r/\lambda_{\rm L} \quad , \quad B' = B/(H_c\sqrt{2}) \quad , \quad A' = A/(\lambda_{\rm L} H_c \sqrt{2}) \\ &\vec{j}' = \frac{4\pi}{c}\frac{\lambda_L}{\sqrt{2}H_c}\,\vec{j} \ . \end{aligned} \tag{50}$$

We also define the reduced energy

$$\mathcal{F}' = \mathcal{F}\left[\frac{\lambda_L^3 H_c^2}{4\pi}\right]^{-1} \tag{51}$$

and the reduced flux quantum

$$\Phi_0' = \frac{\Phi_0}{H_c\sqrt{2}\,\lambda_L^2} = 2\pi\,\frac{\xi}{\lambda_L} = \frac{2\pi}{\kappa} \ . \tag{52}$$

We obtain the Ginsburg-Landau equations in the reduced form (omitting the primes)

$$\left(-i\kappa^{-1}\vec{\nabla} + \vec{A}\right)^2 \Psi - \Psi + |\Psi|^2\Psi = 0 \ , \tag{53}$$

$$\vec{j} = \vec{\nabla} \times \vec{B} = \vec{\nabla} \times (\vec{\nabla} \times \vec{A}) = \frac{i}{2\kappa}\left(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\right) - |\Psi|^2\vec{A} \ , \tag{54}$$

where

$$\kappa = \frac{\lambda_{\rm L}}{\xi} \ . \tag{55}$$

Thus, everything depends on κ.

The free energy in these units reads

$$\mathcal{F}_H = \mathcal{F}_n + \int dV \left\{ -|\Psi|^2 + \frac{1}{2}|\Psi|^4 + \left|\left(-\frac{i\vec{\nabla}}{\kappa} + \vec{A}\right)\Psi\right|^2 + \vec{B}^2 - 2\vec{H}_0\cdot\vec{B} \right\} \ . \tag{56}$$

Integrating by parts, disregarding the boundary, and using the Ginsburg-Landau equations we obtain

$$\mathcal{F}_H = \mathcal{F}_n + \int dV \left\{ -\frac{1}{2}|\Psi|^4 + \vec{B}^2 - 2\vec{B}\cdot\vec{H}_0 \right\} \ . \tag{57}$$

E. Surface energy

Let us estimate the surface energy of an interface between superconducting and normal phases. We assume $H_0 = 1/\sqrt{2}$ (in usual units $H_0 = H_c$), i.e., both phases are possible. In the normal phase we have the critical magnetic field $B = 1/\sqrt{2}$ (in usual units $B = H_c$). In the superconducting phase $B = 0$ and $\Psi = 1$ (in usual units $\Psi = \Psi_0$). In both phases the free energy (106) is given by

$$\mathcal{F}_{H_c} = \mathcal{F}_n + \int dV \left\{-\frac{1}{2}\right\} = \mathcal{F}_n + \int dV \left\{-\vec{H}_0^2\right\} . \tag{58}$$

At the possible border between the two phases both Ψ and $\vec{B}$ are changing from one asymptotic to the other. Such a border is then associated with the energy

$$\mathcal{F}_H - \mathcal{F}_{H_c} = \int dV \left\{-\frac{1}{2}|\Psi|^4 + (\vec{B} - \vec{H}_0)^2\right\} . \tag{59}$$

Far from the border (either $|\Psi| = 0$ and $B = H_0$ or $|\Psi| = 1$ and $B = 0$) the integrand vanishes. Near the border the balance between the two terms is violated. One of them dominates and we obtain the surface energy which is either positive or negative.

The order parameter varies on the scale κ^{-1} (ξ is usual units). The magnetic field varies on the scale 1 (λ_L in usual units).

We consider a quasi-one dimensional situation. All the quantities depend only on x. $\vec{A}$ is along y ($\vec{A} = A(x)\vec{y}$) and, thus, $\vec{B}$ is along z. We can take Ψ to be real. Then

$$\kappa^{-2}\nabla^2\Psi + (1 - A^2)\Psi - \Psi^3 = 0 , \tag{60}$$

$$\nabla^2 A - \Psi^2 A = 0 . \tag{61}$$

Consider 2 cases:

a) $\xi \gg \lambda_L$ ($\kappa \ll 1$)(superconductor of the 1-st type). In this case there is a layer on the interface of thickness ξ where the magnetic field has already vanished and the order parameter has not yet grown, i.e., the state is normal. We see that there is an additional cost of $\sim \xi\frac{H_c^2}{8\pi}$ per unit of area. The logic: the work of expelling the magnetic field has been performed but no energy reduction through the order parameter appearance. Thus the surface energy is positive in this case and the system avoids interfaces.

b) $\xi \ll \lambda_L$ ($\kappa \gg 1$)(superconductor of the 2-nd type). In this case there is a layer of thickness λ_L where the magnetic field is present and also the order parameter has its

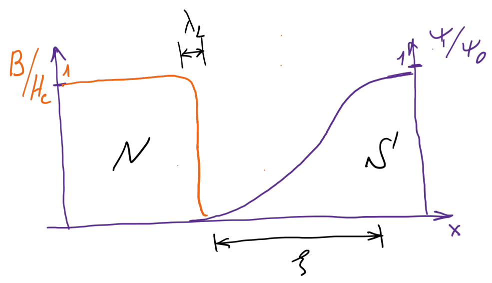

FIG. 4: Surface energy for $\xi \gg \lambda_L$

bulk value. The surface energy is then negative and equal $\sim -\lambda_L \frac{H_c^2}{8\pi}$. The logic: magnetic field not expelled in the layer, thus no energy cost. The energy is reduced by having the superconducting order parameter. Thus the system likes to have interfaces.

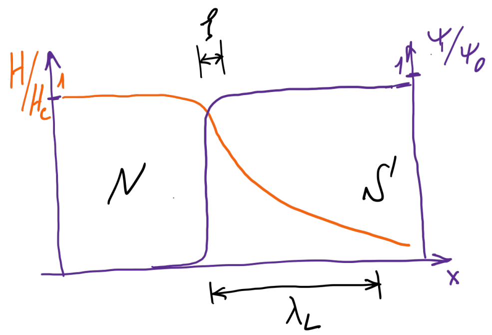

FIG. 5: Surface energy for $\lambda_L \gg \xi$

The critical value of κ at which the surface energy vanishes is given by $\kappa_c = 1/\sqrt{2}$.

F. Type II superconductors, H_{c2}

For $\kappa > \kappa_c = 1/\sqrt{2}$ the surface energy is negative. Thus the system could profit by having a non-homogeneous order parameter. We want to understand at what magnetic field a non-homogeneous superconducting order parameter could start appearing. For this we assume $|\Psi| \ll 1$ (in GL units) and linearize the GL equations.

We consider again a quasi-one dimensional situation. All the quantities depend only on x. $\vec{A}$ is along y ($\vec{A} = A(x)\vec{y}$) and, thus, $\vec{B}$ is along z. We can take Ψ to be real. Then

$$\kappa^{-2}\nabla^2\Psi + (1 - A^2)\Psi - \Psi^3 = 0 \;, \tag{62}$$

$$\nabla^2 A - \Psi^2 A = 0 \;. \tag{63}$$

For $\Psi \ll 1$ we can linearize:

$$\kappa^{-2}\nabla^2\Psi + (1 - A^2)\Psi = 0 \ , \tag{64}$$

$$\nabla^2 A = 0 \ . \tag{65}$$

The last equation gives $A = Bx = H_0 x$. Here H_0 is the external field. The superconductor does not screen yet. Then, from the first equation we obtain

$$\kappa^{-2}\nabla^2\Psi + (1 - H_0^2 x^2)\Psi = 0 \ . \tag{66}$$

We want to find the field H_0 at which an infinitesimal solution with $\Psi \to 0$ for $x \to \pm\infty$ can appear. We rewrite as a Schrödinger equation

$$-\nabla^2\Psi + \kappa^2 H_0^2 x^2 \Psi = \kappa^2 \Psi \ . \tag{67}$$

This equation has the same form as the usual Schrödinger equation of a harmonic oscillator

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + \frac{m\omega^2}{2}\,x^2\Psi = \hbar\omega(n + 1/2)\Psi \ . \tag{68}$$

By comparing the coefficients we get $m = \hbar^2/2$, $\kappa^2 H_0^2 = m\omega^2/2 = \hbar^2\omega^2/4$, and $\kappa^2 = \hbar\omega(n + 1/2)$. We get

$$\hbar\omega = \frac{\kappa^2}{(n + 1/2)} = 2\kappa H_0 \ . \tag{69}$$

Thus solutions exist for

$$H_0 = \frac{\kappa}{2n + 1} \ . \tag{70}$$

We are interested in the biggest possible H_0 at which the infinitesimal solution is possible, i.e., $n = 0$. This gives

$$H_{c2} = \kappa. \tag{71}$$

In the usual units

$$H_{c2} = \kappa\sqrt{2}H_c \ . \tag{72}$$

For $\kappa > 1/\sqrt{2}$ we have $H_{c2} > H_c$.

G. Abrikosov vortex

It turns out that in the mixed phase at fields $H_c < H_0 < H_{c2}$ magnetic field penetrates the superconductor in form of vortices (Abrikosov vortices). Actually, this penetration starts

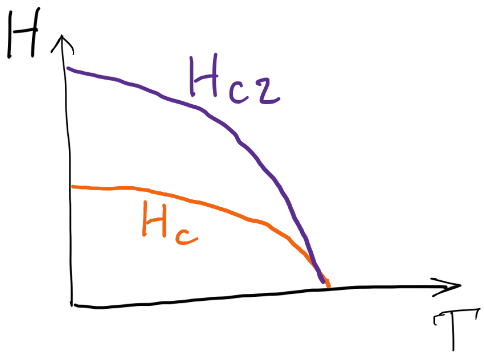

FIG. 6: Type II superconductors. Two critical fields H_c and H_{c2}. Below we will introduce yet another field H_{c1}.

even at a lower field $H_{c1} < H_c$. Each vortex carries the magnetic flux of Φ_0. Here we consider just a single vortex. In reality vortexes form a lattice.

We work in GL units. Consider an Ansatz: $\Psi = f e^{i\chi}$. Then the second GL equation (Eq. (54)) reduces to

$$\vec{j} = -f^2 \vec{v}_s \ , \tag{73}$$

where

$$\vec{v}_s \equiv \kappa^{-1} \vec{\nabla} \chi + \vec{A} \tag{74}$$

is the "superconducting velocity" in the GL units. We introduce polar coordinates (r, φ) and try to find a solution of the form $f = f(r)$, $\vec{v}_s = v(r)\vec{e}_\varphi$, $\vec{A} = a(r)\vec{e}_\varphi$. For a single vortex we take $\chi = -\varphi$. Then $\oint \vec{\nabla}\chi d\vec{l} = -2\pi$. Far from the vortex center we expect no current, this $\vec{v}_s \to 0$. This would mean that $\oint \vec{A} d\vec{l} = 2\pi\,\kappa^{-1} = \Phi_0$ (in the reduced units). Thus the magnetic flux is equal to Φ_0 and our choice corresponds to a single vortex.

From this we obtain (using $\vec{\nabla} = \vec{e}_r \frac{\partial}{\partial r} + \vec{e}_\varphi \frac{1}{r} \frac{\partial}{\partial \varphi}$)

$$\vec{v}_s = \left(-\frac{\kappa^{-1}}{r} + a(r) \right) \vec{e}_\varphi \ , \tag{75}$$

or $v(r) = -(\kappa r)^{-1} + a(r)$ (notice the singularity at $r = 0$). Substituting this Ansatz into the first GL equation (Eq. (53)) we obtain

$$-\kappa^{-2} \left(\frac{d^2 f}{dr^2} + \frac{1}{r}\frac{df}{dr} \right) + v^2 f = f - f^3 \ . \tag{76}$$

We have used the fact that in polar coordinates $\vec{\nabla}^2 = \partial^2/\partial r^2 + (1/r)\partial/\partial r + (1/r^2)\partial^2/\partial\varphi^2$. In our Ansatz $\vec{B} = B(r)\vec{e}_z$. Therefore

$$\vec{\nabla} \times \vec{B} = -\frac{dB}{dr}\vec{e}_\varphi \ . \tag{77}$$

We have used here

$$\vec{\nabla}\times\vec{B} = \left(\frac{1}{r}\frac{\partial B_z}{\partial\varphi} - \frac{\partial B_\varphi}{\partial z}\right)\vec{e}_r + \left(\frac{\partial B_r}{\partial z} - \frac{\partial B_z}{\partial r}\right)\vec{e}_\varphi + \frac{1}{r}\left(\frac{\partial(rB_\varphi)}{\partial r} - \frac{\partial B_r}{\partial\varphi}\right)\vec{e}_z \tag{78}$$

This gives

$$\frac{dB(r)}{dr} = f^2(r)v(r)\ . \tag{79}$$

Finally, using $\vec{A} = a(r)\vec{e}_\varphi$ we obtain

$$\vec{B} = \vec{\nabla}\times\vec{A} = \frac{1}{r}\frac{d}{dr}\left[ra(r)\right]\vec{e}_z \tag{80}$$

Using $v(r) = -(\kappa r)^{-1} + a(r)$ we obtain for $r > 0$

$$B = \frac{1}{r}\frac{d}{dr}\left[rv(r)\right] = dv/dr + (1/r)v\ . \tag{81}$$

The full version of this equation should include $r = 0$. There is a singularity there. Indeed from (75) we get

$$\vec{\nabla}\times\vec{v}_s = -\kappa^{-1}\vec{\nabla}\times\left(\frac{\vec{e}_\varphi}{r}\right) + \vec{\nabla}\times\vec{A} = -\kappa^{-1}2\pi\delta(r)\vec{e}_z + \vec{\nabla}\times\vec{A}\ . \tag{82}$$

Thus the proper equation for $\vec{B}$ reads

$$\vec{B} = \vec{\nabla}\times\vec{A} = \vec{\nabla}\times\vec{v}_s + \kappa^{-1}2\pi\delta(r)\,\vec{e}_z\ . \tag{83}$$

Let us collect the equations for $r > 0$:

$$-\kappa^{-2}\left(\frac{d^2 f}{dr^2} + \frac{1}{r}\frac{df}{dr}\right) + v^2 f = f - f^3\ . \tag{84}$$

$$\frac{dB(r)}{dr} = f^2(r)v(r)\ . \tag{85}$$

$$B = \frac{1}{r}\frac{d}{dr}\left[rv(r)\right] = dv/dr + (1/r)v\ . \tag{86}$$

The last two equations give

$$v'' + v'/r - v/r^2 = f^2 v\ . \tag{87}$$

The boundary conditions read $f(r\to\infty) = 1$, $v(r\to\infty) = 0$. For $r\to 0$ we have to demand that $a(r)$ does not diverge, thus $v(r)\approx -(\kappa r)^{-1}$ for $r\to 0$.

Multiplying (87) by r^2 we obtain

$$r^2 v'' + rv' - (f^2 r^2 + 1)v = 0\ . \tag{88}$$

For $r \gg \kappa^{-1}$ ($r \gg \xi$ in normal units) we have $f \approx 1$ and we get the modified Bessel equation

$$r^2 v'' + r v' - (r^2 + n^2) v = 0 \tag{89}$$

with $n = 1$. The solutions vanishing at $r \to \infty$ are the modified Bessel functions of the second kind $K_n(r)$. Thus we obtain

$$v(r) \propto K_1(r) \tag{90}$$

with the asymptotic behavior at large $r > 1$ ($r > \lambda_L$)

$$K_1(r) \sim \sqrt{\frac{\pi}{2r}}\, e^{-r} \left[1 + O(1/r)\right] \ . \tag{91}$$

The differential equation (89) is linear, thus it does not give the constant in front of $K_1(r)$. To find this constant we use the asymptotic behavior $K_1(r) \approx 1/r$ for $r \ll 1$. Comparing this with $v(r) = -(\kappa r)^{-1} + a(r)$ we obtain

$$v(r) = -K_1(r)/\kappa \ . \tag{92}$$

From this we get

$$B(r) = dv/dr + (1/r)v = K_0(r)/\kappa \ . \tag{93}$$

The asymptotic behavior reads

$$B(r) \approx \frac{1}{\kappa} \ln(1/r) \quad \text{for} \quad 1/\kappa \ll r \ll 1 \ , \tag{94}$$

and

$$B(r) \approx \frac{1}{\kappa} \sqrt{\frac{\pi}{2r}}\, e^{-r} \quad \text{for} \quad r \gg 1 \ . \tag{95}$$

The logarithmic divergency is cut off in the core, for $r < 1/\kappa$. Thus, approximately,

$$B(r) \approx \frac{1}{\kappa} \ln(\kappa) \quad \text{for} \quad r \ll 1/\kappa \ . \tag{96}$$

We now turn to the equation for f:

$$-\kappa^{-2} \left(\frac{d^2 f}{dr^2} + \frac{1}{r} \frac{df}{dr} \right) + v^2 f = f - f^3 \tag{97}$$

and consider the domain $r \ll 1$ ($r \ll \lambda_L$ in normal units). Then $v \approx -(\kappa r)^{-1}$ and we get

$$\kappa^{-2} \left(\frac{d^2 f}{dr^2} + \frac{1}{r} \frac{df}{dr} - \frac{1}{r^2} f \right) = f^3 - f \ . \tag{98}$$

For $1 \gg r \gg \kappa^{-1}$ ($\lambda_L \gg r \gg \xi$) we can expect that f is already close to 1 and thus the derivatives can be neglected. Then

$$\kappa^{-2}\left(-\frac{1}{r^2}f\right) = f^3 - f \ , \tag{99}$$

which has the solution

$$f^2 = 1 - \frac{1}{(\kappa r)^2} \ . \tag{100}$$

This is consistent with the assumption $f \sim 1$.

Finally, for $r \ll \kappa^{-1}$ ($r \ll \xi$) we can assume $f \ll 1$. Then one can try an Ansatz

$$f = C_1(\kappa r) + C_2(\kappa r)^2 + C_3(\kappa r)^3 + \ldots \tag{101}$$

Substituting we get $C_2 = 0$, $C_3 = -C_1/8$. The Ansatz seems to work. The coefficient C_1 one can get from the numerical integration.

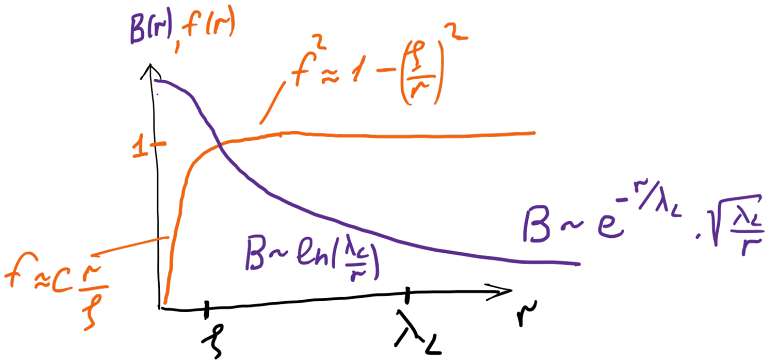

FIG. 7: Abrikosov vortex. Magnetic field $B(r)$ and the order parameter $f(r)$.

H. Energy of the Abrikosov vortex. Field H_{c1}.

We consider type II superconductors with $\kappa \gg 1$. The question is at what field vortices start to appear. A naive ansver would be H_c. It turns out this happens at a lower field $H_{c1} < H_c$. To estimate H_{c1} we have to calculate the free energy of the vortex.

We use again

$$\mathcal{F}_H = \mathcal{F} - \frac{1}{4\pi}\vec{H}_0 \int dV\, \vec{B} \ , \tag{102}$$

where

$$\mathcal{F} = \int dV \left\{ F_n + a|\Psi|^2 + \frac{b}{2}|\Psi|^4 + \frac{1}{4m}\left|\left(-i\hbar\vec{\nabla} + \frac{2e}{c}\vec{A}\right)\Psi\right|^2 + \frac{\vec{B}^2}{8\pi} \right\} \ . \tag{103}$$

In the reduced units, which we will use here these read

$$\mathcal{F}_H = \mathcal{F} - 2\,\vec{H}_0 \int dV\,\vec{B}\ , \tag{104}$$

and

$$\mathcal{F} = \mathcal{F}_n\ + \int dV\ \left\{ -|\Psi|^2 + \frac{1}{2}|\Psi|^4 + \left| \left(-\frac{i\vec{\nabla}}{\kappa} + \vec{A} \right) \Psi \right|^2 + \vec{B}^2 \right\}\ . \tag{105}$$

Integrating by parts, disregarding the boundary, and using the Ginsburg-Landau equations we obtain

$$\mathcal{F} = \mathcal{F}_n\ + \int dV\ \left\{ -\frac{1}{2}|\Psi|^4 + \vec{B}^2 \right\}\ . \tag{106}$$

In the case of a vortex it is very easy to calculate the contribution of the external field. Since the total flux of the magnetic field in the vortex is given by Φ_0 we obtain

$$2\,\vec{H}_0 \int dV\,\vec{B} = 2\,H_0\Phi_0 L\ , \tag{107}$$

where L is the length of the vortex line.

Using the solution obtained above one can calculate the free energy of the vortex per unit length, i.e.,

$$\mathcal{F} = \epsilon L\ . \tag{108}$$

The penetration of vortices starts if the negative contribution due to the external field wins, i.e., if

$$2\,H_0\Phi_0 > \epsilon\ . \tag{109}$$

A calculation (exercise) gives

$$\epsilon \sim \frac{2\pi}{\kappa^2}\ln\kappa\ . \tag{110}$$

For the critical field H_{c1} we should have

$$2\,H_{c1}\Phi_0 = \frac{2\pi}{\kappa^2}\ln\kappa\ . \tag{111}$$

Using $\Phi_0 = 2\pi/\kappa$ (in the reduced units) we get

$$H_{c1} = \frac{1}{2\kappa}\ln\kappa\ . \tag{112}$$

In the usual units this gives

$$H_{c1} \sim \frac{H_c}{\kappa\sqrt{2}}\ln\kappa\ . \tag{113}$$

The phase diagram is shown in Fig. 8

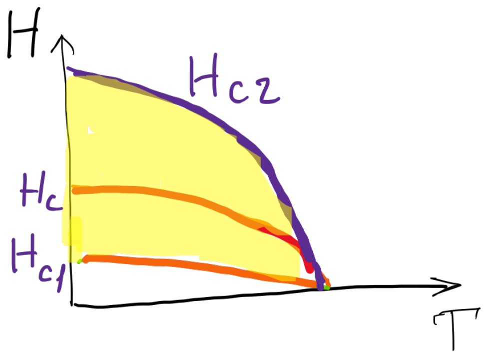

FIG. 8: Phase diagram of type II superconductors for $\kappa \gg 1$. The mixed phase realizes for $H_{c1} < H_0 < H_{c2}$.

I. Pearl vortex

In thin films vortices look differently. Moreover, even in films of type I superconductor such vortices can appear. This limit has been discussed by J. Pearl [1].

Consider a thin film of type II superconductor in the (x,y) plane $(z = 0)$. The thickness of the film is $d \ll \lambda_L$. Then we can consider the current density $\vec{j}$, the order parameter, and the vector potential $\vec{A}$ to be almost independent of z within the film. Recall the London equation

$$\vec{j}_s = -\frac{c}{4\pi\lambda_L^2}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right) \ . \tag{114}$$

Here $\vec{j}_s$ is the 3D current density. The 2D current density in the film is then given by

$$\vec{J}_s = d\vec{j}_s = -\frac{c}{4\pi\Lambda}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right) \ , \tag{115}$$

where $\Lambda \equiv \lambda_L^2/d \gg \lambda_L$ is the so called Pearl length. For the 3D current density we can then write

$$\vec{j}_s(x,r,z) = \vec{J}_s(x,y)\delta(z) = -\frac{c}{4\pi\Lambda}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right)\delta(z) \ . \tag{116}$$

This gives rise to a 3D equation

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{A}) = \frac{4\pi}{c}\vec{j}_s = -\frac{1}{\Lambda}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right)\delta(z) \ . \tag{117}$$

Consider the Coulomb gauge for $\vec{A}$, i.e., $\vec{\nabla}\vec{A} = 0$. Then we obtain

$$(\vec{\nabla}^2)\vec{A} = \frac{1}{\Lambda}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right)\delta(z) \ . \tag{118}$$

We introduce for brevity $\vec{\Phi}(x,y) \equiv \frac{\hbar c}{2e}\vec{\nabla}\phi$. We now perform a 3D Fourier transform of Eq. (118). We introduce $\vec{k} = (\vec{q}, k_z)$, where $\vec{q} = (k_x, k_y)$. We obtain

$$(k_z^2 + q^2)\vec{A}(\vec{k}) = -\frac{1}{\Lambda}\left(\vec{A}_2(\vec{q}) + \vec{\Phi}(\vec{q})\right) \ . \tag{119}$$

Here the 3D Fourier transform reads

$$\vec{A}(\vec{k}) = \int dxdydz\, \vec{A}(x,y,z)e^{-i(k_x x + k_y y + k_z z)} \ , \tag{120}$$

whereas the 2D Fourier transforms are

$$\vec{A}_2(\vec{q}) = \int dxdy\, \vec{A}(x,y,0)e^{-i(k_x x + k_y y)} \ , \tag{121}$$

and

$$\vec{\Phi}(\vec{q}) = \int dxdy\, \vec{\Phi}(x,y)e^{-i(k_x x + k_y y)} \ . \tag{122}$$

Since

$$\vec{A}(x,y,0) = \int \frac{dk_x dk_y dk_z}{(2\pi)^3}\vec{A}(\vec{k})e^{i(k_x x + k_y y)} \tag{123}$$

we obtain

$$\vec{A}_2(\vec{q}) = \int \frac{dk_z}{2\pi}\, \vec{A}(\vec{q}, k_z) \ . \tag{124}$$

From Eq. (119) we obtain

$$\vec{A}(\vec{q}, k_z) = -\frac{1}{q^2 + k_z^2}\frac{1}{\Lambda}\left(\vec{A}_2(\vec{q}) + \vec{\Phi}(\vec{q})\right) \ . \tag{125}$$

Integrating over k_z gives

$$\vec{A}_2(\vec{q}) = -\frac{1}{2\Lambda q}\left(\vec{A}_2(\vec{q}) + \vec{\Phi}(\vec{q})\right) \ . \tag{126}$$

Here $q \equiv |\vec{q}| = \sqrt{q^2}$. This allows us to express both $\vec{A}_2$ and $\vec{A}$ via $\vec{\Phi}$. Namely

$$\vec{A}_2(\vec{q}) = -\frac{\vec{\Phi}(\vec{q})}{1 + 2\Lambda q} \ , \tag{127}$$

and

$$\vec{A}(\vec{q}, k_z) = -\frac{2q\vec{\Phi}(\vec{q})}{(q^2 + k_z^2)(1 + 2\Lambda q)} \ , \tag{128}$$

Recall that $\vec{\Phi}(x,y) \equiv \frac{\hbar c}{2e}\vec{\nabla}\phi$ has as a vector only two components. Thus also $\vec{A}$ (as well as $\vec{A}_2$) has only components A_x and A_y.

For the 2D current density we get

$$\vec{J}(\vec{q}) = -\frac{c}{4\pi\Lambda}\left(\vec{A}_2 + \vec{\Phi}\right) = -\frac{c}{4\pi\Lambda}\vec{\Phi}(\vec{q})\,\frac{2\Lambda q}{1 + 2\Lambda q} \ . \tag{129}$$

Let us consider a single vortex: $\phi(x,y) = -\varphi = \cos^{-1}(x/\sqrt{x^2+y^2})$. Here φ is the angle in the polar coordinates. As we have already seen in the discussion about the Abrikosov vortices (using $\vec{\nabla} = \vec{e}_r \frac{\partial}{\partial r} + \vec{e}_\varphi \frac{1}{r} \frac{\partial}{\partial \varphi}$) we obtain $\vec{\Phi} = -\frac{\Phi_0}{2\pi r}\, \vec{e}_\varphi$ and $\vec{\nabla} \times \vec{\Phi} = -\Phi_0 \delta(x)\delta(y)\vec{e}_z$. The Fourier image of this relation reads

$$[\vec{\nabla} \times \vec{\Phi}]_{\vec{q}} = i\vec{q} \times \vec{\Phi} = -\Phi_0 \vec{e}_z \ . \tag{130}$$

Both $\vec{q}$ and $\vec{\Phi}$ lie in the x, y plain. Thus

$$\vec{\Phi}(\vec{q}) = -i\Phi_0 [\vec{q} \times \vec{e}_z]/q^2 \ . \tag{131}$$

We obtain

$$\vec{A}_2(\vec{q}) = -\frac{\vec{\Phi}(\vec{q})}{1+2\Lambda q} = i\Phi_0 \frac{[\vec{q} \times \vec{e}_z]}{q^2(1+2\Lambda q)} \ , \tag{132}$$

For the magnetic field at $z = 0$ we obtain

$$\vec{B}_2(\vec{q}) = i\vec{q} \times \vec{A}_2(\vec{q}) = \frac{\Phi_0 \vec{e}_z}{1+2\Lambda q} \ . \tag{133}$$

One can perform the Fourier transforms and obtain the current, the vector potential and the magnetic field in the coordinate representation (exercise). However it is already clear that the behavior changes at a distance of order Λ from the vortex core. If $r \ll \Lambda$ this corresponds roughly to $q \gg 1/\Lambda$. Then from

$$\vec{J}(\vec{q}) = -\frac{c}{4\pi\Lambda}\left(\vec{A}_2 + \vec{\Phi}\right) = -\frac{c}{4\pi\Lambda}\vec{\Phi}(\vec{q})\,\frac{2\Lambda q}{1+2\Lambda q} \approx -\frac{c}{4\pi\Lambda}\vec{\Phi}(\vec{q}) \tag{134}$$

we see that the contribution of $\vec{A}_2$ can be neglected and the current is fully determined by the gradient of the phase of the order parameter $\vec{\Phi}$. In this regime $|\vec{J}| \propto 1/r$. For $r \gg \Lambda$ one can show that $|\vec{J}| \propto 1/r^2$.

For superconductor of type I the same theory applies as long as $\Lambda \gg \xi$. For this we need $\lambda_L^2/d \gg \xi$, i.e., $d \ll \lambda_L^2/\xi$.

The theory presented above does not describe the core of the vortex, where the order parameter is suppressed.

J. Josephson Effect from GL theory

Consider a bridge geometry as shown in Fig. 9.

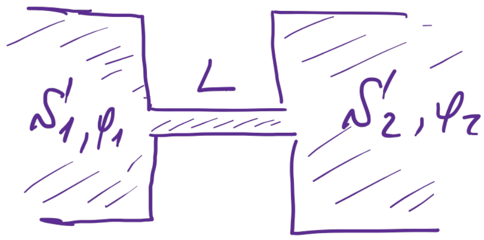

FIG. 9: A bridge geometry leading to Josephson effect.

The GL equation in normal units reads

$$\frac{1}{4m}\left(-i\hbar\vec{\nabla}+\frac{2e}{\hbar c}\vec{A}\right)^2\Psi + a\Psi + b|\Psi|^2\Psi = 0 \tag{135}$$

In the bridge is Ψ only on x dependent. We consider zero magnetic field, i.e., $\vec{A}=0$. Thus:

$$-\frac{\hbar^2}{4m}\frac{\partial^2}{\partial x^2}\Psi + a\Psi + b|\Psi|^2\Psi = 0\ . \tag{136}$$

We introduce $f(x) = \Psi(x)/\Psi_0$, where $\Psi_0^2 = -a/b$ (remember $a < 0$). We divide in addition by $|a|$. This gives

$$-\xi^2\frac{\partial^2}{\partial x^2}f - f + |f|^2 f = 0\ . \tag{137}$$

As boundary conditions we take

$$\begin{aligned} f(x=0) &= e^{i\phi_1}\ , \\ f(x=L) &= e^{i\phi_2}\ . \end{aligned} \tag{138}$$

Assume the bridge is much shorter than the coherence length, $L \ll \xi$. Then the first term is dominant and we should solve $-\xi^2\frac{\partial^2}{\partial x^2}f = 0$. The solution is straightforward:

$$f(x) = \left(1-\frac{x}{L}\right)e^{i\phi_1} + \frac{x}{L}\,e^{i\phi_2}\ . \tag{139}$$

Note that such a solution corresponds to a suppression of the order parameter in the middle of the bridge. Indeed

$$|f(x)|^2 = \left(1-\frac{x}{L}\right)^2 + \left(\frac{x}{L}\right)^2 + 2\left(1-\frac{x}{L}\right)\left(\frac{x}{L}\right)\cos(\Delta\phi)\ , \tag{140}$$

where $\Delta\phi = \phi_2 - \phi_1$. For example, for $\Delta\phi = \pi/2$, we have $|f(L/2)|^2 = 1/2$.

Let us calculate the current

$$\vec{j} = \frac{2ie\hbar}{4m}\left(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\right)\ . \tag{141}$$

We obtain

$$\vec{j} = -\frac{e\hbar}{mL}\Psi_0^2 \sin(\Delta\phi) \ . \tag{142}$$

For the total current we multiply by the cross section area S and obtain

$$I = -I_c \sin(\Delta\phi) \quad , \quad \text{where} \quad I_c = \frac{e\hbar\Psi_0^2 S}{mL} \ . \tag{143}$$

The minus sign here is consistent with the London equation in the bulk of a superconductor:

$$\vec{j}_s = -\frac{c}{4\pi\lambda_L^2}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right) \ . \tag{144}$$

VII. BCS THEORY

A. Attraction due to phonons

A somewhat simplified description of the interaction between electrons and phonons is provided by the following Fröhlich Hamiltonian:

$$H_{el-ph} = \sum_{k,q,\sigma} M(\vec{q})\, c^\dagger_{k+q,\sigma} c_{k,\sigma} \left[a_{\vec{q}} + a^\dagger_{-\vec{q}}\right] \ . \tag{145}$$

The main simplifications here the neglecting of the umklapp processes and the restriction to a single phonon mode (longitudinal, acoustic). The matrix element $M(\vec{q})$ must satisfy $M(-\vec{q}) = M(\vec{q})^*$.

Consider a process (Fig. 10) in which an electron with momentum $\vec{k}_1$ emits virtually a phonon with momentum $\vec{q}$, so that its new momentum is $\vec{k}_1 - \vec{q}$. Then an electron with momentum $\vec{k}_2$ absorbs the photon and its momentum becomes $\vec{k}_2 + \vec{q}$.

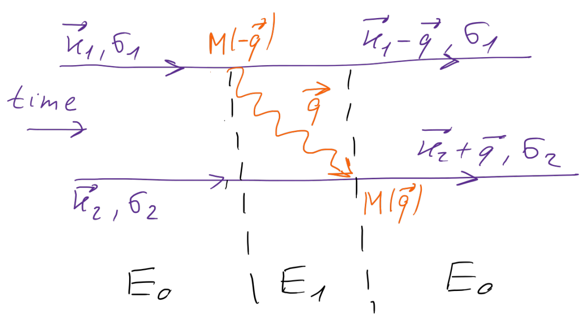

FIG. 10: .

In the initial state the energy is $E_0 = \epsilon_{\vec{k}_1} + \epsilon_{\vec{k}_2}$. In the virtual state the energy is $E_1 = \epsilon_{\vec{k}_1 - \vec{q}} + \epsilon_{\vec{k}_2} + \hbar\omega_q$.

The second order amplitude of this process reads

$$\frac{|M(\vec{q})|^2}{E_0 - E_1} = \frac{|M(\vec{q})|^2}{\epsilon_{\vec{k}_1} - \epsilon_{\vec{k}_1-\vec{q}} - \hbar\omega_q} \tag{146}$$

Another process which interferes with the first one is as follows. Electron with momentum

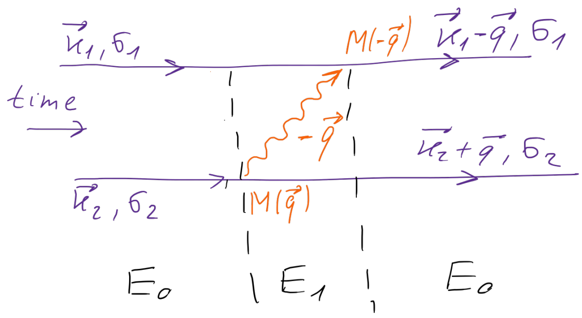

FIG. 11: .

$\vec{k}_2$ emits a phonon with momentum $-\vec{q}$. Then electron with momentum $\vec{k}_1$ absorbs the phonon. The energy E_1 of the intermediate state in this case reads $E_1 = \epsilon_{\vec{k}_1} + \epsilon_{\vec{k}_2+\vec{q}} + \hbar\omega_q$. The amplitude reads

$$\frac{|M(\vec{q})|^2}{E_0 - E_1} = \frac{|M(\vec{q})|^2}{\epsilon_{\vec{k}_2} - \epsilon_{\vec{k}_2+\vec{q}} - \hbar\omega_q} \tag{147}$$

Conservation of energy requires $\epsilon_{\vec{k}_1} + \epsilon_{\vec{k}_2} = \epsilon_{\vec{k}_1-\vec{q}} + \epsilon_{\vec{k}_2+\vec{q}}$. The total amplitude reads

$$\begin{aligned} & \frac{|M(\vec{q})|^2}{\epsilon_{\vec{k}_1} - \epsilon_{\vec{k}_1-\vec{q}} - \hbar\omega_q} + \frac{|M(\vec{q})|^2}{\epsilon_{\vec{k}_2} - \epsilon_{\vec{k}_2+\vec{q}} - \hbar\omega_q} \\ = & \frac{2|M(\vec{q})|^2\hbar\omega_q}{(\epsilon_{\vec{k}_1} - \epsilon_{\vec{k}_1-\vec{q}})^2 - (\hbar\omega_q)^2} \end{aligned} \tag{148}$$

We observe that if $|\epsilon_{\vec{k}_1} - \epsilon_{\vec{k}_1-\vec{q}}| \ll \omega_q$ the sign of the interaction matrix element is negative, i.e., we obtain attraction. We take into account that around the Fermi surface $\epsilon_{\vec{k}} \approx \hbar v_F(|\vec{k}| - k_F)$. In addition $\omega_q \approx cq$, where c is the sound velocity. We notice that $c \ll v_F$ and the highest density of state of phonons is around $q \sim q_D$, or $\omega_q \sim \omega_D$. Since the Debye momentum is very large (of order k_F), we can satisfy the condition $|\epsilon_{\vec{k}_1} - \epsilon_{\vec{k}_1-\vec{q}}| \ll \omega_q$ only if both $\epsilon_{\vec{k}_1}$ and $\epsilon_{\vec{k}_1-\vec{q}}$ are near the Fermi surface. That is, even if $q \sim q_D$ (the typical case) we have $\hbar c q_D = \hbar\omega_D \ll \epsilon_F$. Therefore $\epsilon_{\vec{k}_1}$ and $\epsilon_{\vec{k}_1-\vec{q}}$ should be within $\hbar\omega_D$ from ϵ_F.

We introduce

$$V_{k_1,k_2,q} = \frac{2|M(\vec{q})|^2\hbar\omega_q}{(\epsilon_{\vec{k}_1} - \epsilon_{\vec{k}_1-\vec{q}})^2 - (\hbar\omega_q)^2} = \frac{g_{k_1,k_2,q}}{V} \tag{149}$$

(Introduction of g is convenient since g does not contain extensive quantities like V or N. The dimensionality of g is *energy* $\times$ *volume*). This amplitude is only taken on-shell as far as electrons are concerned. Thus

$$(\epsilon_{\vec{k}_1} - \epsilon_{\vec{k}_1-\vec{q}})^2 = (\epsilon_{\vec{k}_2} - \epsilon_{\vec{k}_2+\vec{q}})^2$$

.

That is the effective second quantized interaction between electrons due to phonons reads

$$H_{el-el-ph} = \frac{1}{2V} \sum_{k_1,\sigma_1,k_2,\sigma_2,q} g_{k_1,k_2,q}\, c^\dagger_{k_1+q,\sigma_1}\, c^\dagger_{k_2-q,\sigma_2}\, c_{k_2,\sigma_2}\, c_{k_1,\sigma_1} \tag{150}$$

The noninteracting Hamiltonian reads

$$H_0 = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma}\, c_{k,\sigma} \tag{151}$$

B. Cooper problem (L. Cooper 1955)

The interaction is attractive and considerable as long as the energy transfer $|\epsilon_{\vec{k}_1} - \epsilon_{\vec{k}_1-\vec{q}}| \ll \hbar\omega_q \leq \hbar\omega_D$. We simplify the model as follows:

$$g_{k_1,k_2,q} = \begin{cases} -g & \text{if} \quad |\epsilon_{\vec{k}_1} - \epsilon_F| \leq \hbar\omega_D \text{ and } |\epsilon_{\vec{k}_1-\vec{q}} - \epsilon_F| \leq \hbar\omega_D \\ 0 & \text{otherwise} \end{cases} \tag{152}$$

Cooper considered a pair of electrons above the filled Fermi sphere. That is the Fermi sphere is given by

$$|\Phi_0\rangle = \prod_{k\leq k_F,\sigma} c^\dagger_{k,\sigma}\, |0\rangle \ , \tag{153}$$

Cooper explored the following state

$$|\Phi\rangle = \sum_{k_1>k_F,\sigma_1,k_2>k_F,\sigma_2} \psi(k_1,\sigma_1,k_2,\sigma_2) c^\dagger_{k_1,\sigma_1} c^\dagger_{k_2,\sigma_2}\, |\Phi_0\rangle \tag{154}$$

The wave function $\psi(k_1,\sigma_1,k_2,\sigma_2)$ is antisymmetric, i.e, $\psi(k_1,\sigma_1,k_2,\sigma_2) = -\psi(k_2,\sigma_2,k_1,\sigma_1)$ (indeed the second quantization is organized so that even if we use here not an antisymmetric function, only the antisymmetric part will be important). We use $\psi(k_1,\sigma_1,k_2,\sigma_2) = \alpha(k_1,k_2)\chi(\sigma_1,\sigma_2)$. Further we restrict ourselves to the states with zero total momentum,

$\vec{k}_1 + \vec{k}_2 = 0$. We also restrict ourselves to the layer of states with energies $[E_F, E_F + \hbar\omega_D]$. Any pair out of this layer interacts with any other pair. Thus

$$|\Phi\rangle = \sum_{E_F<\epsilon_k<E_F+\hbar\omega_D,\sigma_1,\sigma_2} \alpha(\vec{k})\chi(\sigma_1,\sigma_2)c^\dagger_{k,\sigma_1}c^\dagger_{-k,\sigma_2}|\Phi_0\rangle \tag{155}$$

The Schrödinger equation reads

$$E|\Phi\rangle = (H_0 + H_{el-el-ph})|\Phi\rangle \tag{156}$$

We count the energy from the energy of the filled Fermi sphere. Then

$$\begin{aligned} E|\Phi\rangle &= \sum_{k,\sigma_1,\sigma_2} 2\epsilon_k\alpha(\vec{k})\chi(\sigma_1,\sigma_2)c^\dagger_{k,\sigma_1}c^\dagger_{-k,\sigma_2}|\Phi_0\rangle \\ &- \frac{g}{V}\sum_{k,\sigma_1,\sigma_2,q} \alpha(\vec{k})\chi(\sigma_1,\sigma_2)c^\dagger_{k+q,\sigma_1}c^\dagger_{-k-q,\sigma_2}|\Phi_0\rangle \end{aligned} \tag{157}$$

This gives

$$(2\epsilon_k - E)\alpha(k) = \frac{g}{V}\sum_{E_F<\epsilon_{k_1}<E_F+\hbar\omega_D} \alpha(k_1) \tag{158}$$

We denote

$$C \equiv \frac{1}{V}\sum_{E_F<\epsilon_{k_1}<E_F+\hbar\omega_D} \alpha(k_1) \tag{159}$$

and obtain

$$\alpha(k) = \frac{gC}{(2\epsilon_k - E)} \tag{160}$$

Summing this equation we obtain

$$C = \frac{1}{V}\sum_{E_F<\epsilon_{k_1}<E_F+\hbar\omega_D} \frac{gC}{(2\epsilon_k - E)} \tag{161}$$

We obtain equation for E

$$1 = \int_{E_F}^{E_F+\hbar\omega_D} d\epsilon \frac{\nu(\epsilon)g}{(2\epsilon - E)} \tag{162}$$

Approximating the density of states by a constant $\nu(\epsilon) = \nu_0$ (this is density of states per spin) we obtain

$$\frac{1}{g\nu_0} = \frac{1}{2}\ln\frac{E_F + \hbar\omega_D - E/2}{E_F - E/2} \tag{163}$$

Thus

$$\frac{2E_F + 2\hbar\omega_D - E}{2E_F - E} = e^{\frac{2}{g\nu_0}} \tag{164}$$

$$(2E_F - E)(e^{\frac{2}{g\nu_0}} - 1) = 2\hbar\omega_D \tag{165}$$

For weak coupling $g\nu_0 \ll 1$ we obtain

$$2E_F - E = 2\hbar\omega_D e^{-\frac{2}{g\nu_0}} \tag{166}$$

$$E = 2E_F - 2\hbar\omega_D e^{-\frac{2}{g\nu_0}} \tag{167}$$

The binding energy per electron is then found from $E = 2E_F - 2\Delta$

$$\Delta = \hbar\omega_D e^{-\frac{2}{g\nu_0}} \tag{168}$$

1. *Symmetry*

Since $\alpha(k) = \alpha(-k)$, i.e, symmetric, the spin part of the wave function χ must be antisymmetric - singlet. That is $\chi(\uparrow\uparrow) = \chi(\downarrow\downarrow) = 0$ and $\chi(\uparrow\downarrow) = -\chi(\downarrow\uparrow) = 1/\sqrt{2}$.

C. BCS state (J. Bardeen, L. Cooper, and R. Schrieffer (BCS), 1957)

1) Everything done in the grand canonical ensemble. The grand canonical partition function

$$Z_\Omega = \sum_{n,N} e^{-\beta(E_{n,N} - \mu N)} \tag{169}$$

shows that at $T = 0$ one has to minimize $H_G = H - \mu N$.

We obtain

$$H_G = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma}\, c_{k,\sigma} - \frac{1}{2}\frac{g}{V} \sum_{k_1,\sigma_1,k_2,\sigma_2,q} c^\dagger_{k_1+q,\sigma_1}\, c^\dagger_{k_2-q,\sigma_2}\, c_{k_2,\sigma_2}\, c_{k_1,\sigma_1} \tag{170}$$

where the interaction term works only if the energy transfer $\epsilon_{k_1+q} - \epsilon_{k_1}$ is smaller than the Debye energy $\hbar\omega_D$. One can also see (Fig. 12) that under this restriction the phase space available for the interaction is maximal if $\vec{K} \equiv \vec{k}_1 + \vec{k}_2 \approx 0$.

Although the Hamiltonian conserves the number of particles, BCS constructed a trial wave function which is a superposition of different numbers of particles:

$$|BCS\rangle = \prod_k (u_k + v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow})\, |0\rangle \ . \tag{171}$$

with the purpose to use u_k and v_k as variational parameters and minimize $\langle BCS|\, H_G\, |BCS\rangle$.

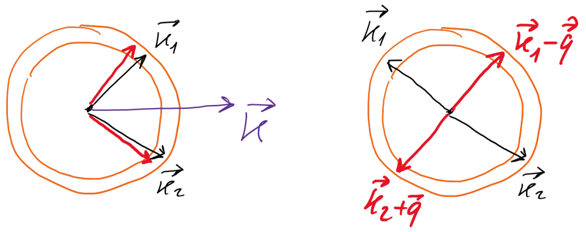

FIG. 12: For $\vec{K} \approx 0$ the phase space available for interaction is much bigger.

For this purpose one can introduce a reduced BSC Hamiltonian. Only terms of this Hamiltonian will contribute to the average with BCS trial functions. The reduced Hamiltonian is the one in which $k_1 = -k_2$ and $\sigma_1 = -\sigma_2$:

$$H_{\mathrm{BCS}} = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma} - \frac{1}{2}\frac{g}{V} \sum_{k,q,\sigma} c^\dagger_{k+q,\sigma} c^\dagger_{-k-q,-\sigma} c_{-k,-\sigma} c_{k,\sigma} \ . \tag{172}$$

Renaming $k' = k + q$ we obtain

$$H_{\mathrm{BCS}} = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma} - \frac{1}{2}\frac{g}{V} \sum_{k,k',\sigma} c^\dagger_{k',\sigma} c^\dagger_{-k',-\sigma} c_{-k,-\sigma} c_{k,\sigma} \ , \tag{173}$$

or

$$H_{\mathrm{BCS}} = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma} - \frac{g}{V} \sum_{k,k'} c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} c_{-k,\downarrow} c_{k,\uparrow} \ , \tag{174}$$

Also the condition on k and k' gets simplified. We just demand that

$$\mu - \hbar\omega_D < \epsilon_k, \epsilon_{k'} < \mu + \hbar\omega_D \ . \tag{175}$$

1. *Averages*

Normalization:

$$\begin{aligned} 1 &= \langle BCS|\, BCS\rangle = \langle 0| \prod_{k_2} (u^*_{k_2} + v^*_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow}) \prod_{k_1} (u_{k_1} + v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow})\, |0\rangle \\ &= \prod_k (|u_k|^2 + |v_k|^2) \ . \end{aligned} \tag{176}$$

We further restrict ourselves to real u_k and v_k such that $u_k^2 + v_k^2 = 1$. Thus only one of them is independent. The following parametrization is helpful: $u_k = \cos\phi_k$, $v_k = \sin\phi_k$.

We obtain

$$
\begin{aligned}
&\langle BCS| \, c^\dagger_{k,\uparrow} \, c_{k,\uparrow} \, |BCS\rangle \\
&= \langle 0| \prod_{k_2} (u_{k_2} + v_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow}) c^\dagger_{k,\uparrow} \, c_{k,\uparrow} \prod_{k_1} (u_{k_1} + v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow}) \, |0\rangle \\
&= v_k^2
\end{aligned} \tag{177}
$$

$$
\begin{aligned}
&\langle BCS| \, c^\dagger_{k,\downarrow} \, c_{k,\downarrow} \, |BCS\rangle \\
&= \langle 0| \prod_{k_2} (u_{k_2} + v_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow}) c^\dagger_{k,\downarrow} \, c_{k,\downarrow} \prod_{k_1} (u_{k_1} + v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow}) \, |0\rangle \\
&= v_{-k}^2
\end{aligned} \tag{178}
$$

$$
\begin{aligned}
&\langle BCS| \, c^\dagger_{k',\uparrow} \, c^\dagger_{-k',\downarrow} \, c_{-k,\downarrow} \, c_{k,\uparrow} \, |BCS\rangle \\
&= \langle 0| \prod_{k_2} (u_{k_2} + v_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow}) \, c^\dagger_{k',\uparrow} \, c^\dagger_{-k',\downarrow} \, c_{-k,\downarrow} \, c_{k,\uparrow} \prod_{k_1} (u_{k_1} + v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow}) \, |0\rangle \\
&= u_k v_k u_{k'} v_{k'}
\end{aligned} \tag{179}
$$

This gives

$$
\langle BCS| \, H_{\mathrm{BCS}} \, |BCS\rangle = 2 \sum_k (\epsilon_k - \mu) v_k^2 - \frac{g}{V} \sum_{k,k'} u_k v_k u_{k'} v_{k'} \tag{180}
$$

or in terms of the angle ϕ_k

$$
\langle BCS| \, H_{\mathrm{BCS}} \, |BCS\rangle = 2 \sum_k \xi_k \sin^2 \phi_k - \frac{1}{4} \frac{g}{V} \sum_{k,k'} \sin(2\phi_k) \sin(2\phi_{k'}) \ . \tag{181}
$$

where $\xi_k \equiv \epsilon_k - \mu$.

We vary with respect to ϕ_k

$$
\frac{\partial}{\partial \phi_k} \langle BCS| \, H_{\mathrm{BCS}} \, |BCS\rangle = 2\xi_k \sin(2\phi_k) - \frac{g}{V} \cos(2\phi_k) \sum_{k'} \sin(2\phi_k) = 0 \ . \tag{182}
$$

(note extra factor 2 in the second term due to the permutation $k \leftrightarrow k'$).

We introduce $\Delta \equiv \frac{g}{V} \sum_{k'} u_{k'} v_{k'} = \frac{g}{2V} \sum_{k'} \sin(2\phi_{k'})$ and obtain

$$
\xi_k \sin(2\phi_k) = \Delta \cos(2\phi_k) \ , \tag{183}
$$

or in terms of v_k and u_k

$$2\xi_k v_k u_k = \Delta(u_k^2 - v_k^2) \ . \tag{184}$$

Trivial solution: $\Delta = 0$. E.g., the Fermi sea: $u_k = 0$ and $v_k = 1$ for $\epsilon_k < \mu$ and $u_k = 1$ and $v_k = 0$ for $\epsilon_k > \mu$.

We look for nontrivial solutions: $\Delta \neq 0$. Then from $\xi_k \sin 2\phi_k = \Delta \cos 2\phi_k$ we obtain

$$\sin 2\phi_k = 2u_k v_k = \frac{\Delta}{\sqrt{\Delta^2 + \xi_k^2}} \ , \tag{185}$$

$$\cos 2\phi_k = u_k^2 - v_k^2 = \frac{\xi_k}{\sqrt{\Delta^2 + \xi_k^2}} \ . \tag{186}$$

It is now possible to find v_k^2 and v_k^2.

$$v_k^2 = \sin^2 \phi_k = \frac{1 - \cos 2\phi_k}{2} = \frac{1}{2} - \frac{\xi_k}{2\sqrt{\Delta^2 + \xi_k^2}} \tag{187}$$

$$u_k^2 = 1 - v_k^2 = \frac{1}{2} + \frac{\xi_k}{2\sqrt{\Delta^2 + \xi_k^2}} \ . \tag{188}$$

These functions are shown in Fig. 13.

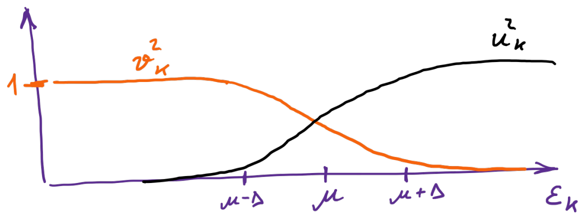

FIG. 13: Functions v_k^2 and v_k^2.

From the definition of $\Delta = \frac{g}{V}\sum_k u_k v_k$ we obtain the self-consistency equation

$$\Delta = \frac{g}{2V}\sum_k \frac{\Delta}{\sqrt{\Delta^2 + \xi_k^2}} \tag{189}$$

or

$$\begin{aligned} 1 \ &= \ \frac{g}{2V}\sum_k \frac{1}{\sqrt{\Delta^2 + (\epsilon_k - \mu)^2}} = \frac{g\nu_0}{2}\int\limits_{-\hbar\omega_D}^{\hbar\omega_D} d\xi \frac{1}{\sqrt{\Delta^2 + \xi^2}} \\ &= \ g\nu_0 \int\limits_0^{\hbar\omega_D/\Delta} dx \frac{1}{\sqrt{1+x^2}} = g\nu_0 \ \ln(\sqrt{1+x^2} + x)\Big|_0^{\hbar\omega_D/\Delta} \approx g\nu_0 \ln \frac{2\hbar\omega_D}{\Delta} \end{aligned} \tag{190}$$

We have assumed $\Delta \ll \hbar\omega_D$.

This gives

$$\Delta = 2\hbar\omega_D e^{-\frac{1}{\nu_0 g}} \tag{191}$$

2. Total energy

We want to convince ourselves that the total energy of the new state is lower that the energy of the trivial solution (fully filled Fermi sphere).

$$
\begin{aligned}
E_{BCS} &= \langle BCS| H_{\rm BCS} |BCS\rangle = 2\sum_k (\epsilon_k - \mu) v_k^2 - \frac{g}{V}\sum_{k,k'} u_k v_k u_{k'} v_{k'} \\
&= 2\sum_k (\epsilon_k - \mu) v_k^2 - \Delta \sum_k u_k v_k \ ,
\end{aligned} \tag{192}
$$

whereas

$$
E_{Norm} = \langle Norm| H_{\rm BCS} |Norm\rangle = 2\sum_k (\epsilon_k - \mu)\theta(\mu - \epsilon_k) \ . \tag{193}
$$

We obtain

$$
\Delta E = E_{BCS} - E_{Norm} = 2\sum_k (\epsilon_k - \mu)(v_k^2 - \theta(\mu - \epsilon_k)) - \Delta \sum_k u_k v_k \ , \tag{194}
$$

With $\xi_k = \epsilon_k - \mu$,

$$
v_k^2 = \sin^2 \phi_k = \frac{1 - \cos 2\phi_k}{2} = \frac{1}{2} - \frac{\xi_k}{2\sqrt{\Delta^2 + \xi_k^2}} \tag{195}
$$

and

$$
u_k v_k = \frac{\Delta}{2\sqrt{\Delta^2 + \xi_k^2}} \tag{196}
$$

we obtain

$$
\Delta E = \sum_k \left(2\xi_k \left[\frac{1}{2} - \frac{\xi_k}{2\sqrt{\Delta^2 + \xi_k^2}} - \theta(-\xi_k) \right] - \frac{\Delta^2}{2\sqrt{\Delta^2 + \xi_k^2}} \right) \tag{197}
$$

$$
\begin{aligned}
\Delta E &= V \int\limits_{-\hbar\omega_D}^{\hbar\omega_D} \nu_0 d\xi \left(2\xi \left[\frac{1}{2} - \frac{\xi}{2\sqrt{\Delta^2 + \xi^2}} - \theta(-\xi) \right] - \frac{\Delta^2}{2\sqrt{\Delta^2 + \xi^2}} \right) \\
&= 2V \int\limits_{0}^{\hbar\omega_D} \nu_0 d\xi \left[\xi - \frac{\xi^2}{\sqrt{\Delta^2 + \xi^2}} - \frac{\Delta^2}{2\sqrt{\Delta^2 + \xi_k^2}} \right] \\
&= 2V\nu_0\Delta^2 \int\limits_{0}^{\hbar\omega_D/\Delta} dx \left(x - \sqrt{1 + x^2} + \frac{1}{2\sqrt{1 + x^2}} \right)
\end{aligned} \tag{198}
$$

The last integral is convergent and for $\hbar\omega_D \gg \Delta$ can be taken to ∞. The integral gives $-1/4$. Thus

$$
\Delta E = -V\,\frac{\nu_0 \Delta^2}{2} \ . \tag{199}
$$

Roughly energy Δ per electron in window of energies of order Δ.

D. Excitations

We want to consider the BCS ground state as vacuum and find the quasiparticle excitations above it. Let us start with the normal state, i.e., $v_k = \theta(-\xi_k)$ and $u_k = \theta(\xi_k)$. For $\xi_k > 0$ we have

$$c_{k,\sigma} |Norm\rangle = 0 \tag{200}$$

while for $\xi_k < 0$

$$c^\dagger_{k,\sigma} |Norm\rangle = 0 \tag{201}$$

we introduce

$$\alpha_{k,\sigma} \equiv \begin{cases} c_{k,\sigma} & \text{if} \quad \xi_k > 0 \\ \pm c^\dagger_{-k,-\sigma} & \text{if} \quad \xi_k < 0 \end{cases} \tag{202}$$

or equivalently

$$\alpha_{k,\sigma} = u_k c_{k,\sigma} \pm v_k c^\dagger_{-k,-\sigma} \tag{203}$$

(the sign to be chosen).

We see, thus, that $\alpha_{k,\sigma} |Norm\rangle = 0$, whereas

$$\alpha^\dagger_{k,\sigma} = u_k c^\dagger_{k,\sigma} \pm v_k c_{-k,-\sigma} \tag{204}$$

creates an excitation of energy $|\xi_k|$.

For the BCS state we obtain

$$\alpha_{k,\sigma} |BCS\rangle = (u_k c_{k,\sigma} \pm v_k c^\dagger_{-k,-\sigma}) \prod_q (u_q + v_q c^\dagger_{q,\uparrow} c^\dagger_{-q,\downarrow}) |0\rangle \tag{205}$$

We see that the proper choice of sign is

$$\alpha_{k,\sigma} = u_k c_{k,\sigma} - \sigma v_k c^\dagger_{-k,-\sigma} \tag{206}$$

and

$$\alpha_{k,\sigma} |BCS\rangle = 0 \ . \tag{207}$$

The conjugated (creation) operator reads

$$\alpha^\dagger_{k,\sigma} = u_k c^\dagger_{k,\sigma} - \sigma v_k c_{-k,-\sigma} \tag{208}$$

One can check the commutation relations

$$\left\{\alpha_{k,\sigma}, \alpha^\dagger_{k',\sigma'}\right\}_+ = \delta_{k,k'}\delta_{\sigma,\sigma'} \tag{209}$$

$$\{\alpha_{k,\sigma}, \alpha_{k',\sigma'}\}_+ = 0 \quad \left\{\alpha^\dagger_{k,\sigma}, \alpha^\dagger_{k',\sigma'}\right\}_+ = 0 \tag{210}$$

The inverse relations read:

$$c_{k,\sigma} = u_k \alpha_{k,\sigma} + \sigma v_k \alpha^\dagger_{-k,-\sigma} \quad , \quad c^\dagger_{k,\sigma} = u_k \alpha^\dagger_{k,\sigma} + \sigma v_k \alpha_{-k,-\sigma} \tag{211}$$

We can show now that in the BCS ground state the expectation values $\langle c_{-k,\downarrow}\, c_{k,\uparrow}\rangle$ and $\langle c^\dagger_{k,\uparrow}\, c^\dagger_{-k,\downarrow}\rangle$ do not vanish. They can be calculated explicitly

Using

$$\begin{aligned} c^\dagger_{k,\uparrow}\, c^\dagger_{-k,\downarrow} &= (u_k \alpha^\dagger_{k,\uparrow} + v_k \alpha_{-k,\downarrow})(u_k \alpha^\dagger_{-k,\downarrow} - v_k \alpha_{k,\uparrow}) \\ &= u_k^2 \alpha^\dagger_{k,\uparrow} \alpha^\dagger_{-k,\downarrow} - v_k^2 \alpha_{-k,\downarrow} \alpha_{k,\uparrow} + u_k v_k (1 - \alpha^\dagger_{k,\uparrow} \alpha_{k,\uparrow} - \alpha^\dagger_{-k,\downarrow} \alpha_{-k,\downarrow}) \end{aligned} \tag{212}$$

and

$$c_{-k,\downarrow} c_{k,\uparrow} = u_k^2 \alpha_{-k,\downarrow} \alpha_{k,\uparrow} - v_k^2 \alpha^\dagger_{k,\uparrow} \alpha^\dagger_{-k,\downarrow} + u_k v_k (1 - \alpha^\dagger_{k,\uparrow} \alpha_{k,\uparrow} - \alpha^\dagger_{-k,\downarrow} \alpha_{-k,\downarrow}) \tag{213}$$

we obtain in the BCS ground state $\langle c_{-k,\downarrow}\, c_{k,\uparrow}\rangle = v_k u_k$ and $\langle c^\dagger_{k,\uparrow}\, c^\dagger_{-k,\downarrow}\rangle = v_k u_k$. This follows from $\alpha_{k,\sigma} |BCS\rangle = 0$ and $\langle BCS|\, \alpha^\dagger_{k,\sigma} = 0$.

1. *Mean field*

We adopt the mean field approximation for the BCS Hamiltonian.

$$H_{\rm BCS} = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma}\, c_{k,\sigma} - \frac{g}{V} \sum_{k,k'} c^\dagger_{k',\uparrow}\, c^\dagger_{-k',\downarrow}\, c_{-k,\downarrow}\, c_{k,\uparrow} \; . \tag{214}$$

Note that in the interaction the terms with $k = k'$ are absent, since the matrix element of the electron-phonon interaction is proportional to the momentum transfer $q = k - k'$. Thus the only averages we can extract in the interaction term are $\langle c_{-k,\downarrow}\, c_{k,\uparrow}\rangle$ and $\langle c^\dagger_{k,\uparrow}\, c^\dagger_{-k,\downarrow}\rangle$.

We use

$$AB = \langle A\rangle \langle B\rangle + \langle A\rangle (B - \langle B\rangle) + (A - \langle A\rangle) \langle B\rangle + (A - \langle A\rangle)(B - \langle A\rangle)$$

and neglect the last term, which leads to

$$AB \approx \langle A\rangle \langle B\rangle + \langle A\rangle (B - \langle B\rangle) + (A - \langle A\rangle) \langle B\rangle = \langle A\rangle B + \langle B\rangle A - \langle A\rangle \langle B\rangle$$

. We introduce $\Delta \equiv \frac{g}{V}\sum_k \langle c_{-k,\downarrow}\, c_{k,\uparrow}\rangle = \frac{g}{V}\sum_k \langle c^\dagger_{k,\uparrow}\, c^\dagger_{-k,\downarrow}\rangle$. The mean field Hamiltonian reads

$$
\begin{aligned}
H^{\mathrm{MF}}_{\mathrm{BCS}} &= \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma}\, c_{k,\sigma} + \frac{g}{V}\sum_{k,k'} \langle c^\dagger_{k',\uparrow}\, c^\dagger_{-k',\downarrow}\rangle\, \langle c_{-k,\downarrow}\, c_{k,\uparrow}\rangle \\
&- \frac{g}{V}\sum_{k,k'} \langle c^\dagger_{k',\uparrow}\, c^\dagger_{-k',\downarrow}\rangle\, c_{-k,\downarrow}\, c_{k,\uparrow} - \frac{g}{V}\sum_{k,k'} c^\dagger_{k',\uparrow}\, c^\dagger_{-k',\downarrow}\, \langle c_{-k,\downarrow}\, c_{k,\uparrow}\rangle \\
&= \sum_{k,\sigma} \xi_k c^\dagger_{k,\sigma}\, c_{k,\sigma} - \sum_k \Delta c_{-k,\downarrow}\, c_{k,\uparrow} - \sum_k \Delta c^\dagger_{k,\uparrow}\, c^\dagger_{-k,\downarrow} + V\frac{\Delta^2}{g}
\end{aligned}
\tag{215}
$$

Substituting the expressions for c operators in terms of α operators we obtain a diagonal Hamiltonian (exercise)

$$
H = \sum_{k,\sigma} E_k \alpha^\dagger_{k,\sigma}\, \alpha_{k,\sigma} + const.\ , \tag{216}
$$

where $E_k = \sqrt{\Delta^2 + \xi_k^2}$.

For proof one needs

$$
\begin{aligned}
& c^\dagger_{k,\uparrow}\, c_{k,\uparrow} + c^\dagger_{-k,\downarrow}\, c_{-k,\downarrow} = (u_k \alpha^\dagger_{k,\uparrow} + v_k \alpha_{-k,\downarrow})(u_k \alpha_{k,\uparrow} + v_k \alpha^\dagger_{-k,\downarrow}) \\
& + (u_k \alpha^\dagger_{-k,\downarrow} - v_k \alpha_{k,\uparrow})(u_k \alpha_{-k,\downarrow} - v_k \alpha^\dagger_{k,\uparrow}) \\
& = (u_k^2 - v_k^2)(\alpha^\dagger_{k,\uparrow}\alpha_{k,\uparrow} + \alpha^\dagger_{-k,\downarrow}\alpha_{-k,\downarrow}) + 2v_k^2 + 2u_k v_k (\alpha^\dagger_{k,\uparrow}\alpha^\dagger_{-k,\downarrow} + \alpha_{-k,\downarrow}\alpha_{k,\uparrow})
\end{aligned}
\tag{217}
$$

2. *Nambu formalism*

Another way to get the same is to use the Nambu spinors. First we obtain

$$
H^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_k \begin{pmatrix} c^\dagger_{k,\uparrow} & c_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} \xi_k & -\Delta \\ -\Delta & 0 \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c^\dagger_{-k,\downarrow} \end{pmatrix} + \sum_k \xi_k c^\dagger_{k,\downarrow}\, c_{k,\downarrow} + V\frac{\Delta^2}{g} \tag{218}
$$

Next we rewrite $\sum_k \xi_k c^\dagger_{k,\downarrow}\, c_{k,\downarrow} = \sum_k \xi_k (1 - c_{k,\downarrow}\, c^\dagger_{k,\downarrow}) = \sum_k \xi_k (1 - c_{-k,\downarrow}\, c^\dagger_{-k,\downarrow})$. This gives

$$
H^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_k \begin{pmatrix} c^\dagger_{k,\uparrow} & c_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c^\dagger_{-k,\downarrow} \end{pmatrix} + \sum_k \xi_k + V\frac{\Delta^2}{g} \tag{219}
$$

The eigenvalues of the matrix $\begin{pmatrix} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{pmatrix}$ read $\pm E_k$, where $E_k = \sqrt{\Delta^2 + \xi_k^2}$. For the eigenvectors we get

$$
\begin{pmatrix} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{pmatrix} \begin{pmatrix} u_k \\ -v_k \end{pmatrix} = E_k \begin{pmatrix} u_k \\ -v_k \end{pmatrix} \tag{220}
$$

and

$$\begin{pmatrix} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{pmatrix} \begin{pmatrix} v_k \\ u_k \end{pmatrix} = -E_k \begin{pmatrix} v_k \\ u_k \end{pmatrix} \tag{221}$$

Thus

$$U^\dagger \begin{pmatrix} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{pmatrix} U = \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} , \tag{222}$$

where

$$U \equiv \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \tag{223}$$

We obtain

$$H_{\rm BCS}^{\rm MF} = \sum_k \begin{pmatrix} c_{k,\uparrow}^\dagger & c_{-k,\downarrow} \end{pmatrix} U U^\dagger \begin{pmatrix} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{pmatrix} U U^\dagger \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix} + \sum_k \xi_k + V \frac{\Delta^2}{g} \tag{224}$$

We use the diagonalization (222) and the Bogoliubov transformation written in the matrix form as

$$\begin{pmatrix} \alpha_{k,\uparrow} \\ \alpha_{-k,\downarrow}^\dagger \end{pmatrix} = U^\dagger \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix} \tag{225}$$

to obtain

$$H_{\rm BCS}^{\rm MF} = \sum_k \begin{pmatrix} \alpha_{k,\uparrow}^\dagger & \alpha_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \alpha_{k,\uparrow} \\ \alpha_{-k,\downarrow}^\dagger \end{pmatrix} + \sum_k \xi_k + V \frac{\Delta^2}{g} \tag{226}$$

Using again the commutation relations for the α operators we obtain

$$H_{\rm BCS}^{\rm MF} = \sum_{k,\sigma} E_k \alpha_{k,\sigma}^\dagger \alpha_{k,\sigma} + \sum_k (\xi_k - E_k) + V \frac{\Delta^2}{g} . \tag{227}$$

3. 4X4 Nambu formalism

In the 2X2 Nambu formalism presented above we have explicitly broken the symmetry between spin up and spin down. There is a way to do the same without breaking the symmetry. Introduce a 4-spinor $\begin{pmatrix} c_{k,\uparrow} & c_{k,\downarrow} & c_{-k,\downarrow}^\dagger & -c_{-k,\uparrow}^\dagger \end{pmatrix}$. Then

$$H_{\rm BCS}^{\rm MF} = \sum_k \begin{pmatrix} c_{k,\uparrow}^\dagger & c_{k,\downarrow}^\dagger & c_{-k,\downarrow} & -c_{-k,\uparrow} \end{pmatrix} \begin{pmatrix} \xi_k & 0 & -\Delta & 0 \\ 0 & \xi_k & 0 & 0 \\ -\Delta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \\ c_{-k,\downarrow}^\dagger \\ -c_{-k,\uparrow}^\dagger \end{pmatrix} + V \frac{\Delta^2}{g} . \tag{228}$$

One observes, however, that there is a redundancy here and we can rewrite

$$
\begin{aligned}
H_{\mathrm{BCS}}^{\mathrm{MF}} &= \sum_k \left(c_{k,\uparrow}^\dagger \ c_{k,\downarrow}^\dagger \ c_{-k,\downarrow} \ -c_{-k,\uparrow} \right) \begin{pmatrix} \xi_k & 0 & -\Delta/2 & 0 \\ 0 & \xi_k & 0 & -\Delta/2 \\ -\Delta/2 & 0 & 0 & 0 \\ 0 & -\Delta/2 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \\ c_{-k,\downarrow}^\dagger \\ -c_{-k,\uparrow}^\dagger \end{pmatrix} \\
&+ V\frac{\Delta^2}{g} \ . \qquad (229)
\end{aligned}
$$

Also the kinetic energy can be written in a more symmetric form

$$
\begin{aligned}
H_{\mathrm{BCS}}^{\mathrm{MF}} &= \frac{1}{2}\sum_k \left(c_{k,\uparrow}^\dagger \ c_{k,\downarrow}^\dagger \ c_{-k,\downarrow} \ -c_{-k,\uparrow} \right) \begin{pmatrix} \xi_k & 0 & -\Delta & 0 \\ 0 & \xi_k & 0 & -\Delta \\ -\Delta & 0 & -\xi_k & 0 \\ 0 & -\Delta & 0 & -\xi_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \\ c_{-k,\downarrow}^\dagger \\ -c_{-k,\uparrow}^\dagger \end{pmatrix} \\
&+ \sum_k \xi_k + V\frac{\Delta^2}{g} \ . \qquad (230)
\end{aligned}
$$

E. Finite temperature

We obtained the energy spectrum $E_k = \sqrt{\Delta^2 + \xi_k^2}$ in the mean-field approximation assuming that $\langle c_{-k,\downarrow} c_{k,\uparrow} \rangle = v_k u_k$, where the averaging is in the ground state, i.e., there are no quasi-particles excited. For $T > 0$ some quasi-particles get excited and the value of $\langle c_{-k,\downarrow} c_{k,\uparrow} \rangle$ changes. Namely, we obtain

$$
\langle c_{-k,\downarrow} c_{k,\uparrow} \rangle = v_k u_k (1 - 2n_k) \ , \qquad (231)
$$

where $n_k = f(E_k) = \frac{1}{e^{\beta E_k + 1}}$.

If we still want to have the Hamiltonian diagonalized by the Bogoliubov transformation, we have to redefine Δ as

$$
\Delta = \frac{g}{V}\sum_k \langle c_{-k,\downarrow} c_{k,\uparrow} \rangle = \frac{g}{V}\sum_k u_k v_k (1 - 2n_k) \qquad (232)
$$

Then, however, Δ is temperature dependent and thus $E_k = \sqrt{\Delta^2 + \xi_k^2}$ is also temperature dependent. We must do everything self-consistently.

From

$$
u_k v_k = \frac{\Delta}{2\sqrt{\Delta^2 + \xi_k^2}} \qquad (233)
$$

we obtain the new self-consistency equation

$$\Delta = \frac{g}{2V}\sum_k \frac{\Delta}{\sqrt{\Delta^2+\xi_k^2}}\,\tanh\frac{\beta E_k}{2} \tag{234}$$

To find the critical temperature T_c we assume that $\Delta(T_c) = 0$. This gives

$$1 = \frac{g}{2V}\sum_k \frac{1}{|\xi_k|}\,\tanh\frac{\beta|\xi_k|}{2} = g\nu_0 \int_0^{\hbar\omega_D} d\xi\,\frac{\tanh\frac{\beta\xi}{2}}{\xi} = g\nu_0 \int_0^{\beta\hbar\omega_D/2} dx\frac{\tanh x}{x} \tag{235}$$

Assuming $y \equiv \hbar\omega_D/(2k_{\rm B}T_c) \gg 1$ we can roughly estimate

$$\int_0^y dx\frac{\tanh x}{x} \approx \int_{1/2}^y \frac{dx}{x} = \ln[2y]\ . \tag{236}$$

This gives

$$1 \approx g\nu_0 \ln\frac{\hbar\omega_D}{k_{\rm B}T_c} \tag{237}$$

or

$$k_{\rm B}T_c = \hbar\omega_D e^{-\frac{1}{g\nu_0}} = \frac{\Delta(T=0)}{2} \tag{238}$$

More precise calculation gives

$$k_{\rm B}T_c = 1.14\hbar\omega_D e^{-\frac{1}{g\nu_0}} = \frac{\Delta(T=0)}{1.76} \tag{239}$$

For $T \sim T_c$ and $T < T_c$ one can obtain

$$\Delta(T) \approx 3.06 k_{\rm B}T_c\sqrt{1-\frac{T}{T_c}} \tag{240}$$

1. *More precise derivation*

We have to minimize the grand canonical potential $\Omega = U - \mu N - TS = \langle H_{BCS}\rangle - TS$. For the density matrix we take (the variational ansatz)

$$\rho = \frac{1}{Z}\,e^{-\beta\sum_{k,\sigma}E_k n_{k,\sigma}}\ , \tag{241}$$

where $n_{k,\sigma} = \alpha^\dagger_{k,\sigma}\alpha_{k,\sigma}$ are the occupation number operators of the quasi-particles while E_k are the energies of the quasiparticles (to be determined). Here

$$\alpha_{k,\sigma} = u_k c_{k,\sigma} - \sigma v_k c^\dagger_{-k,-\sigma} \tag{242}$$

with $v_k = \sin\phi_k$ and $u_k = \cos\phi_k$ and ϕ_k is another variational parameter.

We thus obtain

$$\begin{aligned}\langle H_{BCS}^{MF}\rangle &= \sum_{k,\sigma}\xi_k\langle c^\dagger_{k,\sigma}\,c_{k,\sigma}\rangle - \frac{g}{V}\sum_{k,k'}\langle c^\dagger_{k',\uparrow}\,c^\dagger_{-k',\downarrow}\rangle\,\langle c_{-k,\downarrow}\,c_{k,\uparrow}\rangle \\ &= \sum_k 2\xi_k\left[(u_k^2 - v_k^2)f(E_k) + v_k^2\right] - \frac{g}{V}\left(\sum_k u_k v_k(1-2f(E_k))\right)^2 \end{aligned} \tag{243}$$

For the entropy we have

$$S = -2k_\mathrm{B}\sum_k\left[f(E_k)\,\ln f(E_k) + (1-f(E_k))\,\ln(1-f(E_k))\right] \tag{244}$$

We vary with respect to ϕ_k and with respect to E_k independently. This gives

$$\begin{aligned}\frac{\partial\Omega}{\partial\phi_k} &= 4\xi_k u_k v_k(1-2f(E_k)) \\ &- \frac{2g}{V}\left(\sum_k u_k v_k(1-2f(E_k))\right)(1-2f(E_k))\,(u_k^2 - v_k^2) = 0 \end{aligned} \tag{245}$$

Introducing

$$\Delta = \frac{g}{V}\sum_k\langle c_{-k,\downarrow}c_{k,\uparrow}\rangle = \frac{g}{V}\sum_k u_k v_k(1-2n_k) \tag{246}$$

we obtain the old equation

$$\xi_k\sin 2\phi_k = \Delta\cos 2\phi_k \tag{247}$$

Thus all the formula remain but with new Δ.

$$\begin{aligned}\frac{\partial\Omega}{\partial E_k} &= \frac{\partial\langle H_{BCS}^{MF}\rangle}{\partial E_k} - T\frac{\partial S}{\partial E_k} \\ &= 2\xi_k(u_k^2 - v_k^2)\frac{\partial f}{\partial E_k} + 4\Delta u_k v_k\frac{\partial f}{\partial E_k} - T\frac{\partial S}{\partial E_k} \\ &= 2\sqrt{\xi_k^2 + \Delta^2}\,\frac{\partial f}{\partial E_k} - 2E_k\,\frac{\partial f}{\partial E_k} = 0. \end{aligned} \tag{248}$$

Thus we obtain

$$E_k = \sqrt{\xi_k^2 + \Delta^2} \tag{249}$$

F. Heat capacity

$$C_V = T\left(\frac{\partial S}{\partial T}\right)_V . \tag{250}$$

Using for S Eq. (244) we obtain

$$C_V = -2k_\mathrm{B}T\sum_k(-\beta E_k)\frac{\partial f}{\partial T} = 2\sum_k E_k\,\frac{\partial f}{\partial T} \tag{251}$$

Let's introduce $g(x) = \frac{1}{e^x+1}$. Then $f(E_k) = g(\beta E_k)$.

$$\frac{\partial f}{\partial E_k} = \beta g' \tag{252}$$

$$\frac{\partial f}{\partial T} = g'\cdot\left(E_k\frac{\partial\beta}{\partial T} + \beta\frac{\partial E_k}{\partial T}\right) = g'\cdot\left(-E_k\frac{\beta}{T} + \beta\frac{\partial E_k}{\partial T}\right) = \frac{\partial f}{\partial E_k}\left(-\frac{E_k}{T} + \frac{\Delta}{E_k}\frac{\partial\Delta}{\partial T}\right) \tag{253}$$

Thus

$$C_V = 2\sum_k E_k\left(-\frac{E_k}{T} + \frac{\Delta}{E_k}\frac{\partial\Delta}{\partial T}\right)\frac{\partial f}{\partial E_k} \tag{254}$$

First, we analyze at $T \to T_c$. There $E_k \approx \xi_k$.

With

$$\frac{\partial f}{\partial E} \approx -\delta(E) - \frac{\pi^2}{6}\,(k_\mathrm{B}T)^2\delta''(E)\ , \tag{255}$$

and

$$\Delta(T) \approx 3.06k_\mathrm{B}T_c\sqrt{1-\frac{T}{T_c}} \tag{256}$$

We obtain for $T = T_c - 0$

$$\begin{aligned} C_V(T_c-0) &= 2\nu_0\int d\xi\left(-\frac{\xi^2}{T}\right)\frac{\partial f}{\partial\xi} + \nu_0\int d\xi\frac{\partial\Delta^2}{\partial T}\frac{\partial f}{\partial\xi} \\ &= \frac{2\pi^2\nu_0k_\mathrm{B}^2}{3}T_c + (3.06)^2\nu_0k_\mathrm{B}^2T_c = C_V(T_c+0) + \Delta C_V \end{aligned} \tag{257}$$

Thus one obtains

$$\frac{\Delta C_V}{C_V(T_c+0)} \approx 1.43 \tag{258}$$

Jump in $\frac{\partial\Delta}{\partial T}$ leads to jump in C_V (see Fig. 3).

For $k_\mathrm{B}T \ll k_\mathrm{B}T_c \sim \Delta(0)$ one obtains $C_V \propto e^{-\frac{\Delta}{k_\mathrm{B}T}}$.

G. Microscopic derivation of London equation

We consider the BSC ground state (with real Δ) and add a small vector potential to the kinetic energy. In the first quantisation

$$H_{kin} = \frac{\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2}{2m} \tag{259}$$

with $\vec{p} = -i\hbar\vec{\nabla}$. It is more convenient to start the derivation in the coordinate representation. We define the field

$$\Psi_\sigma(r) = \frac{1}{\sqrt{V}} \sum_k c_{k,\sigma} e^{ikr} \ . \tag{260}$$

This gives in the second quantised form

$$H_{kin} = \sum_\sigma \int dV \, \Psi^\dagger_\sigma(r) \frac{\left(-i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}\right)^2}{2m} \Psi_\sigma(r) = H_{0,kin} + H_1 + O(A^2) \ , \tag{261}$$

where

$$\begin{aligned} H_1 &= \frac{e}{2mc} \sum_\sigma \int dV \, \Psi^\dagger_\sigma(r) \, \left(\vec{A}\vec{p} + \vec{p}\vec{A}\right) \, \Psi_\sigma(r) & (262) \\ &= \frac{e}{mc} \sum_\sigma \int dV \, \Psi^\dagger_\sigma(r) \, \left(\vec{A}\vec{p}\right) \, \Psi_\sigma(r) & (263) \end{aligned}$$

(the order of operators $\vec{A}$ and $\vec{p}$ unimportant since $\vec{\nabla} \cdot \vec{A} = 0$).

Current. The current density is defined as follows

$$\vec{j}(\vec{r}) = -c \, \frac{\delta H_{kin}}{\delta \vec{A}(\vec{r})} \ . \tag{264}$$

One obtains

$$\begin{aligned} -c\delta H_{kin} = \ & -e \sum_\sigma \int dV \, \Psi^\dagger_\sigma(r) \frac{\left(-i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}\right) \delta\vec{A}(r)}{2m} \Psi_\sigma(r) \\ & -e \sum_\sigma \int dV \, \Psi^\dagger_\sigma(r) \frac{\delta\vec{A}(r) \left(-i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}\right)}{2m} \Psi_\sigma(r) \ . \end{aligned} \tag{265}$$

We obtain $\vec{j} = \vec{j}_p + \vec{j}_d$, where

$$\vec{j}_p \equiv \frac{ie\hbar}{2m} \sum_\sigma \left(\Psi^\dagger_\sigma(r) \left[\vec{\nabla}\Psi_\sigma(r)\right] - \left[\vec{\nabla}\Psi^\dagger_\sigma(r)\right] \Psi_\sigma(r) \right) \tag{266}$$

is usually called the paramagnetic contribution, whereas

$$\vec{j}_d(r) \equiv -\frac{e^2}{cm} \vec{A}(r) \sum_\sigma \Psi^\dagger_\sigma(r) \Psi_\sigma(r) \tag{267}$$

is usually called the diamagnetic contribution. Note that the $\vec{j}_d$ contribution immediately gives the London equation:

$$\vec{j}_d = -\frac{e^2 n}{mc} \vec{A} \tag{268}$$

with the full electron density n.

Another contribution linear in $\vec{A}$ could come from $\vec{j}_p$. In order to calculate $\vec{j}_p$ we have to look closer at the effect of the perturbation H_1. We assume the vector potential is a plane wave with a transversal polarization

$$\vec{A} = \vec{a}_q e^{i\vec{q}\vec{r}} \tag{269}$$

and $\vec{q}\cdot\vec{a}_q = 0$ (this corresponds to $\vec{\nabla}\vec{A} = 0$). Since we study the linear response, the response to a general $\vec{A} = \sum_q \vec{a}_q e^{i\vec{q}\vec{r}}$ can be calculated as a superposition. Using $\Psi_\sigma = \frac{1}{\sqrt{V}} \sum_k c_{k,\sigma} e^{ikr}$ and the symmetrised form (262) we obtain

$$H_1 = \frac{\hbar e}{2mc} \sum_{k,\sigma} c^\dagger_{k+q,\sigma} c_{k,\sigma} ((2\vec{k} + \vec{q})\vec{a}_q) = \frac{\hbar e}{mc} \sum_{k,\sigma} c^\dagger_{k+q,\sigma} c_{k,\sigma} (\vec{k}\vec{a}_q) \ . \tag{270}$$

It is necessary to express H_1 via the creation and annihilation operators of the quasiparticles. We use the Bogoliubov relations

$$c_{k,\sigma} = u_k \alpha_{k,\sigma} + \sigma v_k \alpha^\dagger_{-k,-\sigma} \quad , \quad c^\dagger_{k,\sigma} = u_k \alpha^\dagger_{k,\sigma} + \sigma v_k \alpha_{-k,-\sigma} \tag{271}$$

Then

$$H_1 = \frac{\hbar e}{mc} \sum_{k,\sigma} (u_{k+q} \alpha^\dagger_{k+q,\sigma} + \sigma v_{k+q} \alpha_{-k-q,-\sigma})(u_k \alpha_{k,\sigma} + \sigma v_k \alpha^\dagger_{-k,-\sigma})(\vec{k}\vec{a}_q) \ . \tag{272}$$

We divide H_1 to two parts:

$$\begin{aligned} H_1^a &= \frac{\hbar e}{mc} \sum_{k,\sigma} \left(u_{k+q} u_k \alpha^\dagger_{k+q,\sigma} \alpha_{k,\sigma} + v_{k+q} v_k \alpha_{-k-q,-\sigma} \alpha^\dagger_{-k,-\sigma} \right) (\vec{k}\vec{a}_q) \ , \\ &= \frac{\hbar e}{mc} \sum_{k,\sigma} \left(u_{k+q} u_k \alpha^\dagger_{k+q,\sigma} \alpha_{k,\sigma} - v_{k-q} v_k \alpha_{k-q,\sigma} \alpha^\dagger_{k,\sigma} \right) (\vec{k}\vec{a}_q) \ , \\ &= \frac{\hbar e}{mc} \sum_{k,\sigma} \left(u_{k+q} u_k \alpha^\dagger_{k+q,\sigma} \alpha_{k,\sigma} + v_{k-q} v_k \alpha^\dagger_{k,\sigma} \alpha_{k-q,\sigma} \right) (\vec{k}\vec{a}_q) \ , \end{aligned} \tag{273}$$

and

$$H_1^b = \frac{\hbar e}{mc} \sum_{k,\sigma} (\sigma u_{k+q} v_k \alpha^\dagger_{k+q,\sigma} \alpha^\dagger_{-k,-\sigma} + \sigma v_{k+q} u_k \alpha_{-k-q,-\sigma} \alpha_{k,\sigma})(\vec{k}\vec{a}_q) \ . \tag{274}$$

In what follows we will also need the current operator $\vec{j}_p$ expressed with the help of quasiparticle operators. We are interested in the Fourier component $\vec{q}$ of $\vec{j}_p$, i.e.,

$$\vec{j}_p(\vec{q}) = \int d^3r \, \vec{j}_p(\vec{r}) e^{-i\vec{q}\vec{r}} \ . \tag{275}$$

From (266) we get

$$\vec{j}_p(\vec{q}) = -\frac{e\hbar}{2m}\sum_{k,\sigma}(2\vec{k}+\vec{q})c^{\dagger}_{k,\sigma}c_{k+q,\sigma}\ . \tag{276}$$

We obtain

$$\vec{j}_p(\vec{q}) = -\frac{e\hbar}{2m}\sum_{k,\sigma}(2\vec{k}+\vec{q})\left(u_k\alpha^{\dagger}_{k,\sigma}+\sigma v_k\alpha_{-k,-\sigma}\right)\left(u_{k+q}\alpha_{k+q,\sigma}+\sigma v_{k+q}\alpha^{\dagger}_{-k-q,-\sigma}\right)\ . \tag{277}$$

Only H_1^b can generate corrections to the BCS ground state $|0\rangle = |BCS\rangle$. The first order correction reads

$$|\Phi_1\rangle = \sum_{l\neq 0}|l\rangle\frac{\langle l|\,H_1^b\,|0\rangle}{E_0-E_l} \tag{278}$$

The linear in $\vec{A}$ contribution to $\vec{j}_p$ then reads

$$\langle\vec{j}_p\rangle = \langle\Phi_1|\,\vec{j}_p\,|0\rangle + \langle 0|\,\vec{j}_p\,|\Phi_1\rangle\ . \tag{279}$$

This gives

$$\langle\vec{j}_p\rangle = 2\mathrm{Re}\sum_{l\neq 0}\frac{\langle 0|\,\vec{j}_p\,|l\rangle\,\langle l|\,H_1^b\,|0\rangle}{E_0-E_l}\ . \tag{280}$$

To calculate $|\Phi_1\rangle$ we need the matrix elements $\langle l|\,H_1\,|0\rangle$, where $|l\rangle$ is an excited state. Let us consider an excited state with two quasiparticles, namely

$$|l\rangle = \alpha^{\dagger}_{k_1+q_1,\sigma_1}\alpha^{\dagger}_{-k_1,-\sigma_1}\,|0\rangle\ , \tag{281}$$

$$\langle l| = \langle 0|\,\alpha_{-k_1,-\sigma_1}\alpha_{k_1+q_1,\sigma_1}\ . \tag{282}$$

We obtain

$$\langle l|\,H_1^b\,|0\rangle = \frac{\hbar e}{mc}\sum_{k,\sigma}(\vec{k}\vec{a}_q)\sigma u_{k+q}v_k\,\langle 0|\,\alpha_{-k_1,-\sigma_1}\alpha_{k_1+q_1,\sigma_1}\alpha^{\dagger}_{k+q,\sigma}\alpha^{\dagger}_{-k,-\sigma}\,|0\rangle \tag{283}$$

We realize that the relevant terms are either those with $k = k_1$, $q = q_1$, $\sigma = \sigma_1$ or those with $-k = k_1 + q_1$, $q = q_1$, $\sigma = -\sigma_1$. Thus only states $|l\rangle$ with $q_1 = q$ are of relevance. For this particular $|l\rangle$ we, thus, obtain

$$\begin{aligned}\langle l|\,H_1^b\,|0\rangle &= \frac{\hbar e}{mc}\left((\vec{k}_1\vec{a}_q)\sigma_1 u_{k_1+q}v_{k_1} + ((-\vec{k}_1-\vec{q})\vec{a}_q)\sigma_1 u_{k_1}v_{k_1+q}\right)\\ &= \frac{\hbar e}{mc}\,(\vec{k}_1\vec{a}_q)\sigma_1\,\left(u_{k_1+q}v_{k_1} - u_{k_1}v_{k_1+q}\right)\end{aligned} \tag{284}$$

For $\vec{q}\to 0$ we see that the matrix element vanishes. Together with the fact that $|E_0-E_l| > 2\Delta$ this gives "rigidity" and

$$\langle\vec{j}_p\rangle = 0 \tag{285}$$

To calculate the current we need also $\langle 0|\, \vec{j}_p \,|l\rangle$. We obtain

$$\langle 0|\, \vec{j}_p(q) \,|l\rangle = -\frac{e\hbar}{2m} \sum_{k,\sigma} (2\vec{k}+\vec{q})\sigma v_k u_{k+q} \langle 0|\, \alpha_{-k,-\sigma}\alpha_{k+q,\sigma}\alpha^\dagger_{k_1+q,\sigma_1}\alpha^\dagger_{-k_1,-\sigma_1} \,|0\rangle \tag{286}$$

Again there are two options: 1) $k = k_1$, $\sigma = \sigma_1$ or 2) $-k = k_1 + q$, $\sigma = -\sigma_1$. We obtain

$$\langle 0|\, \vec{j}_p(q) \,|l\rangle = -\frac{e\hbar}{2m}(2\vec{k}_1 + \vec{q})\sigma_1(v_{k_1}u_{k_1+q} - v_{k_1+q}u_{k_1}) \ . \tag{287}$$

This gives

$$\begin{aligned} \langle \vec{j}_p(q)\rangle &= 2\mathrm{Re}\left[\frac{e^2\hbar^2}{2m^2c}\sum_{k,\sigma}\frac{(\vec{k}\vec{a}_q)(2\vec{k}+\vec{q})(v_k u_{k+q} - v_{k+q}u_k)^2}{E_k + E_{k+q}}\right] \\ &= \frac{e^2\hbar^2}{m^2c}\sum_{k,\sigma}\frac{(\vec{k}\vec{a}_q)(2\vec{k}+\vec{q})(v_k u_{k+q} - v_{k+q}u_k)^2}{E_k + E_{k+q}} \ . \end{aligned} \tag{288}$$

Substituting $\vec{k} = -\vec{k}' - \vec{q}$ and using the symmetry of E_k, v_k and u_k we obtain (after dropping the prime in $\vec{k}'$)

$$\langle \vec{j}_p(q)\rangle = \frac{e^2\hbar^2}{m^2c}\sum_{k,\sigma}\frac{(\vec{k}\vec{a}_q)(2\vec{k}-\vec{q})(v_k u_{k+q} - v_{k+q}u_k)^2}{E_k + E_{k+q}} \ . \tag{289}$$

Thus the term $\vec{q}$ from $2\vec{k}+\vec{q}$ drops and we obtain

$$\langle \vec{j}_p(q)\rangle = \frac{2e^2\hbar^2}{m^2c}\sum_{k,\sigma}\frac{\vec{k}(\vec{k}\vec{a}_q)(v_k u_{k+q} - v_{k+q}u_k)^2}{E_k + E_{k+q}} \ . \tag{290}$$

This can be in general written as

$$\langle j_{p,\alpha}(\vec{q})\rangle = -\sum_\beta Q^p_{\alpha,\beta}(\vec{q})A_\beta(\vec{q}) \ . \tag{291}$$

This contribution adds to the one due to the diamagnetic current. In general the relation between the current and the vector potential reads

$$\langle j_\alpha(\vec{q})\rangle = -\sum_\beta Q_{\alpha,\beta}(\vec{q})A_\beta(\vec{q}) \ . \tag{292}$$

Here $Q_{\alpha,\beta} = Q^d_{\alpha,\beta} + Q^p_{\alpha,\beta}$, where $Q^d_{\alpha,\beta} = \frac{e^2 n}{mc}\delta_{\alpha,\beta}$.

In coordinate representation this reads

$$j_\alpha(\vec{r}) = -\sum_\beta \int d^3r' Q_{\alpha,\beta}(\vec{r}-\vec{r}')A_\beta(\vec{r}') \ . \tag{293}$$

This is called Pippard relation.

H. Pippard vs. London, coherence length.

The matrix element (284) vanishes for $q \to 0$. Let us analyze it more precisely. We have

$$u_{k+q}v_k - u_k v_{k+q} = \sqrt{\frac{1}{2} + \frac{\xi_{k+q}}{2E_{k+q}}}\sqrt{\frac{1}{2} - \frac{\xi_k}{2E_k}} - \sqrt{\frac{1}{2} + \frac{\xi_k}{2E_k}}\sqrt{\frac{1}{2} - \frac{\xi_{k+q}}{2E_{k+q}}} \ . \tag{294}$$

For $\xi_k \ll E_k \sim \Delta$ we obtain

$$u_{k+q}v_k - u_k v_{k+q} \approx \frac{1}{2\Delta}\left(\xi_{k+q} - \xi_k\right) \approx \frac{\hbar v_F q}{2\Delta} \ . \tag{295}$$

This introduces the coherence length:

$$\xi \equiv \frac{\hbar v_F}{\Delta} \tag{296}$$

(one usually defines $\xi_0 = \frac{\hbar v_F}{\pi\Delta}$). Interpretation: ξ is the size of a Cooper pair.

We conclude that the kernel Q in (293) decays at the distance of order ξ. Indeed Q^d is local, whereas Q^p decays at ξ. Two limits: $\xi < \lambda_L$ - London limit, $\xi > \lambda_L$ - Pippard limit.

I. Superconducting density

At $T = 0$ we obtained

$$\vec{j} = -\frac{e^2 n}{mc}\vec{A} \tag{297}$$

Here n is the total electron density. Note that transition to pairs does not change the result. Namely the substitution $n \to n/2$, $m \to 2m$, and $e \to 2e$ leaves the result unchanged.

At $T > 0$ not all the electrons participate in the super current. One introduces the superconducting density $n_s(T)$ and the normal density $n_n(T)$, such that $n_s + n_n = n$. Thus

$$\vec{j}_s = -\frac{e^2 n_s}{mc}\vec{A} \tag{298}$$

Calculations show that near the critical temperature, i.e., for $T_c - T \ll T_c$

$$\frac{n_s}{n} \approx 2\left(1 - \frac{T}{T_c}\right) \tag{299}$$

The new penetration depth is defined as

$$\lambda_L(T) = \sqrt{\frac{c^2 m}{4\pi n_s e^2}} \approx \frac{\lambda_L(T=0)}{\sqrt{2}}\left(1 - \frac{T}{T_c}\right)^{-1/2} \tag{300}$$

Proof. Here we concentrate on the part of the perturbation (272), which conserves the number of quasiparticles, namely H_1^a given by (273). In the limit $q \to 0$ and using $u_k^2 + v_k^2 = 1$ this reduces to

$$H_1^a \underset{q \to 0}{=} \frac{\hbar e}{mc} \sum_{k,\sigma} \alpha_{k,\sigma}^{\dagger} \alpha_{k,\sigma} (\vec{k}\vec{a}_q) \ . \tag{301}$$

This can be interpreted as a shift of the energy of the quasiparticles, namely $E_k \to E_k' = E_k + \frac{\hbar e}{mc}(\vec{k}\vec{a}_q)$. Also the paramagnetic current density (277) in the limit $q \to 0$ can be written as

$$\vec{j}_p(\vec{q} \to 0) = -\frac{e\hbar}{m} \sum_{k,\sigma} \vec{k} \alpha_{k,\sigma}^{\dagger} \alpha_{k,\sigma} \ . \tag{302}$$

The idea is now that due to the perturbation (301) the occupation numbers of the quasiparticles are changed. Namely

$$\langle \alpha_{k,\sigma}^{\dagger} \alpha_{k,\sigma} \rangle = f \left[E_k + \frac{\hbar e}{mc}(\vec{k}\vec{a}_q) \right] \ . \tag{303}$$

Here $f[\ldots]$ is the Fermi function. This gives rise to a finite paramagnetic current

$$\langle \vec{j}_p(\vec{q} \to 0) \rangle = -\frac{e\hbar}{m} \sum_{k,\sigma} \vec{k} f \left[E_k + \frac{\hbar e}{mc}(\vec{k}\vec{a}_q) \right] \ . \tag{304}$$

We expand in $\vec{a}_q$ and notice that the unperturbed result is zero. This gives

$$\langle \vec{j}_p(\vec{q} \to 0) \rangle = -\frac{e^2\hbar^2}{m^2 c} \sum_{k,\sigma} \vec{k}(\vec{k}\vec{a}_q) \, \frac{\partial f}{\partial E}|_{E_k} \ . \tag{305}$$

The derivative $\partial f / \partial E$ is non-zero only in the vicinity of the Fermi energy. Thus we can take $|\vec{k}| = k_F$. Introducing the angle θ_k such that $\vec{k}\vec{a} = |a| k_F \cos\theta_k$ and averaging over the 3D solid angles we obtain

$$\langle \vec{j}_p(\vec{q} \to 0) \rangle = -\vec{a}_q \, \frac{2e^2\hbar^2}{3m^2 c} k_F^2 \nu_0 \int d\xi \frac{\partial f}{\partial E} \ . \tag{306}$$

Using

$$\nu_0 = \frac{k_F m}{2\pi^2 \hbar^2} \quad , \quad n = \frac{k_F^3}{3\pi^2} \tag{307}$$

we obtain

$$\langle \vec{j}_p(\vec{q} \to 0) \rangle = -\vec{a}_q \, \frac{n e^2}{mc} \int d\xi \frac{\partial f}{\partial E} \ . \tag{308}$$

Combining with the contribution of the diamagnetic current we obtain

$$\langle \vec{j}(\vec{q} \to 0) \rangle = -\vec{a}_q \, \frac{n e^2}{mc} \left[1 + \int_{-\infty}^{\infty} d\xi \frac{\partial f}{\partial E} \right] = -\vec{a}_q \, \frac{n_s e^2}{mc} \ , \tag{309}$$

where the superconducting density is given by

$$n_s = n \left[1 + \int_{-\infty}^{\infty} d\xi \frac{\partial f}{\partial E} \right] \ . \tag{310}$$

We recall that $E = \sqrt{\Delta^2 + \xi^2}$. Thus

$$n_s = n \left[1 + 2 \int_{\Delta}^{\infty} dE \frac{E}{\sqrt{E^2 - \Delta^2}} \frac{\partial f}{\partial E} \right] \ . \tag{311}$$

For $T = 0$ this gives $n_s = n$.

For $T \ll T_c$ one obtains $n_s = n(1 - O(e^{-\Delta/T}))$

For $T \to T_c$ (Abrikosov)

$$\frac{n_s}{n} \approx 2 \left(1 - \frac{T}{T_c} \right) \tag{312}$$

J. Critical field

One applies external magnetic field H. It is known that the field is expelled from the superconductor (Meissner effect). That is inside the superconductor $B = 0$. When the field reaches the critical field H_c the superconductivity is destroyed and the field penetrates the metal.

Naive (but correct) argument: The total (free) energy of a cylindrical superconductor consists of the bulk free energy F_s and the energy of the induced currents screening the external magnetic field. We have $B = 0 = B_{\text{ext}} + B_{\text{induced}}$ (recall that $H = B_{\text{ext}}$). The energy of the induced currents is given by $B^2_{\text{induced}}/(8\pi)$. Thus the total energy of a superconductor reads $F_s + H^2/(8\pi)$. For $H = H_c$ the free energy of a superconductor and of a normal metal should be equal

$$F_s + \frac{H_c^2}{8\pi} = F_n \ . \tag{313}$$

The less naive thermodynamic argument involves the free enthalpy $G = F - HB/(4\pi)$ (see the book by Abrikosov).

At zero temperature ($F = U - TS$) we have

$$F_n - F_s = \frac{\nu_0 \Delta^2}{2} \tag{314}$$

Thus we find

$$H_c(T = 0) = 2\sqrt{\pi \nu_0} \Delta(T = 0) \tag{315}$$

In particular also for H_c we have the isotope effect, $H_c \propto M^{-1/2}$.

For $T \to T_c - 0$ one obtains (no proof)

$$H_c(T) = 1.735 H_c(0)\left(1 - \frac{T}{T_c}\right) \tag{316}$$

K. Order parameter, phase

Thus far Δ was real. We could however introduce a different BCS groundstate:

$$|BCS(\phi)\rangle = \prod_k (u_k + e^{i\phi} v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}) |0\rangle \ . \tag{317}$$

Exercise: check that

$$|BCS(N)\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi} \, |BCS(\phi)\rangle \, e^{-iN\phi} \tag{318}$$

gives a state with a fixed number of electrons N.

We obtain for Δ

$$\Delta = \frac{g}{V} \sum_k \langle c_{-k,\downarrow} c_{k,\uparrow} \rangle = \frac{g}{V} \sum_k u_k v_k e^{i\phi} = |\Delta| e^{i\phi} \tag{319}$$

This can be understood as follows. The BCS Hamiltonian (174) is invariant under the transformation

$$\begin{aligned} c_{k,\sigma} &\to \tilde{c}_{k,\sigma} = e^{-i\phi/2} c_{k,\sigma} \ , \\ c^\dagger_{k,\sigma} &\to \tilde{c}^\dagger_{k,\sigma} = e^{i\phi/2} c_{k,\sigma} \ . \end{aligned} \tag{320}$$

Under this transformation also the BCS ground state gets transformed:

$$|BCS\rangle \to |BCS\rangle' = \prod_k (u_k + v_k \tilde{c}^\dagger_{k,\uparrow} \tilde{c}^\dagger_{-k,\downarrow}) |0\rangle = \prod_k (u_k + e^{i\phi} v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}) |0\rangle \ . \tag{321}$$

A general gauge transformation reads:

$$\vec{A} \to \vec{A}' = \vec{A} + \vec{\nabla}\chi \tag{322}$$

$$\Psi \to \Psi' = \Psi e^{-\frac{ie}{\hbar c}\chi} \tag{323}$$

Comparing with (320) we see that (320) is the gauge transformation with a constant ($\vec{r}$-independent) phase. We, thus, identify

$$\frac{\phi}{2} = \frac{e}{\hbar c}\chi \tag{324}$$

Now we generalize to an $\vec{r}$-dependent phase $\phi(\vec{r})$. This dependence should be sufficiently slow. Then the gauge transformation reads

$$\vec{A} \to \vec{A}' = \vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi \ , \tag{325}$$

$$\Psi \to \Psi' = \Psi e^{-\phi/2} \ . \tag{326}$$

Assume in the $'$ frame the order parameter is real. Then for the current we obtain

$$\vec{j}_s = -\frac{e^2 n_s}{mc}\vec{A}' \tag{327}$$

In the original frame the London equation becomes

$$\vec{j}_s = -\frac{e^2 n_s}{mc}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right) \ . \tag{328}$$

It is a gauge invariant equation.

L. BCS state with N Cooper pairs

Above we have introduced (317,318) a BCS ground state with a phase ϕ:

$$|BCS(\phi)\rangle = \prod_k (u_k + e^{i\phi} v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow})\,|0\rangle \ . \tag{329}$$

We have argued that state

$$|BCS(N)\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi}\ |BCS(\phi)\rangle\, e^{-iN\phi} \tag{330}$$

gives a state with a fixed number of Cooper pairs N.

Here we try to see if the state $|BCS(N)\rangle$ corresponds to the same expectation value of the energy as the state $|BCS(\phi)\rangle$. First we discuss the normalization. Generalising Eqs. (176) we obtain

$$\begin{aligned}\langle\, BCS(\phi_2)|\, BCS(\phi_1)\rangle \ &= \ \langle 0|\prod_{k_2}(u_{k_2} + e^{-i\phi_2}\, v_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow}) \prod_{k_1}(u_{k_1} + e^{i\phi_1}\, v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow})\,|0\rangle \\ &= \ \prod_k (u_k^2 + e^{i(\phi_1-\phi_2)}\, v_k^2) \ . \end{aligned} \tag{331}$$

Thus,

$$\langle BCS(N)|\,BCS(N)\rangle = \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\, \langle BCS(\phi_2)|\,BCS(\phi_1)\rangle$$

$$= \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\, \prod_k (u_k^2 + e^{i(\phi_1-\phi_2)}\, v_k^2)$$

$$= \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\, e^{\sum_k \ln(u_k^2 + e^{i(\phi_1-\phi_2)}\, v_k^2)}$$

$$= \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\, e^{\sum_k \ln(1+\left[e^{i(\phi_1-\phi_2)}-1\right]\, v_k^2)}\ . \tag{332}$$

Assuming $N \gg 1$ we can use the stationary phase approximation and expand in $\phi_1 - \phi_2$. We obtain

$$\langle BCS(N)|\,BCS(N)\rangle = \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\, e^{\sum_k \left[i(\phi_1-\phi_2)v_k^2 - \frac{(\phi_1-\phi_2)^2}{2}(v_k^2 - v_k^4)\right]}\ . \tag{333}$$

We estimate $\sum_k v_k^2 \sim N(\mu)$, where $N(\mu)$ is (half) the number of electrons in a Fermi gas with chemical potential μ. Further,

$$A \equiv \sum_k (v_k^2 - v_k^4) = \sum_k \frac{1}{4}\, \frac{\Delta^2}{\Delta^2 + \xi_k^2} \approx \frac{\pi}{4} V\nu_0\Delta\ , \tag{334}$$

where ν_0 is the density of states (per spin direction) at the Fermi surface and V is the volume. In sufficiently large systems $V\nu_0\Delta \gg 1$. (Moreover, if the system is so small that $V\nu_0\Delta < 1$, the superconductivity becomes impossible.) This gives

$$\begin{aligned}\langle BCS(N)|\,BCS(N)\rangle &= \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-i(N-N(\mu))(\phi_1-\phi_2) - \frac{A(\phi_1-\phi_2)^2}{2}} \\ &\approx \frac{1}{\sqrt{2\pi A}} \exp\left[-\frac{(N-N(\mu))^2}{2A}\right]\end{aligned} \tag{335}$$

Thus, we see that if $|N - N(\mu)| \ll \sqrt{V\nu_0\Delta}$ the properly normalized state is

$$|BCS(N)\rangle_{\text{Norm}} = (2\pi A)^{1/4} \int_0^{2\pi} \frac{d\phi}{2\pi}\ |BCS(\phi)\rangle\, e^{-iN\phi} \tag{336}$$

Analogously to Eqs. (177,178,179) we obtain

$$
\begin{aligned}
&\langle BCS(\phi_2)|\, c^\dagger_{k,\uparrow}\, c_{k,\uparrow}\, |BCS(\phi_1)\rangle \\
&= \langle 0| \prod_{k_2} (u_{k_2} + e^{-i\phi_2}\, v_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow}) c^\dagger_{k,\uparrow}\, c_{k,\uparrow} \prod_{k_1} (u_{k_1} + e^{i\phi_1}\, v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow})\, |0\rangle \\
&= v_k^2 e^{i(\phi_1-\phi_2)} \prod_{q\neq k} (u_q^2 + e^{i(\phi_1-\phi_2)}\, v_q^2)
\end{aligned}
\tag{337}
$$

$$
\begin{aligned}
&\langle BCS(\phi_2)|\, c^\dagger_{k,\downarrow}\, c_{k,\downarrow}\, |BCS(\phi_1)\rangle \\
&= \langle 0| \prod_{k_2} (u_{k_2} + e^{-i\phi_2}\, v_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow}) c^\dagger_{k,\downarrow}\, c_{k,\downarrow} \prod_{k_1} (u_{k_1} + e^{i\phi_1}\, v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow})\, |0\rangle \\
&= v_{-k}^2 e^{i(\phi_1-\phi_2)} \prod_{q\neq -k} (u_q^2 + e^{i(\phi_1-\phi_2)}\, v_q^2)
\end{aligned}
\tag{338}
$$

$$
\begin{aligned}
&\langle BCS(\phi_2)|\; c^\dagger_{k',\uparrow}\, c^\dagger_{-k',\downarrow}\, c_{-k,\downarrow}\, c_{k,\uparrow}\, |BCS(\phi_1)\rangle \\
&= \langle 0| \prod_{k_2} (u_{k_2} + e^{-i\phi_2}\, v_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow})\; c^\dagger_{k',\uparrow}\, c^\dagger_{-k',\downarrow}\, c_{-k,\downarrow}\, c_{k,\uparrow} \prod_{k_1} (u_{k_1} + e^{i\phi_1}\, v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow})\, |0\rangle \\
&= u_k v_k u_{k'} v_{k'}\, e^{i(\phi_1-\phi_2)} \prod_{q\neq k, q\neq k'} (u_q^2 + e^{i(\phi_1-\phi_2)}\, v_q^2)
\end{aligned}
\tag{339}
$$

This gives (we introduce $\delta\phi \equiv \phi_1 - \phi_2$ for brevity)

$$
\begin{aligned}
\langle BCS(\phi_2)|\, H_{\mathrm{BCS}}\, |BCS(\phi_1)\rangle = e^{i\delta\phi} \Bigg\{ & 2 \sum_k (\epsilon_k - \mu) v_k^2 \prod_{q\neq k} (u_q^2 + e^{i\delta\phi}\, v_q^2) \\
& - \frac{g}{V} \sum_{k,k'} u_k v_k u_{k'} v_{k'} \prod_{q\neq k, q\neq k'} (u_q^2 + e^{i\delta\phi}\, v_q^2) \Bigg\}\ .
\end{aligned}
\tag{340}
$$

and

$$
\begin{aligned}
&\langle BCS(N)|\, H_{\mathrm{BCS}}\, |BCS(N)\rangle = \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-iN\delta\phi}\, \langle BCS(\phi_2)|\, H_{\mathrm{BCS}}\, |BCS(\phi_1)\rangle \\
&= \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-i(N-1)\delta\phi} \Bigg\{ 2 \sum_k (\epsilon_k - \mu) v_k^2 \prod_{q\neq k} (u_q^2 + e^{i\delta\phi}\, v_q^2) \\
&- \ \frac{g}{V} \sum_{k,k'} u_k v_k u_{k'} v_{k'} \prod_{q\neq k, q\neq k'} (u_q^2 + e^{i\delta\phi}\, v_q^2) \Bigg\}\ .
\end{aligned}
\tag{341}
$$

In a sufficiently large system we can approximate

$$
\prod_{q\neq k} (u_q^2 + e^{i\delta\phi}\, v_q^2) \approx \prod_q (u_q^2 + e^{i\delta\phi}\, v_q^2)\ ,
\tag{342}
$$

$$\prod_{q\neq k, q\neq k'} (u_q^2 + e^{i\delta\phi}\, v_q^2) \approx \prod_q (u_q^2 + e^{i\delta\phi}\, v_q^2) \ . \tag{343}$$

Thus we obtain

$$\langle BCS(N)|\, H_{\rm BCS}\, |BCS(N)\rangle = \left\{ 2\sum_k (\epsilon_k - \mu) v_k^2 - \frac{g}{V}\sum_{k,k'} u_k v_k u_{k'} v_{k'} \right\}$$
$$\int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-i(N-1)\delta\phi}\, \prod_q (u_q^2 + e^{i\delta\phi}\, v_q^2) \ . \tag{344}$$

The double integral is the same as in (332) (up to an immaterial $N \to N-1$). Thus we observe that if $|N - N(\mu)| \ll \sqrt{V\nu_0\Delta}$

$$\langle BCS(N)|\, H_{\rm BCS}\, |BCS(N)\rangle = \left\{ 2\sum_k (\epsilon_k - \mu) v_k^2 - \frac{g}{V}\sum_{k,k'} u_k v_k u_{k'} v_{k'} \right\} \frac{1}{\sqrt{2\pi A}} \ . \tag{345}$$

Changing to $|BCS(N)\rangle_{\rm Norm}$ we obtain the expectation value equal to $\langle BCS(\phi)|\, H_{\rm BCS}\, |BCS(\phi)\rangle$. In conclusion, the projection of the BCS wave function on a state with a fixed number of particles works well if this number is sufficiently close to the one dictated by the chemical potential.

VIII. TUNNEL JUNCTION

Consider a tunnel junction. The Hamiltonian reads $H = H_L + H_R + H_T$, where

$$H_T = \sum_{k,p} t_{k,p} c_k^\dagger d_p + h.c. \ . \tag{346}$$

We use the Golden Rule to calculate the rate of tunnelling from left to right and vice versa:

$$\begin{aligned} \Gamma_{L\to R} &= \frac{2\pi}{\hbar}\sum_{k,p} |t|^2 f_L(\epsilon_k)(1 - f_R(\epsilon_p))\delta(\epsilon_k - \epsilon_p) \\ &= \frac{2\pi}{\hbar}|t|^2 \int d\epsilon\, \rho_L(\epsilon)\rho_R(\epsilon) f_L(\epsilon)(1 - f_R(\epsilon)) \\ &= \frac{2\pi}{\hbar}|t|^2 \int d\epsilon\, \rho_L(\epsilon)\rho_R(\epsilon) f(\epsilon - \mu_L)(1 - f(\epsilon - \mu_R)) \\ &= \frac{2\pi}{\hbar}|t|^2 \rho_L\rho_R\, \frac{\Delta\mu}{1 - e^{-\beta\Delta\mu}} \ , \end{aligned} \tag{347}$$

where $\Delta\mu \equiv \mu_L - \mu_R$. For simplicity we assume the absolute value of the tunnelling amplitudes to be constant, i.e., $|t_{k,p}| \equiv |t|$. We observe that the tunnelling rate is not vanishing if $\Delta\mu = 0$ and even if $\Delta\mu < 0$, if the temperature is finite $T > 0$. This is the reason for the thermal noise. Identifying the voltage as $\Delta\mu = -eV$ we obtain the current

$$I = -e(\Gamma_{L\to R} - \Gamma_{R\to L}) = V\frac{e^2}{h}\,(2\pi)^2|t|^2\rho_L\rho_R\ . \tag{348}$$

Thus we obtain the Ohm's law $I = G_T V$, where the tunnelling conductance $G_T = 1/R_T$ is given by $G_T = g_T G_K$, where

$$g_T \equiv (2\pi)^2|t|^2\rho_L\rho_R \tag{349}$$

is the dimensionless tunnelling conductance and $G_K = 1/R_K = e^2/h = e^2/(2\pi\hbar)$ is the conductance quantum.

For electrons with spin we effectively have 2 parallel channels, since

$$H_T = \sum_{k,p,\sigma} t_{k,p} c^\dagger_{k,\sigma} d_{p,\sigma} + h.c.\ . \tag{350}$$

Thus we obtain $g_T = 2 \times (2\pi)^2|t|^2\rho_L\rho_R$, where $\rho_{L/R}$ are the orbital densities of states.

A. Josephson effect

We consider now a tunnel junction between two superconductors with different phases ϕ_L and ϕ_R. The Hamiltonian reads

$$H = H_{BCS,L} + H_{BCS,R} + H_T\ , \tag{351}$$

where the tunnelling Hamiltonian reads

$$H_T = \sum_{k_1,k_2,\sigma} T\left[R^\dagger_{k_1,\sigma} L_{k_2,\sigma} + L^\dagger_{k_2,\sigma} R_{k_1,\sigma}\right]\ . \tag{352}$$

Here $R_{k,\sigma} \equiv c^{(R)}_{k,\sigma}$ is the annihilation operator of an electron in the right superconductor. Two important things: 1) microscopically the electrons and not the quasiparticles tunnel; 2) tunnelling conserves spin.

A gauge transformation $L_{k,\sigma} \to e^{i\phi_L/2} L_{k,\sigma}$ and $R_{k,\sigma} \to e^{i\phi_R/2} R_{k,\sigma}$ "removes" the phases from the respective BCS wave functions (making v_k, u_k, and Δ real) and renders the tunneling Hamiltonian

$$H_T = \sum_{k_1,k_2,\sigma} T\left[R^\dagger_{k_1,\sigma} L_{k_2,\sigma} e^{-i\phi/2} + L^\dagger_{k_2,\sigma} R_{k_1,\sigma} e^{i\phi/2}\right]\ , \tag{353}$$

where $\phi \equiv \phi_R - \phi_L$. This choice of sign corresponds to a gradient of phase in the bulk of the superconductor.

Josephson [2] used (353) and calculated the tunneling current. We do so here for a time-independent phase difference ϕ. The current operator is given by time derivative of the number of particles in the right lead $N_R = \sum_{k,\sigma} R^\dagger_{k,\sigma} R_{k,\sigma}$

$$I = -e\dot{N}_R = -\frac{ie}{\hbar}[H_T, N_R] = \frac{ie}{\hbar}\sum_{k_1,k_2,\sigma} T\left[R^\dagger_{k_1,\sigma} L_{k_2,\sigma} e^{-i\phi/2} - L^\dagger_{k_2,\sigma} R_{k_1,\sigma} e^{i\phi/2}\right] . \tag{354}$$

The first order time-dependent perturbation theory gives for the density matrix of the system in the interaction representation

$$\rho(t) = T e^{-i\int_{-\infty}^{t} dt' H_T(t')} \rho_0 \tilde{T} e^{i\int_{-\infty}^{t} dt' H_T(t')} \approx -i\int_{-\infty}^{t} dt' [H_T(t'), \rho_0] . \tag{355}$$

For the expectation value of the current this gives

$$\begin{aligned}\langle I(t)\rangle &= \mathrm{Tr}\{\rho(t)I(t)\} = -i\int_{-\infty}^{t} dt'\, \mathrm{Tr}\left\{[H_T(t'), \rho_0]I(t)\right\} = -i\int_{-\infty}^{t} dt'\, \mathrm{Tr}\left\{[I(t), H_T(t')]\,\rho_0\right\} \\ &= -i\int_{-\infty}^{t} dt'\, \langle [I(t), H_T(t')]\rangle_0 .\end{aligned} \tag{356}$$

The proper way to perform this calculation is to introduce the "adiabatic switching" of the tunnelling Hamiltonian, i.e., $H_T(t') \to H_T(t')e^{\delta t'}$, where $\delta > 0$ and $\delta \to 0$. Equivalently $H_T(t') \to H_T(t')e^{-\delta(t-t')}$. This makes all the integrals converging.

In particular, at zero temperature $\langle \ldots \rangle_0$ corresponds to averaging over BCS states in both superconductors. We obtain

$$\begin{aligned}&[I(t), H_T(t')] = \frac{ie}{\hbar}T^2 \sum_{k_1,k_2,\sigma,q_1,q_2,\gamma} \\ &\left[\left(R^\dagger_{k_1,\sigma}(t)L_{k_2,\sigma}(t)e^{-i\phi/2} - L^\dagger_{k_2,\sigma}(t)R_{k_1,\sigma}(t)e^{i\phi/2}\right), \left(R^\dagger_{q_1,\gamma}(t')L_{q_2,\gamma}(t')e^{-i\phi/2} + L^\dagger_{q_2,\gamma}(t')R_{q_1,\gamma}(t')e^{i\phi/2}\right)\right]\end{aligned} \tag{357}$$

To get Josephson current we collect only the terms in which the phase ϕ does not disappear. The other terms contribute only if ϕ is time-dependent. We, thus, are left with

$$\begin{aligned}&[I(t), H_T(t')] = \cdots + \frac{ie}{\hbar}T^2 \sum_{k_1,k_2,\sigma,q_1,q_2,\gamma} \\ &e^{-i\phi}\left[\left(R^\dagger_{k_1,\sigma}(t)L_{k_2,\sigma}(t)\right), \left(R^\dagger_{q_1,\gamma}(t')L_{q_2,\gamma}(t')\right)\right] - e^{i\phi}\left[\left(L^\dagger_{k_2,\sigma}(t)R_{k_1,\sigma}(t)\right), \left(L^\dagger_{q_2,\gamma}(t')R_{q_1,\gamma}(t')\right)\right] ,\end{aligned} \tag{358}$$

where ... stands for omitted terms.

Upon averaging we obtain

$$\langle [I(t), H_T(t')] \rangle_0 = \cdots - \frac{ie}{\hbar} T^2 \sum_{k_1,k_2,\sigma} [$$
$$e^{-i\phi} \left\{ \langle R^\dagger_{k_1,\sigma}(t) R^\dagger_{-k_1,-\sigma}(t') \rangle_0 \langle L_{k_2,\sigma}(t) L_{-k_2,-\sigma}(t') \rangle_0 - \langle R^\dagger_{k_1,\sigma}(t') R^\dagger_{-k_1,-\sigma}(t) \rangle_0 \langle L_{k_2,\sigma}(t') L_{-k_2,-\sigma}(t) \rangle_0 \right\}$$
$$-e^{i\phi} \left\{ \langle L^\dagger_{k_2,\sigma}(t) L^\dagger_{-k_2,-\sigma}(t') \rangle_0 \langle R_{k_1,\sigma}(t) R_{-k_1,-\sigma}(t') \rangle_0 - \langle L^\dagger_{k_2,\sigma}(t') L^\dagger_{-k_2,-\sigma}(t) \rangle_0 \langle R_{k_1,\sigma}(t') R_{-k_1,-\sigma}(t) \rangle_0 \right\}$$
$$] \ . \tag{359}$$

At zero temperature we use

$$\begin{aligned} &\langle c^\dagger_{k,\sigma}(t_1)\, c^\dagger_{-k,-\sigma}(t_2) \rangle_0 = \langle BCS|\, c^\dagger_{k,\sigma}(t_1)\, c^\dagger_{-k,-\sigma}(t_2)\, |BCS\rangle \\ &= \langle BCS| \left(u_k \alpha^\dagger_{k,\sigma}(t_1) + \sigma v_k \alpha_{-k,-\sigma}(t_1) \right) \left(u_k \alpha^\dagger_{-k,-\sigma}(t_2) - \sigma v_k \alpha_{k,\sigma}(t_2) \right) |BCS\rangle \\ &= \sigma v_k u_k e^{-iE_k(t_1-t_2)} \ , \end{aligned} \tag{360}$$

and

$$\begin{aligned} &\langle BCS|\, c_{k,\sigma}(t_1)\, c_{-k,-\sigma}(t_2)\, |BCS\rangle \\ &= \langle BCS| \left(u_k \alpha_{k,\sigma}(t_1) + \sigma v_k \alpha^\dagger_{-k,-\sigma}(t_1) \right) \left(u_k \alpha_{-k,-\sigma}(t_2) - \sigma v_k \alpha^\dagger_{k,\sigma}(t_2) \right) |BCS\rangle \\ &= -\sigma v_k u_k e^{-iE_k(t_1-t_2)} \ , \end{aligned} \tag{361}$$

After some algebra we obtain (from the anomalous correlators, the rest gives zero)

$$\begin{aligned} \langle I(t) \rangle = & \quad 2eT^2 e^{-i\phi} \int_{-\infty}^{t} dt' \sum_{k_1,k_2} v_{k_1} u_{k_1} v_{k_2} u_{k_2} \left[e^{-i(E_{k_1}+E_{k_2})(t-t')} - e^{i(E_{k_1}+E_{k_2})(t-t')} \right] e^{-\delta(t-t')} \\ & - \ 2eT^2 e^{i\phi} \int_{-\infty}^{t} dt' \sum_{k_1,k_2} v_{k_1} u_{k_1} v_{k_2} u_{k_2} \left[e^{-i(E_{k_1}+E_{k_2})(t-t')} - e^{i(E_{k_1}+E_{k_2})(t-t')} \right] e^{-\delta(t-t')} \\ & = \ -8eT^2 \sin(\phi) \sum_{k_1,k_2} \frac{v_{k_1} u_{k_1} v_{k_2} u_{k_2}}{E_{k_1} + E_{k_2}} = -2eT^2 \sin(\phi) \sum_{k_1,k_2} \frac{\Delta^2}{E_{k_1} E_{k_2} (E_{k_1} + E_{k_2})} \\ & = \ -2\pi^2 T^2 \nu^2 e \Delta \hbar^{-1} \sin(\phi) = -I_c \sin(\phi) \ , \end{aligned} \tag{362}$$

where the Josephson critical current is given by

$$I_c = \frac{g_T e \Delta}{4\hbar} = \frac{\pi \Delta}{2eR_T} \ , \tag{363}$$

where $g_T = 2 \times 4\pi^2 T^2 \nu^2$ is the dimensionless conductance of the tunnel junction (factor 2 accounts for spin), while the tunnel resistance is given by $R_T = \frac{h}{e^2} \frac{1}{g_T}$. This is the famous

Ambegaokar-Baratoff relation [3] (see also erratum [4]). At finite temperature the relation reads (no derivation is provided, see Ref. [4]):

$$I_c = \frac{\pi\Delta(T)}{2eR_T}\tanh\left(\frac{\beta\Delta(T)}{2}\right) \ , \tag{364}$$

where $\Delta(T)$ is the temperature dependent gap.

Thus we have obtained the first Josephson relation $I = -I_c \sin\phi = -I_c \sin(\phi_R - \phi_L)$. The minus sign here corresponds to the London equation in the bulk of a superconductor

$$\vec{j}_s = -\frac{c}{4\pi\lambda_L^2}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right) \ . \tag{365}$$

We have introduced the variable ϕ as the difference of two phases $\phi = \phi_R - \phi_L$. The gauge invariant definition reads

$$\phi = \phi_R - \phi_L + \frac{2e}{\hbar c}\int_L^R \vec{A}d\vec{l} \ . \tag{366}$$

As a shortest way to the second Josephson relation we assume that an electric field exists in the junction and that it is only due to the time-dependence of $\vec{A}$. Then we obtain

$$\dot{\phi} = \frac{2e}{\hbar c}\int_L^R \left[\frac{\partial}{\partial t}\vec{A}\right] d\vec{l} = -\frac{2e}{\hbar}\int_L^R \vec{E}d\vec{l} = -\frac{2e}{\hbar}V \ , \tag{367}$$

where V is the voltage (note that voltage is usually defined as $V = V_L - V_R$). An alternative way to derive this is to start with a difference of (time-dependent) electro-chemical potentials

$$H = H_L + H_R - eV_L(t)\sum_{k,\sigma} L^\dagger_{k,\sigma}L_{k,\sigma} - eV_R(t)\sum_{k,\sigma} R^\dagger_{k,\sigma}R_{k,\sigma} + H_T \ , \tag{368}$$

where $V_{L/R}$ are the applied electric potentials (in addition to the constant chemical potential μ, which is included in H_L and H_R). A time-dependent gauge ransformation with

$$U = e^{-\frac{ie}{\hbar}\hat{N}_L \int^t V_L(t')dt'}\, e^{-\frac{ie}{\hbar}\hat{N}_R \int^t V_R(t')dt'} \tag{369}$$

leads to the new Hamiltonian

$$\tilde{H} = i\dot{U}U^{-1} + UHU^{-1} \ . \tag{370}$$

the terms with V_L and V_R are cancelled and instead the electronic operators are replaced by, e.g,

$$L \to ULU^{-1} = Le^{i\phi_L/2} \ , \tag{371}$$

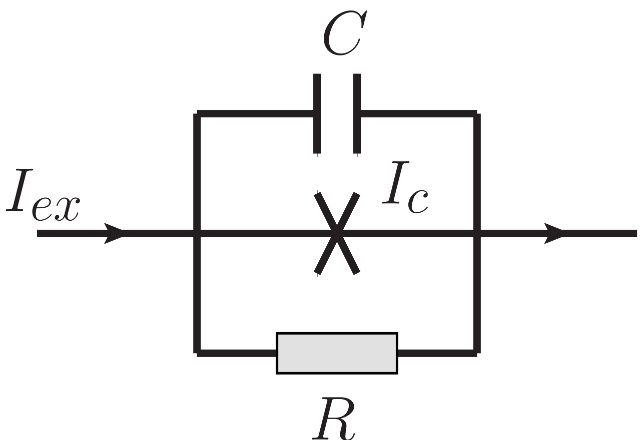

FIG. 14: RSJ Circuit.

where $\phi_L = const. + \frac{2e}{\hbar}\int^t V_L(t')dt'$ and, thus, $\dot\phi = \dot\phi_R - \dot\phi_L = \frac{2e}{\hbar}(V_R - V_L) = -\frac{2e}{\hbar}V$.

It is of course more convenient to abandon the logic of London relation and to define the phase drop on the Josephson contact as

$$\phi' \equiv \phi_L - \phi_R \ . \tag{372}$$

Then we get the usual Josephson relations

$$I = I_c \sin(\phi') \quad , \quad \dot\phi' = \frac{2e}{\hbar}V \ . \tag{373}$$

Later we will drop the prime.

IX. MACROSCOPIC QUANTUM PHENOMENA

1. *Resistively shunted Josephson junction (RSJ) circuit*

Consider a circuit of parallelly connected Josephson junction and a shunt resistor R. A Josephson junction is simultaneously a capacitor. An external current I_{ex} is applied. The Kirchhoff rules lead to the ecquation

$$I_c \sin\phi + \frac{V}{R} + \dot Q = I_{ex} \ . \tag{374}$$

As $Q = CV$ and $V = \frac{\hbar}{2e}\dot\phi$. Thus we obtain

$$I_c \sin\phi + \frac{\hbar}{2eR}\,\dot\phi + \frac{\hbar C}{2e}\,\ddot\phi = I_{ex} \ . \tag{375}$$

It is very convenient to measure the phase in units of magnetic flux, so that $V = \frac{1}{c}\dot{\Phi}$ (in SI units $V = \dot{\Phi}$):

$$\Phi = \frac{c\hbar}{2e}\,\phi = \frac{\Phi_0}{2\pi}\,\phi \quad , \quad \phi = 2\pi\frac{\Phi}{\Phi_0} \ . \tag{376}$$

Then the Kirchhoff equation reads

$$I_c \sin\left(2\pi\frac{\Phi}{\Phi_0}\right) + \frac{\dot{\Phi}}{cR} + \frac{C\ddot{\Phi}}{c} = I_{ex} \ , \tag{377}$$

or in SI units

$$I_c \sin\left(2\pi\frac{\Phi}{\Phi_0}\right) + \frac{\dot{\Phi}}{R} + C\ddot{\Phi} = I_{ex} \ . \tag{378}$$

There are two regimes. In case $I_{ex} < I_c$ there exists a stationary solution $\phi = \arcsin(I_{ex}/I_c)$. All the current flows through the Josephson contact as a super-current. Indeed $V \propto \dot{\phi} = 0$. At $I_{ex} > I_c$ at least part of the current must flow through the resistor. Thus a voltage develops and the phase starts to "run".

2. *Particle in a washboard potential*

The equation of motion (378) can be considered as an equation of motion of a particle with the coordinate $x = \Phi$. We must identify the capacitance with the mass, $m = C$, the inverse resistance with the friction coefficient $\gamma = R^{-1}$. Then we have

$$m\ddot{x} = -\gamma\dot{x} - \frac{\partial U}{\partial x} \ , \tag{379}$$

where for the potential we obtain

$$U(\Phi) = -E_J \cos\left(2\pi\frac{\Phi}{\Phi_0}\right) - I_{ex}\Phi \ , \tag{380}$$

where

$$E_J \equiv \frac{I_c\Phi_0}{2\pi} = \frac{\hbar I_c}{2e} \tag{381}$$

is called the Josephson energy. The potential energy $U(\Phi)$ has a form of a washboard and is called a washboard potential. In Fig. 15 the case $I_{ex} < I_c$ is shown. In this case the potential has minima and, thus, classically stationary solutions are possible.

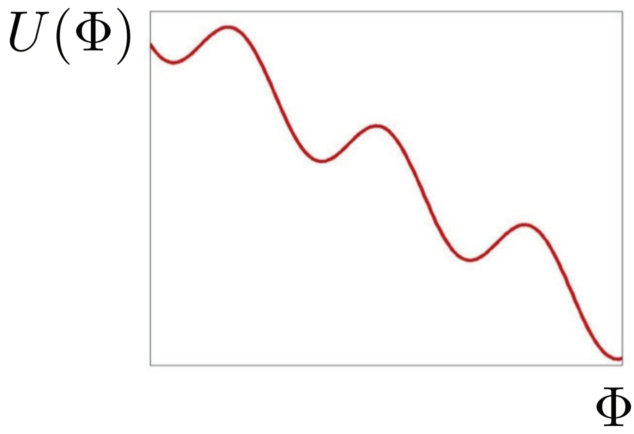

FIG. 15: Washboard potential.

3. *Over-damped case*

We rewrite (378) in terms of dimensionless phase $\phi = 2\pi\Phi/\Phi_0$:

$$\frac{C\hbar}{2e}\ddot{\phi} + \frac{\hbar}{2eR}\dot{\phi} + I_c \sin\phi = I_{ex} \ . \tag{382}$$

Assume we can neglect the first term in comparison with the second. This will be the case if the RC time is shorter than a characteristic time of the $\phi(t)$ time-evolution: over-damped case. We will determine the applicability domain of this approximation later. In the over-damped case the equation of motion reads

$$\frac{\hbar}{2eR}\dot{\phi} + I_c \sin\phi = I_{ex} \ . \tag{383}$$

For $I_{ex} < I_c$ the stationary solution reads $\dot{\phi} = 0$, $\sin\phi = I_{ex}/I_c$. We now try to find the stationary (running) solution for $I_{ex} > I_c$. This solution should have the form

$$\phi(t) = \frac{2\pi}{T}t + \delta\phi(t) \ , \tag{384}$$

such that $\delta\phi(t)$ is periodic: $\delta\phi(t+T) = \delta\phi(t)$. That is the "period" T is the time over which the phase changes by 2π. We rewrite (383) as

$$\frac{d\phi}{dt} = \frac{2eRI_{ex}}{\hbar}(1 - (I_c/I_{ex})\sin\phi) \ . \tag{385}$$

Further we use separation of variables

$$\frac{d\phi}{(1 - (I_c/I_{ex})\sin\phi)} = \frac{2eRI_{ex}}{\hbar}dt \ . \tag{386}$$

We integrate over one period T and use that fact that $\sin\phi$ is periodic. Further we use the integral

$$\int_0^{2\pi} d\phi \, \frac{1}{1 - a\sin\phi} = \frac{2\pi}{\sqrt{1-a^2}} \tag{387}$$

for $0 < a < 1$. Thus we find the period T:

$$\frac{2\pi}{\sqrt{1 - I_c^2/I_{ex}^2}} = \frac{2eRI_{ex}}{\hbar} T \ , \tag{388}$$

or

$$\frac{2\pi}{T} = \frac{2eR}{\hbar}\sqrt{I_{ex}^2 - I_c^2} \ . \tag{389}$$

This immediately gives the average voltage

$$\langle V \rangle = \left\langle \dot{\Phi} \right\rangle = \frac{\Phi_0}{2\pi}\left\langle \dot{\phi} \right\rangle = \frac{\Phi_0}{2\pi}\frac{2\pi}{T} = R\sqrt{I_{ex}^2 - I_c^2} \ . \tag{390}$$

It is also possible to find analytically the full time-dependent voltage $V(t)$ (see the book by Abrikosov). Clearly, $V(t)$ oscillates around $\langle V \rangle$ with period T.

Now we are also ready to formulate the condition for the over-damped dynamics. One possible criterium would be (Abrikosov) $RC \ll T/2\pi$, then we obtain

$$\frac{2\pi RC}{T} = \frac{2eR^2C}{\hbar}\sqrt{I_{ex}^2 - I_c^2} \ll 1 \ . \tag{391}$$

This seems to fail for $I_{ex} \to \infty$.

Alternatively (Tinkham), we can rewrite (382)

$$\frac{C\hbar}{2eI_c}\ddot{\phi} + \frac{\hbar}{2eRI_c}\dot{\phi} + \sin\phi = I_{ex}/I_c \ . \tag{392}$$

The coefficient in front of the first term has dimensions of $[t]^2$. This allows us to introduce the frequency

$$\omega_p^2 \equiv \frac{2eI_c}{C\hbar} = \frac{(2e)^2 E_J}{C\hbar^2} \ . \tag{393}$$

This is the plasma frequency of small oscillations in the case of no damping $R \to \infty$ and no bias current $I_{ex} = 0$. In what follows we will introduce the charging energy (for Cooper pairs) $E_C = (2e)^2/2C$. Then $\omega_p^2 = 2E_JE_C/\hbar^2$. We introduce now dimensionless time $\tau = \omega_p t$. Then the equation of motion reads

$$\frac{d^2\phi}{d\tau^2} + Q^{-1}\frac{d\phi}{d\tau} + \sin\phi = (I_{ex}/I_0) \ . \tag{394}$$

Here Q is the quality factor given by

$$Q = \frac{2eRI_c}{\hbar\omega_p} = \omega_p RC \ . \tag{395}$$

The condition for the over-damped dynamics reads $Q \ll 1$.

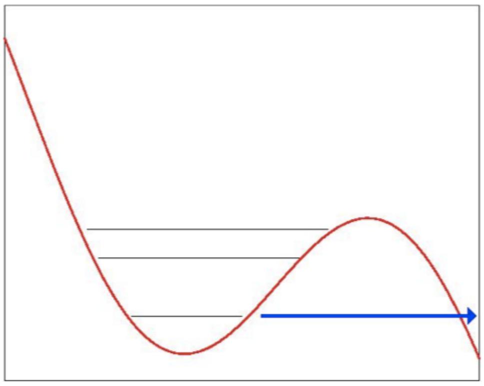

FIG. 16: Macroscopic Quantum Tunneling (MQT).

4. ac-Josephson effect, Shapiro steps

.....

5. MQT

When the external current is close to the critical value a situation shown in Fig. 16 emerges. If we allow ourselves to think of this situation quantum mechanically, then we would conclude that only a few quantum levels should remain in the potential well. Moreover a tunneling process out of the well should become possible. This tunneling process was named Macroscopic Quantum Tunneling because in the 80-s and the 90-s many researchers doubted the fact one can apply quantum mechanics to the dynamics of the "macroscopic" variable Φ. It was also argued that a macroscopic variable is necessarily coupled to a dissipative bath which would hinder the tunneling.

6. dc-SQUID

The simplest dc-SQUID (Superconducting QUantum Interference Device) is shown in Fig. 17. It consists of two Josephson junctions in a superconducting ring. The current bias is applied. The simplest case is when the superconducting parts of the ring are thick (thicker than the London penetration depth λ_L). Then along the dashed line in Fig. 17 the

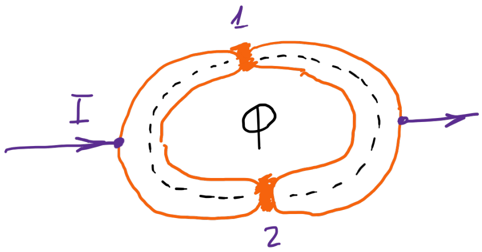

FIG. 17: dc-SQUID. The superconducting parts assumed thicker that λ_L. The dashed line is deep in the superconducting parts so that the superconducting velocity there vanishes. This is used for the discussion of the flux dependence.

superconducting velocity vanishes. That is

$$\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right) = 0 \tag{396}$$

along the dashed line (in the electrodes) but not in the junctions. Integrating along a closed contour we obtain for the total flux Φ:

$$\begin{aligned} \Phi &= \oint \vec{A}d\vec{l} = \int_{electrodes} \vec{A}d\vec{l} + \int_{junctions} \vec{A}d\vec{l} \\ &= -\frac{\Phi_0}{2\pi}\int_{electrodes} \vec{\nabla}\phi\, d\vec{l} + \int_{junctions} \vec{A}d\vec{l} \end{aligned} \tag{397}$$

The phase of the order parameter is single valued $(mod(2\pi))$. Therefore

$$\int_{electrodes} \vec{\nabla}\phi\, d\vec{l} + \Delta\phi_1 + \Delta\phi_2 = 0[mod(2\pi)]. \tag{398}$$

Here $\Delta\phi_1$ and $\Delta\phi_2$ are the phase drops counted according to the integration direction (later on the contour minus earlier on the contour). This gives

$$\frac{\Phi_0}{2\pi}\Delta\phi_1 + \int_{junction\ 1} \vec{A}d\vec{l} + \frac{\Phi_0}{2\pi}\Delta\phi_2 + \int_{junction\ 2} \vec{A}d\vec{l} = \Phi[mod(\Phi_0)]\ . \tag{399}$$

This can be written as

$$\phi_1 + \phi_2 = \frac{2\pi\Phi}{\Phi_0}\ , \tag{400}$$

where ϕ_1 and ϕ_2 are the gauge invariant phase drops on the junctions (counted in the direction of the contour). Here we use a clockwise contour in Fig. 17 and, thus, a positive magnetic flux "goes into the picture". Recalling the discussion on the signs of the phase drops at the end of Sec. VIII A we obtain for the current (from left to right)

$$I = -I_c \sin\phi_1 + I_c \sin\phi_2\ . \tag{401}$$

For simplicity we assume here that the two critical currents are equal.

Of course, we can now change the signs of ϕ_1 and ϕ_2 (as at the end of Sec.VIII A) and get the commonly used

$$I = I_c \sin\phi_1 - I_c \sin\phi_2 \ . \tag{402}$$

This gives

$$I = 2I_c \sin\frac{\phi_1 - \phi_2}{2} \cdot \cos\frac{\phi_1 + \phi_2}{2} = 2I_c \cos\frac{\pi\Phi}{\Phi_0} \cdot \sin\frac{\phi_1 - \phi_2}{2} \tag{403}$$

The combination $(\phi_1 - \phi_2)/2$ is the effective phase drop in the SQUID considered as an effective Josephson junction. The effective critical current is given by

$$I_c^{SQUID} = 2I_c \left|\cos\frac{\pi\Phi}{\Phi_0}\right| \ . \tag{404}$$

7. Quantization

We write down the Lagrangian that would give the equation of motion (379 or 378). Clearly we cannot include the dissipative part in the Lagrange formalism. Thus we start from the limit $R \to \infty$. The Lagrangian reads

$$L = \frac{C\dot{\Phi}^2}{2} - U(\Phi) = \frac{C\dot{\Phi}^2}{2} + E_J \cos\left(2\pi\frac{\Phi}{\Phi_0}\right) + I_{ex}\Phi \ . \tag{405}$$

We transform to the Hamiltonian formalism and introduce the canonical momentum

$$Q \equiv \frac{\partial L}{\partial\dot{\Phi}} = C\dot{\Phi} \ . \tag{406}$$

The Hamiltonian reads

$$H = \frac{Q^2}{2C} + U(\Phi) = \frac{Q^2}{2C} - E_J \cos\left(2\pi\frac{\Phi}{\Phi_0}\right) - I_{ex}\Phi \ . \tag{407}$$

The canonical momentum corresponds to the charge on the capacitor (junction). The usual commutation relations should be applied

$$[\Phi, Q] = i\hbar \ . \tag{408}$$

In the Hamilton formalism it is inconvenient to have an unbounded from below potential. Thus we try to transform the term $-I_{ex}\Phi$ away. This can be achieved by the following canonical transformation

$$R = \exp\left[-\frac{i}{\hbar}Q_{ex}(t)\Phi\right] \ , \tag{409}$$

where $Q_{ex}(t) \equiv \int^{t} I_{ex}(t')dt'$. Indeed the new Hamiltonian reads

$$\tilde{H} = RHR^{-1} + i\hbar\dot{R}R^{-1} = \frac{(Q - Q_{ex}(t))^2}{2C} - E_J \cos\left(2\pi\frac{\Phi}{\Phi_0}\right) \ . \tag{410}$$

The price we pay is that the new Hamiltonian is time-dependent. The Hamiltonian (410) is very interesting. Let us investigate the operator

$$\cos\left(2\pi\frac{\Phi}{\Phi_0}\right) = \cos\left(\frac{2e}{\hbar}\,\Phi\right) = \frac{1}{2}\,\exp\left[\frac{i}{\hbar}\,2e\,\Phi\right] + h.c. \tag{411}$$

We have

$$\exp\left[\frac{i}{\hbar}\,2e\,\Phi\right]\,|Q\rangle = |Q + 2e\rangle \quad , \quad \exp\left[-\frac{i}{\hbar}\,2e\,\Phi\right]\,|Q\rangle = |Q - 2e\rangle \ . \tag{412}$$

Thus in this Hamiltonian only the states differing by an integer number of Cooper pairs get connected. The constant offset charge remains undetermined. This, however, can be absorbed into the bias charge Q_{ex}. Thus, we can restrict ourselves to the Hilbert space $|Q = 2em\rangle$.

8. *Josephson energy dominated regime*

In this regime $E_J \gg E_C$, where $E_C = \frac{(2e)^2}{2C}$ is the Cooper pair charging energy. Let us first neglect E_C completely, i.e., put $C = \infty$. Recall that C plays the role of the mass. Then the Hamiltonian reads $H = -E_J \cos\left(2\pi\frac{\Phi}{\Phi_0}\right)$. On one hand it is clear that the relevant state are those with a given phase, i.e., $|\Phi\rangle$. On the other hand, in the discrete charge representation the Hamiltonian reads

$$H = -\frac{E_J}{2}\sum_m \left(|m+1\rangle\,\langle m| + |m\rangle\,\langle m+1|\right) \ . \tag{413}$$

The eigenstates of this tight-binding Hamiltonian are the Bloch waves $|k\rangle = \sum_m e^{ikm}\,|m\rangle$ with the wave vector k belonging to the first Brillouin zone $-\pi \le k \le \pi$. The eigenenergy reads $E_k = -E_J\cos(k)$. Thus we identify $k = \phi = \frac{2\pi\Phi}{\Phi_0}$.

9. *Charging energy dominated regime*

In this regime $E_J \ll E_C$. The main term in the Hamiltonian is the charging energy term

$$H_C = \frac{(Q - Q_{ex}(t))^2}{2C} = \frac{(2em - Q_{ex})^2}{2C} \ . \tag{414}$$

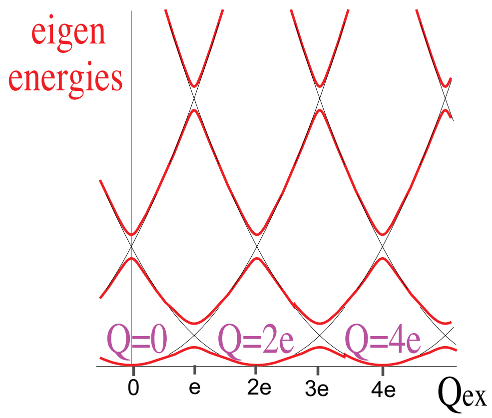

FIG. 18: Eigen levels in the coulomb blockade regime. Different parabolas correspond to different values of $Q = 2em$. The red lines represent the eigenlevels with the Josephson energy taken into account. The Josephson tunneling lifts the degeneracy between the charge states.

The eigenenergies corresponding to different values of m form parabolas as functions of Q_{ex} (see Fig. 18). The minima of the parabolas are at $Q_{ex} = 0, 2e, 4e, \ldots$. The Josephson tunneling term serves now as a perturbation $H_J = -E_J \cos\left(2\pi \frac{\Phi}{\Phi_0}\right)$. It lifts the degeneracies, e.g., at $Q_{ex} = e, 3e, 5e, \ldots$.

If a small enough external current is applied, $Q_{ex} = I_{ex}t$ the adiabatic theorem holds and the system remains in the ground state. Yet, one can see that between the degeneracies at $Q_{ex} = e, 3e, 5e, \ldots$ the capacitance is charged and discharged and oscillating voltage $V = \partial E_0 / \partial Q_{ex}$ appears. Here $E_0(Q_{ex})$ is the energy of the ground state. The Cooper pairs tunnel only at the degeneracy points. In between the Coulomb blockade prevents the Cooper pairs from tunneling because this would cost energy.

X. VARIOUS QUBITS

A. Charge qubit

We start by considering the so called Cooper pair box shown in Fig. 19. We derive the Hamiltonian starting from the Lagrangian

$$L = \frac{C_J \dot{\Phi}_J^2}{2} + \frac{C_g \dot{\Phi}_g^2}{2} - U_J(\Phi_J) \ , \tag{415}$$

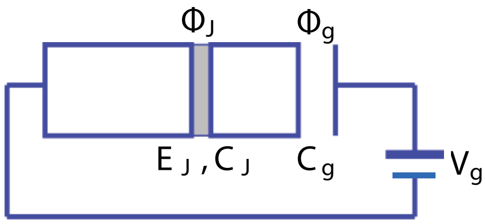

FIG. 19: Cooper Pair Box. The Josephson tunnel junction is characterized by the Josephson energy E_J and by the capacitance C_J. The superconducting island is controlled by the gate voltage V_g via the gate capacitance C_g. To derive the system's Lagrangian and Hamiltonian we introduce the phase drop on the Josephson junction Φ_J and the phase drop on the gate capacitor Φ_g.

where $U_J = -E_J \cos\left(2\pi \frac{\Phi_J}{\Phi_0}\right)$. The sum of all the phases along the loop must vanish and the phase on the voltage source is given by $const. + V_g t$. Thus we obtain

$$\dot{\Phi}_g = -\dot{\Phi}_J - V_g \tag{416}$$

and the Lagrangian in terms of the only generalized coordinate Φ_J reads

$$\begin{aligned} L &= \frac{C_J \dot{\Phi}_J^2}{2} + \frac{C_g(\dot{\Phi}_J + V_g)^2}{2} - U_J(\Phi_J) \\ &= \frac{(C_J + C_g)\dot{\Phi}_J^2}{2} + C_g \dot{\Phi}_J V_g - U_J(\Phi_J) + const. \ . \end{aligned} \tag{417}$$

The conjugated momentum (charge) reads

$$Q = \frac{\partial L}{\partial \dot{\Phi}_J} = (C_J + C_g)\dot{\Phi}_J + C_g V_g \ . \tag{418}$$

Since $C_J \dot{\Phi}_J$ is the charge on the Josephson junction capacitance while $C_g \dot{\Phi}_J + C_g V_g = -C_g \dot{\Phi}_g$ is minus the charge on the gate capacitance we conclude that $Q = 2em$ is the charge on the island (we disregard here the possibility to have an odd number of electrons on the island). We obtain

$$\dot{\Phi}_J = \frac{Q - C_g V_g}{C_J + C_g} \ . \tag{419}$$

The Hamiltonian reads

$$\begin{aligned} H = Q\,\dot{\Phi}_J - L &= \frac{(Q - C_g V_g)^2}{2(C_J + C_g)} + U_J(\Phi_J) \\ &= \frac{(Q - C_g V_g)^2}{2(C_J + C_g)} - E_J \cos\left(2\pi \frac{\Phi_J}{\Phi_0}\right) \ . \end{aligned} \tag{420}$$

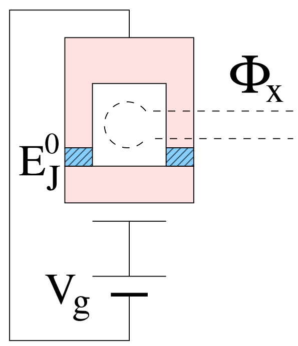

FIG. 20: Charge quit with controllable Josephson energy.

This is exactly the Hamiltonian (410) with $Q_{ex} = C_g V_g$. The two level system is formed by the two lowest levels around $C_g V_g = e + 2eN$.

In Hamiltonian (420) the interplay of two energy scales determines the physical regime. These are 1) Josephson energy E_J; 2) Charging energy $E_C \equiv \frac{(2e)^2}{2(C_J+C_g)}$. In the simplest regime $E_J \ll E_C$ and for $Q_{ex} \sim e$ one can restrict the Hilbert space to two charge states with lowest charging energies $|\uparrow\rangle = |Q = 0\rangle$ and $|\downarrow\rangle = |Q = 2e\rangle$. In this Hilbert space we have

$$\cos\left(2\pi \frac{\Phi_J}{\Phi_0}\right) = \frac{1}{2}\sigma_x \ , \tag{421}$$

and

$$Q = e(1 - \sigma_z) \ . \tag{422}$$

Substituting these to (420) and disregarding constant energy shifts we obtain

$$H = -\frac{1}{2}\left(1 - \frac{Q_{ex}}{e}\right) E_C\,\sigma_z - \frac{1}{2} E_J\,\sigma_x \ . \tag{423}$$

Thus we obtain an effective spin-1/2 in a magnetic field whose z-component can be controlled by the gate voltage.

In Fig. 20 a charge qubit is shown in which the Josephson junction was replaced by a dc-SQUID. A straightforward derivation (assuming the geometrical inductance of the SQUID loop being vanishingly small) gives again the Hamiltonian (420) with $C_J \to 2C_J$ (just because there are two junctions instead of one) and

$$E_J \to 2E_J^{(0)} \cos\left(\frac{\pi\Phi_x}{\Phi_0}\right) \ . \tag{424}$$

Here $E_J^{(0)}$ is the Josephson energy of a single junction. We assume the two junctions of the SQUID to be identical. Now we can control also the x-component of the effective magnetic field.

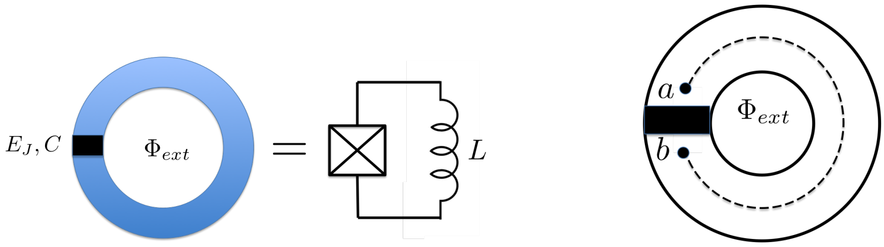

FIG. 21: RF-SQUID.

1. *Transmon*

A "Transmon" qubit is essentially a charge qubit shunted by a large capacitance in order to decrease the charging energy. The Hamiltonian can be written as

$$H = E_C(n - q_g)^2 - E_J \cos\phi \ , \tag{425}$$

where $q_g \equiv Q_g/2e = C_g V_g/2e$ is the dimensionless gate charge. The quantization is provided by the relation $e^{i\phi}|n\rangle = |n+1\rangle$. The system is controlled by the time-dependent $q_g(t)$. Due to the shunt capacitance one decreases the charging energy and reaches the regime $E_C < E_J$. In this case it is not sufficient to consider only two charge states.

B. Flux qubit

1. *RF-SQUID*

The simplest flux qubit is called RF-SQUID (Radio-Frequency-Superconducting-QUantum-Interference-Device) and is shown in Fig. 21 We recall the London equation $\vec{j}_s = -\frac{e^2 n_s}{mc}\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right)$ and the fact that the super-current density $\vec{j}_s$ vanishes in the bulk of the superconductor. Thus assuming the ring in thick and integrating along the line which is in the middle of the ring (see Fig. 21) we obtain (we integrate clockwise along the dashed line)

$$0 = \int_a^b \left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right) d\vec{l} = \int_a^b \vec{A}d\vec{l} + \frac{\hbar c}{2e}(\phi_b - \phi_a) \ , \tag{426}$$

$$\frac{\hbar c}{2e}(\phi_a - \phi_b) = \int_a^b \vec{A}d\vec{l} \ . \tag{427}$$

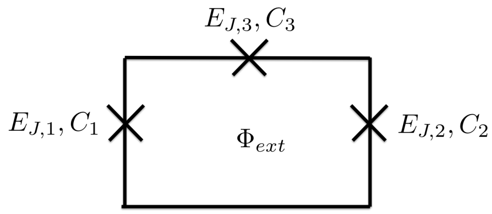

FIG. 22: 3-junction flux qubit. Proposed by J.E. Mooij et al.

$$\frac{\hbar c}{2e}(\phi_a - \phi_b) + \int_b^a \vec{A}d\vec{l} = \int_a^b \vec{A}d\vec{l} + \int_b^a \vec{A}d\vec{l} = \oint \vec{A}d\vec{l} = \Phi \ , \tag{428}$$

where Φ is the total flux through the ring. Thus the gauge invariant phase drop across the Josephson junction reads:

$$\Delta\phi = (\phi_a - \phi_b) + \frac{2e}{\hbar c}\int_b^a \vec{A}d\vec{l} = \frac{2e}{\hbar c}\Phi = 2\pi\frac{\Phi}{\Phi_0} \ . \tag{429}$$

As before it may be more convenient to change the sign of $\Delta\phi$: $\Delta\phi' = -\Delta\phi = 2\pi\frac{\Phi}{\Phi_0}$. The Josephson energy can be written then as $-E_J\cos(\Delta\phi') = -E_J\cos(2\pi\Phi/\Phi_0)$. For the inductive energy we observe that the flux created by the current in the ring is given by $\Phi - \Phi_{ext}$. Indeed Φ is the total flux (and the dynamical variable of our theory). Part of it is due to Φ_{ext}. The rest must be created by the current flowing in the ring. Thus the inductive energy reads $(\Phi - \Phi_{ext})^2/2L$. Finally the energy of the electric field reads $C\dot{\Phi}^2/2$. Thus, the Lagrangian of the system reads:

$$\mathcal{L} = \frac{C\dot{\Phi}^2}{2} - U(\Phi) \ , \tag{430}$$

where

$$U(\Phi) = \frac{(\Phi - \Phi_{ext})^2}{2L} - E_J\cos\left(\frac{2\pi\Phi}{\Phi_0}\right) \ . \tag{431}$$

At $\Phi_{ext} = \Phi_0/2$ we obtain a double-well potential if $I_c L > \Phi_0/2\pi$ (here $I_c = 2\pi E_J/\Phi_0$). One needs then a relatively large inductance. Purely geometric inductance can be achieved by increasing the size, which usually brings problems with noise.

C. 3-junction flux qubit

For a loop with three junction (a qubit proposed by J.E. Mooij, Fig 22) there are three gauge invariant phase drops across the three junctions (measured in units of flux), Φ_1, Φ_2,

Φ_3 and the argument similar to the provided for the RF-SQUIS gives (here we have already flipped the signs of the phase differences)

$$\Phi_1 + \Phi_2 + \Phi_3 = -\Phi \ , \tag{432}$$

where Φ is the total flux in the ring. Neglecting the geometric inductance of the ring we have $\Phi = \Phi_{ext}$. Thus we are left with two dynamical variables Φ_1 and Φ_2, whereas $\Phi_3 = -\Phi_{ext} - \Phi_1 - \Phi_2$. The Lagrangian reads

$$\mathcal{L} = K - U \ , \tag{433}$$

where

$$K = \frac{C_1 \dot{\Phi}_1^2}{2} + \frac{C_2 \dot{\Phi}_2^2}{2} + \frac{C_3 (\dot{\Phi}_1 + \dot{\Phi}_2)^2}{2} \ , \tag{434}$$

and

$$U = -E_{J,1} \cos\left(\frac{2\pi\Phi_1}{\Phi_0}\right) - E_{J,2} \cos\left(\frac{2\pi\Phi_2}{\Phi_0}\right) - E_{J,3} \cos\left(\frac{2\pi(\Phi_1 + \Phi_2 + \Phi_{ext})}{\Phi_0}\right) \ . \tag{435}$$

An interesting regime arises for $E_{J,1} = E_{J,2}$ and $E_{J,3} = \alpha E_{J,1}$, where $\alpha \sim 0.7$.

D. Fluxonium

The Lagrangian is the same as that of an RF-SQUID

$$\mathcal{L} = \frac{C\dot{\Phi}^2}{2} - \frac{(\Phi - \Phi_{ext})^2}{2L} + E_J \cos\left(\frac{2\pi\Phi}{\Phi_0}\right) \ , \tag{436}$$

which gives the Hamiltonian

$$\mathcal{H} = \frac{Q^2}{2C} - \frac{(\Phi - \Phi_{ext})^2}{2L} + E_J \cos\left(\frac{2\pi\Phi}{\Phi_0}\right) \ . \tag{437}$$

XI. BOGOLIUBOV-DE GENNES FORMALISM

We need this formalism to describe non-homogeneous structures including superconductors, e.g., Normal metal - Superconductor (NS) interfaces or Superconductor - Normal metal -Superconductor (SNS) constrictions.

One starts from the Hamiltonian (170) with an attraction due to phonons.

$$H_G = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma}\, c_{k,\sigma} - \frac{1}{2}\,\frac{g}{V} \sum_{k_1,\sigma_1,k_2,\sigma_2,q} c^\dagger_{k_1+q,\sigma_1}\, c^\dagger_{k_2-q,\sigma_2}\, c_{k_2,\sigma_2}\, c_{k_1,\sigma_1} \tag{438}$$

If we forget for a moment about the restrictions on the energies and momenta of electrons participating in the interaction, this can be written as a contact interaction in the r-space. Namely, introducing

$$\psi_\sigma(r) = \frac{1}{\sqrt{V}} \sum_k c_{k,\sigma} e^{ikr} \ , \tag{439}$$

we can rewrite (170) as

$$H_G = \int dV\, \psi^\dagger_{\sigma_1}(r) \left[h^{(1)}_{\sigma_1,\sigma_2}\right] \psi_{\sigma_2}(r) - g \int dV\, \psi^\dagger_\uparrow(r)\psi^\dagger_\downarrow(r)\psi_\downarrow(r)\psi_\uparrow(r) \ . \tag{440}$$

Here $h^{(1)}_{\sigma_1,\sigma_2}$ is the single-particle Hamiltonian. In (170) this is $h^{(1)}_{\sigma_1,\sigma_2} = \left[\epsilon(-i\vec{\nabla}) - \mu\right] \delta_{\sigma_1,\sigma_2}$. However, in general, more complicated situations are possible (e.g., with spin-orbit interaction, with external magnetic field, with inhomogeneous external (scalar) potential etc.).

In the mean-field approximation this gives

$$\begin{aligned} H^{MF} &= \int dV\, \psi^\dagger_{\sigma_1}(r) \left[h^{(1)}_{\sigma_1,\sigma_2}\right] \psi_{\sigma_2}(r) + \int dV \frac{|\Delta(r)|^2}{g} \\ &- \int dV\, \Delta(r)\psi^\dagger_\uparrow(r)\psi^\dagger_\downarrow(r) - \int dV\, \Delta^*(r)\psi_\downarrow(r)\psi_\uparrow(r) \ , \end{aligned} \tag{441}$$

where

$$\Delta(r) \equiv g\langle \psi_\downarrow(r)\psi_\uparrow(r)\rangle \ . \tag{442}$$

Introducing a spinor

$$\Psi(r) = [\psi_\uparrow(r), \psi_\downarrow(r), \psi^\dagger_\downarrow(r), -\psi^\dagger_\uparrow(r)]^T = \begin{pmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \\ \psi^\dagger_\downarrow(r) \\ -\psi^\dagger_\uparrow(r) \end{pmatrix} \tag{443}$$

we can rewrite

$$H^{MF} = \int dV\, \Psi^\dagger(r) \begin{pmatrix} \hat{h}^{(1)} & -\Delta/2 \\ -\Delta^*/2 & 0 \end{pmatrix} \Psi(r) + \int dV \frac{|\Delta(r)|^2}{g} \ . \tag{444}$$

We now want to make the matrix more symmetric. Since the operator $h^{(1)}$ contains derivatives (momentum operator) it is more convenient to think of it as a non-local one and write the diagonal part as

$$\int dr_1 dr_2 \sum_{\sigma_1,\sigma_2} \psi^\dagger_{\sigma_1}(r_1) h^{(1)}(r_1, \sigma_1; r_2, \sigma_2) \psi_{\sigma_2}(r_2) \ . \tag{445}$$

We can now commute ψ and $\psi^\dagger$ and obtain

$$-\int dr_1 dr_2 \sum_{\sigma_1,\sigma_2} \psi_{\sigma_2}(r_2) h^{(1)}(r_1,\sigma_1;r_2,\sigma_2)\psi^\dagger_{\sigma_1}(r_1) + \int dr \sum_\sigma h^{(1)}(r,\sigma;r,\sigma) \ . \tag{446}$$

The last term is a (possibly infinite) constant, whereas the first term can be written as

$$-\int dr_1 dr_2 \sum_{\sigma_1,\sigma_2} \psi_{\sigma_1}(r_1) \left[h^{(1)}\right]^T (r_1,\sigma_1;r_2,\sigma_2)\psi^\dagger_{\sigma_2}(r_2) \ . \tag{447}$$

We also use the fact, that the second half of the spinor (443) is given by

$$\begin{pmatrix} \psi^\dagger_\downarrow \\ -\psi^\dagger_\uparrow \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi^\dagger_\uparrow \\ \psi^\dagger_\downarrow \end{pmatrix} = i\sigma_y \begin{pmatrix} \psi^\dagger_\uparrow \\ \psi^\dagger_\downarrow \end{pmatrix} \tag{448}$$

Thus we obtain (up to a constant)

$$H^{MF} = \frac{1}{2}\int dV\, \Psi^\dagger(r) \begin{pmatrix} \hat{h}^{(1)} & -\Delta \\ -\Delta^* & -\sigma_y \left[\hat{h}^{(1)}\right]^T \sigma_y \end{pmatrix} \Psi(r) + \int dV \frac{|\Delta(r)|^2}{g} \ . \tag{449}$$

The transposition operator in $\left[\hat{h}^{(1)}\right]^T$ relates to all indexes of $h^{(1)}$, that is to coordinate and spin indexes.

We define

$$h_{BdG} = \begin{pmatrix} \hat{h}^{(1)} & -\Delta \\ -\Delta^* & -\sigma_y \left[\hat{h}^{(1)}\right]^T \sigma_y \end{pmatrix} \ . \tag{450}$$

This is a Hermitian operator, which should have a complete basis of eigenstates, $h_{BdG}\Phi_n = E_n\Phi_n$. These eigenstates are 4-spinors:

$$\Phi_n(r) = \begin{pmatrix} \Phi_{1,n}(r) \\ \Phi_{2,n}(r) \\ \Phi_{3,n}(r) \\ \Phi_{4,n}(r) \end{pmatrix} \tag{451}$$

Inserting $\sum_n \Phi_n(r)\Phi_n^\dagger(r')$ left and right of h_{BdG} (we should again consider h_{BdG} as a matrix $h_{BdG}(r,r')$ in the coordinate space as well) we obtain

$$H^{MF} = \frac{1}{2}\sum_n E_n \alpha_n^\dagger \alpha_n + \int dV \frac{|\Delta(r)|^2}{g} \ , \tag{452}$$

where

$$\begin{aligned} \alpha_n &\equiv \int dr\, \Phi_n^\dagger(r)\Psi(r) \\ &= \int dr\, \Big(\Phi^*_{1,n}(r)\psi_\uparrow(r) + \Phi^*_{2,n}(r)\psi_\downarrow(r) + \Phi^*_{3,n}(r)\psi^\dagger_\downarrow(r) - \Phi^*_{4,n}(r)\psi^\dagger_\uparrow(r)\Big) \end{aligned} \tag{453}$$

are annihilation operators of the BdG states. Multiplying this relation by $\Phi_n(r')$ from the left, summing of n and using $\sum_n \Phi_n(r')\Phi_n^\dagger(r) = \delta(r-r')\hat{1}_4$ (here $\hat{1}_4$ is a 4×4 unity matrix) we get

$$\Psi(r) = \sum_n \Phi_n(r)\alpha_n \ . \tag{454}$$

A. Particle-hole symmetry

Consider an operator given by

$$C = \begin{pmatrix} 0 & -i\sigma_y \\ i\sigma_y & 0 \end{pmatrix} = \tau_y\sigma_y \ . \tag{455}$$

It's easy to see that $C^{-1} = C^\dagger = C$. We observe the property

$$C^{-1}h_{BdG}C = -h_{BdG}^* \ . \tag{456}$$

From this one observes that is Φ_n is an eigenstate of h_{BdG} with the eigenvalue E_n, then the state $C\Phi_n^*$ is an eigenstate with eigenvalue $-E_n$. Indeed

$$h_{BdG}C\Phi_n^* = CC^{-1}h_{BdG}C\Phi_n^* = C(-h_{BdG}^*)\Phi_n^* = -E_nC\Phi_n^* \ . \tag{457}$$

To each eigenstate with positive energy there corresponds an eigenstate with opposite negative energy. It is convenient to introduce the notation $\Phi_{-n} \equiv C\Phi_n^*$ and $E_{-n} = -E_n$. This allows us to organize the indexes so that positive n correspond to positive energies and negative n to negative energies. This particle-hole symmetry is completely analogous to the particle-antiparticle symmetry of the Dirac theory and is called there charge conjugation symmetry.

However, the superconductivity has an extra property. Namely, it is easy to observe that the field Ψ (see (443)) is self-conjugate, namely

$$C\Psi = (\Psi^\dagger)^T \tag{458}$$

From this we obtain (using $C^T = C$)

$$\begin{aligned} \alpha_{-n} &= \int dr\, \Phi_{-n}^\dagger(r)\Psi(r) = \int dr\, (C\Phi_n^*)^\dagger\Psi = \int dr\, \Phi_n^T C\Psi = \int dr\, \Phi_n^T(\Psi^\dagger)^T \\ &= \int dr\, \Psi^\dagger\Phi_n \ . \end{aligned} \tag{459}$$

Therefore

$$\alpha^\dagger_{-n} = \int dr\, \Phi^\dagger_n \Psi = \alpha_n \ . \tag{460}$$

This very important property is closely related to Majorana physics in high energy, i.e., particles and antiparticles are the same. We finally obtain

$$H^{MF} = \sum_{n>0} E_n \alpha^\dagger_n \alpha_n - \frac{1}{2}\sum_{n>0} E_n + \int dV \frac{|\Delta(r)|^2}{g} \ . \tag{461}$$

B. Self-consistency condition

The order parameter has been introduced as

$$\Delta(r) \equiv g\langle \psi_\downarrow(r)\psi_\uparrow(r)\rangle \ . \tag{462}$$

Using $\Psi(r) = \sum_n \Phi_n(r)\alpha_n$ we get $\psi_\uparrow(r) = \sum \Phi_{1,n}(r)\alpha_n$ and $\psi_\downarrow(r) = \sum \Phi_{2,n}(r)\alpha_n$. This gives

$$\Delta(r) \equiv g\sum_{n,m} \Phi_{2,m}(r)\Phi_{1,n}(r)\langle \alpha_m\alpha_n\rangle \ . \tag{463}$$

Using the property $\alpha^\dagger_{-n} = \alpha_n$ we obtain

$$\begin{aligned}\Delta(r) \ &= \ g\sum_{n>0} \Phi_{2,-n}(r)\Phi_{1,n}(r)\langle \alpha^\dagger_n\alpha_n\rangle \\ &+ \ g\sum_{n>0} \Phi_{2,n}(r)\Phi_{1,-n}(r)\langle \alpha_n\alpha^\dagger_n\rangle \ .\end{aligned} \tag{464}$$

Using $\Phi_{-n} \equiv C\Phi^*_n$ and

$$C = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \tag{465}$$

we obtain

$$\begin{aligned}\Delta(r) \ &= \ g\sum_{n>0} \Phi^*_{3,n}(r)\Phi_{1,n}(r)\langle \alpha^\dagger_n\alpha_n\rangle \\ &- \ g\sum_{n>0} \Phi_{2,n}(r)\Phi^*_{4,n}(r)\langle \alpha_n\alpha^\dagger_n\rangle \ .\end{aligned} \tag{466}$$

C. Spin-independent case

The simplest case is when $\hat{h}^{(1)}$ is spin independent (diagonal in spin indexes), i.e. . Then h_{BdG} can be written as

$$h_{BdG} = \begin{pmatrix} h^{(1)} & 0 & -\Delta & 0 \\ 0 & h^{(1)} & 0 & -\Delta \\ -\Delta^* & 0 & -[h^{(1)}]^* & 0 \\ 0 & -\Delta^* & 0 & -[h^{(1)}]^* \end{pmatrix} \tag{467}$$

The problem factorizes into two equivalent blocks (1-3) and (2-4). In each block the Hamiltonian reads

$$h^{(2)}_{BdG} = \begin{pmatrix} h^{(1)} & -\Delta \\ -\Delta^* & -[h^{(1)}]^* \end{pmatrix} \tag{468}$$

This $2X2$ block is still particle-hole symmetric, i.e.,

$$C^{-1} h^{(2)}_{BdG} C = -h^{(2)*}_{BdG} \;, \tag{469}$$

where now $C = \tau_y$.

We can look for the eigenvectors of $h^{(2)}_{BdG}$ in the form $(u_n(r), -v_n^*(r))^T$. That is

$$\begin{pmatrix} h^{(1)} & -\Delta \\ -\Delta^* & -[h^{(1)}]^* \end{pmatrix} \begin{pmatrix} u_n \\ -v_n^* \end{pmatrix} = E_n \begin{pmatrix} u_n \\ -v_n^* \end{pmatrix} \;. \tag{470}$$

It is important to realize that such a solution provides two degenerate eigenvectors of the 4×4 problem. That is

$$\Phi^{(1)}_n = \begin{pmatrix} u_n \\ 0 \\ -v_n^* \\ 0 \end{pmatrix} \;, \quad \Phi^{(2)}_n = \begin{pmatrix} 0 \\ u_n \\ 0 \\ -v_n^* \end{pmatrix} \;. \tag{471}$$

Then, from (466) we get

$$\Delta(r) = g \sum_{n>0} u_n(r) v_n(r) \tanh\left(\frac{\beta E_n}{2}\right) \;. \tag{472}$$

1. Homogenous case

In the simplest case when everything (Δ, μ, external potential) is homogenous, we recover our earlier results. Namely (470) can be solved using plain waves:

$$\begin{pmatrix} u_n(r) \\ -v_n^*(r) \end{pmatrix} = \begin{pmatrix} u_k \\ -v_k^* \end{pmatrix} \frac{e^{ikr}}{\sqrt{V}} \; . \tag{473}$$

Assuming $h^{(1)}e^{ikr} = [h^{(1)}]^* e^{ikr} = \xi_k e^{ikr}$ we get

$$\begin{pmatrix} \xi_k & -\Delta \\ -\Delta^* & -\xi_k \end{pmatrix} \begin{pmatrix} u_k \\ -v_k^* \end{pmatrix} = E_k \begin{pmatrix} u_k \\ -v_k^* \end{pmatrix} \; . \tag{474}$$

This differs from (220) only by the fact that Δ is complex. Assuming $\Delta = |\Delta| e^{i\phi}$ we can solve by putting $u_k = u_{k0} \geq 0$, $v_k = v_{k0} e^{i\phi}$, where $v_{k0} > 0$. For u_{k0}, v_{k0} we obtain

$$\begin{pmatrix} \xi_k & -|\Delta| \\ -|\Delta| & -\xi_k \end{pmatrix} \begin{pmatrix} u_{k0} \\ -v_{k0} \end{pmatrix} = E_k \begin{pmatrix} u_{k0} \\ -v_{k_0} \end{pmatrix} \; , \tag{475}$$

which coincides with (470). The solution is then $E_k = \sqrt{\xi_k^2 + |\Delta|^2}$ and

$$v_{k0} = \sqrt{\frac{1}{2} - \frac{\xi_k}{2E_k}} \tag{476}$$

$$u_{k0} = \sqrt{\frac{1}{2} + \frac{\xi_k}{2E_k}} \; . \tag{477}$$

The quasiparticle annihilation operators are then given by

$$\alpha_k^{(1)} = \alpha_{k,\uparrow} = \frac{1}{\sqrt{V}} \int dr \, \left[u_{k0} e^{-ikr} \psi_\uparrow(r) - v_{k0} e^{-ikr} e^{i\phi} \psi_\downarrow^\dagger(r) \right] = u_{k0} c_{k,\uparrow} - e^{i\phi} v_{k0} c_{-k,\downarrow}^\dagger \; , \tag{478}$$

and

$$\alpha_k^{(2)} = \alpha_{k,\downarrow} = \frac{1}{\sqrt{V}} \int dr \, \left[u_{k0} e^{-ikr} \psi_\downarrow(r) + v_{k0} e^{-ikr} e^{i\phi} \psi_\uparrow^\dagger(r) \right] = u_{k0} c_{k,\downarrow} + e^{i\phi} v_{k0} c_{-k,\uparrow}^\dagger \; . \tag{479}$$

These are the same Bogoliubov relations as in (206) or (225), except for the non-vanishing phase of the order parameter and, correspondingly, the factor $e^{i\phi}$ multiplying the BCS coefficient v_{k0}.

2. *Number and phase again*

The factors $e^{i\phi}$ in (478) and (479) can be given a very important interpretation. On the first sight the operators $\alpha^\dagger_{k,\sigma} = u_{k0} c^\dagger_{k,\sigma} - \sigma e^{-i\phi} v_{k0} c_{-k,-\sigma}$ acting on a state with a given number of particles M creates a superposition of a state with $M+1$ particles and a state with $M-1$ particles. However, this is not so. Let us recall the role of the operator $e^{-i\phi}$. From the analysis of Sec. VII L we can conclude that the operator $e^{-i\phi}$ increases the number of Cooper pairs in the condensate by one (the fact that $e^{-i\phi}$ and not $e^{i\phi}$ increases the number has to do with the signs chosen in Sec. VII L). Thus the proper interpretation should read

$$\alpha^\dagger_{k,\sigma} = u_{k0} c^\dagger_{k,\sigma} - \sigma S^\dagger v_{k0} c_{-k,-\sigma} \ , \tag{480}$$

where $S^\dagger = e^{-i\phi}$ creates an extra Cooper pair in the condensate. This way the operator $\alpha^\dagger_{k,\sigma}$ adds a single electron to the system and creates a quasi-particle excitation. Of course one can also define another operator

$$\tilde{\alpha}^\dagger_{k,\sigma} = S \alpha^\dagger_{k,\sigma} = S u_{k0} c^\dagger_{k,\sigma} - \sigma v_{k0} c_{-k,-\sigma} \ . \tag{481}$$

This operator removes one electron from the system and creates a quasi-particle excitation. This issues are discussed in the book by Tinkham and in the very important paper by Blonder, Tinkham and Klapwijk [5] (BTK theory).

D. Non-homogeneous situation

The BdG equation in general (spin-diagonal case) read (cf. 470)

$$\begin{pmatrix} h^{(1)} & -\Delta \\ -\Delta^* & -[h^{(1)}]^* \end{pmatrix} \begin{pmatrix} u_n \\ -v_n^* \end{pmatrix} = E_n \begin{pmatrix} u_n \\ -v_n^* \end{pmatrix} \ . \tag{482}$$

This can be rewritten as

$$\begin{pmatrix} h^{(1)} & \Delta \\ \Delta^* & -[h^{(1)}]^* \end{pmatrix} \begin{pmatrix} u_n \\ v_n^* \end{pmatrix} = E_n \begin{pmatrix} u_n \\ v_n^* \end{pmatrix} \ . \tag{483}$$

Usually in the literature one uses also $v_n^* \to v_n$. We will keep v_n as in (483) so that the phase of v_n coincides with that of Δ in the homogeneous case.

For the simplest situation

$$h^{(1)} = [h^{(1)}]^* = -\frac{\hbar^2 \nabla^2}{2m} - \mu \tag{484}$$

E. NS contact, Andreev reflection

Consider a contact in which $\Delta = 0$ for $x < 0$ and $\Delta = |\Delta| e^{i\phi}$ for $x > 0$. We will start with a quasi one dimensional setup, in which the transverse movement in y and z directions is restricted by a potential $V(y,z)$. That is

$$h^{(1)} = [h^{(1)}]^* = -\frac{\hbar^2 \nabla_x^2}{2m} - \frac{\hbar^2(\nabla_y^2 + \nabla_z^2)}{2m} + V(y,z) - \mu \ . \tag{485}$$

Then one first solves the transverse Schrödinger equation

$$\left[-\frac{\hbar^2(\nabla_y^2 + \nabla_z^2)}{2m} + V(y,z) \right] \psi_m(y,z) = \epsilon_m \psi_m(y,z) \ . \tag{486}$$

Here, m counts the transverse channels. The wave functions $\psi_m(y,z)$ can be choses real.

To solve the full problem one makes an ansatz

$$\begin{pmatrix} u(r) \\ v^*(r) \end{pmatrix} = \psi_m(y,z) \begin{pmatrix} u_m(x) \\ v_m^*(x) \end{pmatrix} \tag{487}$$

For $u(x)$ and $v(x)$ (we drop the index m and focus on a single channel) we obtain the following BdG equations

$$\begin{pmatrix} -\frac{\hbar^2 \nabla_x^2}{2m} - \tilde{\mu} & \Delta(x) \\ \Delta^*(x) & \frac{\hbar^2 \nabla_x^2}{2m} + \tilde{\mu} \end{pmatrix} \begin{pmatrix} u \\ v^* \end{pmatrix} = E \begin{pmatrix} u \\ v^* \end{pmatrix} \ . \tag{488}$$

Here, $\tilde{\mu} = \mu - \epsilon_m$ is the effective chemical potential for transverse channel m.

We look for solutions with $E > 0$. Most important is the regime $E \ll \tilde{\mu}$. For $x < 0$ and $x > 0$ the solutions are plain waves.

1. *Spectrum on the normal side*

For $x < 0$ we have $\Delta = 0$ and there are 4 solutions:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{\pm i k_e x} \quad , \quad E = \frac{\hbar^2 k_e^2}{2m} - \tilde{\mu} \ , \tag{489}$$

and

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{\pm i k_h x} \quad , \quad E = \tilde{\mu} - \frac{\hbar^2 k_h^2}{2m} \ . \tag{490}$$

We introduce the Fermi momentum $\hbar k_F = \sqrt{2m\tilde{\mu}}$. Then, from $E > 0$ follows $|k_e| > k_F$ and $|k_h| < k_F$. This spectrum is shown in Fig. 23.

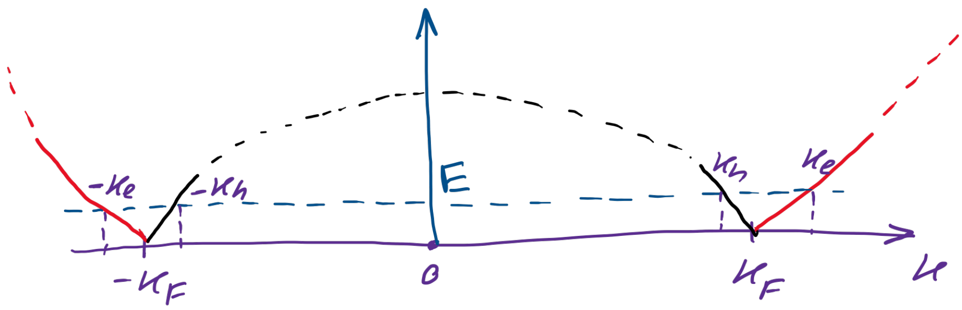

FIG. 23: Spectrum on the normal side of the NS contact.

2. *Spectrum on the superconducting side*

For $x > 0$ we look for solutions of the form

$$\begin{pmatrix} u_k \\ v_k^* \end{pmatrix} e^{ikx} \ . \tag{491}$$

This gives an algebraic equation

$$\begin{pmatrix} \xi_k & \Delta \\ \Delta^* & -\xi_k \end{pmatrix} \begin{pmatrix} u_k \\ v_k^* \end{pmatrix} = E \begin{pmatrix} u_k \\ v_k^* \end{pmatrix} \ , \tag{492}$$

where $\xi_k = \frac{\hbar^2 k^2}{2m} - \tilde{\mu}$. The situation differs for $E > |\Delta|$ and $E < |\Delta|$.

Case $E > |\Delta|$. For $E > |\Delta|$ we obtain the usual BCS coherence factors u and v. Namely $E = \sqrt{|\Delta|^2 + \xi_k^2}$ and

$$v_k = e^{i\phi} v_{k0} = e^{i\phi} \sqrt{\frac{1}{2} - \frac{\xi_k}{2E}} \ , \tag{493}$$

$$u_k = u_{k0} = \sqrt{\frac{1}{2} + \frac{\xi_k}{2E}} \ . \tag{494}$$

The equation $E = \sqrt{|\Delta|^2 + \xi_k^2}$ has four solutions for k as shown in Fig. 24. This can be found from $\xi_k = \pm\sqrt{E^2 - |\Delta|^2}$. The two solutions with $\xi_k > 0$ are particle-like and the two solutions with $\xi_k < 0$ are hole-like. We obtain

$$\frac{\hbar^2 k_e^2}{2m} = \tilde{\mu} + \sqrt{E^2 - |\Delta|^2} \ , \tag{495}$$

$$\frac{\hbar^2 k_h^2}{2m} = \tilde{\mu} - \sqrt{E^2 - |\Delta|^2} \ . \tag{496}$$

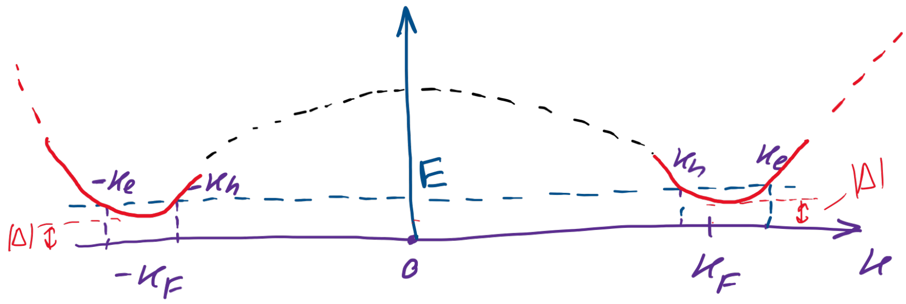

FIG. 24: Spectrum on the superconducting side of the NS contact.

Case $E < |\Delta|$. We need also solutions for $E < |\Delta|$ to match with the corresponding solutions for $x < 0$. These will be evanescent waves. Of course only waves decaying at $x \to \infty$ are important. In this case $\xi_k^2 < 0$ and $\xi_k = \pm i\sqrt{|\Delta|^2 - E^2}$. We can still take the solutions

$$u_k = \sqrt{\frac{1}{2} + \frac{\xi_k}{2E}} \ . \tag{497}$$

$$v_k^* = e^{-i\phi}\sqrt{\frac{1}{2} - \frac{\xi_k}{2E}} \quad , \quad v_k = e^{i\phi}\sqrt{\frac{1}{2} + \frac{\xi_k}{2E}} = e^{i\phi} u_k \ . \tag{498}$$

These are no longer normalized, i.e., $|u_k|^2 + |v_k|^2 \neq 1$, rather $|u_k| = |v_k|$ and $u_k^2 + (e^{i\phi} v_k^*)^2 = 1$. The equation $\xi_k = \pm i\sqrt{|\Delta|^2 - E^2}$ has 4 solutions for k. Two of these ($\xi_k = +i\sqrt{|\Delta|^2 - E^2}$) satisfy

$$\frac{\hbar^2 k^2}{2m} = \tilde{\mu} + i\sqrt{|\Delta|^2 - E^2} \ . \tag{499}$$

Only one with $\mathrm{Im}[k] > 0$ should be kept. Namely

$$k_1 = k_F \sqrt{1 + i\frac{\sqrt{|\Delta|^2 - E^2}}{\tilde{\mu}}} \ . \tag{500}$$

For the other two ($\xi_k = -i\sqrt{|\Delta|^2 - E^2}$) we have

$$\frac{\hbar^2 k^2}{2m} = \tilde{\mu} - i\sqrt{|\Delta|^2 - E^2} \ . \tag{501}$$

Again only one with $\mathrm{Im}[k] > 0$ should be kept. Namely

$$k_2 = -k_F \sqrt{1 - i\frac{\sqrt{|\Delta|^2 - E^2}}{\tilde{\mu}}} \ . \tag{502}$$

What is left is to match the solutions using usual boundary conditions.

3. Andreev reflection for $E < |\Delta|$ in an ideal contact.

For $E < |\Delta|$ the free propagating solutions exist only for $x < 0$. For scattering problems it is convenient to normalize the wave functions to a unit flux of particles by multiplying with $v_g^{-1/2}$, where $v_g = \hbar^{-1}\partial E_k/\partial k$ is the group velocity. The incoming waves should have positive v_g for $x < 0$ and negative v_g for $x > 0$. The outgoing wave should have negative v_g for $x < 0$ and positive v_g for $x > 0$. For an incoming electron-like particle the possible processes are shown in Fig. 25. For an incoming hole-like particle the possible processes

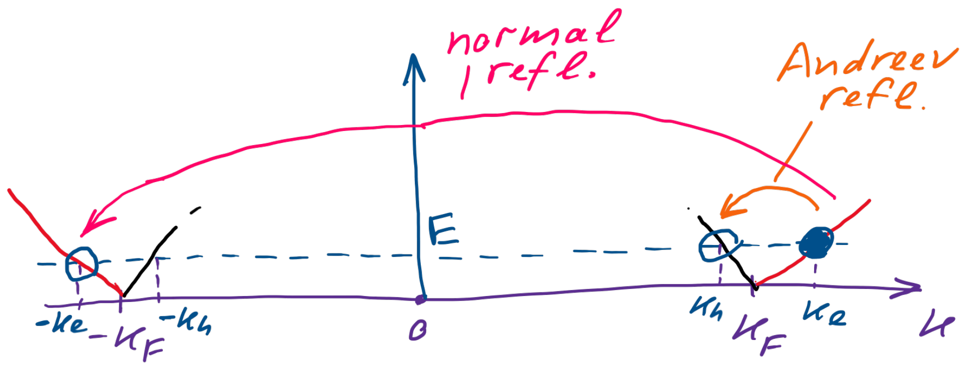

FIG. 25: Andreev and normal reflections for incoming electron at $E < |\Delta|$.

are shown in Fig. 26. The conversion of electron into hole or vice versa is called Andreev

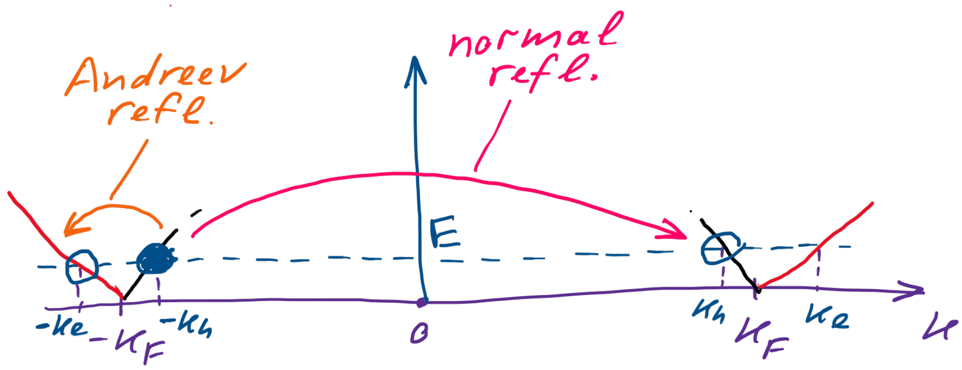

FIG. 26: Andreev and normal reflections for incoming hole at $E < |\Delta|$.

reflection (A.F. Andreev, 1964).

Let us consider the process in Fig. 25 (incoming electron) and assume $E, |\Delta| \ll \tilde{\mu}$. Then the absolute values of the group velocities off all three modes involved are approximately equal to $|v_g| = v_F = \hbar k_F/m$. The wave function for $x < 0$ is then given by

$$\Psi(x<0) = \frac{1}{\sqrt{v_F}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_e x} + \frac{r_N}{\sqrt{v_F}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ik_e x} + \frac{r_A}{\sqrt{v_F}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik_h x} \ . \tag{503}$$

For the evanescent wave for $x > 0$ we can write

$$\Psi(x>0) = A \begin{pmatrix} U_g \\ e^{-i\phi} U_g^* \end{pmatrix} e^{ik_1 x} + B \begin{pmatrix} U_g^* \\ e^{-i\phi} U_g \end{pmatrix} e^{ik_2 x} \ , \tag{504}$$

where

$$U_g \equiv \sqrt{\frac{E + i\sqrt{|\Delta|^2 - E^2}}{2E}} \ . \tag{505}$$

It is not necessary to normalize the evanescent wave functions. For $E, |\Delta| \ll \tilde{\mu}$ we have

$$k_1 \approx k_F + i\frac{\sqrt{|\Delta|^2 - E^2}}{\hbar v_F} \quad , \quad k_2 \approx -k_F + i\frac{\sqrt{|\Delta|^2 - E^2}}{\hbar v_F} \ . \tag{506}$$

In an ideal contact the wave functions and their derivatives should be continuos. The continuity of the wave functions gives

$$\begin{aligned} \frac{1 + r_N}{\sqrt{v_F}} &= AU_g + BU_g^* \ , \\ \frac{r_A}{\sqrt{v_F}} &= (AU_g^* + BU_g) e^{-i\phi} \ . \end{aligned} \tag{507}$$

For the derivatives we approximately put $|k_e| \approx |k_h| \approx |k_1| \approx |k_2| \approx k_F$. Then

$$\begin{aligned} \frac{1 - r_N}{\sqrt{v_F}} &= AU_g - BU_g^* \ , \\ \frac{r_A}{\sqrt{v_F}} &= (AU_g^* - BU_g) e^{-i\phi} \ . \end{aligned} \tag{508}$$

The solution reads $B = 0$, $r_N = 0$, $AU_g = 1/\sqrt{v_F}$, $r_A = \sqrt{v_F} AU_g^* e^{-i\phi} = (U_g^*/U_g) e^{-i\phi}$. We have

$$\frac{U_g^*}{U_g} = \sqrt{\frac{E - i\sqrt{|\Delta|^2 - E^2}}{E + i\sqrt{|\Delta|^2 - E^2}}} = \exp\left[-i \arccos(E/|\Delta|)\right] \ . \tag{509}$$

Thus, in this approximation we have a 100% Andreev reflection: $r_N = 0$ and

$$r_A = e^{-i\phi} e^{-i\gamma(E)} \ , \tag{510}$$

where $\gamma(E) \equiv \arccos(E/|\Delta|)$.

Coming back to the discussion of Sec. XI C 2 we write down the corresponding quasiparticle creation operator for $x < 0$. This reads (cf. 453, we use here a different normalization)

$$\alpha^\dagger = \frac{1}{\sqrt{v_F}} \int\limits_{x<0} dx \, \left[\left\{ e^{ik_e x} + r_N e^{-ik_e x} \right\} \psi_\uparrow^\dagger(x) - r_A e^{ik_h x} \psi_\downarrow(x) \right] + \text{evanescent part} \ . \tag{511}$$

The fact that r_A contain the phase factor $e^{-i\phi}$ means in the spirit of Sec. XI C 2 that an extra Cooper pair is created. Thus an electron in reflected to a hole and the charge is conserved as an extra Cooper pair is added to the condensate at $x > 0$.

F. Andreev reflection in 2D or 3D, propagation direction of the reflected hole

We consider now a 2D ideal NS contact between 3D normal metal and 3D superconductor. The BdG equations read

$$\begin{pmatrix} -\frac{\hbar^2 \vec{\nabla}^2}{2m} - \mu & \Delta(r) \\ \Delta^*(r) & \frac{\hbar^2 \vec{\nabla}^2}{2m} + \mu \end{pmatrix} \begin{pmatrix} u \\ v^* \end{pmatrix} = E \begin{pmatrix} u \\ v^* \end{pmatrix} \ , \tag{512}$$

where $\Delta(r) = \theta(x)|\Delta|e^{i\phi}$. On the normal side ($x < 0$), where $\Delta = 0$ the solutions are

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i\vec{k}\vec{r}} \quad , \quad E = \frac{\hbar^2 \vec{k}^2}{2m} - \mu > 0 \quad , \quad |\vec{k}| > k_F \ , \tag{513}$$

and

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{i\vec{k}\vec{r}} \quad , \quad E = \mu - \frac{\hbar^2 \vec{k}^2}{2m} > 0 \quad , \quad |\vec{k}| < k_F \ . \tag{514}$$

Upon reflection the y and z components of the wave vector are conserved. Thus possible scattering processes are shown in Fig. 27. As we can see, the Andreev reflected hole propagates in the direction opposite to that of the incoming electron. In contrast, a normally reflected electron undergoes a usual specular reflection.

G. SNS contacts, Andreev bound states, Josephson current

1. *Byers–Yang theorem*

The relation between the phase drop in an SNS contact and the current can be discussed in the framework of the so called Byers–Yang theorem. This was first formulated by N. Byers

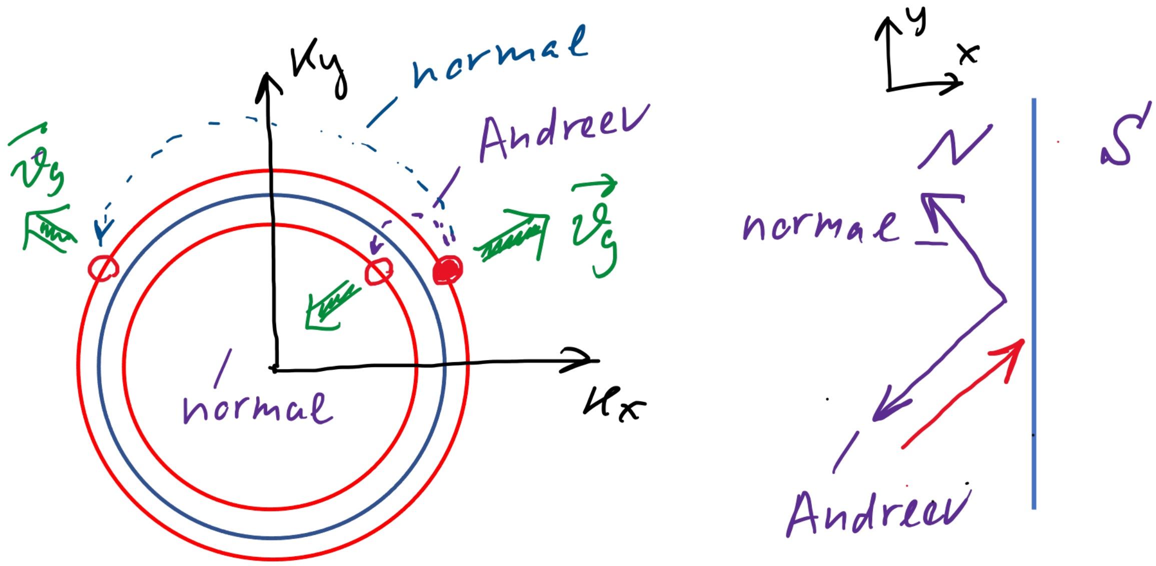

FIG. 27: Andreev reflection in 2D.

and C. N. Yang in Ref. [6]. A version with a much wider application domain was provided by F. Bloch in Ref. [7]. We will follow F. Bloch. Consider a (superconducting) ring. The current flowing in the ring can, in principle, create its own (internal) magnetic field (vector potential $\vec{A}_{in}$). In addition an external magnetic field (flux) is applied. Thus, one can split the magnetic field and the vector potential into the internal $\vec{A}_{in}$ and the external $\vec{A}_{ex}$ ones.

$$\vec{A} = \vec{A}_{in} + \vec{A}_{ex} \ . \tag{515}$$

The simplest (theoretically) situation arises if the external magnetic flux is concentrated in the opening of the ring such that the external magnetic field vanishes in the body of the ring itself. Thus in the body of the ring $\vec{\nabla} \times \vec{A}_{ex} = 0$. Thus, locally, in the body of the ring $\vec{A}_{ex} = \vec{\nabla}\chi$. However, $\chi(r)$ is not single valued in general. Indeed

$$\oint \vec{A}_{ex} d\vec{l} = \Phi_{ex} \ , \tag{516}$$

where the integration contour is in the body of the ring.

Consider the many-body Hamiltonian of interacting electrons (here first quantization)

$$H = H[\vec{p}_j + e\vec{A}(\vec{r}_j)/c, \vec{r}_j] \ . \tag{517}$$

Here $\vec{p}_j = -i\hbar\vec{\nabla}_j$. This Hamiltonian should in principle also include the degrees of freedom corresponding to the internal field $\vec{A}_{in}$. The support of the many-body wave function $\psi(\vec{r}_j)$

is in the body of the ring. We can perform there a gauge transformation:

$$\psi(\vec{r}_j) = \psi_0(\vec{r}_j) \exp\left[-\frac{ie}{\hbar c}\sum_j \chi(r_j)\right] . \tag{518}$$

Upon this gauge transformation the Hamiltonian for ψ_0 will not contain $\vec{A}_{ex}$, i.e.,

$$H_0 = H[\vec{p}_j + e\vec{A}_{in}(\vec{r}_j)/c, \vec{r}_j] . \tag{519}$$

However, the new wave function ψ_0 has a non-trivial boundary condition. Since ψ is single valued, ψ_0 is multiplied by a factor

$$\exp\left[\frac{ie}{\hbar c}\Phi_{ex}\right] \tag{520}$$

when particle with coordinate $\vec{r}_j$ is brought around the ring. If, however, $\Phi_{ex} = 2\pi n\hbar c/e$, the wave function ψ_0 is periodic and ψ. This shows the the (many-body) spectrum does not change upon addition of $2\pi\hbar c/e$ to the external flux. In other words spectrum and, thus, all thermodynamic quantities are periodic functions of Φ_{ex}. The period is in general $2\pi\hbar c/e$. However, if the system is superconducting and the electrons are paired into Cooper pairs of charge $2e$, the period is halved and is given by $\Phi_0 = 2\pi\hbar c/2e$. This is the essence of Byers–Yang theorem: the free energy $F(\Phi_{ex})$ is a periodic function with period of $\Phi_0^{\text{normal}} = 2\Phi_0$ in general and Φ_0 if the ring is superconducting.

More important for us now is the relation between $F(\Phi_{ex})$ and the current in the ring. The integral of the *external* electric field (EMF, voltage) is given by

$$V_{ex} = -\frac{1}{c}\frac{d\Phi_{ex}}{dt} . \tag{521}$$

From $dF/dt = IV_{ex}$ (at constant temperature, thus free energy and not just energy) one gets $dF = -Id\Phi_{ex}/c$ and

$$I = -c\frac{\partial F}{\partial \Phi_{ex}} . \tag{522}$$

2. Josephson current through an SNS contact

Consider the following theoretical trick. Put formally an SNS contact into an ideal thick (thicker than London penetration length) superconducting ring. Apply an infinitesimal external flux $\delta\Phi_{ex}$ as in the construction above (no magnetic field in the body of the ring).

Repeating the arguments used in flux quantization we conclude that the gauge invariant phase drop on the SNS contact gets an addition of $\delta\Phi_{ex}$. After the sign flip (as above) we conclude that the phase drop is changed as $\Phi \to \Phi - \delta\Phi_{ex}$. Thus from $I = -c\partial F/\partial\Phi_{ex}$ follows

$$I = c\,\frac{\partial F}{\partial \Phi}\ . \tag{523}$$

(If we would not flip the sign of phase drop, we would get a minus sign here.)

Thus, solving the BdG equations ang obtaining the spectrum of positive eigen-energies $E_n(\Phi)$ we can calculate the Josephson current. Using

$$H^{MF} = \sum_{n>0} E_n \alpha_n^\dagger \alpha_n - \frac{1}{2}\sum_{n>0} E_n + \int dV \frac{|\Delta(r)|^2}{g}\ , \tag{524}$$

and assuming the last term does not depend on Φ we obtain

$$F(\Phi) = -k_{\rm B}T \ln \left[\prod_{n>0}\left(e^{\beta E_n/2} + e^{-\beta E_n/2}\right)\right] = -\beta^{-1}\sum_{n>0} \ln\left(2\cosh(\beta E_n/2)\right)\ . \tag{525}$$

Thus

$$I = -\frac{c}{2}\sum_{n>0} \tanh\left(\frac{\beta E_n}{2}\right)\frac{\partial E_n}{\partial \Phi}\ . \tag{526}$$

At zero temperature this gives

$$I = -\frac{c}{2}\sum_{n>0} \frac{\partial E_n}{\partial \Phi}\ . \tag{527}$$

H. Ideal SNS contact, Andreev bound states. Short junction limit.

Consider an SNS contact similar to the NS contact considered above. The normal part ($\Delta = 0$) extends form $x = -L/2$ to $x = L/2$. For $x > L/2$ we have a superconductor with $\Delta = |\Delta| e^{i\phi_R}$, for $x < -L/2$ we have a superconductor with $\Delta = |\Delta| e^{i\phi_L}$. Both NS contacts are ideal and no scattering happens in the normal part. We will first consider the limit of short junction. Namely we will disregard the phase difference acquired by the electron and hole wave at distance L. The precise criterium will be specified below.

We consider eigenstates of the Bogoliubov-de Gennes hamiltonian with $E < |\Delta|$. Such states are bound to the normal part and are called Andreev bound states.

First solution. We can consider Andreev bound state, in which the electron propagates to the right and the hole propagates to the left. Since, as we know from Sec. XI E 3, the Andreev reflection is perfect at $E < |\Delta|$, these two waves would constantly transform to each other on both boundaries. Thus no other waves are generated. The wave function for $-L/2 < x < L/2$ reads

$$\Psi(-L/2 < x < L/2) = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{ik_e x} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ik_h x} \ . \tag{528}$$

(Normalization is not important here.) In the approximation $k_e \approx k_h \approx k_F$ the solution is simple. The Andreev reflection (as analyzed above, see Eq. 510) at $x = L/2$ provides the relation

$$b = e^{-i\phi_R} e^{-i\gamma(E)} a \ . \tag{529}$$

The dual Andreev reflection at $x = -L/2$ gives (left as an exercise)

$$a = e^{i\phi_L} e^{-i\gamma(E)} b \ . \tag{530}$$

These two equations are compatible only if

$$e^{i(\phi_L - \phi_R)} e^{-2i\gamma(E)} = 1 \ . \tag{531}$$

We obtain the quantization condition

$$(\phi_L - \phi_R) - 2\gamma(E) = 0 \ \mathrm{mod}(2\pi) \ . \tag{532}$$

We use the relation (509):

$$e^{-i\gamma(E)} = \frac{U_g^*}{U_g} = \sqrt{\frac{E - i\sqrt{|\Delta|^2 - E^2}}{E + i\sqrt{|\Delta|^2 - E^2}}} = \exp\left[-i \arccos(E/|\Delta|)\right] \ . \tag{533}$$

Since $\cos\gamma = E/|\Delta| > 0$ and $\sin\gamma = \sqrt{|\Delta|^2 - E^2}/|\Delta| > 0$ we conclude that $0 < \gamma(E) < \pi/2$ for $E > 0$. Thus, a positive energy solution exists only if $0 < (\phi_L - \phi_R) < \pi$. There

$$\gamma(E) = \frac{(\phi_L - \phi_R)}{2} \ . \tag{534}$$

and

$$E = |\Delta| \cos\frac{(\phi_L - \phi_R)}{2} \ . \tag{535}$$

For $\pi < (\phi_L - \phi_R) < 2\pi$ the solution found here is still a legitimate solution, but with $E < 0$. Its positive energy counterpart will be found next.

Second solution. Another possible solution is the one, in which the electron moves to the left and the hole moves to the right. The wave function in the normal domain reads

$$\Psi(-L/2 < x < L/2) = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ik_e x} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{-ik_h x} \; . \tag{536}$$

Solving the Andreev reflexion problem again (left as an exercise) we get at $x = L/2$

$$a = e^{i\phi_R} e^{-i\gamma(E)} b \; . \tag{537}$$

Considering now the boundary at $x = -L/2$ we obtain (exercise)

$$b = e^{-i\phi_L} e^{-i\gamma(E)} a \; . \tag{538}$$

We obtain again a slightly different quantization condition

$$(\phi_L - \phi_R) + 2\gamma(E) = 0 \bmod(2\pi) \; . \tag{539}$$

Since again $0 < \gamma(E) < \pi/2$ for $E > 0$ we obtain that positive energy solution exist only if $-\pi < (\phi_L - \phi_R) < 0$ and

$$\gamma(E) = -\frac{(\phi_L - \phi_R)}{2} \; . \tag{540}$$

If we want to have $0 < (\phi_L - \phi_R) < 2\pi$, we should shift by 2π. Then we get

$$\gamma(E) = -\frac{(\phi_L - \phi_R)}{2} + \pi \; , \tag{541}$$

where now $\pi < (\phi_L - \phi_R) < 2\pi$. Thus, finally

$$E = -|\Delta| \cos\frac{(\phi_L - \phi_R)}{2} > 0 \tag{542}$$

for $\pi < (\phi_L - \phi_R) < 2\pi$. This solution is still a legitimate one for $0 < (\phi_L - \phi_R) < \pi$. However, in this domain it has a negative energy.

Short junction condition. In our consideration we have neglected the difference of phases acquired by the electron and hole wave over the distance L. That is we assumed $[k_e(E) - k_h(E)]L \ll 2\pi$. Since

$$k_e = \frac{1}{\hbar}\sqrt{2m(\mu + E)} \approx k_F + \frac{k_F E}{2\mu} = k_F + \frac{E}{\hbar v_F} \; , \tag{543}$$

and

$$k_h = \frac{1}{\hbar}\sqrt{2m(\mu - E)} \approx k_F - \frac{k_F E}{2\mu} = k_F - \frac{E}{\hbar v_F} \; , \tag{544}$$

the condition of short junction reads

$$\frac{2EL}{\hbar v_F} \ll 2\pi \ . \tag{545}$$

The maximum relevant value of E for the Andreev bound states is $|\Delta|$. Thus the condition is satisfied if

$$L \ll \frac{\pi\hbar v_F}{|\Delta|} \sim \xi. \tag{546}$$

Here ξ is the superconducting coherence length.

Summary. Collecting the results we get two Andreev bound states. The first one has the energy

$$E_1 = |\Delta| \cos\frac{(\phi_L - \phi_R)}{2} \ , \tag{547}$$

which is positive for $0 < (\phi_L - \phi_R) < \pi$. The second solution has the energy

$$E_2 = -|\Delta| \cos\frac{(\phi_L - \phi_R)}{2} \ , \tag{548}$$

which is positive for $\pi < (\phi_L - \phi_R) < 2\pi$. These results are summarized in Fig. 28. Using

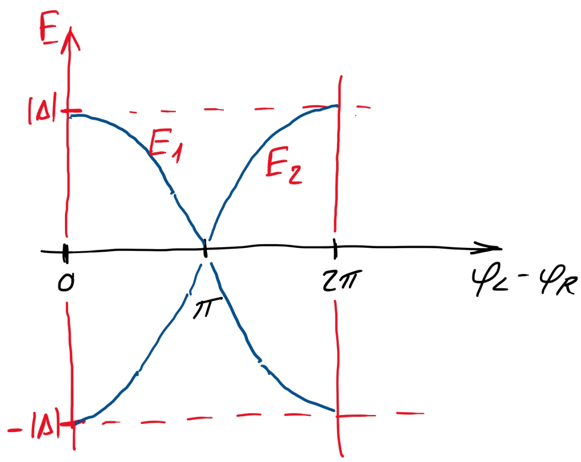

FIG. 28: Andreev Bound States in an ideal SNS junction.

(526) we can now calculate the contribution of theses Andreev bound states to the Josephson current. We obtain (at $T = 0$)

$$\begin{aligned} I_{\text{ABS}} &= -\frac{2\pi c}{2\Phi_0}\sum_{n>0}\frac{\partial E_n}{\partial(\phi_L - \phi_R)} = -\frac{2e}{2\hbar}\sum_{n>0}\frac{\partial E_n}{\partial(\phi_L - \phi_R)} \\ &= \begin{cases} \frac{|\Delta| e}{\hbar}\sin\frac{\phi_L - \phi_R}{2} & \text{for} \quad 0 < \phi_L - \phi_2 < \pi \ , \\ -\frac{|\Delta| e}{\hbar}\sin\frac{\phi_L - \phi_R}{2} & \text{for} \quad \pi < \phi_L - \phi_2 < 2\pi \ . \end{cases} \end{aligned} \tag{549}$$

I. Long junction limit.

We now consider the case $L > \xi$. Let us reconsider the problem of Andreev reflection for the case of the boundary located at $x = L/2$. Equations (507) and (508) then should be rewritten as

$$\frac{e^{ik_eL/2} + r_N e^{-ik_eL/2}}{\sqrt{v_F}} = AU_g e^{ik_1 L/2} + BU_g^* e^{ik_2 L/2} \ ,$$
$$\frac{r_A e^{ik_h L/2}}{\sqrt{v_F}} = (AU_g^* e^{ik_1 L/2} + BU_g e^{ik_2 L/2}) e^{-i\phi} \ . \tag{550}$$

$$\frac{e^{ik_eL/2} - r_N e^{-ik_eL/2}}{\sqrt{v_F}} = AU_g e^{ik_1 L/2} - BU_g^* e^{ik_2 L/2} \ ,$$
$$\frac{r_A e^{ik_h L/2}}{\sqrt{v_F}} = (AU_g^* e^{ik_1 L/2} - BU_g e^{ik_2 L/2}) e^{-i\phi} \ . \tag{551}$$

Solving these we obtain

$$r_A = e^{i(k_e - k_h)L/2} e^{-i\phi} e^{-i\gamma(E)} \ . \tag{552}$$

For the problem of Andreev Bound State considered above we obtain the relations

$$b = e^{-i\phi_R} e^{-i\gamma(E)} e^{i(k_e-k_h)L/2} a \ . \tag{553}$$

The dual Andreev reflection at $x = -L/2$ gives (left as an exercise)

$$a = e^{i\phi_L} e^{-i\gamma(E)} e^{i(k_e-k_h)L/2} b \ . \tag{554}$$

Thus, the quantization condition reads

$$(\phi_L - \phi_R) - 2\gamma(E) + (k_e - k_h)L = 0 \ \mathrm{mod}(2\pi). \tag{555}$$

This leads to

$$(\phi_L - \phi_R) - 2\gamma(E) + \frac{2EL}{\hbar v_F} = 2\pi N. \tag{556}$$

In the limit $L > \xi$ there are multiple solutions possible (for different values of N).

J. Majorana bound states

We consider a model proposed by Kitaev [8], a 1-D p-wave superconductor. The Hamiltonian reads

$$H = \sum_{j=1}^{N-1} \left[-t c_j^\dagger c_{j+1} + \Delta c_j c_{j+1} + h.c. \right] \ . \tag{557}$$

We assume the order parameter Δ to be real. We introduce the Majorana operators (not really related to Majorana particles)

$$
\begin{aligned}
c_j &= \frac{1}{2}(\gamma_{A,j} + i\gamma_{B,j}) \\
c_j^\dagger &= \frac{1}{2}(\gamma_{A,j} - i\gamma_{B,j}) \ .
\end{aligned} \tag{558}
$$

The inverse relations read

$$
\begin{aligned}
\gamma_{A,j} &= c_j + c_j^\dagger \\
\gamma_{B,j} &= -i(c_j - c_j^\dagger) \ .
\end{aligned} \tag{559}
$$

The commutation relations of the Majorana operators read $\{\gamma_{\alpha,j}, \gamma_{\alpha',j'}\}_+ = 2\delta_{\alpha,\alpha'}\delta_{j,j'}$. Here $\alpha, \alpha' = A/B$. In particular $\gamma_{\alpha,j}^2 = 1$. Also these operators are Hermitian, $\gamma_{\alpha,j}^\dagger = \gamma_{\alpha,j}$. Substituting we obtain

$$
H = \frac{1}{4}\sum_{j=1}^{N-1}\left[-t(\gamma_{A,j} - i\gamma_{B,j})(\gamma_{A,j+1} + i\gamma_{B,j+1}) + \Delta(\gamma_{A,j} + i\gamma_{B,j})(\gamma_{A,j+1} + i\gamma_{B,j+1}) + h.c.\right] \ . \tag{560}
$$

The AA and BB terms vanish and we are left with

$$
H = \frac{i}{2}\sum_{j=1}^{N-1}\left[(-t+\Delta)\gamma_{A,j}\gamma_{B,j+1} + (t+\Delta)\gamma_{B,j}\gamma_{A,j+1}\right] \ . \tag{561}
$$

An interesting situation arises if $\Delta = t$. We obtain

$$
H = i\sum_{j=1}^{N-1} t\gamma_{B,j}\gamma_{A,j+1} \ . \tag{562}
$$

Two Majoranas are not involved in this Hamiltonian and, thus, commute with it. These are $\gamma_L \equiv \gamma_{A.1}$ and $\gamma_R \equiv \gamma_{B,N}$. This means that all the eigenstates including the ground state are double degenerate. Indeed from γ_L and γ_R we can form a new pair of Fermi operators

$$
d \equiv \frac{1}{2}(\gamma_L + i\gamma_R) \quad \text{and} \quad d^\dagger \equiv \frac{1}{2}(\gamma_L - i\gamma_R) \ . \tag{563}
$$

The operators d and $d^\dagger$ commute with the Hamiltonian. The doubling of the states in according to the occupation number $d^\dagger d$. If there exist a ground state $|g0\rangle$ such that $d\,|g0\rangle = 0$, then also the state $|g1\rangle = d^\dagger\,|g0\rangle$ is a ground state, i.e., it has the same energy.

Consider a more general model

$$
H = -\mu\sum_n c_n^\dagger c_n + \sum_n\left[-tc_{n+1}^\dagger c_n + h.c.\right] + \sum_n\left[\Delta c_n c_{n+1} + h.c.\right] \ . \tag{564}
$$

An infinite (periodic) system can be diagonalized by transforming to the Fourier space. Namely, we introduce

$$c_n = \frac{1}{\sqrt{N}} \sum_k c_k e^{ikn} \,, \tag{565}$$

where N is the number of sights. Substituting we obtain

$$H = -\mu \sum_k c_k^\dagger c_k + \sum_k \left[-t c_k^\dagger c_k e^{-ik} + h.c. \right] + \sum_k \left[\Delta c_{-k} c_k e^{ik} + h.c. \right] \,. \tag{566}$$

Symmetrizing with respect to $k \leftrightarrow -k$ we obtain

$$H = -\mu \sum_k c_k^\dagger c_k + \sum_k \left[-2t \cos(k) c_k^\dagger c_k \right] + \sum_k \left[i\Delta c_{-k} c_k \sin(k) + h.c. \right] \,. \tag{567}$$

Rewrite this in a matrix form

$$H = \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \begin{pmatrix} -\mu - 2t\cos k & -i\Delta \sin k \\ i\Delta \sin k & 0 \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \tag{568}$$

And in a symmetric form

$$H = \frac{1}{2} \sum_k \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \begin{pmatrix} -\mu - 2t\cos k & -2i\Delta \sin k \\ 2i\Delta \sin k & \mu + 2t\cos k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} + const. \tag{569}$$

We can rewrite the BdG Hamiltonian using the Pauli matrices

$$h_{BdG} = \left(-\mu - 2t\cos k \right) \tau_z + 2\Delta \sin k \, \tau_y \,. \tag{570}$$

This Hamiltonian possesses the particle-hole symmetry

$$C^{-1} h_{BdG} C = -h_{BdG}^* \,. \tag{571}$$

with $C = \tau_x$. To see this one has to take into account that complex conjugation involves $k \to -k$, i.e., $h_{BdG}^* = h_{BdG}^*(-k)$. Also the field

$$\Psi_n = \begin{pmatrix} c_n \\ c_n^\dagger \end{pmatrix} = \frac{1}{\sqrt{N}} \sum_k \begin{pmatrix} c_k e^{ikn} \\ c_k^\dagger e^{-ikn} \end{pmatrix} = \frac{1}{\sqrt{N}} \sum_k \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} e^{ikn} \tag{572}$$

satisfies, of course,

$$C\Psi_n = \left(\Psi_n^\dagger \right)^T \,. \tag{573}$$

The Majorana edge states appear in the so-called topological phase. The simplest way to identify this phase is to write h_{BdG} as

$$h_{BdG} = \vec{d}(k)\vec{\tau} \,, \tag{574}$$

and follow the trajectory of vector $\vec{d}(k) = (0, 2\Delta \sin k, -\mu - 2t\cos k)$ in the Brillouin zone: $k = [-\pi, \pi]$. The eigenenergies are given by

$$E(k) = \pm\sqrt{\left[\vec{d}(k)\right]^2} = \pm\sqrt{(-\mu - 2t\cos k)^2 + (2\Delta \sin k)^2}\ . \tag{575}$$

The topological and the trivial phases are shown in Fig. 29. The topological phase occurs

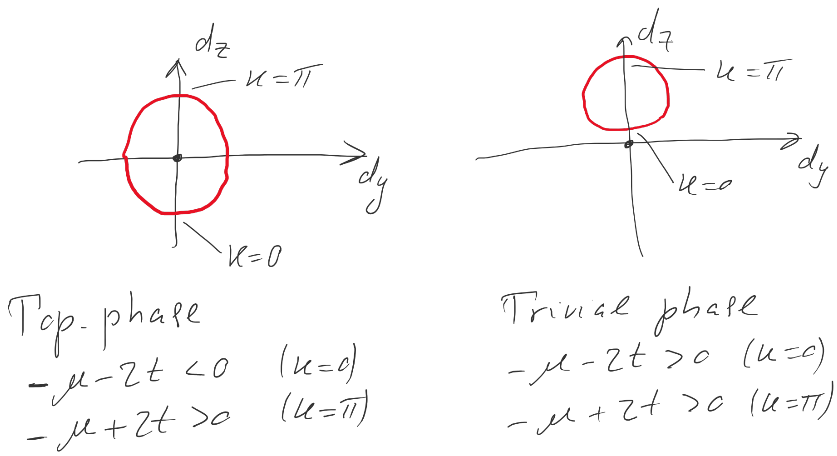

FIG. 29: Topological and trivial phases of the Kitaev model.

for $-2t < \mu < 2t$. A transition between the phases requires closing the gap either at $k = 0$ or at $k = \pi$.

1. *Domain wall and a zero (Majorana) mode.*

Consider the long-wave limit $k \approx 0$ in the vicinity of the phase transition $\mu \approx -2t$. We linearize (570) and obtain

$$h_{BdG} = (-\mu - 2t\cos k)\,\tau_z + 2\Delta \sin k\,\tau_y \approx m\tau_z + 2\Delta k\tau_y\ . \tag{576}$$

Here $m \equiv -\mu - 2t$. We can go back to the (continuous) coordinate representation. We consider a smooth domain wall $m(x)$ such that $m(x \to -\infty) = -m$ (topological phase) and $m(x \to \infty) = m$ (trivial phase). The Hamiltonian can be written as

$$h_{BdG} = m(x)\tau_z - i\hbar v(\partial/\partial x)\tau_y\ . \tag{577}$$

Here $v = 2\Delta/\hbar$ (in proper units $2\Delta a/\hbar$, where a is the lattice constant) is the velocity. The zero mode can be found solving

$$0 = h_{BdG}\Phi = m(x)\tau_z\Phi(x) - i\hbar v(\partial/\partial x)\tau_y\Phi(x)\ , \tag{578}$$

where $\Phi(x) = (\phi_1(x), \phi_2(x))^T$ is a two-component (spinor) wave function. This gives

$$(\partial/\partial x)\Phi = \frac{m(x)}{\hbar v}\tau_x \Phi \ . \tag{579}$$

Two possible solutions are proportional to the eigenvectors of τ_x. Namely

$$\Phi(x) = e^{\pm\frac{1}{\hbar v}\int\limits_0^x dx\, m(x)} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \ . \tag{580}$$

In our case only the variant with minus converge at both limits, thus

$$\Phi(x) = e^{-\frac{1}{\hbar v}\int\limits_0^x dx\, m(x)} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \ . \tag{581}$$

2. Physical realizations of Majorana wires.

Wire with strong spin orbit interaction, magnetic field and proximity induced superconducting correlations [9–11]

$$h_{\rm BdG} = \left(\frac{p^2}{2m} - \mu + up\,\sigma_y\right)\tau_z + B\sigma_z - \Delta_0\tau_x \tag{582}$$

Particle-hole symmetry with $C = \tau_y\sigma_y$. One considers the regime in which $B \gg \Delta_0$ and $B \gg mu^2$. In this case one can reduce to a single spin component

$$h_{\rm BdG} = \left(\frac{p^2}{2m} - \mu_{\rm eff}\right)\tau_z - vp\tau_y \tag{583}$$

Particle-hole symmetry with $C = \tau_x$. Here $v \sim \frac{u\Delta_0}{B}$.

$$\hat{\mathcal{H}} = \frac{1}{2}\int {\rm d}x \begin{pmatrix} \hat{\psi}(x) \\ \hat{\psi}^\dagger(x) \end{pmatrix}^\dagger \begin{pmatrix} -\frac{1}{2m}\partial_x^2 - \mu(x) & v\,\partial_x \\ -v\,\partial_x & \frac{1}{2m}\partial_x^2 + \mu(x) \end{pmatrix} \begin{pmatrix} \hat{\psi}(x) \\ \hat{\psi}^\dagger(x) \end{pmatrix} \tag{584}$$

The BdG equations read

$$\begin{pmatrix} -\frac{1}{2m}\partial_x^2 - \mu(x) & v\,\partial_x \\ -v\,\partial_x & \frac{1}{2m}\partial_x^2 + \mu(x) \end{pmatrix} \begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} = \epsilon_n \begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} \ . \tag{585}$$

The two-component wave function

$$\Phi_n = \begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} \ . \tag{586}$$

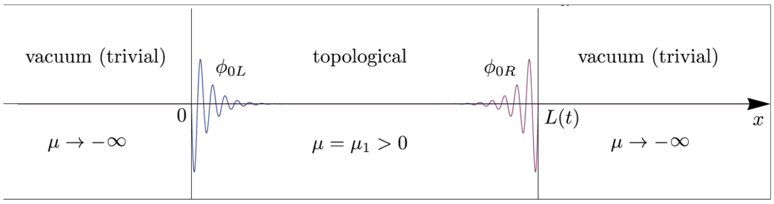

FIG. 30: Wave functions of the Majorana edge modes.

The quasiparticle operators read

$$\alpha_n \equiv \int dx\, \Phi_n^\dagger(x)\Psi(x) = \int dx\, \begin{pmatrix} f_n^*(x) & g_n^*(x) \end{pmatrix} \begin{pmatrix} \hat\psi(x) \\ \hat\psi^\dagger(x) \end{pmatrix}$$
$$= \int dx\, \left(f_n^*(x)\hat\psi(x) + g_n^*(x)\hat\psi^\dagger(x) \right) \ . \tag{587}$$

Particle-hole symmetry

$$\Phi_{-n} = C\Phi_n^* = \begin{pmatrix} g_n^*(x) \\ f_n^*(x) \end{pmatrix} \quad , \quad \epsilon_{-n} = -\epsilon_n \ , \tag{588}$$

and

$$\alpha_{-n} = \int dx\, \left(g_n(x)\hat\psi(x) + f_n(x)\hat\psi^\dagger(x) \right) = \alpha_n^\dagger \ . \tag{589}$$

If $\epsilon_1 = \epsilon_{-1} = 0$ one can form superpositions of these two. For example we can construct (real) Majorana operators

$$\gamma_L = \alpha_1 + \alpha_1^\dagger \quad , \quad i\gamma_R = \alpha_1 - \alpha_1^\dagger \ . \tag{590}$$

The corresponding wave functions are easy to find:

$$\gamma_{L/R} = \int dx\, \Phi_{L/R}^\dagger(x)\Psi(x) \ , \tag{591}$$

where

$$\Phi_L = \Phi_1 + \Phi_{-1} = \begin{pmatrix} f_1(x) + g_1^*(x) \\ g_1(x) + f_1^*(x) \end{pmatrix} \ , \tag{592}$$

$$\Phi_R = \frac{\Phi_1 - \Phi_{-1}}{i} = \frac{1}{i} \begin{pmatrix} f_1(x) - g_1^*(x) \\ g_1(x) - f_1^*(x) \end{pmatrix} \ . \tag{593}$$

The wave functions $\Phi_{L/R}$ satisfy $\Phi_L = C\Phi_L^*$ and $\Phi_R = C\Phi_R^*$. They are eigenvectors of the BdG Hamiltonian with zero energy. Most importantly they are localized at different edges of the wire.

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