Ecole GDR MICO
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Introduction to Superconductivity Theory

Indranil Paul

indranil.paul@grenoble.cnrs.fr

www.neel.cnrs.fr

Free Electron System

Hamiltonian $H = \sum_i p_i^2/(2m) - \mu N, \; i=1,\ldots,N$.
μ is the chemical potential. N is the total particle number.

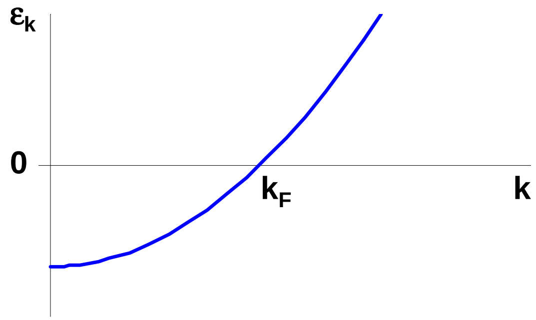
Momentum $\hbar k$ and spin σ are good quantum numbers.
$H = 2 \sum_k \varepsilon_k n_k$. The factor 2 is due to spin degeneracy.

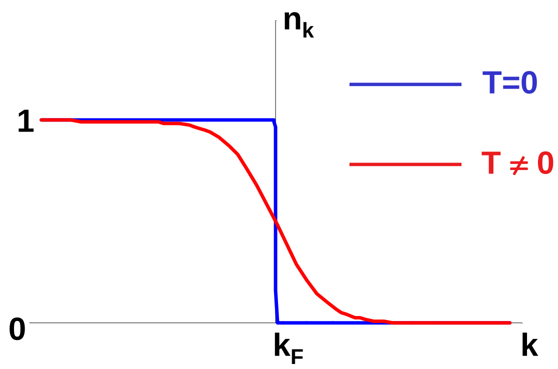
$\varepsilon_k = (\hbar k)^2/(2m) - \mu$, is the single particle spectrum.

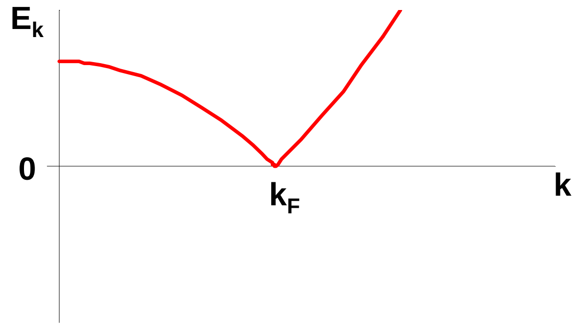
n_k is the Fermi-Dirac distribution. $n_k = 1/[e^{\varepsilon_k/(k_B T)} + 1]$

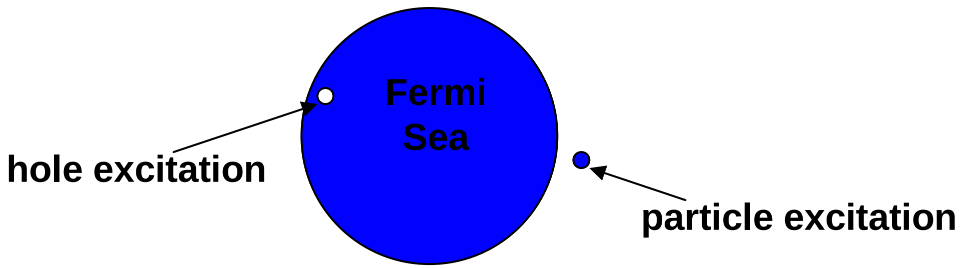
The ground state is a filled Fermi sea (Pauli exclusion).
Fermi wave-vector $k_F = (2\, m\, \mu)^{1/2}$.

Particle- and hole- excitations around k_F have vanishingly low energies. Excitation spectrum $E_K = |k^2 - k_F^2|/(2m)$.
Finite density of states at the Fermi level.







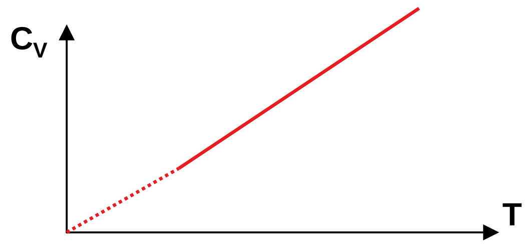


Metals: Nearly Free "Electrons"

The electrons in a metal interact with one another with a short range repulsive potential (screened Coulomb). The phenomenological theory for metals was developed by L. Landau in 1956 (Landau Fermi liquid theory). This system of interacting electrons is adiabatically connected to a system of free electrons. There is a one-to-one correspondence between the energy eigenstates and the energy eigenfunctions of the two systems. Thus, for all practical purposes we will think of the electrons in a metal as non-interacting fermions with renormalized parameters, such as $m \to m^*$. (remember Thierry's lecture)

(i) <u>Specific heat</u> (C_V): At finite-T the volume of excitations $\sim 4\pi k_F^2 \Delta k$, where $E_k \sim (\hbar^2 k_F/m)\,\Delta k \sim k_B T$. This gives free energy $F \propto -T^2$.

$C_V = \gamma T$.

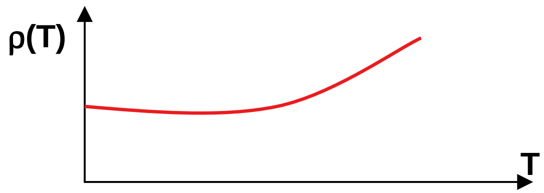


(ii) <u>Landau Diamagnetism</u> (χ_L): A uniform magnetic field H affects the orbital motion of the electrons (Lorentz force). $H = \sum_i (p_i - eA/c)^2/(2m)$.

$M = \chi_L H$, $\chi_L = -(e^2 k_F)/(12\pi^2 mc^2)$. M is anti-parallel to H.

Real metals are weakly diamagnetic.

(iii) <u>Finite resistivity</u> (ρ): Metals carry current following Ohm's law $E = \rho J$. There is a corresponding voltage drop V. Usually ρ increases with temperature. (remember Kamran's lecture)



A quick reminder: magnets, paramagnets & diamagnets

$B = H + 4\pi M$ (constitutive relation).

H is the external magnetic field.

M is the magnetization in a material in response to H.
(dM/dH) is the magnetic susceptibility (χ_m).

B is the “net” magnetic field in the system. Also called magnetic field induction.

In a non-magnetic material (such as vacuum, M=0 no matter what) B = H.

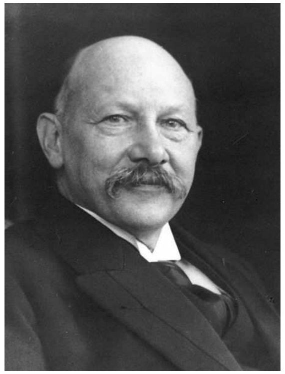
(a) Magnet: $M \neq 0$ even when H is zero.
E.g.: Fe, Ni (ferromagnet) and Cr (antiferromagnet).

(b) Paramagnet: when χ_m is positive. In response to H there is a M in the same direction. Most metals are here.

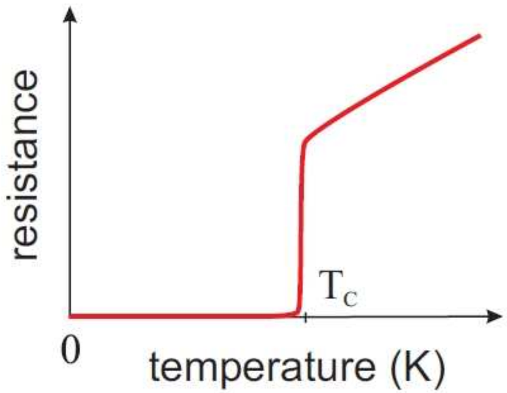
(c) Diamagnet: when χ_m is negative. In response to H there is a M in the opposite direction. Eg: Bismuth.

Electrons have two sources of M: (i) electron spin [Zeeman term $H(n_\uparrow - n_\Downarrow)$]
(ii) orbital contribution: $p \rightarrow (p - eA/c)$ (remember Lorentz force).

Discovery of Superconductivity



Nobel Prize 1913



In 1908 Heike Kamerlingh Onnes liquified He. In 1911 he discovered superconductivity in Hg. For temperatures below $T_c \approx 4K$ the resistance goes to zero.

Can we think of a superconductor as an ideal conductor for which $\rho = 0$?
The answer is NO.
The response of a superconductor to a magnetic field (Meissner effect) is different from that of an ideal conductor.

Maxwell's Equations

1. $\nabla \cdot \mathbf{E} = 4\pi n$ (Gauss's law)

2. $\nabla \times \mathbf{E} = - \partial \mathbf{B}/(c\, \partial t)$ (Faraday's law of induction)

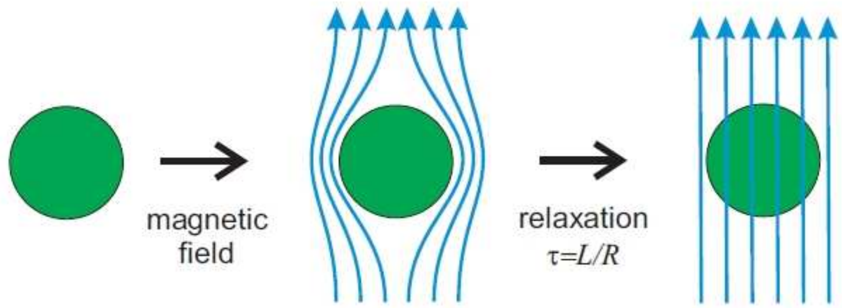
3. $\nabla \cdot \mathbf{B} = 0$ (no magnetic-monopole)

4. $\nabla \times \mathbf{B} = (4\pi/c)\, \mathbf{J} + \partial \mathbf{E}/(c\, \partial t)$ (Ampere's law + Maxwell's correction)

Conductors in a Magnetic Field

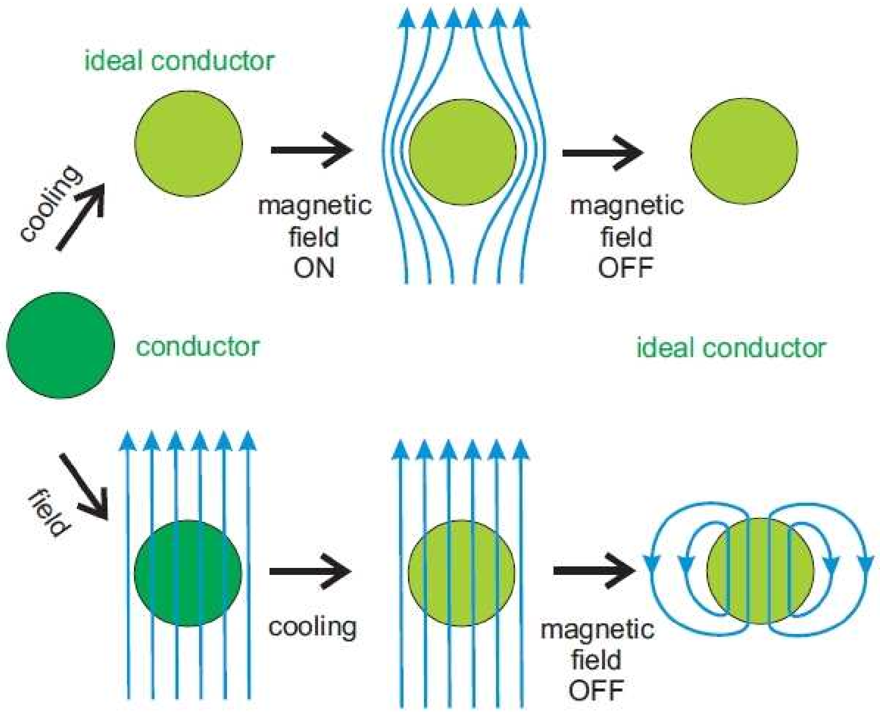
A real conductor in a magnetic field

A magnetic field induces a screening current [Faraday's' law, $\nabla \times E = - \partial B/(c \partial t)$]. In a real conductor the screening current decays, and in equilibrium the magnetic field penetrates almost entirely into the metal (weak diamagnetism).

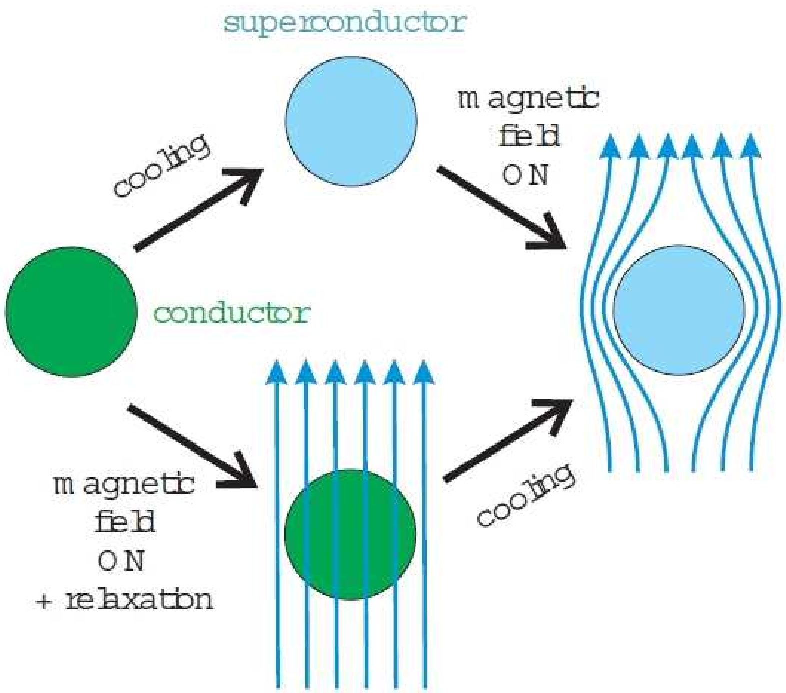


An ideal conductor in a magnetic field

$E = \rho J = 0$.
Thus, $\partial B/(c \partial t) = - \nabla \times E = 0$.
B = constant, inside an ideal conductor.
The final state depends on whether the system was cooled below T_c in the presence/absence of a magnetic field.



Superconductor in a Magnetic Field: Meissner Effect



Irrespective of whether the system was cooled below T_c in the presence/absence of a magnetic field, B = 0 inside a superconductor (a perfect diamagnet).

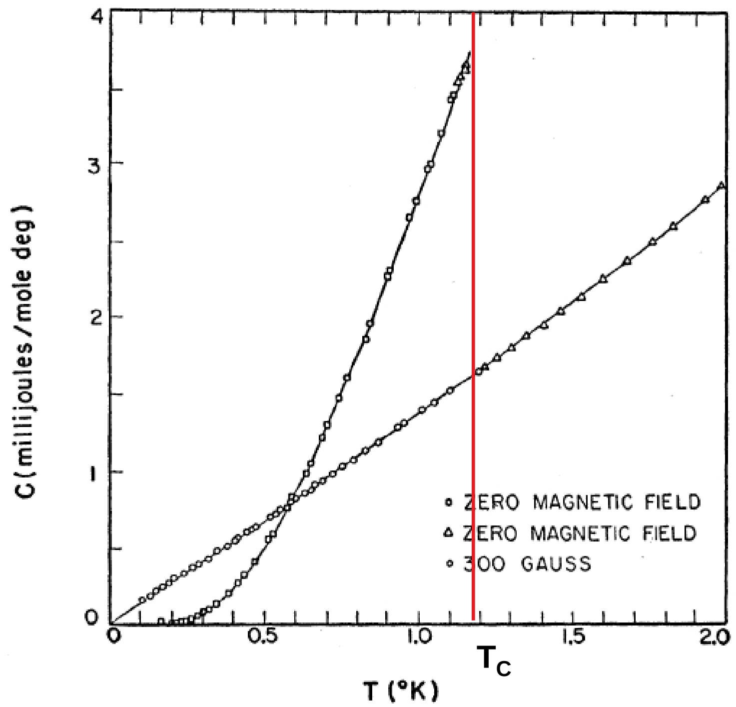
This remarkable property of a superconductor was discovered by W. Meissner and R. Ochsenfeld in 1933.

Later we will understand it as a consequence of phase rigidity in a superconductor.

Thermodynamic property: Specific heat

(i) For $T > T_C$, $C_V \approx \gamma T$.

(ii) At T_C the specific heat jumps (typical signature of a mean field type phase transition).
As $T \to 0$, $C_V \approx A\, e^{-\Delta/(k_B T)}$, with $\Delta \approx 1.44\, k_B T_C$.
Evidence for an energy gap between the ground state and the excited states of a superconductor (very different from a metal).



Specific heat of Al with $T_C \approx 1.2$ K.
N. E. Phillips, Phys. Rev. 114, 676 (1959)

Note: A magnetic field H = 0.03 T suppresses T_C and the appearance of the superconducting state. Sufficiently large magnetic fields destroy superconductivity and brings back metallicity.

Summary

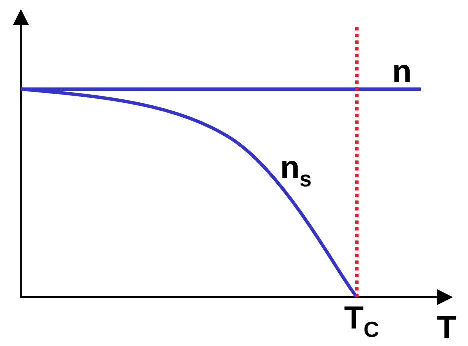
1. A superconductor is a zero resistance state (a resolution limited statement).

2. It is a perfect diamagnet. B=0 in the bulk irrespective of how the state was prepared. Different from an ideal metal (perfect diamagnet only if there is field-after-cooling); and certainly very different from any realistic metal (weak diamagnets).

3. Evidence of an energy gap between the ground state and the excited states of a superconductor.

A superconductor is a new phase of matter compared to a metal.

London equations & the two-fluid model (1935)



For $T < T_C$, the total density of electrons $n = n_s + n_n$.
n_s = density of superconducting electrons;
n_n = density of normal electrons.
For $T \to 0$, $n_s \to n$; and for $T \to T_C$, $n_s \to 0$.
The normal electrons conduct with finite resistance, while the superconducting electrons have dissipationless flow.

$m\,(dv_s)/(dt) = -\,eE$ (Newton's 2nd law). Since $J = -\,e n_s v_s$,

$$dJ/dt = n_s e^2/m\, E \qquad \text{(1st London equation)}$$

Combined with Maxwell eqn $\nabla \times E = -\,\partial B/(c\,\partial t)$ gives $\partial/\partial t\,[\nabla \times J + n_s e^2/(mc)\, B] = 0$. Trivially satisfied for static B and J. Thus, it does not necessarily imply B=0 inside a superconductor (Meissner effect).

$$\nabla \times J + n_s e^2/(mc)\, B = 0 \qquad \text{(2nd London equation)}$$

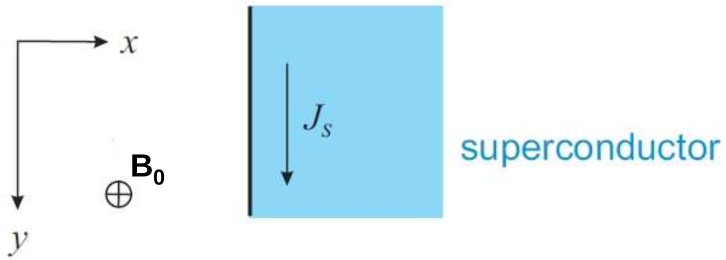
The 2nd London equation implies Meissner effect.

Does a perfect diamagnet imply an ideal conductor?
Derive 1st London eqn from the 2nd London eqn.

B-field expulsion: London penetration depth

The London eqn $\nabla \times J = -n_s e^2/(mc)B$ combined with Maxwell eqn $\nabla \times B = (4\pi/c)J$ gives

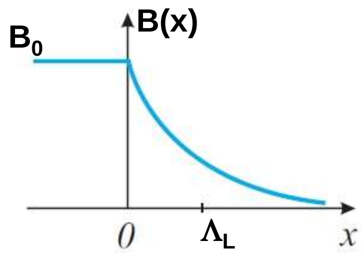
$\nabla^2 B = \Lambda_L^{-2} B, \nabla^2 J = \Lambda_L^{-2} J,$ $\Lambda_L = [mc^2/(4\pi n_s e^2)]^{1/2}$ (London penetration depth).



Eqn: $d^2B/(dx^2) = \Lambda_L^{-2} B(x)$.

Solution:

$$\begin{cases} B(x) = B_0\, e^{-x/\Lambda_L}. \\ J(x) = c B_0/(4\pi\Lambda_L)\, e^{-x/\Lambda_L}. \end{cases}$$



Meissner effect: In response to B_0, the superconductor develops a supercurrent J at the surface which screens the B-field.

Currents & B-fields exist only within a boundary layer of thickness Λ_L.

How do we justify the 2nd London equation?

Ginzburg Landau theory ......

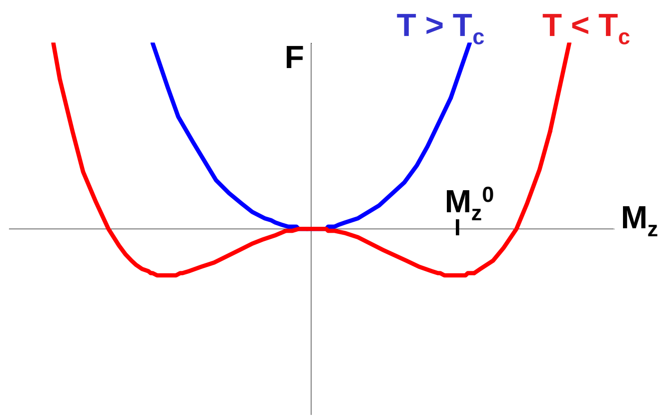
Landau's theory of phase transitions

A phase transition between a symmetrical high-T phase & a symmetry-broken low-T phase is described by an order parameter (OP). The OP is zero in the symmetrical phase and is non-zero in the symmetry-broken phase. Near T_C the free energy can be expressed in powers of the OP, keeping only those terms that are allowed by the symmetries of the system. The equilibrium value of the OP is obtained by minimizing the free energy with respect to the OP.

Example: paramagnet-ferromagnet transition
Let us assume that there is strong magnetic anisotropy and the magnetic moments order along the z-direction (easy axis).
In this case the relevant symmetry is time reversal symmetry.
The order parameter is M_z (magnetization along z-direction).

$F[M_z] = a\, M_z^2/2 + b\, M_z^4/4 + \cdots$.   Why isn't M_z^3 allowed?

At the phase transition "a" changes sign: $a = a'\,(T - T_C)$.
Below T_C a spontaneous magnetization $M_z^0 = (-a/b)^{1/2}$ develops.



Ginzburg Landau theory

The order parameter to describe the phase transition between a high-T metallic phase and a low-T superconducting state is a complex-valued function $\Psi(r)$.

Physical meaning of $\Psi(r)$

We will learn later that the basic building blocks of a superconductor are bound pairs of electrons (Cooper pairs). $\Psi(r)$ is the wave-function describing the centre of mass motion of a Cooper pair. All the pairs are in the same quantum state (a condensate). A single wave-function describes the superconducting electrons.

$\Psi = (n_s/2)^{1/2}\, e^{i\,\Phi}$ ($|\Psi|^2$ gives density of superconducting electrons).

Symmetry: In a superconductor U(1) symmetry is broken. This is associated with particle number conservation. $F[\Psi]$ must be invariant under $\Psi \rightarrow \Psi\, e^{i\,\alpha}$.

Homogeneous case: $F = F_n + a\,|\Psi|^2 + b\,|\Psi|^4/2$, and $a = a'\,(T\text{-}T_c)$.

Calculate the specific heat discontinuity at T_c.

How to include B-field and write down the current J in terms of $\Psi(r)$?

Ginzburg Landau theory & Meissner effect

Finite B-field produces variations in $\Psi(r)$. for slow variations add a term
$c \int dV\, |\nabla\Psi(r)|^2$ to the free energy. Variations of the order parameter cost energy.

GL: $c = \hbar^2/[2(2m)]$!! (c is not any arbitrary constant)

Note: this theory has no dynamics and is not quantum mechanical per se.
The notion of quantum mechanics enters through the coefficient c.

Justification: With this choice of c the term looks like $\int \Psi^* \, p^2/(4m)\, \Psi \, dV$ which is like the "kinetic energy" of an entity with mass 2m. Gives the notion of current.

Add magnetic field via gauge invariance: $p \to p - 2eA/c$ (please note the 2e)

$$F = F_n(B=0) + \int dV \, [\, B^2/(8\pi) + \hbar^2/(4m)|(\nabla - 2ieA/(\hbar c))\Psi(r)|^2 + a|\Psi|^2 + b|\Psi|^4/2 \,].$$

For low-B field n_s is homogeneous.

$$F_s = F_s(B=0) + \int dV \, [\, B^2/(8\pi) + \hbar^2 n_s/(8m)\, (\nabla\Phi - 2eA/(\hbar c))^2].$$

Note: Energy depends upon the gradient of the phase (phase stiffness).

cont.....

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Minimizing free energy with respect to A gives

$$\nabla \times \mathbf{B} = 4\pi/c \underbrace{[\hbar e n_s/(2m)\,(\nabla\Phi - 2e\mathbf{A}/(\hbar c))]}_{\mathbf{J}\ \text{(Maxwell eqn: } \nabla \times \mathbf{B} = 4\pi/c\ \mathbf{J})}.$$

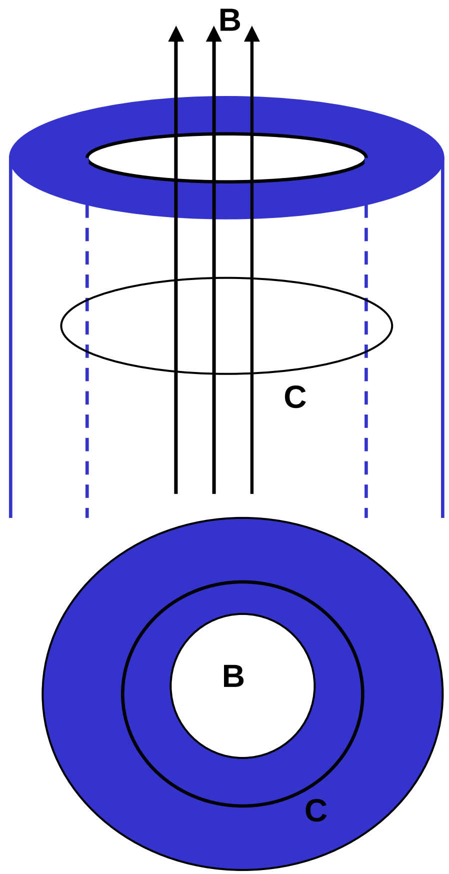
According to GL theory: $\mathbf{J} = \hbar e n_s/(2m)\,[\nabla\Phi - 2e\mathbf{A}/(\hbar c)]$.

$\nabla \times \mathbf{J} = - n_s e^2/(mc)\,\mathbf{B}$, which is the 2nd London eqn.

Summary: GL theory correctly identifies the order parameter for the metal-superconductor phase transition. It gives a correct description of the electromagnetic response of a superconductor, particularly the Meissner effect.

Note: Minimizing the free energy with respect to Ψ gives a 2nd GL equation. This is important to study how $\Psi(r)$ varies spatially in a magnetic field or at a boundary.

Flux quantization



Flux quantization is a beautiful consequence of phase stiffness.

Imagine a metal with a hole at $T > T_c$. Put B-field through the hole. The magnetic flux is $\Phi_B = \int B \cdot dS$.
Φ_B varies continuously as B is changed.

The situation is dramatically different in the superconducting phase. Φ_B changes discretely as B is changed continuously!

GL eqn for current: $J = \hbar e n_s/(2m)\,[\nabla\Phi - 2eA/(\hbar c)]$.

Consider a closed loop C deep inside the superconductor.
$\int_C J \cdot dL = 0$ (currents cannot exist in the bulk).

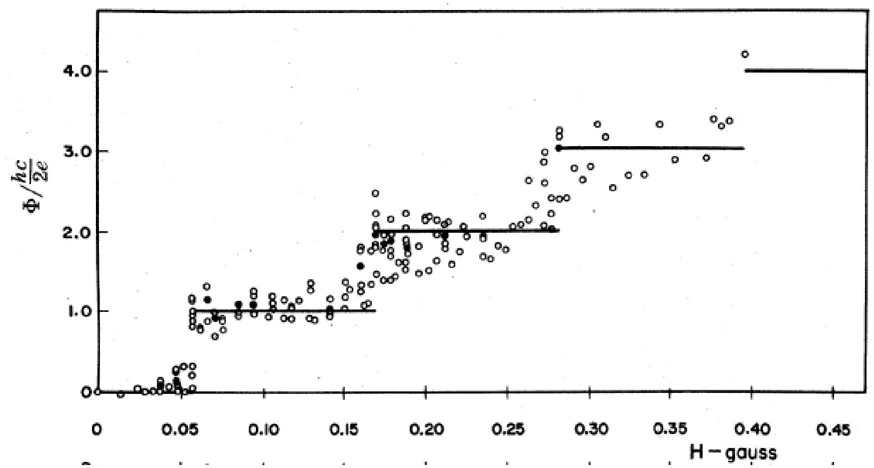
$\int_C \nabla\Phi \cdot dL = (2e/\hbar c) \int_C A \cdot dL = (2e/\hbar c)\, \Phi_B$.

Since $\Psi(r) = (n_s/2)^{1/2} e^{i\Phi}$ is single valued,
$\int_c \nabla\Phi \cdot dL = 2\pi n$, where n is an integer.

$$\boxed{\Phi_B = n\, \Phi_0,}$$

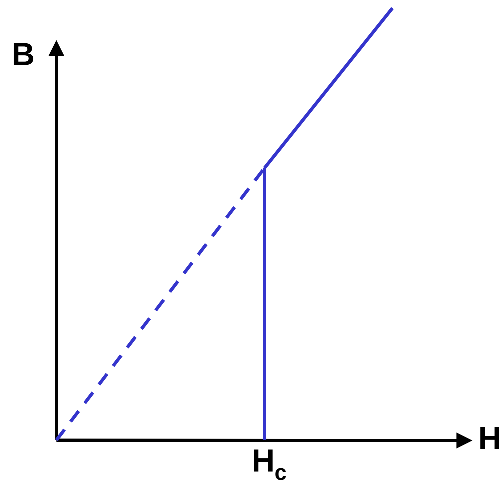
where $\Phi_0 = hc/(2e)$ is the flux quantum.

Deaver & Fairbank, PRL 7, 43 (1961).



Critical H_c and type-I superconductors

Does Meissner effect (expulsion of B-field) continue indefinitely as external field H is increased?



The answer is NO.

For homogeneous systems there is a critical external field H_c above which superconductivity is destroyed. These are called type-I superconductors.

<u>Thermodynamic justification</u>

In an external field H the Gibbs free energy G(T,H) is minimized.

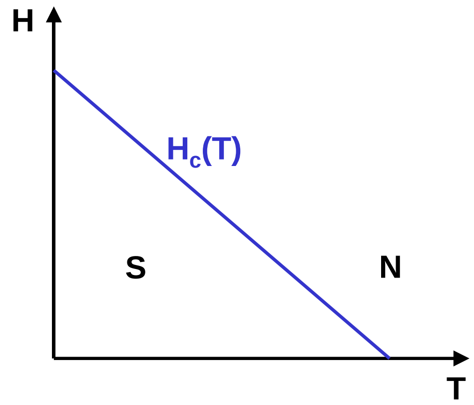
$G(T,H) = F(T,B) - B(r)\cdot H/(4\pi)$.

For a superconductor B=0.

$G_s(T,H) = a\,|\Psi|^2 + b\,|\Psi|^4/2 = -\,a^2/(2b)$.

Ignoring weak diamagentism in a metal B = H.

$G_n(T,H) = -\,H^2/(8\pi)$.



$G_s(T,H) - G_n(T,H) = -a^2/(2b) + H^2/(8\,\pi)$.

$H_c = (4\pi/b)^{1/2}\,a'\,(T_c - T)$.

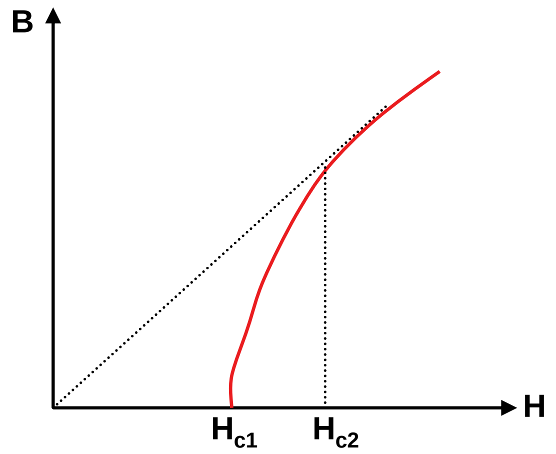
The normal metal is thermodynamically more stable for $H > H_c$.

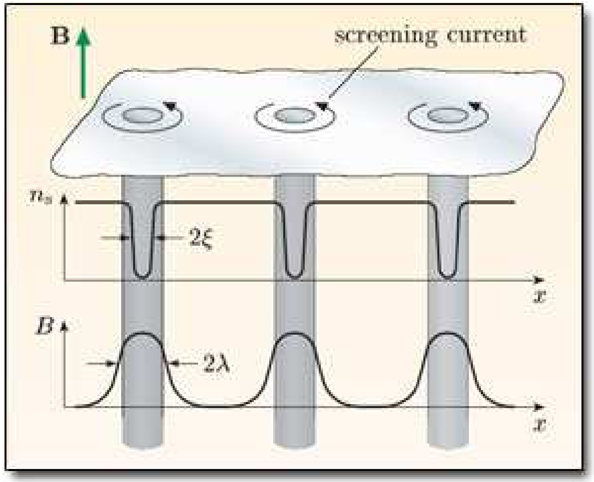
For pure metals H_c is very small ($\sim$ 0.01T).

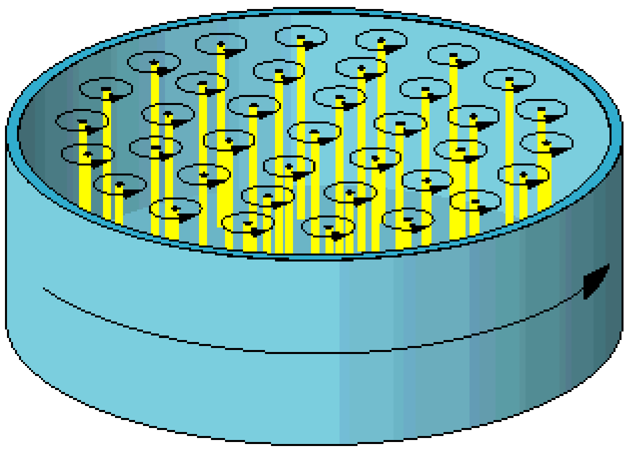
Type-II superconductors

In type-II superconductors there is a mixed phase in between the superconductor and the metal phases ($H_{c1} < H < H_{c2}$).

In this phase the B-field enters partially in the system in the form of thin filaments of magnetic flux. Within each filament the B-field is high ($B \sim H$) and the material is metallic. This is the core. A vortex of screening supercurrent circulates around the core. (Proposed by A. A. Abrikosov, Nobel prize 2003)

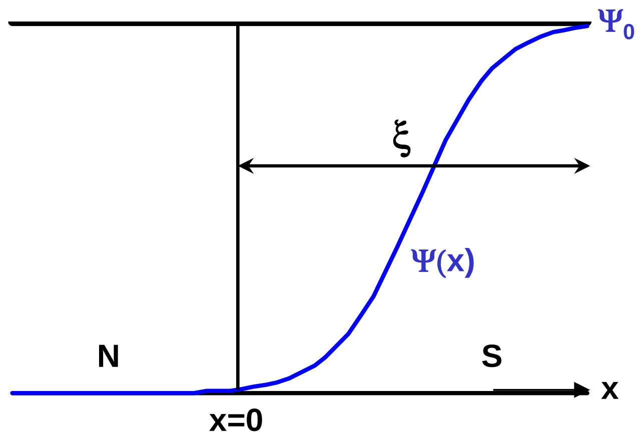






To understand the existence of the mixed phase one needs to study the boundary between a normal metal and a superconductor and the energy associated with it.

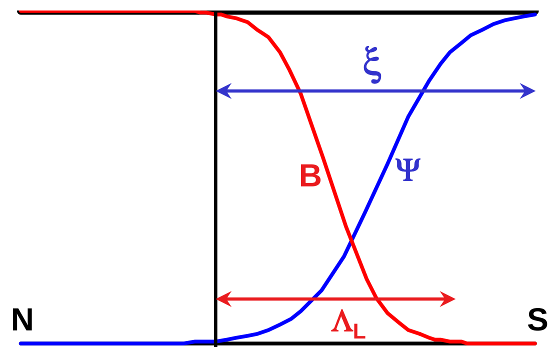
Coherence length ξ and penetration depth Λ_L



Variation of $\Psi(x)$ at a S-N boundary

GL eqn: $-\hbar^2\nabla^2/(4m)\Psi + a\Psi + b\Psi^3 = 0$.
Near boundary $\Psi \approx 0$, well inside S $\Psi = \Psi_0 = (-a/b)^{1/2}$.
Writing $\Psi = \Psi_0 - \Psi_1(x)$, we get $\Psi_1(x) = \Psi_0\, e^{-\sqrt{2}\, x/\xi}$.
$\xi = \hbar/2(m|a|)^{1/2} \propto (T_c - T)^{1/2}$. (coherence length)

Implicit in the GL eqns are two length scales:
Λ_L & ξ both proportional to $(T_c - T)^{-1/2}$. ξ is the scale over which Ψ varies and Λ_L is the scale over which B-field varies.



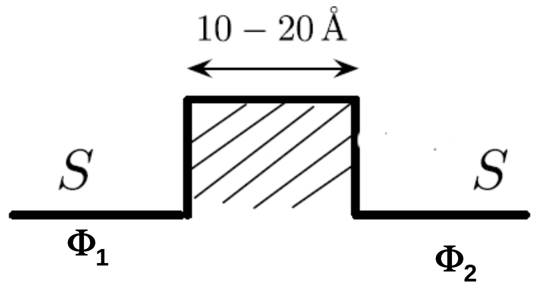
In an external field H_c the bulk Gibbs free energies are equal $G_s(H_c) = G_n(H_c) = -H_c^2/(8\pi)$. Boundary is stable. The surface energy is

$$\sigma_{ns} = \left[\underbrace{\int_{-\infty}^{\Lambda_L} dx}_{\text{magnetic energy}} + \underbrace{\int_{\xi}^{\infty} dx}_{\text{condensate energy}} - \underbrace{\int_{-\infty}^{\infty} dx}_{\text{no boundary}} \right] (-H_c^2/8\pi) = (\xi - \Lambda_L) H_c^2/8\pi$$

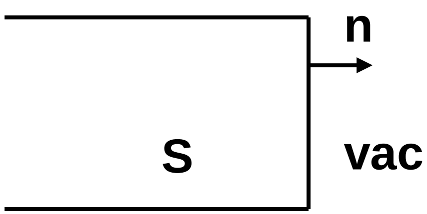
For $\xi < \sqrt{2}\,\Lambda_L$ boundaries are energetically favourable. Gives type-II superconductors.

Josephson Effect

If two superconductors are separated by a thin insulating layer, there is tunneling of Cooper pairs which sets up a dissipationless current.



$I = I_0 \sin[\Phi_2 - \Phi_1]$ (DC Josephson effect)

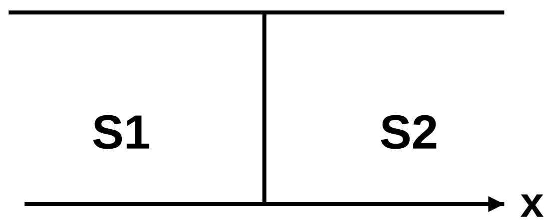


No current flows perpendicular to the boundary:

$$\mathbf{n} \cdot \underbrace{[\, -i\,\hbar\nabla\Psi - (2e/c)\, A\, \Psi]}_{\text{gauge invariant momentum}} = 0$$

$$\partial\, \psi_1/(\partial\, x) - 2ie/(\hbar c)\, A_x\, \Psi_1 = -\Psi_2/\lambda$$

$$\partial\, \Psi_2/(\partial\, x) - 2ie/(\hbar\, c)\, A_x\, \Psi_2 = \Psi_1/\lambda$$



Put this relation in the equation for current.

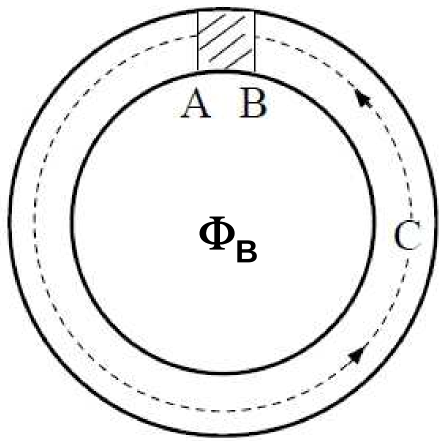
$$J = J_0 \sin(\Phi_2 - \Phi_1)$$

cont...

In the presence of a finite voltage across the junction the phase difference increases linearly in time.

$$V = \hbar/(2e)\, \partial[\Phi_2 - \Phi_1]/(\partial t)$$

In the presence of a finite voltage the supercurrent oscillates in time with frequency $2eV/\hbar$.



From flux quantization condition

$$\Phi_B - \Phi_A = 2\pi\, \Phi_B/\Phi_0$$

Differentiate with respect to time:

$$\partial[\Phi_B - \Phi_A]/(\partial t) = 2\pi/\Phi_0\, \partial/(\partial t) \int B \cdot dS$$

$$= (2e/\hbar)V$$

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Introduction to Superconductivity Theory
Part II

Indranil Paul

indranil.paul@grenoble.cnrs.fr

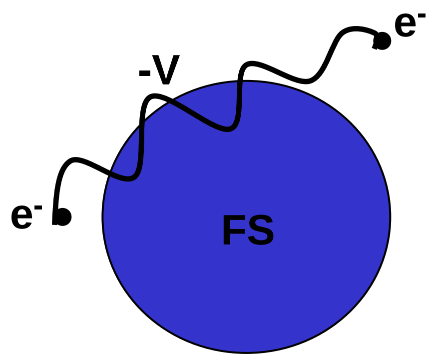
www.neel.cnrs.fr

Beginning of a microscopic theory: Cooper problem

The ground state of electrons interacting repulsively is adiabatically connected to the ground state of a system of free electrons. Pauli principle has a profound effect.
What happens when electrons attract each other?
In 1957 Leon Cooper discovered that the situation is qualitatively different: even for a small attractive force the Fermi surface becomes unstable!

<u>Cooper problem</u>

Imagine a system of N non-interacting electrons forming a Fermi sea (FS). In this background if two electrons interact attractively, what is the ground state eigen-function & eigen-energy?

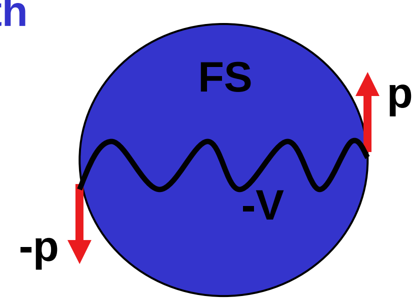


What is the ground state?

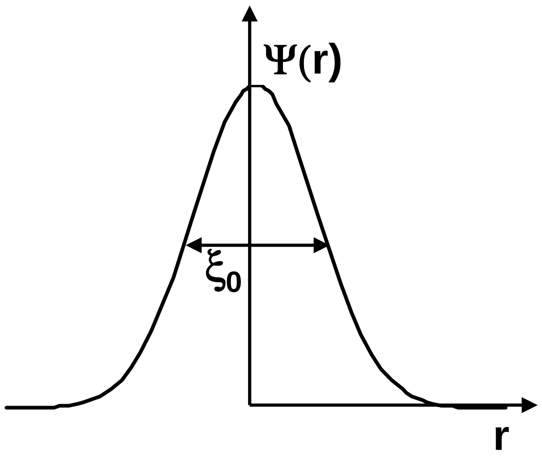
With no interaction $\Psi(r_1, r_2) \sim e^{ik_1 r_1} e^{ik_2 r_2}$; $|k_1| = |k_2| = k_F$.
$E = 2E_F$ and wavefunction is plane-wave like.

<u>Cooper's answer</u>

The two electrons form a bound state with net momentum zero.
$E = 2E_F - \Delta$, Δ is binding energy.
$\Psi(r) \to 0$, as $r \to \infty$.
$\Psi(r)$ has a spatial extent $\xi_0 = \hbar v_F/\Delta$.
ξ_0 = Pippard coherence length.



With attractive interaction two electrons form a bound state



Bound state wavefunction

Cooper pair formation: eigen-value problem

$\Psi(r_1, r_2)$ = two-electron wavefunction. Assume attractive interaction is $V(r_1 - r_2)$.

$R = (r_1 + r_2)/2$ = centre of mass coordinate; $r = (r_1 - r_2)$ = relative coordinate.
Separable: $\Psi(r_1, r_2) = \Psi(r)\,\Phi(R)$.

In the R-coordinate there is no interaction, $\Phi(R) = e^{i\,P\cdot R}$, P = total momentum.
Ground state should have zero total momentum, $\Phi(R) = 1$.
(N+2)-body problem $\rightarrow$ (N+1)-body problem.

$[-\hbar^2/(2m)(\nabla_1^2 + \nabla_2^2) + V(r)]\,\Psi(r_1 - r_2) = E\,\Psi(r_1 - r_2)$
Is this a 1-body problem?
Where is information about the remaining N-electrons?

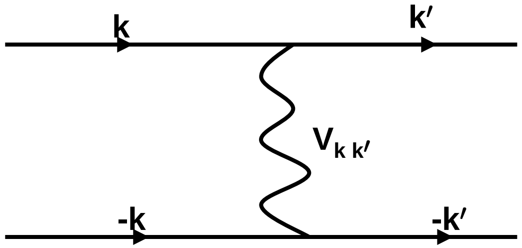
$\Psi(r_1 - r_2) = \sum_k g(k) \exp[i\,k\cdot(r_1 - r_2)]$.
g(k) = probability amplitude to find one electron in the plane-wave state $\exp[ik\cdot r_1]$ with momentum $\hbar k$, and a 2nd electron in the state $\exp[-ik\cdot r_2]$ with momentum $-\hbar k$.

$g(k) = 0, \quad \text{for } k < k_F.$

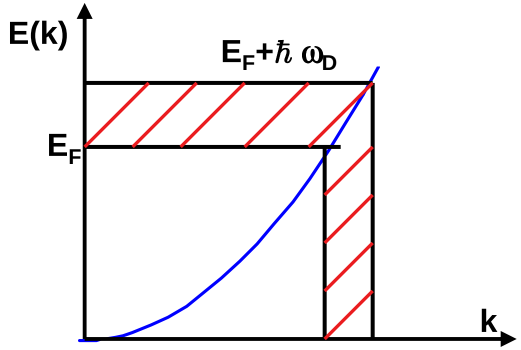
Pauli principle takes care of the N-electrons. Makes the problem truly many-body. Qualitatively different from standard 2-body bound state problems.

cont...

Fourier transform the interaction: $V_{kk'} = \int d^3(r_1-r_2)\, V(r_1-r_2)\, \exp[-i(k-k')\cdot(r_1-r_2)]$
$V_{kk'}$ = scattering amplitude of a pair $(k, -k) \rightarrow (k', -k')$.
Due to the presence of the attractive interaction, the relative momentum is not a good quantum number.



$\hbar^2 k^2/m\, g(k) + \sum_{k'}' V_{kk'}\, g(k') = E\, g(k)$.



Simplify interaction:
$V_{kk'} = -V$, for $E_F < \hbar^2 k^2/(2m), \hbar^2 k'^2/(2m) < E_F + \hbar\omega_D$
$= 0$, otherwise.
The interaction is attractive & constant in an energy interval $\hbar\omega_D$. Later we will identify $\hbar\omega_D$ as a typical energy scale of the phonons.

Write $E = 2E_F + \Delta$, where Δ is binding energy given by:

$$1 = VN_0 \int_0^{\hbar\omega_D} \frac{d\xi}{2\xi - \Delta},$$

N_0 = Density of states at E_F

$\Delta \approx -2\hbar\omega_D \exp[-2/N_0 V]$.

The two electrons form a bound state and gain energy Δ compared to plane-wave states at k_F. So they prefer to disregard the Fermi wavevector!

Comments on Cooper pairing

1. The binding energy $\Delta \sim \exp[-2/N_0 V]$ is non-analytic function of V.
The problem is intrinsically non-perturbative.

2. The bound state forms even for very small V! This is a consequence of it being a many-body problem rather than a two-body problem.

For the two-body problem no Fermi surface, i.e., $k_F = 0$. Then $N(\xi) \propto \xi^{1/2}$, $1 = V \int \xi^{1/2} \, d\xi \,/\, (2\xi - \Delta)$, is satisfied only for sufficiently large V (the log singularity is lost).

3. What about the spin of the two electrons?
We assumed V(r) is spin independent. Total spin is a good quantum number.

$g(k) = C/(E - \hbar^2 k^2/2m) \;\Rightarrow\; g(-k) = g(k)$.
The spatial part of the Cooper wavefunction is symmetric under $r_1 \leftrightarrow r_2$.
The spin part must be antisymmetric.
$\chi_{spin} = (\uparrow\Downarrow - \Downarrow\uparrow)/\sqrt{2}$, i.e., S=0 (singlet).

4. The average size of a Cooper pair is given by
the Pippard coherence length $\xi_0 = \hbar v_F/\Delta$.

$\langle r^2 \rangle = (\int d^3 r \, |\Psi(r)|^2 \, r^2)/(\int d^3 r \, |\Psi(r)|^2) = 2\,\xi_0/\sqrt{3}$.

How to generalize Cooper's answer?

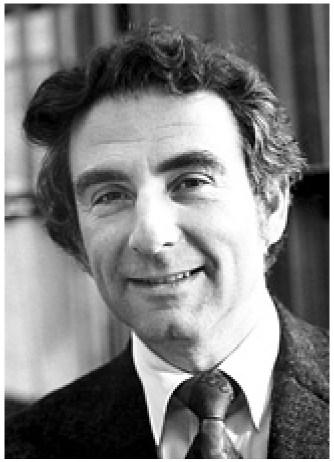
The Cooper problem showed us that when two electrons interact attractively
in the presence of a Fermi sea (filled by N other electrons), they form a bound state.

How to generalize this idea for N-electrons? How to treat them all in the same way?

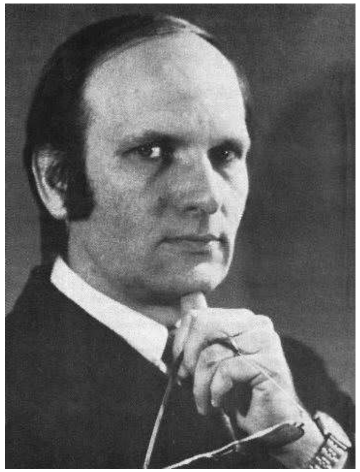
Note: In Cooper's treatment the two electrons are distinguishable from the remaining electrons forming the FS. The wavefunction is not antisymmetrized between a "soup" electron and a "chosen" electron.

Within one year of Cooper's work, in 1957 John Bardeen, Leon Cooper and Robert Schrieffer generalized the Cooper solution. With this the microscopic theory of SC was born. Nobel prize 1972.

J. Bardeen

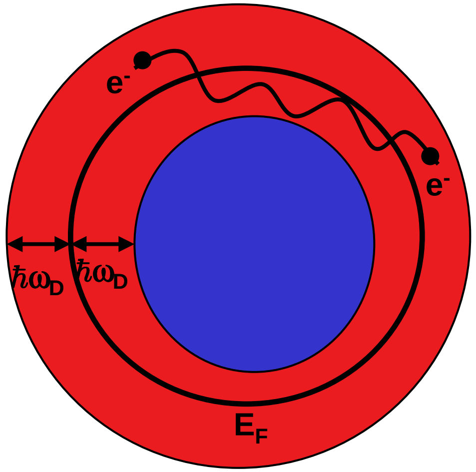


L. Cooper



R. Schrieffer

Variational Idea



Hamiltonian (H): **A system of electrons with kinetic energy $p^2/(2m)$ (H_0) and a two-particle attractive interaction (V). The interaction is "on" only for electrons within an energy range $\hbar\omega_D$ of the Fermi energy.**

We will try to find the ground state using variational method.

Strategy

1. We will propose a trial wavefunction $\Psi(\alpha, \beta....)$ in terms of parameters α, β etc.

2. We will calculate average energy $E(\alpha, \beta) = \langle \Psi | H | \Psi \rangle$.

3. We will fix the parameters α, β etc by minimizing E: $\partial E/(\partial \alpha) = 0$.

Justification

If our initial guess is good Ψ_{app} will have a lot of overlap with the exact ground state wavefunction Ψ_{ex}, i.e., $\langle \Psi_{app} | \Psi_{ex} \rangle \approx 1$.

We will know the guess is good if we can explain experimental facts.

Ψ - cookbook

A natural generalization of Copper's solution is to pair N-electrons keeping the centre of mass momentum zero.

Let us 1st pair two electrons, 1 & 2, in a state $\Phi(r_1 - r_2; \sigma_1\, \sigma_2)$.
We assume Φ is antisymmetric under $1 \leftrightarrow 2$.

Next we pair electrons 3 & 4 in the same state Φ, i.e., $\Phi(r_3 - r_4; \sigma_3\, \sigma_4)$.

And so on ...

$$\Psi_N = A\,[\Phi(r_1 - r_2; \sigma_1\, \sigma_2)\, \Phi(r_3 - r_4; \sigma_3\, \sigma_4) \cdots]$$

Expand Φ in Fourier series: $\Phi(r_1 - r_2) = \sum_k g(k)\, \overbrace{\exp[ik\cdot(r_1 - r_2)}^{\text{plane waves } (k,\, -k)}\, \underbrace{(\uparrow \Downarrow - \Downarrow \uparrow)/\sqrt{2}}_{\text{singlet}}$.

To be consistent : $g(k) = g(-k)$

$$\Phi(r_1 - r_2; \sigma_1\, \sigma_2) = \sum_k g(k)\, \underbrace{[\,|\,k\uparrow\ ; -k\Downarrow> - |k\Downarrow\ ; -k\uparrow>]/\sqrt{2}}_{|1,1>_k}. = \sum_k g(k)\, |1,1>_k = \sum_k g(k)\, c^{\dagger}_{k\uparrow}\, c^{\dagger}_{-k\Downarrow}\, |0>$$

Note: Unlike the Cooper problem the sum over k is over all momenta.

cont...

$$\Psi_N = \sum_{k_1 \cdots k_{N/2}} g(k_1) \cdots g(k_{N/2}) \; [\, |1,1>_{k_1} \otimes |1,1>_{k_2} \cdots |1,1>_{k_{N/2}} \,]$$

Turns out that for technical reasons it is difficult to work with wavefunctions with fixed number of pairs.

BCS recipe

Write a wavefunction which is a linear superposition of states with 1, 2, ⋯, N, ⋯, ∞ number of pairs.

$$\Psi_{BCS} = \lambda_2\Psi_2 + \lambda_4\Psi_4 + \cdots + \lambda_N\Psi_N + \cdots$$

$$= \prod_{\text{all } k} [\, u_k\, |0,0>_k + v_k\, |1,1>_k \,] \quad = \prod_k (u_k + v_k\, c^\dagger_{k\uparrow}\, c^\dagger_{-k\Downarrow})|0>$$

Either the pair of states (k, -k) is unoccupied with probability amplitude u_k, or both are occupied with probablility amplitude v_k. (u_k, v_k) are variational parameters we will determine.

$u_k^2 + v_k^2 = 1$ (normalization); (u_{-k}, v_{-k}) = (u_k, v_k) (even parity)

Note: $u_k = 1$ for $|k| > k_F$, $v_k = 1$ for $|k| < k_F$, and all else zero gives the ground state of non-interacting electrons (the filled Fermi sea).

Does it make physical sense?

Ψ_{BCS} is a wavefunction which is a superposition of states with different particle numbers. Is this physical?

--- in a truly isolated system this is indeed unphysical.

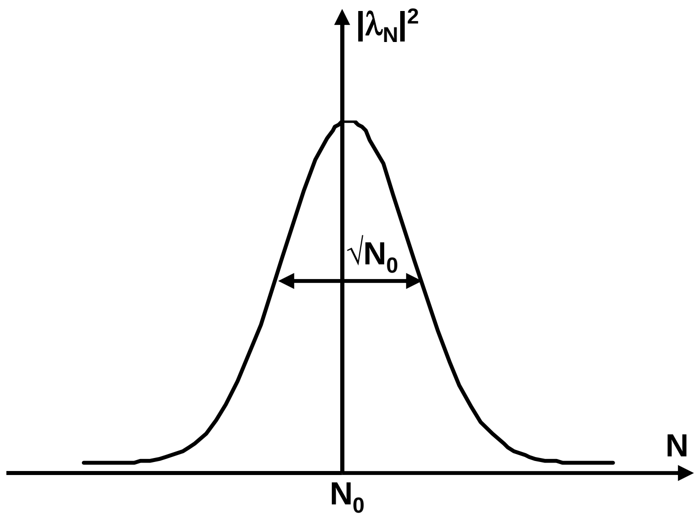
--- most experimental setups are "open" systems, such as a metal with current leads. Then particle number can fluctuate.

$\Psi_{BCS} = \sum_N \lambda_N \Psi_N$

The probability $|\lambda_N|^2$ is sharply peaked around N_0, the average particle number.

$<\Psi_{BCS}| O | \Psi_{BCS}> = <\Psi_N | O |\Psi_N> + (1/\sqrt{N})$-corrections

In the thermodynamic limit they give the same result.

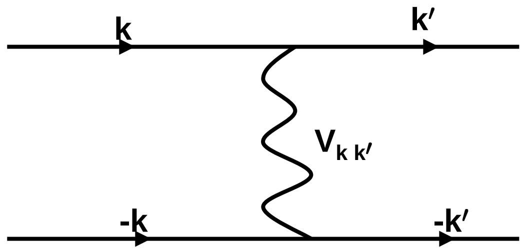


Probability $|\lambda_N|^2$ is sharply peaked

BCS equations at T=0

In Ψ_{BCS} the probability for occupying the state k (and –k) is v_k^2.

$\langle H_0 \rangle = \langle \Psi_{BCS} | H_0 | \Psi_{BCS} \rangle = 2 \sum_k \xi_k v_k^2$, ξ_k = energy of state k measured from μ.



How to calculate $\langle V \rangle$?

V describes scattering of a pair from (k, -k) to (k′, -k′) as well as scattering of unpaired electrons. But only the 1st type of scattering enter $\langle V \rangle$.

Before the scattering (k, -k) is full while (k′, -k′) is empty. Gives the amplitude ($v_k u_{k'}$).
After scattering (k, -k) is empty while (k′, -k′) is full. Gives the amplitude ($u_k v_{k'}$).

$\langle V \rangle = \langle \Psi_{BCS} | V | \Psi_{BCS} \rangle = \sum_{k,k'} V_{kk'} u_k v_k u_{k'} v_{k'}$.

We discover the existence of a new quantity called the gap function Δ_k, and an associated energy $E_k = (\xi_k^2 + \Delta_k^2)^{1/2}$.

$u_k^2 = (1 + \xi_k/E_k)/2$ and $v_k^2 = (1 - \xi_k/E_k)/2$.

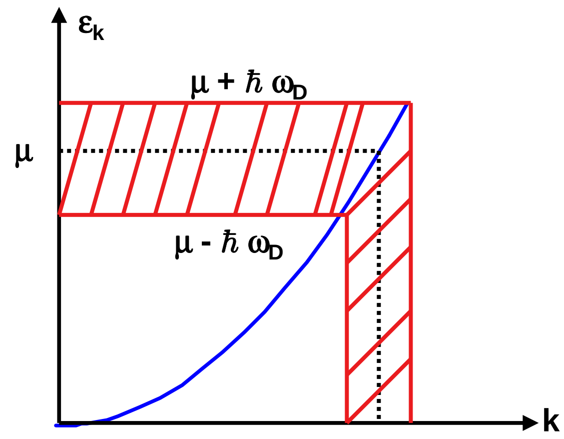
Δ_k is given by the famous BCS gap-eqn at T=0: $\Delta_k = -\sum_{k'} V_{kk'} \Delta_{k'} / (2 E_{k'})$.

A normal state is $\Delta_k = 0$, and a SC is $\Delta_k \neq 0$.

Physical Consequences

1. Simple model:

$V_{kk'} = -V$ for $|\xi_k|, |\xi_{k'}| < \hbar\omega_D$
$= 0$ outside



Interaction is isotropic $\Rightarrow \Delta_k = \Delta_0$.

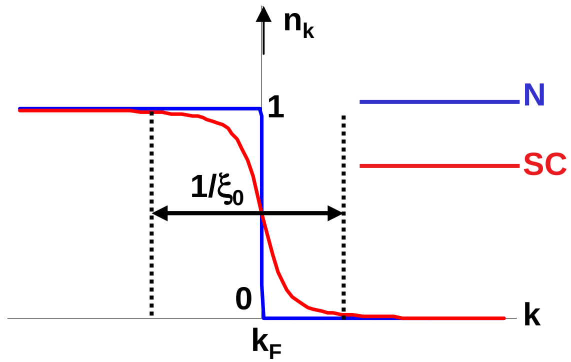
$$\Delta_0 \approx 2\,\hbar\,\omega_D \exp[-1/N_0 V]$$

Any finite attractive interaction opens a gap.

2. The ground state energy difference between SC ($\Delta \neq 0$) and the normal state ($\Delta = 0$) is
$E_S - E_N = -N_0\,\Delta_0^2/2$
Lowering of energy due to Cooper pairing.

3. The electrons with opposite momentum pair up in bound states. The concept of a FS is destroyed. What remains is the concept of a chemical potential.

4. The occupation probability is $n_k = v_k^2$.
The concept of a FS is smeared out.
SC involves electrons around k_F within a width $1/\xi_0$.

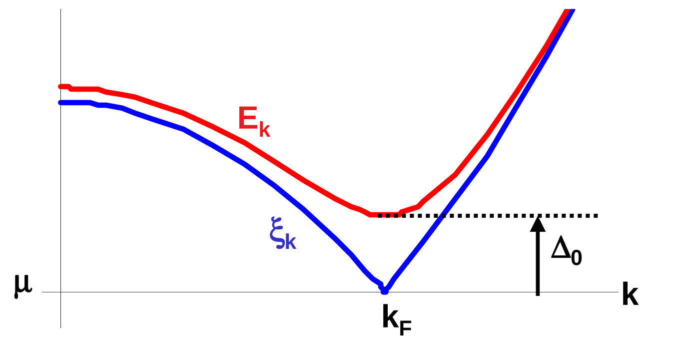


Meaning of the gap Δ_k

1. **Simplest excitation:** Obtained by breaking a pair. Either remove ($k\uparrow$) or ($-k, \Downarrow$).

Excitation energy = Loss of binding energy of ($k\uparrow, -k\Downarrow$) pair + gain in KE of single e^- at k.

Loss = $-\left[2\,\xi_k v_k^2 + 2\sum_{kk'} V_{kk'}\, u_k v_k\, u_{k'} v_{k'}\right]$,   Gain= ξ_k



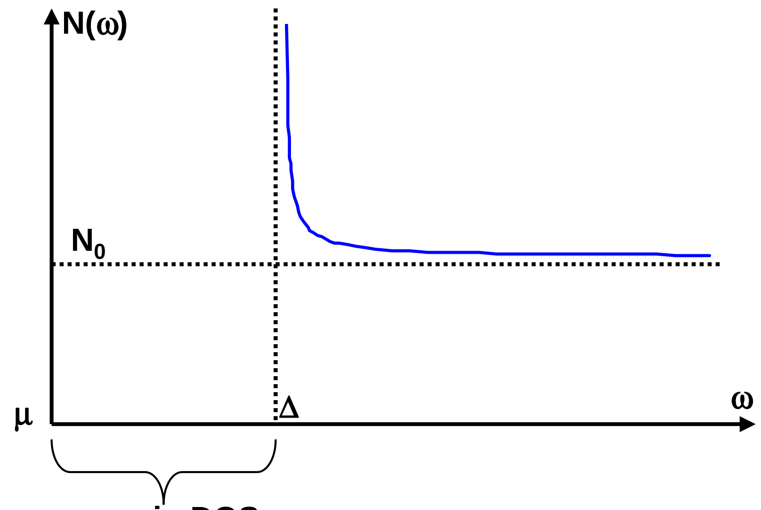
Gap in single particle excitation spectrum

Excitation energy = $E_k = (\xi_k^2 + \Delta_k^2)^{1/2}$ (Bogoliubov modes)

2. **Density of states (DOS):** The gap shows in the density of states (can be measured by tunneling spectroscopy) ---- remember the course of D. Roditchev.

$N_S(\omega) = 0$ for $\omega < \Delta$

$= N_0\, \omega/(\omega^2 - \Delta^2)^{1/2}$ for $\omega > \Delta$



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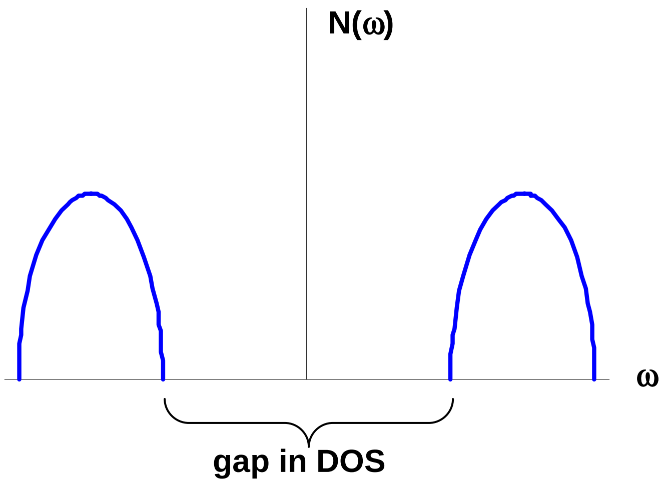
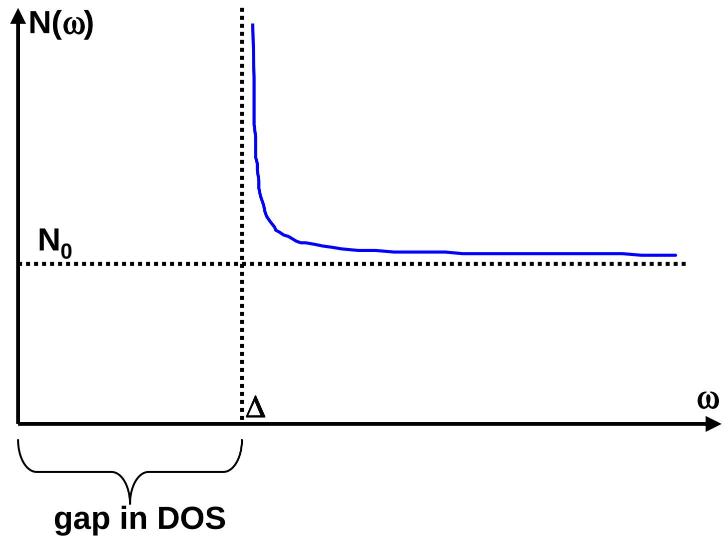


DOS of an insulator

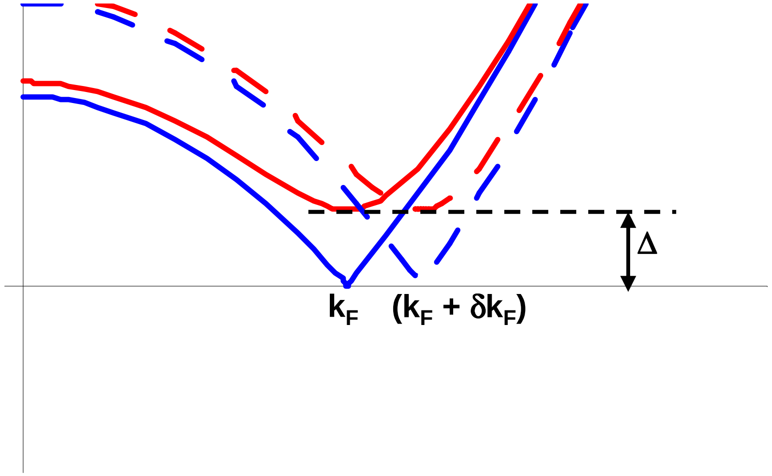


DOS of a superconductor

Even in an insulator an energy gap opens in the single particle spectrum.
How is a superconductor different from an insulator?

In an insulator $\partial N/(\partial \mu) = 0$.
Is this also true for a superconductor?

cont...



The BCS gap Δ is tied to the chemical potential. It does not change with the chemical potential.

$\partial N/(\partial \mu) \neq 0$. (It takes the value of the normal state)

BCS theory at finite T

1. BCS gap eqn (obtained by minimizing the free energy and not just the ground state energy) at finiteT:

$$\Delta_k = - \sum_{k'} V_{kk'} \Delta_{k'}/(2E_{k'}) \; [1 - 2 f(E_{k'})],$$

$f(E) = 1/(\exp[E/k_B T] + 1)$

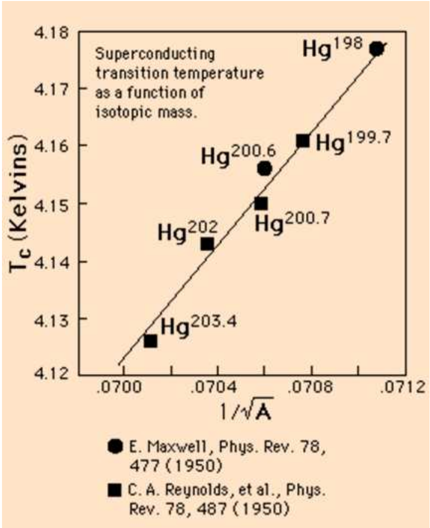
This makes Δ_k T-dependent. T_c can be calculated using the gap eqn.

$(k_B T_c)/\Delta \approx 0.5$.

2. Entropy $S = -2k_B \sum_k [(1-f_k) \mathrm{Log}(1-f_k) + f_k \mathrm{Log}\, f_k]$

$C = T\, dS/dT \propto \exp[-\Delta/(k_B T)]$, at the lowest temperature.

Attractive interaction: role of phonons

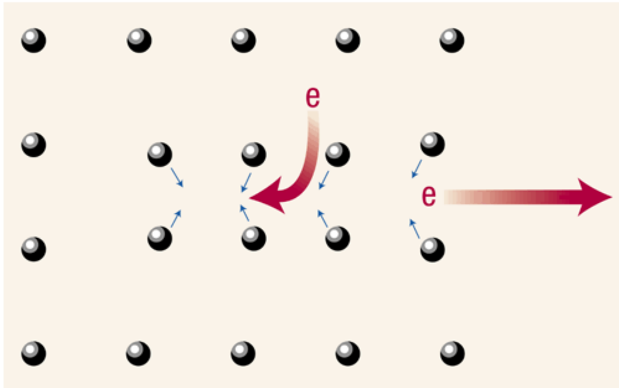


Isotope effect (1950): $T_c \propto 1/\sqrt{M}$.
M = mass of the ions forming the lattice.

The lattice plays a role in establishing SC.

When an e^- moves away from a region it leaves behind a net +ve charge. The lattice tries to adjust but it moves very slow compared to the electrons.
The net +ve charge attracts a 2nd e^- in the vicinity.

$D(\omega, q) \approx 1/(\omega^2 - \omega_q^2)$. For small ω, $D < 0$.



Persistent current

1. In Ψ_{BCS} we pair states with equal & opposite momenta ($k\uparrow$, $-k\Downarrow$). A Cooper pair has zero centre of mass momentum.

2. Let us give a momentum boost to all els$^-$. $\hbar k \to \hbar k + p$. This is steady current-carrying state $J = nep/m$.

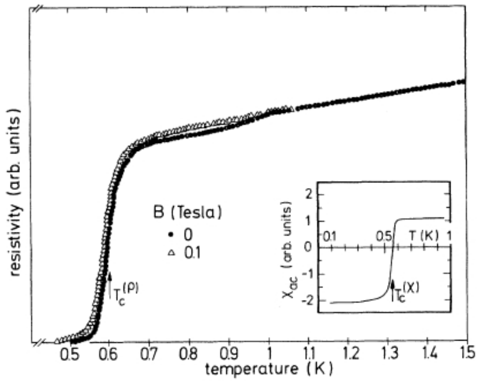
3. In this state Cooper pairs form between ($k+p/\hbar \uparrow$, $-k+p \Downarrow$), i.e., between electrons with relative momentum $2\hbar k$ just as in $p=0$ case. Since the bound state formation and the gain in binding energy takes place in the relative coordinate, all the earlier arguments are still valid. Therefore, value of gap Δ is unchanged even though $p \neq 0$.

4. The only cost of energy by creating the current state is $p^2/(2m)$ per electron. As long as the KE is less than the binding energy, $\Psi_{BCS}(p)$ is still the ground state with els$^-$ in pairs.

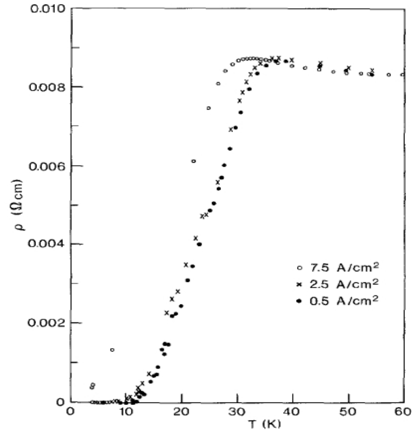
5. In a normal metal the source of resistance is scattering with $k \to -k$ (back-scattering). In a SC for this to happen one has to 1st break the pairs. This costs energy Δ. For $T < \Delta$, the only available excitations are modes $\hbar\,\omega \sim T$. These modes do not have enough energy to break the pair. The current state cannot decay momentum.

Beyond BCS

"The theory of Bardeen Cooper and Scrieffer - the BCS theory - has explained so much that we can say that we now understand the superconducting state almost as well as we do the 'normal' state" ----- J. Ziman, 1963, *Principles of the theory of Solids*



Steglich, et al, PRL 43, 1892 (79)



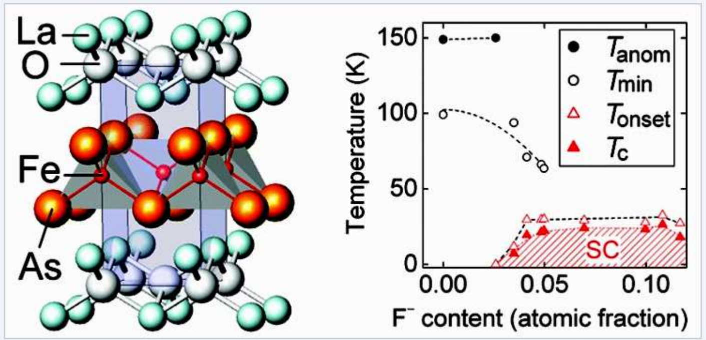
Bednorz & Müller, Z. Phys B 64, 189 (86)

Surprises:

1. Discovery of superconductivity in the rare earth compound $CeCu_2Si_2$. $T_c \approx 0.5$ K. Should not be superconducting according to BCS logic.

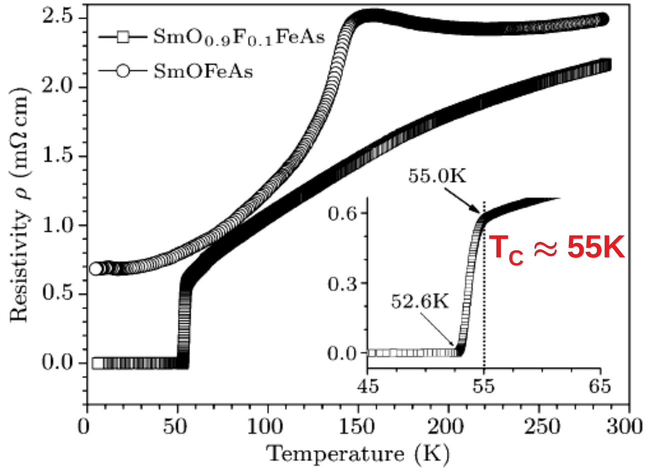
2. In 1986 Bednorz & Müller discovered superconductivity in Ba-La-Cu-O. $T_c \approx 30$ K.

Latest excitement: Fe-based superconductors



We report that a layered iron-based compound LaOFeAs undergoes superconducting transition under doping with F^- ions at the O^{2-} site. The transition temperature (T_c) exhibits a trapezoid shape dependence on the F^- content, with the highest T_c of ~26 K at ~11 atom %.

Kamihara et al, J. Am. Chem. Soc 130, 3296 (08)



Ren et al, Chin. Phys. Lett. 25, 2215 (08)

Several classes: ReOFeAs [Re = La, Ce, Sm...]; $AeFe_2As_2$ [Ae = Ba, Sr, Ca]; MFeAs [M = Li, Na]; FeCh [Ch = Se, Te].

Motivation to look beyond the standard BCS paradigm....

Superconductivity in unconventional situation

Conventional = Situation where electron-phonon mediated BCS type superconductivity theory & and its strong coupling generalization works.

What are the various ingredients in the BCS theory?
We can think of unconventionality arising due to the lack of one or more of those ingredients.

Causes of unconventionality

1. Multiband system
E.g. : MgB_2, Fe-based pnictide superconductors.
MgB_2 is a two-band superconductor ($T_c \approx 39$ K). Everything else is conventional.
The bands have two different gap functions ($\Delta_1 \approx 10\ \Delta_2$), both s-wave.
But a single transition temperature (can be understood from symmetry).
Choi et al, Nature 418, 758 (02).

2. Other bosonic (non-phonon) excitation mediated superconductivity
E.g. : Spin fluctuation mediated pairing in superfluid He-3. Possibly in Sr_2RuO_4.
What about the cuprates?
Spin fluctuation = collective excitations of the fermions. An electron can spin polarize the medium locally. A 2nd electron with the same spin alignment gets attracted if the interaction is ferromagnetic.

Causes of unconventionality (cont.)

3. Anisotropic gap function Δ_k (non s-wave)
The interaction $V_{kk'}$ can depend on the angle $k \cdot k'$.
$V_{k\,k'} = \sum_l V_l P_l (\cos\theta)$. V_l ($l \neq 0$) can be the dominant interaction.

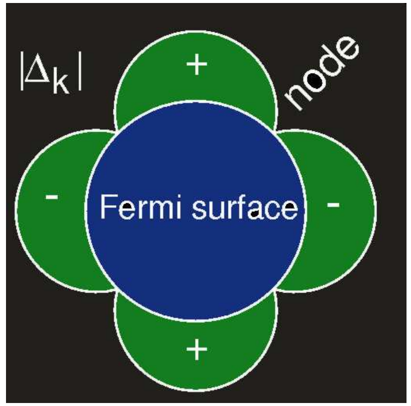
E.g. : (i) The cuprate superconductors have $d_{x^2-y^2}$ (l=2) gap symmetry. $\Delta_k = \Delta_0 (\cos k_x - \cos k_y)$. Gives rise to nodes where gap vanishes and low-energy excitations are possible.
$E_k = (\varepsilon_k^2 + \Delta_k^2)^{1/2}$. The physics of nodal excitations can be important.

(ii) p-wave pairing in He-3 and possibly in Sr_2RuO_4.

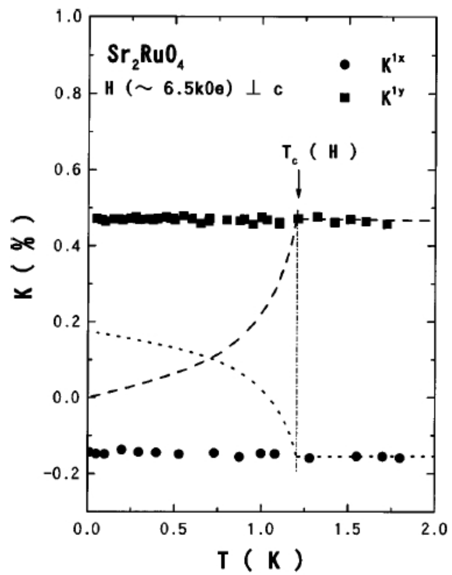
4. Triplet pairing (S=1)
E.g. : He-3, and Sr_2RuO_4.

In standard BCS the Cooper pairs form a spin singlet (S=0).

For S=1 and L=1, 9 independent order parameters to play with! Non-trivial spin susceptibility is expected at least along certain directions of the applied field. In a singlet superconductor the spin susceptibility is zero as $T \to 0$.



$d_{x^2-y^2}$ gap symmetry

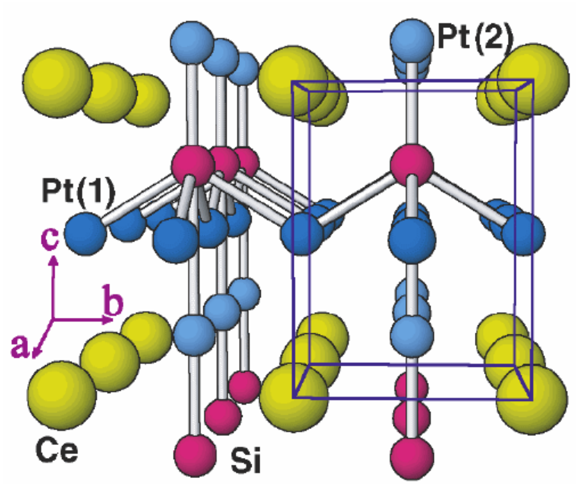


T-dependence of Knight shift
Ishida et al, Nature 396, 658 (98)

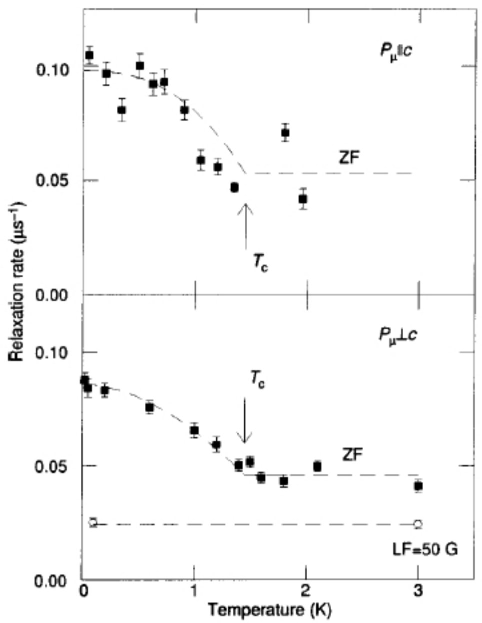
Causes of unconventionality (cont.)

5. Lack of symmetry (broken spontaneously or otherwise)

E.g. (i): Non-centrosymmetric superconductors such as $CePt_3Si$ ($T_c \approx$ 1K), $CeRhSi_3$, $CeIrSi_3$. These systems lack inversion symmetry, which produces spin-orbit coupling of the form e.g., $(p\cdot\sigma)$. Since parity is not a good quantum number the ground state wavefunction has no definite parity. Singlet & triplet Cooper pairs coexist.



Crystal structure of $CePt_3Si$
No c $\rightarrow$ −c symmetry



Muon spin relaxation rate. Evidence of additional magnetic scattering below T_c
Luke et al, Nature 394, 558 (98)

E.g. (ii): Spontaneous breaking of time reversal symmetry in Sr_2RuO_4. $\Delta(k) = (k_x + i\,k_y)(|\uparrow\Downarrow\rangle + |\Downarrow\uparrow\rangle)$ as in A-phase of He-3. L_z=1, and S_z=0. Gives rise to exotic electro-magnetic properties.

In standard BCS pairing is between time reversed pairs $|k\uparrow\rangle$ and $|-k\Downarrow\rangle$. Non-magnetic impurities do not have affect superconductivity (if s-wave)—Anderson's theorem.

Causes of unconventionality (cont.)

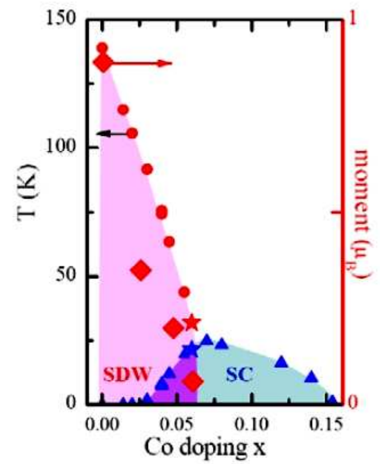
6. Coexistence of superconductivity with other types of order

(i) SC coexisting with antiferromagnetism, such as heavy fermions $CeCu_2Si_2$ doped with Ge, $CeRhIn_5$, $CeIn_3$ (arXiv:0201040, arXiv:0908.3980), newly discovered Fe-pnictide $BaFe_2As_2$ when doped.

(ii) coexistence with ferromagnetism such as UGe_2, URhGe, UCoGe; singlet or triplet? homogeneous or modulating orders?

(iii) coexistence with charge ordering as in $NbSe_2$.

These orders usually compete with one another. In the coexistence regime how do they affect one another?



Phase diagram of $BaFe_2As_2$
Laplace et al, EPJB 73, 161 (10)

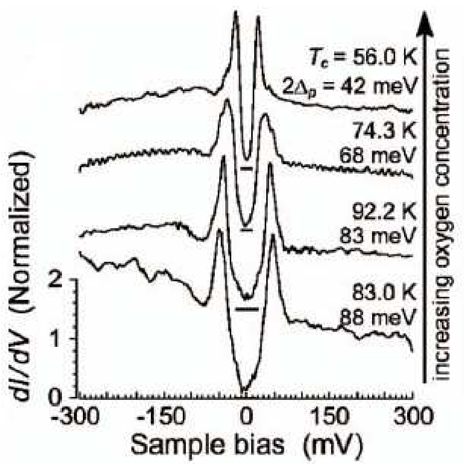
Causes of unconventionality (cont.)

7. Effects of strong correlation

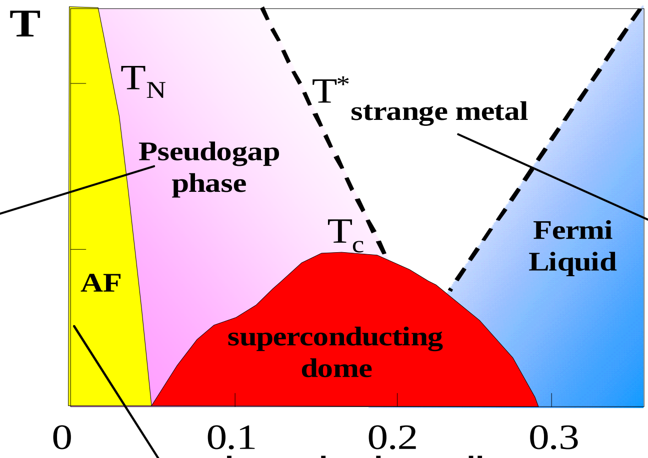
Strong correlation = effects of interaction cannot be understood perturbatively. The parent metallic state itself is unusual. Does the BCS mechanism work even if the metal is not a Landau Fermi liquid?

E.g. : (i) heavy fermions, where superconductivity is often near a QCP; as in $CeCu_2Si_2$, $CeCu_2Ge_2$, $CePd_2Si_2$.

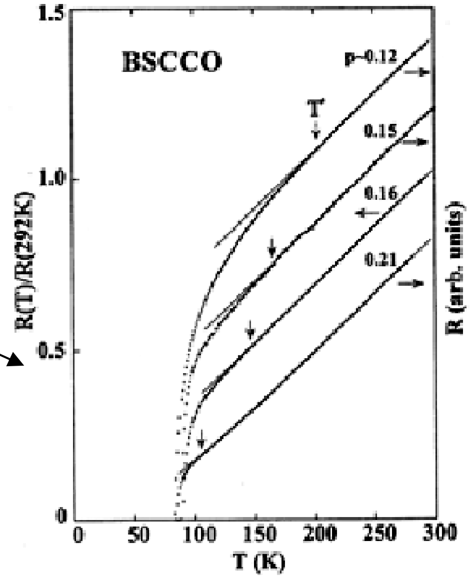
(ii) the CuO based high temperature superconductors.



Vanishing density of states at FS



schematic phase diagram



T-linear resistivity

Fundamental puzzles of the cuprates

(i) why SC develops in the vicinity of an interaction-driven (Mott) insulator and an AFM?

(ii) why is T_c so high?

(iii) how to understand the unusual metal-phase and its relation with SC?

References

1. *Theory of superconductivity*, R. Schrieffer
2. *Superconductivity of metals & alloys*, P. G. de Gennes
3. *Statistical Physics, part-2*, Landau & Lifshitz.
3. Leggett, Rev. Mod. Phys. 47, 331 (1975).
4. Gentle introductions in the last chapters of Ashcroft & Mermin, *Solid state physics*, and in Ziman, *Principles of the theory of solids.*

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1. I took quite a few pictures from the website of Dr. A. V. Ustinov:
http://www.pi.uni-karlsruhe.de/ustinov/

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