Emergence of Quantum Phases in Novel Materials

VII Edition ICMM-CSIC Postgraduate Course

rconductivity

Topology Dirac Topology Chern Majoranas Mott Heavy fermions Topology Chern Majoranas Mott Heavy fermions Movi Chern Majoranas Mott Heavy fermions Movi Chern Majoranas Mott Majoranas M

María José Calderón

mariaj.calderon@csic.es





BIBLIOGRAPHY

"Introduction to Many-body physics" Piers Coleman

"Introduction to superconductivity" Tinkham

SPC history:

"Superconductivity: a very short introduction" S. Blundell

Collection of reviews

•Conventional SPC "Superconductivity" Edited by Parks. 1968.

•Conventional and unconventional SPC "Superconductivity" 2008 (Fe SPC not included)

THE DISCOVERY (1911)





Heike Kamerlingh Onnes liquefied He: 1st person to measure low T resistivity

S. Blundell "Superconductivity: a very short introduction"

THE DISCOVERY (1911)

S. Blundell "Superconductivity: a very short introduction"

And many compounds!

https://www.webelements.com/periodicity/superconductivity_temp/

M.J. Calderón calderon@icmm.csic.es

OUTLINE

- Superconductivity I
 - Properties (zero resistivity, Meissner effect)
 - Understanding (pairing, BCS, Ginzburg-Landau)
 - Electron-phonon interaction (conventional superconductivity)
- Superconductivity II (unconventional superconductivity)
 - What are the new issues.
 - What are (some of) the proposals.

A BIT OF (THE EARLY) HISTORY

1911: Discovery

1933: Meissner effect

1935: London Equations

1937: Superfluidity in ⁴He

1950: Isotope effect

Electron-electron interaction mediated by phonons

Ginzburg-Landau

1953: Pippard's coherence length

1955: Idea of gap (Bardeen)

Bardeen-Pines effective interaction

1956: Cooper pairs

Abrikosov extension of Ginzburg-Landau (vortices)

1957: BCS

1959: Gor'kov derived Ginzburg-Landau theory from BCS

SUPERCONDUCTORS ARE NOT PERFECT CONDUCTORS

New lead: The Meissner-Ochsenfeld effect (1933): SUPERCONDUCTORS ARE PERFECT DIAMAGNETS

Perfect conductor

Superconductor

www.open.edu: Superconductivity

THE MEISSNER-OCHSENFELD EFFECT (1933)

Superconductors expel magnetic fields

www.icmm.csic.es/superconductividad Note: this picture corresponds to the mixed state (see later)

Superconductors produce supercurrents that completely screen out the magnetic field.

M.J. Calderón calderon@icmm.csic.es

LONDON EQUATIONS (1935)

(phenomenological approach)

Ohm's law

(a relation between current and electric field)

London equations

A new relation between electric current and magnetic field (inspiration: Meissner effect)

LONDON EQUATIONS (1935)

(phenomenological approach)

Superconductivity is a macroscopic quantum phenomenon

Long range order of the momentum vector:

A condensation in momentum space (= zero net momentum) rather than in real space

M.J. Calderón calderon@icmm.csic.es

LONDON EQUATIONS (1935)

Without applied magnetic field, the ground state has zero net momentum (condensation in momentum space). If =0 also under an applied field (the wave-function is "rigid"):

n_s is the density of superconducting electrons

M.J. Calderón calderon@icmm.csic.es

LONDON EQUATIONS

velocity against resistance).

$$\Lambda = \frac{m}{n_s e^2}$$

LONDON EQUATIONS

Superconducting electrons do not suffer any scattering. From the Drude model for electrical conductivity

LONDON EQUATIONS

SUPERCURRENT SCREENS MAGNETIC FIELD

+MAXWELL EQUATION

$$\vec{h} = -c\nabla \times \left(\Lambda \vec{J_s}\right) \qquad \nabla \times \vec{h} = 4\pi \vec{J_s}/c$$

$$\nabla^2 \vec{h} = \frac{\vec{h}}{\lambda^2} \longrightarrow \vec{h}(r) = \vec{h}(0)e^{-r/\lambda}$$

$$\Lambda = \frac{m}{n_s e^2} \qquad \lambda^2 = mc^2/4\pi n_s e^2$$

$$\nabla \times (\nabla \times \vec{B}) = \nabla (\nabla \cdot \vec{B}) - \nabla^2 \vec{B} = -\nabla^2 \vec{B}$$

LONDON EQUATIONS

LONDON PENETRATION LENGTH

PIPPARD'S COHERENCE LENGTH

From the uncertainty principle:

Only e- within $k_B T_c$ of E_F participate in superconductivity

$$\Delta p \approx \frac{k_B T_c}{v_F} \qquad \qquad \Delta x \gtrsim \frac{\hbar}{\Delta p} \approx \frac{\hbar v_F}{k_B T_c} \sim \xi_0$$

From a non-local generalization of the London equations

$$\xi_0$$
: wave-function size

$$\xi_0 = 0.15 \frac{\hbar v_F}{k_B T_c}$$

2 characteristic length scales: penetration and coherence lengths

⁴HE SUPERFLUIDITY (1937)

⁴He liquifies at 4.2K
(He I: normal quantum liquid)
At 2.17K, transition to superfluid (He II).
λ transition.

Superfluidity \rightarrow Viscosity=0.

2 fluid model

- normal fluid
- superfluid

Relation to Bose Einstein condensation:

In BEC: no interactions. In superfluid there are interactions (superfluid density is reduced)

SUPERFLUIDITY & SUPERCONDUCTIVITY

A superconductor is a charged superfluid.

Note: What is condensing in the superconductor?? Electrons are fermions, not bosons!! Before 1957, a microscopic theory was still missing.

LANDAU TRANSITION THEORY U(1)

Macroscopic theory in terms of order parameters. Valid close to the critical point. The order parameter description is valid for lengths larger than the coherence length.

$$f[\Psi] = r(\Psi^*\Psi) + \frac{u}{2}(\Psi^*\Psi)^2$$
$$\Psi \equiv \Psi_1 + i\Psi_2 \equiv |\Psi| e^{i\phi}$$
For Tc
$$\Psi = \sqrt{\frac{|r|}{u}} e^{i\phi}$$

A well-defined phase breaks the U(1) continuous symmetry (spontaneous symmetry breaking)

(allows for inhomogeneous order parameters)

New gradient terms. For a superfluid (no charge):

$$f_{GL}[\Psi, \nabla \Psi] = \frac{\hbar^2}{2m} |\nabla \Psi|^2 + r |\Psi|^2 + \frac{u}{2} |\Psi|^4$$

London's phenomenological wavefunction is the complex order parameter.

$$\Psi(x) = |\Psi(x)| e^{i\phi(x)}$$

$$n_s = |\Psi|^2$$

(allows for inhomogeneous order parameters)

New gradient terms. For a superfluid (no charge):

$$f_{GL}[\Psi, \nabla \Psi] = \frac{\hbar^2}{2m} |\nabla \Psi|^2 + r |\Psi|^2 + \frac{u}{2} |\Psi|^4$$

The rigidity of the order parameter is in the gradient term

$$\nabla \Psi = (\nabla |\Psi| + i |\Psi| \nabla \phi) e^{i\phi}$$

$$f_{GL} = \frac{\hbar^2}{2m} |\Psi|^2 (\nabla \phi)^2 + [\frac{\hbar^2}{2m} (\nabla |\Psi|)^2 + r |\Psi|^2 + \frac{u}{2} |\Psi|^4]$$
Phase stiffness

(allows for inhomogeneous order parameters)

New gradient terms. For a superfluid (no charge):

$$f_{GL}[\Psi, \nabla \Psi] = \frac{\hbar^2}{2m} |\nabla \Psi|^2 + r |\Psi|^2 + \frac{u}{2} |\Psi|^4$$

Length scale related to the gradient term: **correlation length** (length scale of the amplitude fluctuations).

At T=0, it is the Pippard's coherence length.

$$\xi(T) = \xi(0) \left| 1 - \frac{T}{T_c} \right|^{-1/2}; \ \xi(0) = \sqrt{\frac{\hbar^2}{2maT_c}}$$

Phase stiffness
$$f_{GL} = \frac{\rho_{\phi}}{2} (\nabla \phi)^2 + \text{constant}$$

Amplitude fluctuations are confined to scales shorter than ξ. For longer lengths those terms are constant.

Calculate the current

$$\vec{J} = -i\frac{\hbar}{2m} \left(\psi^* \vec{\nabla} \psi - \vec{\nabla} \psi^* \psi \right)$$

Using:

$$\psi(x) = \sqrt{n_s(x)} e^{i\phi(x)}$$

$$F[\Psi, \mathbf{A}] = \int d^d x \left[\frac{\hbar^2}{2M} \left| \left(\nabla - \frac{ie^*}{\hbar} \mathbf{A} \right) \Psi \right|^2 + r \left| \Psi \right|^2 + \frac{u}{2} \left| \Psi \right|^4 + \frac{(\nabla \times \mathbf{A})^2}{2\mu_0} \right]$$

The free energy is gauge invariant (any change in the phase of the order parameter can be compensated by a gauge transformation)

$$\psi(x) \to \psi(x)e^{i\alpha(x)} \qquad \mathbf{A} \to \mathbf{A} + \frac{\hbar}{e^*}\nabla\alpha$$

The electromagnetic part of the Free energy has an associated length: the London penetration length λ .

(Note e*. e*=2e only after BCS theory)

 $\mathbf{A} \to \mathbf{A} + \frac{\hbar}{\rho^*} \nabla \alpha$ $\psi(x) \to \psi(x) e^{i\alpha(x)}$

By absorbing the phase of the order parameter, the phase stiffness appears as a mass term (gapped excitation).

ANDERSON-HIGGS MECHANISM

(see section 11.6.2 of Coleman's book for a demonstration)

(in a neutral superfluid you have Goldstone (massless) modes)

$$F[\Psi, \mathbf{A}] = \int d^d x \left[\frac{\hbar^2}{2M} \left[\left(\nabla - \frac{ie^*}{\hbar} \mathbf{A} \right) \Psi \right]^2 + r \left| \Psi \right|^2 + \frac{u}{2} \left| \Psi \right|^4 + \frac{(\nabla \times \mathbf{A})^2}{2\mu_0} \right]$$

Now the current is:

$$\mathbf{J}(x) = \frac{e^*\hbar}{M} |\Psi|^2 \nabla \phi - \frac{e^{*2}}{M} |\psi|^2 \mathbf{A} = e^* n_s \frac{\hbar}{M} \left(\overrightarrow{\nabla} \phi - \frac{e^*}{\hbar} \mathbf{A} \right) = e^* n_s \mathbf{v}_s$$

An external vector potential produces superflow

M.J. Calderón calderon@icmm.csic.es

D.C. JOSEPHSON EFFECT (1962)

A <u>zero voltage</u> supercurrent should flow between two superconducting electrodes connected by a "weak link".

A.C. JOSEPHSON EFFECT

An applied voltage leads to an oscillatory current

$$F[\Psi, \mathbf{A}] = \int d^d x \left[\frac{\hbar^2}{2M} \left| \left(\nabla - \frac{ie^*}{\hbar} \mathbf{A} \right) \Psi \right|^2 + r \left| \Psi \right|^2 + \frac{u}{2} \left| \Psi \right|^4 + \frac{(\nabla \times \mathbf{A})^2}{2\mu_0} \right]$$

The length scale for A: London penetration length λ . The length scale for $(\nabla \psi)^2$ is the coherence length ξ .

Ginzburg Landau parameter: λ/ξ .

M.J. Calderón calderon@icmm.csic.es

CRITICAL FIELD H_C

There is a maximum value of magnetic field H_c that can be applied before superconductivity is destroyed. There is also a critical current I_c .

First superconductors discovered had a low H_c. This is bad news if you want to build magnets with superconducting cables.

Some superconductors (alloys) didn't exclude the magnetic field completely and had much larger critical fields (1930's).

Coleman's book

M.J. Calderón calderon@icmm.csic.es

35

CRITICAL FIELD H_C

TYPE I/TYPE II SUPERCONDUCTORS

The first superconductors were all Type I ($\lambda << \xi$). Abrikosov explored the opposite possibility.

London penetration length

Correlation length

TYPE I/TYPE II SUPERCONDUCTORS

The first superconductors were all Type I ($\lambda << \xi$). Abrikosov explored the opposite possibility.

London penetration length

$$\lambda = \left(\frac{mc^2}{4\pi n_s e^2}\right)^{1/2}$$

London and Ginzburg-Landau considered λ<ξ. The supercurrent that screens the applied magnetic field occurs in a thin layer. The correlation length

$$\xi(T) = \xi(0) \left| 1 - \frac{T}{T_c} \right|^{-1/2}; \xi(0) = \sqrt{\frac{\hbar^2}{2maT_c}}$$

$$\sum_{i=1}^{n} \text{ or } i(x)$$

TYPE I/TYPE II SUPERCONDUCTORS

(X) ⊚







Modifying the wave-function costs a lot of energy. Not much energy gain by allowing H in. N/S interfaces are costly. At H_c there is a first order transition into the normal state.

Modifying the wave-function doesn't cost too much. You gain energy by allowing the magnetic field in. N/S interfaces are favoured. Two critical fields. Vortices.

CRITICAL FIELD H_C



SOME EXAMPLES

ching/			
.uk/teac	Compound	<i>T</i> _c [K]	ξ[n
am.ac.	Al	1.18	160
.phy.c	Pb	7.19	83
/w.qm	Nb	9.25	40
ww//:	Nb ₃ Sn	18.2	3.6
http	YBa ₂ Cu ₃ O _{7-δ}	90	(1.5

Compound	<i>T</i> _c [K]	ξ[nm]	λ[nm]	$\kappa = \lambda / \xi$	
41	1.18	1600	50	0.03	type-I
Pb	7.19	83	39	0.47	type-I
Nb	9.25	40	44	1.1	border
Nb₃ Sn	18.2	3.6	124	34	type-II
YBa ₂ Cu ₃ O _{7-δ}	90	(1.5)	(130)	(87)	type-II

In type II superconductors, part of the field can go through the superconductor. A supercurrent circulates around the magnetic flux to screen it: Vortices.



Superconductivity is suppressed at the vortex core



In type II superconductors, part of the field can go through the superconductor. A supercurrent circulates around the magnetic flux to screen it: Vortices.





Vortices repel each other (they have the same topological charge)

M.J. Calderón calderon@icmm.csic.es

In type II superconductors, part of the field can go through the superconductor. A supercurrent circulates around the magnetic flux to screen it: Vortices.







www.icmm.csic.es/superconductividad



www.icmm.csic.es/superconductividad





In type II superconductors, part of the field can go through the superconductor. A supercurrent circulates around the magnetic flux to screen it: Vortices.

From London eqs: the magnetic flux is quantized. Vortices order in a regular array.

First observation of an array of vortices



Physics Letters 24A, 526 (1967)

Supercurrent exert forces on vortices leading to dissipation. Impurities pin the vortices so they cannot move.

TOWARDS A MICROSCOPIC MODEL

M.J. Calderón calderon@icmm.csic.es

ISOTOPE EFFECT

(C. Reynolds et al, E. Maxwell)

Evidence that superconductivity was related to electron-phonon interaction

$$T_c \propto \omega_D \approx \frac{1}{\sqrt{M}}$$



Independently, Fröhlich suggested that SPC occurs due to electronlattice interaction. Also Bardeen, independently, as soon as he knew about the isotope effect.

$$V_{\text{eff}}(\mathbf{k}, \mathbf{k}') = -g_{\mathbf{k}-\mathbf{k}'}^2 \frac{2\omega_{\mathbf{k}-\mathbf{k}'}}{\omega_{\mathbf{k}-\mathbf{k}'}^2 - (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})^2}$$

Formulation of the electron-phonon interaction. Leads to attractive energy for low-energy transfer.

THE IDEA OF A GAP

Bardeen proposed that a gap in the spectrum would lead to the rigidity of the wave-function. Some experiments were showing a sign of a gap (activated specific heat).

EFFECTIVE INTERACTION

Bardeen-Pines effective interaction:

screened Coulomb +

retarded electron-phonon interaction

Bare Coulomb

$$V(r) = e^2/r \to V_q = 4\pi e^2/q^2$$

Screened Coulomb

$$V(r) = \frac{e^2 e^{-\kappa r}}{\epsilon r} \to V_q = \frac{4\pi e^2}{\epsilon (q^2 + \kappa^2)}$$

Coulomb is always repulsive

EFFECTIVE INTERACTION

Electron-phonon interaction. Phonon of frequency ω_{a} .

$$V_q + |M_q|^2 \left(\frac{1}{\hbar\omega - \hbar\omega_q} + \frac{1}{-\hbar\omega - \hbar\omega_q} \right) = V_q + \frac{2|M_q|^2}{\hbar} \frac{\omega_q}{\omega^2 - \omega_q^2}$$

Change in E M_g: electron-phonon matrix element.

for the e-

If electron-phonon interaction is too weak (good metals), no superconductivity arises

Modification of the dielectric screening by a moving particle in a lattice that can be deformed.

Overscreening: The effective electron-electron interaction can be negative (attractive)

Key issue: the dynamics of the phonons is much slower than the electrons'

EFFECTIVE INTERACTION

Include electron-phonon interaction (must be important due to isotope effect). Phonon of frequency ω_{α} .

$$V_q + |M_q|^2 \left(\frac{1}{\hbar\omega - \hbar\omega_q} + \frac{1}{-\hbar\omega - \hbar\omega_q}\right) = V_q + \frac{2|M_q|^2}{\hbar}\frac{\omega_q}{\omega^2 - \omega_q^2}$$

Attraction if $\omega < \omega_q$



Moving Charge

 $\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet$ $\bullet \quad \bullet \quad \bullet$ $\bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet$ $\bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet$ $\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet$ • • \bullet \bullet • • $\bullet \quad \bullet \quad \bullet \quad \bullet$ $\bullet \quad \bullet \quad \bullet$ $\bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet$ $\bullet \bullet \bullet \bullet \bullet \bullet \bullet \bullet$ $\bullet \quad \bullet \quad \bullet$ $\bullet \quad \bullet \quad \bullet \quad \bullet$ • • Time avoidance

BCS theory (1957)

Bardeen-Cooper-Schrieffer

Interaction-pairs-wavefunction

Nobel prize 1972

Arbitrarily weak attractions can bind pairs of electrons on the Fermi surface (free particles would need an energy minimum).



Add two electrons on top of the Fermi sea

$$|\Psi\rangle = \Lambda^{\dagger} |FS\rangle$$

Assume zero momentum and singlet pairing (expected lowest energy)

With pair creation operator

$$\Lambda^{\dagger} = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}$$

pair wavefunction

(s-wave symmetry for conventional superconductors)

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \hat{V}$$

Define:
$$|\mathbf{k}_{P}\rangle \equiv c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}|FS\rangle$$

$$H|\Psi\rangle = \sum_{|\mathbf{k}|>k_F} 2\epsilon_{\mathbf{k}}\phi_{\mathbf{k}} |\mathbf{k}_p\rangle + \sum_{|\mathbf{k}|,|\mathbf{k}'|>k_F} |\mathbf{k}_p\rangle \langle \mathbf{k}_p |\hat{V}|\mathbf{k}'_p\rangle \phi_{\mathbf{k}'}$$

$$E\phi_{\mathbf{k}} = 2\epsilon_{\mathbf{k}}\phi_{\mathbf{k}} + \sum_{|\mathbf{k}'| > k_{F}} \langle \mathbf{k}_{p} | \hat{V} | \mathbf{k}'_{p} \rangle \phi_{\mathbf{k}'}$$



Coleman's book

56

Simplified model interaction: only attractive within an energy ω_D of the Fermi energy



$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -g_0/V \\ 0 \end{cases}$$

 $(|\epsilon_{\mathbf{k}}|, |\epsilon_{\mathbf{k}'}| < \omega_D)$ (otherwise). Coleman's book

Coleman's book

COOPER PAIRS (1956)

$$E\phi_{\mathbf{k}} = 2\epsilon_{\mathbf{k}}\phi_{\mathbf{k}} + \sum_{|\mathbf{k}'| > k_{F}} \langle \mathbf{k}_{p} | \hat{V} | \mathbf{k}'_{p} \rangle \phi_{\mathbf{k}'}$$

$$(E - \epsilon_{\mathbf{k}})\phi_{\mathbf{k}} = -\frac{g_{0}}{V} \sum_{0 < \epsilon_{\mathbf{k}'} < \omega_{D}} \phi_{\mathbf{k}'}$$

$$\phi_{\mathbf{k}} = -\frac{g_{0}/V}{E - 2\epsilon_{\mathbf{k}}} \sum_{0 < \epsilon_{\mathbf{k}'} < \omega_{D}} \phi_{\mathbf{k}'} \qquad E = -2\omega_{D}e^{\frac{-2}{g_{0}N(0)}}$$

Fermi sea is unstable to the formation of Cooper pairs

- Cooper pair is a bound state beneath the particle-hole continuum.
- Cooper pairs can condensate.

The degeneracy of the Fermi sea N(0) implies pairs form even for a very weak pairing interaction

$$E = -2\omega_D e^{\frac{-2}{g_0 N(0)}}$$

- The Cooper pair has a small smearing in k space \rightarrow a large extension (coherence length) in real space (10⁴ Å for Al).
- Pairs overlap.



nttp://www.qm.phy.cam.ac.uk/teaching/

OBSERVATION OF COOPER PAIRS

The vortex magnetic flux is quantized (London, 1950)

$$\Phi_0 = \frac{h}{e^*} \equiv \frac{h}{2e}$$

Magnetic flux in a cylinder provides a proof for the charge of the Cooper pair.



SCHRIEFFER: BCS WAVE-FUNCTION

Coherent superposition of Cooper pair operators

$$|\Psi_{BCS}\rangle = \exp[\Lambda^{\dagger}]|0\rangle \qquad \Lambda^{\dagger} = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}$$
$$\Psi_{BCS}\rangle = \prod_{\mathbf{k}} \exp[\phi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}]|0\rangle = \prod_{\mathbf{k}} (1 + \phi_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger})|0\rangle$$

(all higher power orders are 0)

And the **BCS** Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}$$

PAIRING HAMILTONIAN

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}$$

Mean field approximation

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle$$

Mean field Hamiltonian

$$H = \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} - \sum_k \left(\Delta_k c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} + \Delta^*_k c_{-k\downarrow} c_{k\uparrow} \right)$$

Tinkham's book

PAIRING HAMILTONIAN

Mean field Hamiltonian

$$H = \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} - \sum_k \left(\Delta_k c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} + \Delta^*_k c_{-k\downarrow} c_{k\uparrow} \right)$$

Pair creation: $e^- + e^- \rightarrow \text{pair}^{2-}$

Note $c_{-\mathbf{k}\downarrow} = h_{\mathbf{k}\downarrow}^{\dagger}$ is a hole creation operator

Andreev reflection:

$$e^- \rightarrow \text{pair}^{2-} + h^+$$



nan's book

EXCITATION SPECTRUM

Diagonalize (Bogoliubov transformation)

٠

$$\alpha_{k\uparrow}^{\dagger} = c_{k\uparrow}^{\dagger} u_k + c_{-k\downarrow} v_k$$
$$\alpha_{-k\downarrow} = c_{-k\downarrow} u_k^* - c_{k\uparrow}^{\dagger} v_k^*$$

$$H = \sum_{k\sigma} E_k \alpha_{k\sigma}^{\dagger} \alpha_{k\sigma}$$
$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$$

The self consistent eq for the gap is:

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{\sqrt{\epsilon_{\mathbf{k}'}^2 + |\Delta_{\mathbf{k}'}|^2}} V_{\mathbf{k},\mathbf{k}'}$$

M.J. Calderón calderon@icmm.csic.es



Excitation spectrum. And reev scattering mixes electron and hole excitation spectra producing the gap $\Delta.$

Excitation energy of quasiparticles

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$$



Coleman's book

Density of Bogoliubov quasiparticles (a) BCS Theory $N_{s}(E) = N_{n}(0) \frac{d |\epsilon_{\mathbf{k}}|}{dE_{\mathbf{k}}} =$ $= N_{n}(0) \left(\frac{E}{\sqrt{E^{2} - |\Delta|^{2}}} \right) \theta(E - |\Delta|)$ N_(E)/N_(0) 60 **Coherence** peak 05 1.01.52.0 E/Δ

BCS THEORY

Explicit equation for Δ (T=0) $\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{\sqrt{\epsilon_{\mathbf{k}'}^2 + |\Delta_{\mathbf{k}'}|^2}} V_{\mathbf{k},\mathbf{k}'}$

Within BCS $V_{kk'} = -V$ within $\hbar \omega_D$ of E_F Then $\Delta_{kk'} = \Delta$ (isotropic)

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

Isotropic pairing function: s-wave



BCS THEORY

For finite T

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{\sqrt{\epsilon_{\mathbf{k}'}^2 + |\Delta_{\mathbf{k}'}|^2}} \tanh\left(\frac{\beta}{2} \sqrt{\epsilon_{\mathbf{k}'}^2 + |\Delta_{\mathbf{k}'}|^2}\right)$$

For weak coupling superconductors

Universal $\Delta(T)$ curve in the weak coupling limit



MIGDAL-ELIASHBERG (INCLUSION OF RETARDATION EFFECTS)

BCS theory included retardation effects in a minimal way by introducing an energy cut-off: the Debye frequency.

Eliashberg treated the electron-phonon interaction including correctly the retardation effects.



Migdal (1957): vertex corrections O(m/M)^{1/2} can be dropped (equivalent to adiabaticity condition)

MIGDAL-ELIASHBERG (INCLUSION OF RETARDATION EFFECTS)

BCS theory included retardation effects in a minimal way by introducing an energy cut-off: the Debye frequency.

Eliashberg treated the electron-phonon interaction including correctly the retardation effects.

$$T_{c} = \mathcal{F}(\alpha^{2} \mathcal{F}(\omega), \mu^{*}) \qquad \Delta = \mathcal{G}(\alpha^{2} \mathcal{F}(\omega), \mu^{*})$$

$$\frac{2\Delta}{k_{B}T_{c}} = 3.53 \left[1 + 12.5 \left(\frac{T_{c}}{\omega_{ln}} \right)^{2} \log \left(\frac{\omega_{ln}}{2T_{c}} \right) \right]$$
Coupling strength PRB 29, 184 (1984)

MIGDAL-ELIASHBERG



MAX T_c FOR PHONON MEDIATED SUPERCONDUCTIVITY

McMillan PR 167, 331

$$T_c \propto \langle \omega_{ph} \rangle \exp[-1/(\lambda - \mu^*)]$$

With the electron phonon coupling constant

TABLE VIII. The predicted maximum superconducting transition temperature for four classes of materials found from the observed T_c and λ and Fig. 11, together with the observed Alloys

Pure metals

Mal	T _e		Tomax	Observed maximum	
Metal	("K)	λ	(°K)	Te	Material
Pb	7.2	1.3	9.2	8.8	Pb–Bi
Nb	9.2	0.82	22	10.8	Zr-Nb
V₃Si	17	0.82	40		
Nb ₃ Sn			28	20	Nb ₃ Al-Nb ₃ Ge

Input: phonon spectrum

$$\lambda = 2\int_{0}^{\infty} \frac{\alpha^{2} F(\omega)}{\omega}$$

Note:

 MgB_2 Tc=40K
Canfield and Crabtree, Physics Today 2003.

$MgB_{2}(2001)$

T_c=39 K.

MULTIBAND SUPERCONDUCTOR

Conventional SPC.

2 differentiated bands.

One very strong phonon (in the B plane) coupled to the conduction electrons.



2 energy gaps with different electron-phonon strengths





RECORD T_C FOR ELECTRON-PHONON MEDIATED SUPERCONDUCTIVITY

H₂S T_c=203 K (at 200 GPa); Nature 525, 73 (2015) LaH₁₀ T_C=250 K at 170 GPa; Nature 569, 528 (2019)

 H_2S leads to H_3S under high pressures. Hydrogen atoms are light → high phonon frequencies expected. Large Tc predicted Ashcroft PRL 21, 1748 (1968); 21, 1748 (2004)

Role of anharmonic phonons.

Errea et al PRL 114, 157004



Recent developments by Ranga Dias (closer to ambient conditions) under discussion.



Mazin, Nature 464, 183 (2010)

MATTHIAS'S RULES (1950's)

- High symmetry (cubic best) is good
- High density of electronic states is good.
- Stay away from oxygen
- Stay away from magnetism (PM impurities destroy superconductivity)
- Stay away from insulators
- Stay away from theorists



OUTLINE

- Superconductivity
 - Properties (zero resistivity, Meissner effect)
 - Understanding (pairing, BCS, Ginzburg-Landau)
 - Electron-phonon interaction (conventional superconductivity)
- Unconventional superconductivity (unsolved)
 - What are the new issues.
 - What are the proposals.

Physics World, Jan 2002

MATTHIAS'S RULES ?

Theory predicted superconductivity in hydrogen compounds (Ashcroft) and semiconductors (SrTiO₃, Cohen).



UNCONVENTIONAL SUPERCONDUCTORS

Not driven by conventional phonons.



Physics World, Jan 2002

UNCONVENTIONAL SUPERCONDUCTORS

The "normal" state is more complicated

- Proximity or coexistence with magnetism
- Strong correlations.
 - Competing orders (stripes).
 - Is there a Fermi surface? Doped Mott insulator. Non-Fermi liquid behaviour. Pseudogap phases.
- Low dimensionality, anisotropies, nematicity.

UNCONVENTIONAL SUPERCONDUCTORS

The superconducting state is different

The pairing function Δ_k may

- Be non-isotropic (including nodes, sign changes)
- Have a finite orbital momentum (p- or d-wave symmetry)
- Be spin-triplet (p-wave symmetry)
- λ>>ξ (type II)
- Anisotropies



Many theories.

2 distinct approaches to the problem:

- Stay within BCS (need a Fermi surface!) but a new pairing (glue) mechanism is needed (maybe spin fluctuations, some kind of electron-phonon interaction).
- Start from the Mott state (no boson exchange required) and see how to gain energy from pairing
 - Resonating valence bonds
 - Kinetic energy driven
 - Quantum criticality...

Many theories.

2 distinct approaches to the problem:

- Stay within BCS (need a Fermi surface!) but a new pairing (glue) mechanism is needed (maybe spin fluctuations, some kind of electron-phonon interaction).
 - A: We know how to deal with it. D: Usually there is no Fermi surface.

Many theories.

2 distinct approaches to the problem:

- Start from the Mott state
 - Resonating valence bonds
 - Kinetic energy driven
 - Quantum criticality...

A: It seems, in principle, more self-consistent. D: We need to properly treat the Mott state first!!

FIRST APPROACH

Assume BCS is valid for non-conventional superconductors.

We need some attractive interaction (but no phonons!) +Very strong electron-electron repulsive interaction. Is there a way around it??

PAIRING SYMMETRY

$$\psi(\vec{r}_{1}s_{1},\vec{r}_{2}s_{2}) = \varphi(\vec{r}_{1},\vec{r}_{2})\chi(s_{1},s_{2})$$

Spatial

Spin

Pair wavefunction must be antisymmetric

Spin singlet \rightarrow even parity orbital wave function s, d Spin triplet \rightarrow odd parity orbital wave-function p, f

Singlet SPC

s-wave: conventional spc d-wave: cuprates d-wave/d-wave: Fe scp p-wave (triplet SPC):

- Superfluidity in ³He
- UPt₃, UTe₂
- Indications in some multilayered graphene systems.
- Proximity effects.

SUPERFLUIDITY IN ³HE (1972)

 $T_{c}=2.7 \text{ mK}$

Pairing cannot be mediated by the lattice. Nuclear forces are strongly repulsive in the core \rightarrow no s-wave possible. Need of wavefunctions that vanish at $r\rightarrow 0$.

High angular momentum pairing (p-wave) was proposed as a way to overcome the short range repulsion (Pitaevskii 1959).

Glue: One possibility is mediation by ferromagnetic spin fluctuations: FM paramagnons (FM fluctuations suppress s-wave and enhance p-wave pairing).

SUPERFLUIDITY IN ³HE

Attractive interactions by ferromagnetic fluctuations:

FM clouds are formed which attract the ³He quasiparticles (something like magnetic polarons instead of lattice polarons)





s wave gap

Gap equation from BCS (T=0)

(spherical symmetry)

$$\Delta_{k} = -\frac{1}{\Omega} \sum_{kk'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}}$$

For $V_{kk'}$ constant and attractive: isotropic gap $\Delta_k \text{=} \Delta$

а





(a)





Gap equation from BCS (T=0)

$$\Delta_{k} = -\frac{1}{\Omega} \sum_{kk'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}}$$

Repulsive $V_{kk'}$ \leftarrow Anisotropic Δ_k with sign change!

$$\operatorname{sign}(\Delta_{\mathbf{k}}) = -\operatorname{sign}(V_{\mathbf{k},\mathbf{k}'})\operatorname{sign}(\Delta_{\mathbf{k}})$$

An anisotropic pair potential leads to an anisotropic gap

$$V_{kk'} = -V_0 \gamma_k \gamma_{k'}$$
$$\Delta_k = \gamma_k \Delta_0$$
form factor

For instance, d-wave

$$\Delta_k = \Delta_0 \cos(2\phi)$$



The gap has nodes and sign changes



SINGLET VERSUS TRIPLET

From Knight shift experiments (nuclear magnetic resonance experiment)



(note Sr₂RuO₄ is currently known not to be a triplet superconductor)

NODES VERSUS NODELESS



Without nodes: activated behavior (λ , specific heat...) With nodes: power law behaviors

Gap without nodes

London penetration length within BCS

 $\left(\frac{T_c}{T}\right)$ ~ **3**.33 $\exp(-1.76T_c/T)$ 300 200 \mathbf{r}_{1} € র্ব в 100 -0 \odot ē 6 Temperature (K)

Pb_{0.95}Sn_{0.05} PRL 70, 3999 (1993)

Gap with nodes

Power law dependencies



www.personal.psu.edu/ewh10 Physica C 320, 9

TUNNELING SPECTROSCOPY





Voltage (mV)

SENSITIVITY TO THE PHASE: JOSEPHSON EFFECT $I_s = I_c \sin \Delta \varphi$



MATERIALS

SOME TYPICAL PHASE DIAGRAMS



HEAVY FERMIONS (1979)

"Our experiments demonstrate for the first time that superconductivity can exist in a metal in which many-body interactions, probably magnetic in origin, have strongly renormalized the properties of the conduction-electron gas."

PRL 43, 1892 (1979)

Coexisting AF + SPC

Reentrant SPC due to competition with Kondo

Quantum criticality Nat. Phys. 4, 186



FERROMAGNETIC SUPERCONDUCTORS



Proximity of quantum critical point can lead to coexistence

Possible triplet pairing UPt₃, UTe₂ Science 365, 684 (2019) URhGe Science 309, 1343 (2005) UCoGe Nature Comm 8, 14480 (2017) PRL 94, 097003 (2005)

CUPRATES

- Layers of CuO₂. Different related structures.
- But note!: SPC requires coherence in 3dim.
- Highest Tc 134K (at ambient pressure).
- Tc increases with number of CuO2 planes in the unit cell (up to n=3).
- Pairs were found to be singlets.
- d-wave pairing was proposed in the cuprates early on. Scalapino, Phys. Rep. 250, 329 (1995)
- Undoped cuprates are correlated insulators and AF (π,π).





CUPRATES: COMPLEX "NORMAL" STATE





Origin?: spin-singlet formation (Anderson), pairing with short range order (preformed pairs), antiferromagnetic fluctuations, charge density wave

Is it due to fluctuations or is it a new phase (with a related broken symmetry)? Transition or crossover?



In other words: Is it a precursor or a competing phase?





Science 307, 901

Norman et al, Adv. Phys. 54, 715 (2005) http://www.msd.anl.gov/files/msd/cuprates-columbia.pdf

105

FE BASED SUPERCONDUCTORS

Many different families discovered, all sharing a Fe plane





An important breakthrough because it could help understand cuprates



Fe-As or Fe-Se planes



108
HIGHEST T_c IN Fe SUPERCONDUCTORS

Single layer FeSe on doped SrTiO₃



Nature Materials 14, 285–289 (2015)

Fe BASED SUPERCONDUCTORS

Differences with cuprates:

- The AF state is metallic (not Mott insulator): Hund metal (correlations).
- Multiorbital system (more than 1 gap possible)
- SPC can be achieved without chemical doping.
- More 3dim-like (less anisotropy in c-direction)

Proposed mechanisms for superconductivity

- Spin fluctuations (π,0)
- Orbital fluctuations
- Possible role of nematicity

Extended BZ (1 Fe unit cell)



Gap symmetry

•	-	-		
	Family	Full gap	Highly anisotropic	Strong nodal
v:1106.3712	ш	$\Pr EeAsO_{1-y}[52K]$ [293] SmFeAs(O,F)[55K] [295]	LaFeAs(O,F)[26K] [214] NdFeAs(O,F) [214]	LaFePO[6K] [203, 204, 294]
	122	$\begin{array}{l} ({\rm Ba}, {\rm K}){\rm Fe}_2{\rm As}_2[40{\rm K}] [146, 236, 296, 242] \\ {\rm Ba}({\rm Fe}, {\rm Co})_2{\rm As}_2 {\rm OP}, 23{\rm K} 238, 208 \end{array}$	$\begin{array}{l} {\rm Ba(Fe,Co)_2As_2} \ [{\rm OD}] \ [238,\ 241]^* \\ {\rm Ba(Fe,Ni)_2As_2} \ [297]^* \\ {\rm Ba(Fe,Co)_2As_2} \ [{\rm UD}] \ [241]^* \end{array}$	$\begin{array}{c} {\rm KFe_2As_2} [4{\rm K}] [211, 309] \\ {\rm BaFe_2(As,P)_2 OP, 31{\rm K} [205, 149]} \\ {\rm (Ba,K)Fe_2Ae_2} [{\rm UD}] [242] \end{array}$
arXi	111	LiFeAs [18K] [298, 258]		LiFeP [6K] [299]
	11		Fe(Se,Te) [27K] [281, 246]	

Fe BASED SUPERCONDUCTORS

Role of <u>nematicity</u>?

Breaks the tetragonal symmetry.

Related to magnetic fluctuations.

Nematic order postulated for the pseudogap in cuprates.



doping http://www.ifsc.usp.br/coloquio/2013/Fernandes.pdf

Fe BASED SUPERCONDUCTORS

Pseudogap

Gap opening due to spin fluctuations: Nat. Comm. **2**, 392 (2011)



MECHANISMS

Spin fluctuations play the role of phonons (à la BCS).

The "normal" state can be described as a nearly AF Fermi liquid (unconventional Fermi liquid close to an AF instability).

Note: calculating the effective interaction is not trivial because vertex corrections can be important (Migdal's theorem doesn't apply)

If the magnetic susceptibility has a peak at q (remember nesting) the interaction is also peaked at q and $\Gamma_s(k, k') = \frac{3}{2}U^2 \frac{\chi_0(q)}{1 - U\chi_0(q)}$ positive.

If you look at the interaction in real space

It changes sign with position!!

Attractive interaction by space avoidance

Scalapino, Phys. Rep. 1995 Hirshfield et al. 1106.3712



115

Square lattice at half-filling:



At $q=(\pi,\pi)$ the spin susceptibility is maximal (nesting)

$$V_{k,k'} = V_{k-k'} = V_q \propto \chi_q > 0 \quad q = (\pi, \pi)$$

To fullfil the gap equation, you need an anisotropic gap such that

$$\Delta_{k} = -\frac{1}{\Omega} \sum_{kk'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}} \qquad \text{sign}(\Delta_{\mathbf{k}}) = -\text{sign}(V_{\mathbf{k},\mathbf{k}'}) \text{sign}(\Delta_{\mathbf{k}})$$

$$d\text{-wave}$$

$$\Delta_{k} = \frac{\Delta_{0}}{2} (\cos k_{x} - \cos k_{y})$$

$$\Delta_{k+(\pi,\pi)} = \frac{\Delta_{0}}{2} (-\cos k_{x} + \cos k_{y}) = -\Delta_{k}$$

116

Correlation between Tc and a typical energy scale of spin fluctuations.

In the Scalapino approach, the t-J model is the basis for understanding.

Moriya-Ueda, Rep. Prog. Phys. 66, 1299 (2003) Scalapino, Rev. Mod. Phys. 84, 1383 (2012)



For a murtiorbital system (as Fe-superconductors)

For instance, spin fluctuations related to nesting between electron and hole pockets: $q=(\pi,0)$





This would lead to an s_{\pm}

(as the order parameter averages to zero on the Fermi surface, you also get "Coulomb avoidance")

ELECTRON-PHONON

Not discarded! For cuprates: Phys. Rev. Lett. 105, 257001 Maybe coupled to other degrees of freedom?

For Fe-superconductors

Spin-phonon?

Adv. in Cond. Matt. Phys. 2010, 164916 (2010)

Orbital fluctuations induced by electron-phonon.

PRL 104, 157001

Interplay of many degrees of freedom may be relevant.



KINETIC ENERGY DRIVEN MECHANISM

Different energy scales involved for underdoped cuprates

T*: Phase transition or crossover (no exp. evidence of phase transition)





KINETIC ENERGY DRIVEN MECHANISM

Carlson et al, Chapter 21

Different energy scales involved for underdoped cuprates At T*_{stripe}: stripe formation. Stripes are rivers of charge where holes can move (gain kinetic energy in 1dim). In between, AF regions where the carriers are localized.

At T^*_{pair} : local pairing (spin-gap) within the 1DEGs (stripes). Pairs can tunnel to neighboring 1DEG (which in principle has another k_F). This way the system gains kinetic energy in a perpendicular direction as well. There is finite Δ but not fixed phase. At T_c : phase coherence sets in (Josephson coupling between

stripes) \rightarrow superconductivity.

T_c< T^{*}_{pair}<T^{*}_{stripe}

QUANTUM PHASE TRANSITIONS



Transition at T=0 with consequences for T>0.

Divergence of time coherence.

Region in which termal and quantum fluctuations are equally important



Taillefer Annu Rev Cond Matter Phys (2010)





Linear T resistivity coming from fluctuations in the pseudogap phase (spin density wave order).

In organic spc and Fe pnictides, similar phenomena coming from spin fluctuations.

HIDDEN ORDER

Idea: the pseudogap phase is in fact a gapped phase (pseudo in experiment due to imperfections or dynamic effects)



PRL 83, 3538



RESONATING VALENCE BONDS

Mottness from the start.

Pairing scale very large (related to T*)

Quantum fluctuations destroy long range order leading to a spin liquid of singlets.

However, spin liquid not found on cuprates.



http://www.msd.anl.gov/files/msd/cuprates-columbia.pdf

(Anderson)

POST HIGH T_c PRINCIPLES TO FIND SPC

MAZIN, NATURE 464, 183 (2010)

- Layered structures
- Carrier density should not be too high (compared to conventional metals)
- Transition metals of the fourth period (3d) are good
- Magnetism is essential
- Proper Fermi surface geometry is essential (in relation to spin excitations)

Corollary: work with solid state chemists (you need complex chemical compounds)

SUPERCONDUCTIVITY IN MULTILAYERED GRAPHENE (2018-)

Moiré systems:



Cao et al, Nature 556, 80 (2018); Nature 556, 43 (2018) Lu, et al Nature 574, 653 (2019) Mirror-symmetric twisted trilayer, quatrilayer and pentalayer graphene D fig (Virm) -0.5

Park et al, Nature 590, 249 (2021) Zhang et al, Science 377, 1538 (2022) Park et al Nat. Mater. 21, 877 (2022) Non-moiré systems:



ABC trilayer: Zhou et al, Nature 598, 429; 598, 434 (2021)

OUTLINE

• Superconductivity

- Properties (zero resistivity, Meissner effect)
- Understanding (pairing, BCS, Ginzburg-Landau)
- Electron-phonon interaction (conventional superconductivity)
- Unconventional superconductivity (unsolved)
 - What are the new issues.
 - What are the proposals.