



BCS Theory

**Huge effect of a small gap:
the BCS theory of supercon-
ductivity**

GSI PhD Seminar, January 31, 2001

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Nobel Prizes



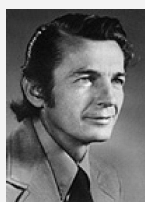
1913 Heike Kamerlingh-Onnes “for his investigations on the properties of matter at low temperatures which led, inter alia to the production of liquid helium”



1962 Lev Davidovich Landau “for his pioneering theories for condensed matter, especially liquid helium”

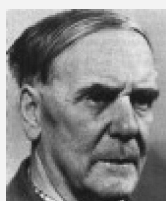


1972 John Bardeen, Leon N. Cooper, J. Robert Schrieffer “for their jointly developed theory of superconductivity, usually called the BCS-theory”

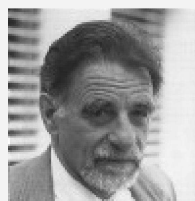
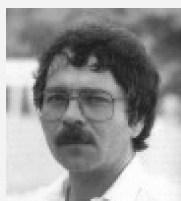


1973 Ivar Giaever “for their experimental discoveries regarding tunneling phenomena in superconductors”

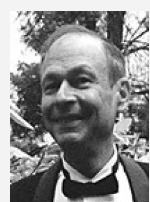
1973 Brian D. Josephson “for his theoretical predictions of the properties of a supercurrent through a tunnel barrier, in particular those phenomena which are generally known as the Josephson effects”



1978 Pyotr Leonidovich Kapitza “for his basic inventions and discoveries in the area of low-temperature physics”



1987 J. Georg Bednorz, K. Alexander Müller “for their important breakthrough in the discovery of superconductivity in ceramic materials”

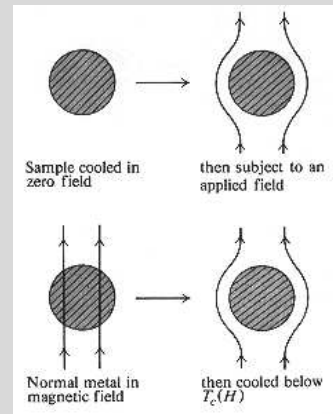


1996 David M. Lee, Douglas D. Osheroff, Robert C. Richardson “for their discovery of superfluidity in helium-3”

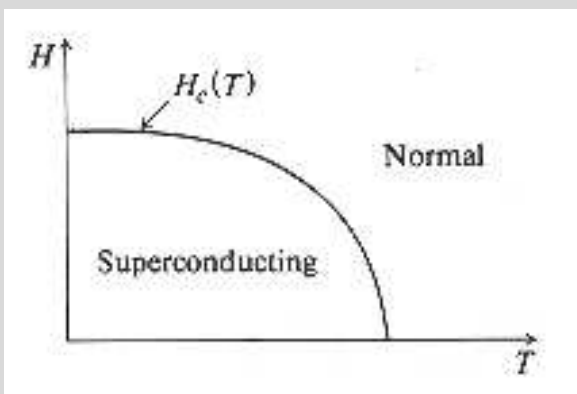
Superconductor Phenomenology

Infinite Conductivity

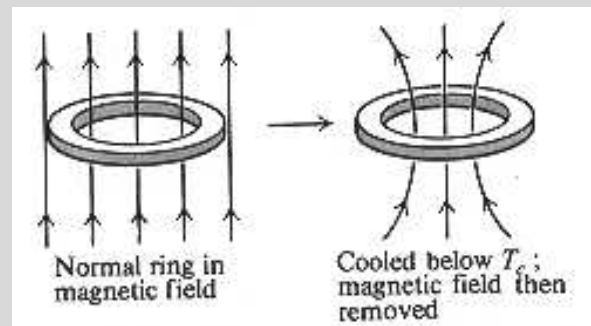
Meissner effect



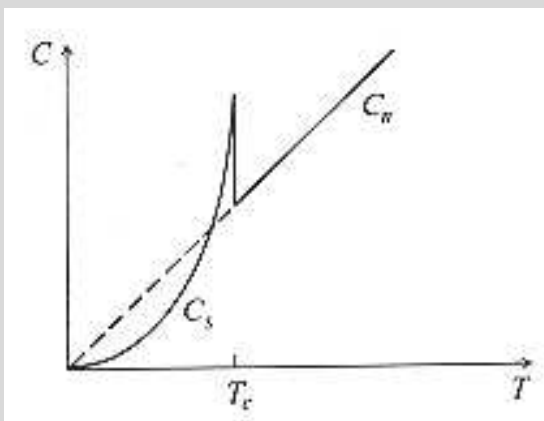
Critical Field



Persistent currents and flux quantization



Specific Heat



Isotope effect

The transition temperature T_c varies with the ionic mass M

$$T_c \propto M^{-1/2}$$

Phenomenological Theories

London Theory

two-fluid model: **normal** and **superconducting** electrons

London equation permits no magnetic field in the interior

$$\nabla \times \mathbf{j} = -\frac{n_s e^2}{mc} \mathbf{B}$$

allow calculation of penetration depth

Ginzburg-Landau Theory

superconductor is characterized by complex **order parameter** $\Psi(\mathbf{r})$ which vanishes above T_c

Free Energy density of the superconductor

$$F_s = F_n + a|\Psi|^2 + \frac{1}{2}b|\Psi|^4 + \frac{1}{2m^*} \left| \left(\frac{\hbar}{i} \nabla + \frac{e^* \mathbf{A}}{c} \right) \Psi \right|^2 + \frac{h^2}{8\pi}$$

allows description of superconductors with nonuniform fields and surface effects, flux quantization and gives description of Type II superconductors

Microscopic BCS Theory

Wanted

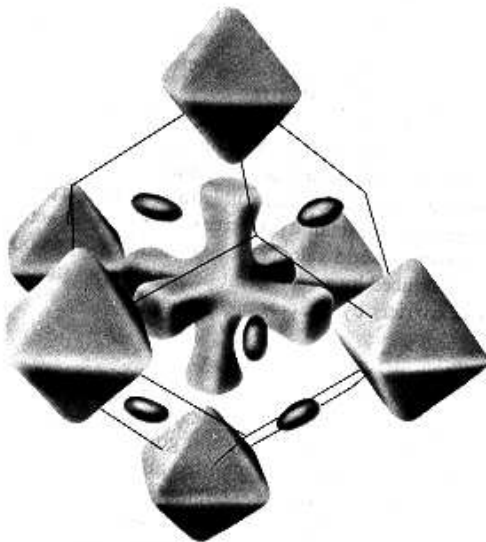
A microscopic theory should describe the phenomenology based on first principles (electron and crystal structure of the metal, Hamiltonian of the system)

The physical nature of the order-parameter should be identified, the special non-classical features of the superconducting phase should be outlined

Simplifications

Superconductivity is observed in many metals, therefore a principle understanding should not depend on the band-structure of the metal and the detailed form of electron-electron and electron-lattice-interaction

The BCS theory will be presented for the $T = 0$ case. A temperature dependent description should make use of thermal Green's functions (see Fetter, Walecka, Quantum Theory of Many-Particle Systems)



tungsten fermi surface

Fermions in a box

Fermi Gas / Fermi Liquid

- Ground-state of fermi-liquid (in which the electrons are described as independent particles) has no correlations between electrons of opposite spin and only statistical, by pauli-principle, correlations for electrons of same spin.
- Single particle excitations are described by moving an electron with momentum \mathbf{k}_i from the the fermi sphere to a momentum \mathbf{k}_j above the fermi sphere.

Two Electrons above the fermi-sphere

- The real electron-electron interaction is weak and slowly varying over the fermi surface.
- The energy involved in the transition to the superconducting state is small
- ✓ only excitations near the fermi-surface play a role
- small attractive interaction between electrons at the fermi surface
- ✓ electrons try to minimize their energy, using the attractive potential, have to pay with kinetic energy
- ✓ widespread relative wavefunction of the order of $10^{-4}cm$, if the interaction is also attractive at short distances the electrons will form a spin-singulett

Cooper Pairs

- Solution of Bethe-Goldstone-equation is possible to solve numerically. Using a simplified interaction, an analytical solution is possible. The Hamilton-Operator of the two electrons

$$\tilde{H} = \frac{1}{2m} \tilde{\mathbf{k}}_1^2 + \frac{1}{2m} \tilde{\mathbf{k}}_2^2 + \tilde{V}$$

- Define binding-energy relative to fermi-energy

$$\tilde{H}|\Psi\rangle = E|\Psi\rangle = (E_B + 2\epsilon_F)|\Psi\rangle$$

- Total momentum is conserved. only states above the fermi surface can be occupied. Therefore pair wavefunction has one electron spin-up, one spin-down (spin-singulett)

$$|\Psi\rangle = \sum_{k_1 > k_F, k_2 > k_F} \langle \mathbf{k}_1, \mathbf{k}_2 | \Psi \rangle = \sum_{|\frac{1}{2}\mathbf{P}+\mathbf{k}| > k_F, |\frac{1}{2}\mathbf{P}-\mathbf{k}| > k_F} \langle \mathbf{P}, \mathbf{k} | \Psi \rangle \quad (1)$$

- Lowest energy for $\mathbf{P} = 0$, therefore use

$$\langle \mathbf{k} | \Psi \rangle = \langle \mathbf{P} = 0, \mathbf{k} | \Psi \rangle$$

$$\langle \mathbf{k} | \tilde{H} | \Psi \rangle = (E_B + 2\epsilon_F) \langle \mathbf{k} | \Psi \rangle$$

$$2\epsilon_k \langle \mathbf{k} | \Psi \rangle + \sum_{\mathbf{k}'} \langle \mathbf{k} | \tilde{V} | \mathbf{k}' \rangle \langle \mathbf{k}' | \Psi \rangle = (E_B + 2\epsilon_F) \langle \mathbf{k} | \Psi \rangle$$

- This is the simplified interaction, attractive in small region at the fermi surface

$$\langle \mathbf{k} | \tilde{V} | \mathbf{k}' \rangle = V(k, k') = -V \Theta(\omega_D - |\epsilon_k - \epsilon_F|) \Theta(\omega_D - |\epsilon_{k'} - \epsilon_F|)$$

Cooper Pairs, continued

- Going from the momentum to the energy basis, using the density of states $N(\epsilon)$

$$(-E_B + 2(\epsilon - \epsilon_F))\langle \epsilon | \Psi \rangle = V \int_{\epsilon_F}^{\epsilon_F + \omega_D} d\epsilon' N(\epsilon') \langle \epsilon' | \Psi \rangle$$

- With the further assumptions $\omega_D \ll \epsilon_F$ and $E_B \ll \omega_D$ we can assume $N(\epsilon) \approx N(\epsilon_F)$

$$E_B = -2\omega_D \exp\left(-\frac{2}{N(\epsilon_F)V}\right)$$

- ✓ There's a bound-state for an arbitrarily small potential. This is a many-body effect.
- ✓ We have an instability of the normal fermi-liquid against the formation of cooper-pairs. The task is now to formulate a self-consistent treatment of all electrons, the electrons are indistinguishable !
- ✓ At higher Temperature $kT \approx \omega_D$ the surface is fuzzy and the instability goes away.

BCS many-particle state

- We have to find a many-particle state, which has two-body correlations in the form of cooper-pairs and respects the fermi character of the electrons.
- To get the correlations in the many-body case we use the variational principle
- We could use in principle an ansatz of the form

$$|\Psi_{\text{BCS}}\rangle = \left(\sum_{\mathbf{k}} g(k) a_{\tilde{\mathbf{k}}\uparrow}^{\dagger} a_{\tilde{\mathbf{k}}\downarrow}^{\dagger} \right)^{(N/2)} |0\rangle$$

- ✗ This ansatz has technical problems. Therefore we use something else.

$$|\Psi_{\text{BCS}}\rangle = \exp\left(\sum_{\mathbf{k}} g(k) a_{\tilde{\mathbf{k}}\uparrow}^{\dagger} a_{\tilde{\mathbf{k}}\downarrow}^{\dagger} \right) |0\rangle$$

- ✗ This state has no definite particle number !

- Using the anticommutation relations of the fermions we get

$$|\Psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} (1 + g(k) a_{\tilde{\mathbf{k}}\uparrow}^{\dagger} a_{\tilde{\mathbf{k}}\downarrow}^{\dagger}) |0\rangle$$

- Usual one uses a slightly different notation

$$|\Psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}} (u_k + v_k a_{\tilde{\mathbf{k}}\uparrow}^{\dagger} a_{\tilde{-\mathbf{k}}\downarrow}^{\dagger}) |0\rangle$$

- The normal ground state (filled fermi sphere) is given in this ansatz by

$$\begin{cases} |v_k| = 1, u_k = 0; \epsilon_k < \epsilon_F \\ v_k = 0, |u_k| = 1; \epsilon_k > \epsilon_F \end{cases}$$

Reduced Interaction

- We are using a reduced Hamiltonian, here only contributions which contain two cooper-pairs are considered. it is assumed that the missing parts of the Hamiltonian don't destroy the structure of the solution - they should give more or less the same contributions in the normal and in the superconducting state

$$\tilde{H}_{\text{red}} = \sum_{\mathbf{k}} \epsilon_k (a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\uparrow} + a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}\downarrow}) + \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger a_{-\mathbf{k}\uparrow} a_{\mathbf{k}\downarrow}$$

- We have no fixed particle number. Introduce chemical potential μ which fixes the expectation value of the particle number

$$\langle \Psi_{\text{BCS}} | \tilde{N} | \Psi_{\text{BCS}} \rangle = N$$

- For the Variation we need the matrix elements of the reduced Hamiltonian. After some tedious algebra we get

$$\langle \Psi_{\text{BCS}} | \Psi_{\text{BCS}} \rangle = \prod_{\mathbf{k}} (|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2)$$

$$\langle \Psi_{\text{BCS}} | \tilde{N} | \Psi_{\text{BCS}} \rangle = 2 \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2 \cdot \prod_{\mathbf{k}' \neq \mathbf{k}} (|u_{\mathbf{k}'}|^2 + |v_{\mathbf{k}'}|^2)$$

$$\begin{aligned} \langle \Psi_{\text{BCS}} | \tilde{H}_{\text{red}} | \Psi_{\text{BCS}} \rangle = & 2 \sum_{\mathbf{k}} \epsilon_k |v_{\mathbf{k}}|^2 \cdot \prod_{\mathbf{k}' \neq \mathbf{k}} (|u_{\mathbf{k}'}|^2 + |v_{\mathbf{k}'}|^2) + \\ & \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} u_{\mathbf{k}'}^* v_{\mathbf{k}}^* u_{\mathbf{k}} v_{\mathbf{k}'} \cdot \prod_{\mathbf{p} \neq \mathbf{k}, \mathbf{p} \neq \mathbf{k}'} (|u_{\mathbf{p}}|^2 + |v_{\mathbf{p}}|^2) \end{aligned}$$

Gap Equation

- To fulfill the normalization

$$|u_k|^2 + |v_k|^2 = 1$$

we make the ansatz

$$u_k = \sin \theta_k, \quad v_k = e^{i\phi_k} \cos \theta_k$$

- The variation procedure now tells us to minimize

$$\langle \Psi_{\text{BCS}} | \tilde{H}_{\text{red}} - \mu \tilde{N} | \Psi_{\text{BCS}} \rangle$$

- The result is

$$\phi_k = \alpha, \quad \tan 2\theta_k = -\frac{e^{-i\alpha} \Delta_k}{\epsilon_k - \mu}$$

with

$$\Delta_k = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'}^* v_{\mathbf{k}'}$$

- We finally arrive at the [gap equation](#)

$$|\Delta_k| = -\frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{|\Delta_{\mathbf{k}'}|}{\sqrt{(\epsilon_k - \mu)^2 + |\Delta_k|^2}}$$

Solution of the Gap Equation

- ✗ The gap equation is for a general potential an integral equation. A simple solution is possible for the electron-electron interaction as discussed for the Cooper Pairs
- Using this simple form of the interaction we get

$$\Delta_k = \begin{cases} \Delta & ; |\epsilon_k - \mu| < \omega_D \\ 0 & ; \textit{elsewhere} \end{cases}$$

$$|\Delta| = 2\omega_D \exp\left(-\frac{1}{N(\epsilon_F)V}\right)$$

and change of the groundstate energy of

$$\frac{\delta E}{\Omega} = -\frac{1}{2}N(\epsilon_F)|\Delta|^2$$

Bogoliubov Transformation

- To describe the excitations of the BCS ground-state the Bogoliubov Transformation to **quasi-particle**-operators $\tilde{\alpha}_k$ and $\tilde{\beta}_k$ are used which “live” on the BCS-vacuum and satisfy the usual anticommutation relations

$$\tilde{\alpha}_{\mathbf{k}} = u_k \tilde{a}_{\mathbf{k}\uparrow} - v_k \tilde{a}_{-\mathbf{k}\downarrow}^\dagger \quad \tilde{\beta}_{-\mathbf{k}} = u_k \tilde{a}_{-\mathbf{k}\downarrow} + v_k \tilde{a}_{\mathbf{k}\uparrow}^\dagger$$

- excitation spectrum has a gap of 2Δ

Outlook

Applications

- High- T_c superconductors
- Liquid ^3He
- neutron stars

Order Parameter

- Bose condensation
- Off-diagonal long-range order
- Meissner effect and Flux Quantization
- Josephson effects

Order Parameter

- Temperature Dependence
- Crystal structure, Fermi surface
- Electron-electron interaction