Superconductivity Lectures

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International Summer School: Topological and Symmetry-Broken Phases in Physics and Chemistry – Theoretical Basics and Phenomena Ranging from Crystals and Molecules to Majorana Fermions, Neutrinos and Cosmic Phase Transitions

14 - 18 August 2017 in Dresden, Germany

Superconductivity

- Topic 1 Review of basics, phenomena and BCS theory (including gauge symmetry breaking and link to Higgs)
- Topic 2 Unconventional superconductivity I, (mainly examples from different materials)
- Topic 3 Unconventional superconductivity II (more formal symmetry classification)
- Topic 4 Topological Superconductivity


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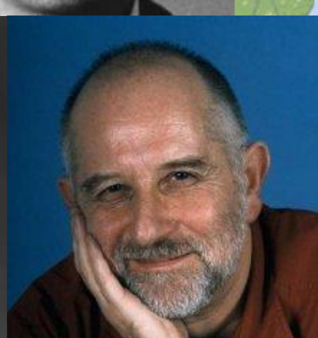
August 8 1902
Birth of Paul Dirac

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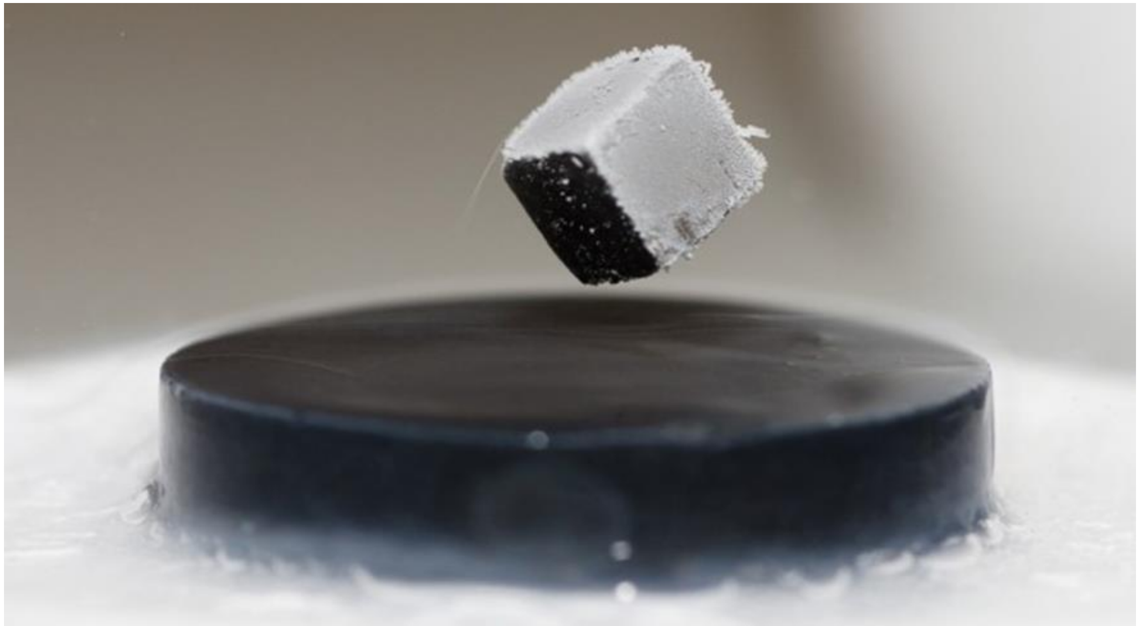
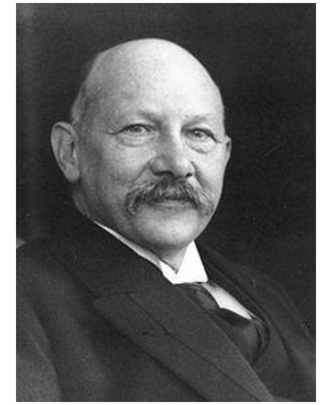
Topic 1: Review of basics, phenomena and BCS theory



Topic 1: Review of pheonomena and BCS theory

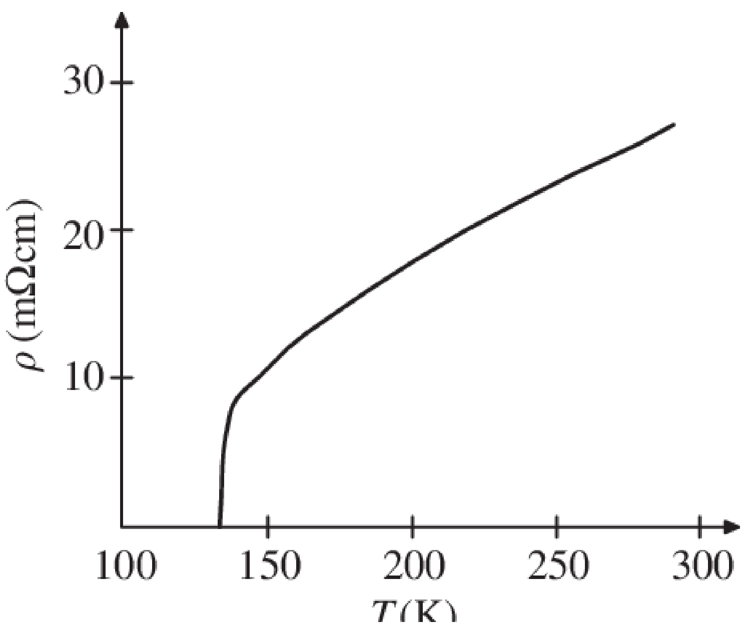
- 100+ years of superconductivity
- Resistance and Meissner effect
- The Cooper problem
- The BCS state
- Energy gap and quasiparticle excitations
- BCS Higgs and the (Anderson)-Higgs boson?

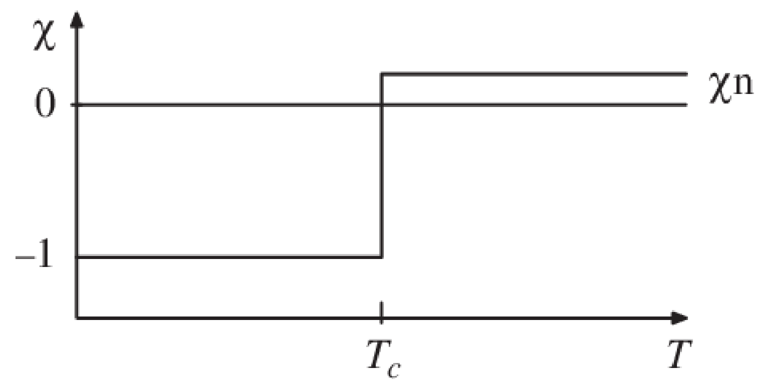
100 years of superconductivity

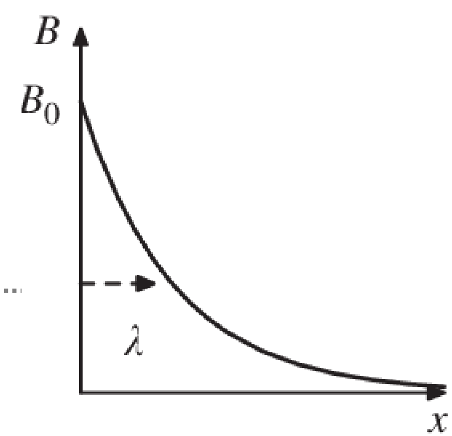


- Discovered in 1911 by Kammelingh Onnes in Hg at 4.2K
- Meissner Ochsenfeld effect 1932
- Bardeen Copper Schrieffer theory 1954
- In 1986 Bendorz and Muller discover 38K superconductivity in $La_{2-x}Ba_x\ CuO_4$
- Eremets 2014 190K superconductivity in H_3S at ultrahigh pressure of > 150GPa

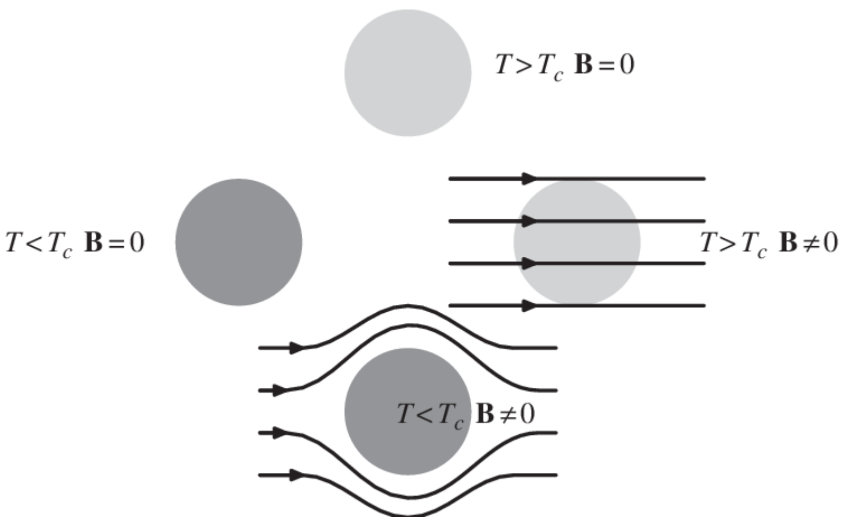
Resistive and Magnetic transitions, penetration depth

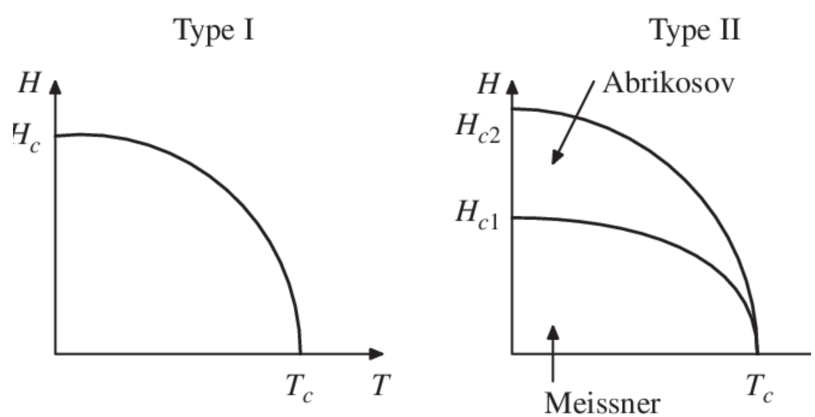


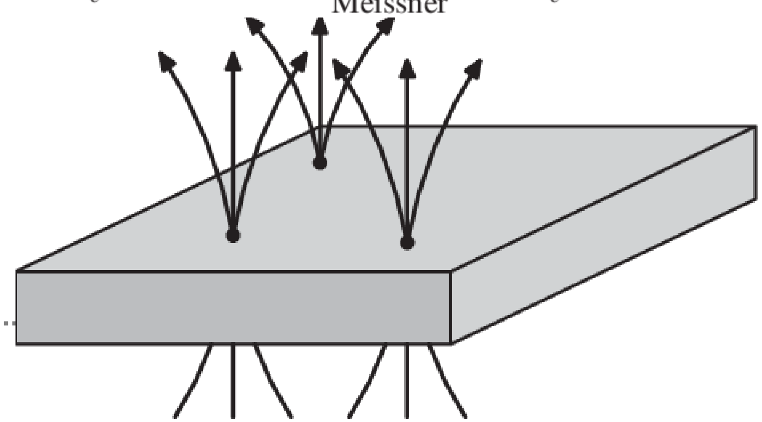




Meissner effect and type I and type II materials



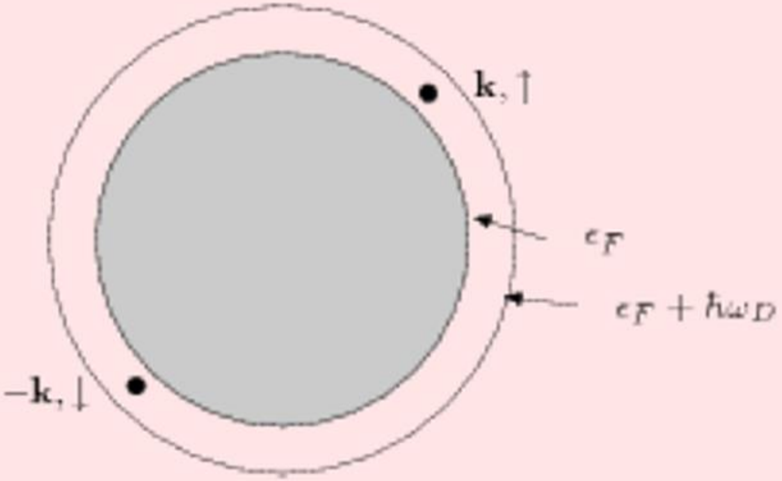




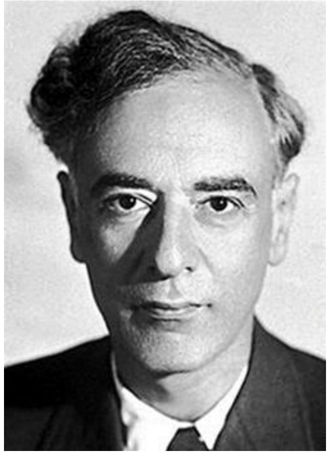
The BCS theory

In 1956 “BCS” finally solved the 40 year old puzzle of superconductivity.
John Bardeen, Leon Cooper and Bob Schrieffer

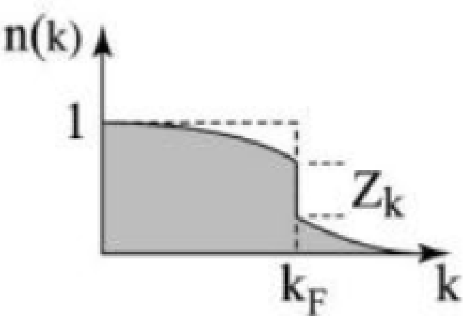
- The theory was in perfect agreement with experiments on simple superconductors such as Al
- The energy gap 2Δ at the Fermi surface was found to obey exactly the BCS prediction $2\Delta = 3.5 k_B T_c$.

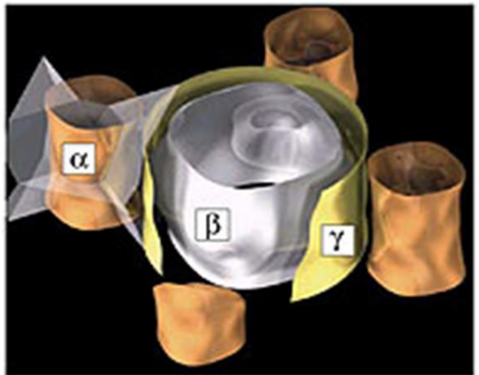


Landau Fermi liquid model of metals



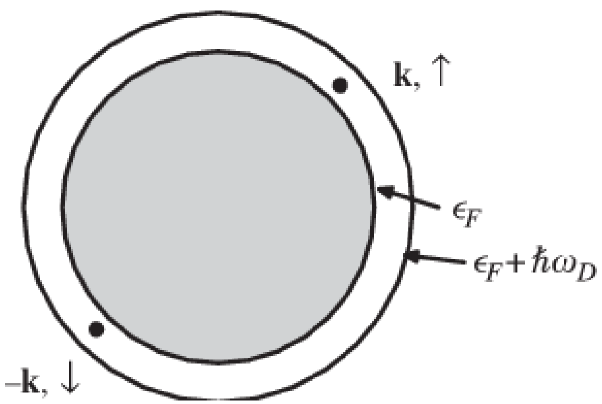
- Normal metals are described by Landau Fermi liquid theory
- The many-body ground state is smoothly connected to the non-interacting Fermi 'sea', retaining the Fermi surface as a sharp discontinuity in momentum density
- Excitations near this ground state are electron-like or hole-like 'quasiparticles' near to the Fermi surface
- These are long-lived weakly interacting excitations, occupied as expected in a Fermi Dirac distribution at temperature T
- Kohn-Sham DFT waves are an approximation to these many-body states, accurate enough for most purposes
- Eg the experimental FS of the superconductor Sr_2Ru O_4





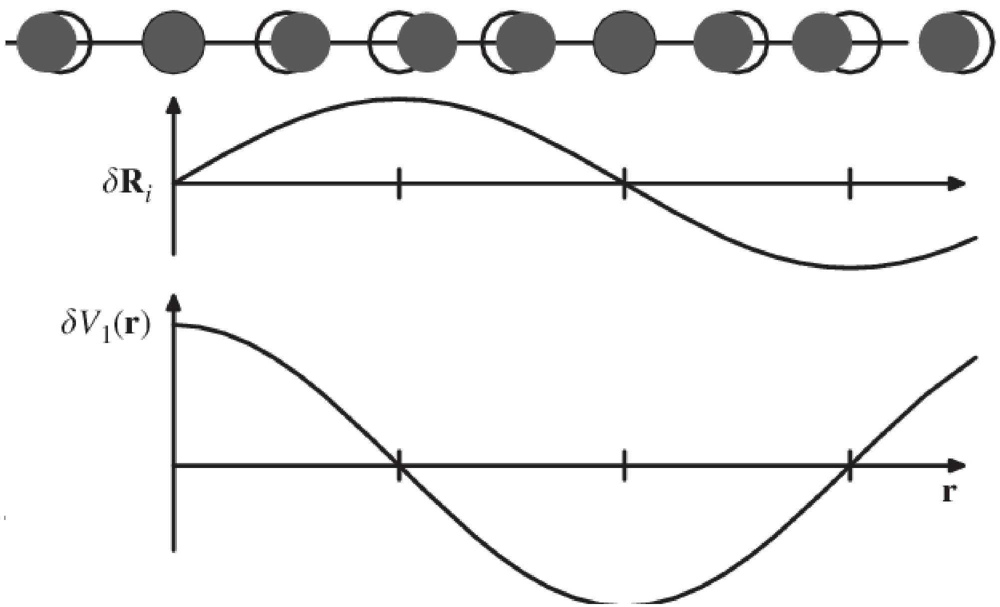
The Cooper problem and instability of the Fermi sea

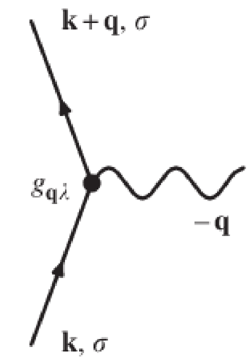
- Fermi liquid theory shows that repulsion between electrons in metals is normally weak (screening of direct Coulomb repulsive forces)
- But Cooper discovered that if an attractive force exists between two quasiparticles outside the Fermi sea, they for a bound state (Cooper pair)
- Surprisingly this occurs HOWEVER WEAK the attraction



Electron phonon interaction

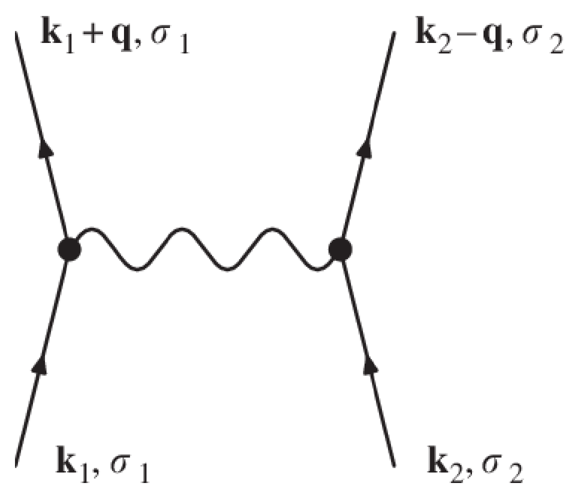
- Consider a static (or 'slow') lattice distortion of wave vector q
- This creates a modulation in the electon potential
- Electrons scatter from k to k+q

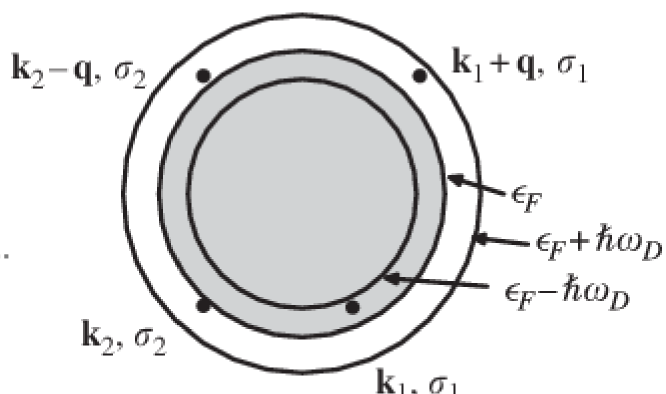




Electron-electron interaction from phonons

- Electrons can exchange virtual phonons
- Process just like exchange of gauge bosons in QED or QCD
- The effective interaction is attractive of all energies a below the phonon Debye frequency





The microscopic order parameter

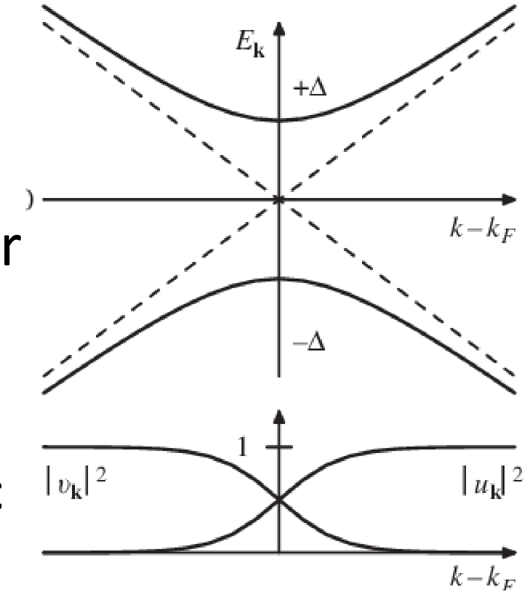
- The coherent state proposed by BCS is a condensate of "Cooper pairs"
- Each pair has zero momentm and spin, but effective charge 2

$$\hat{P}^{+}_{\mathbf{k}} = c^{+}_{\mathbf{k}\uparrow} c^{+}_{-\mathbf{k}\downarrow}. \qquad |\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}} \left(u^{*}_{\mathbf{k}} + v^{*}_{\mathbf{k}} \hat{P}^{+}_{\mathbf{k}} \right))|0\rangle,$$

The BCS state has indefinite particle number, and therefore violates gauge symmetry for an exact N-body quantum state

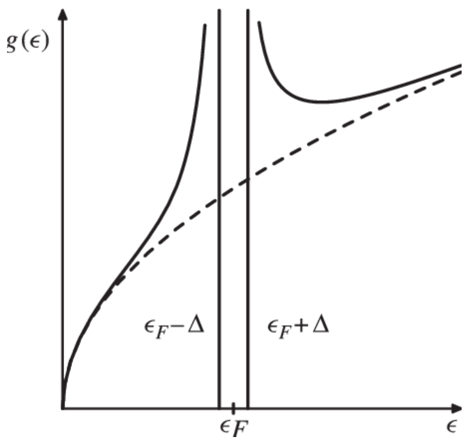
The Bogoliubov quasiparticle spectra

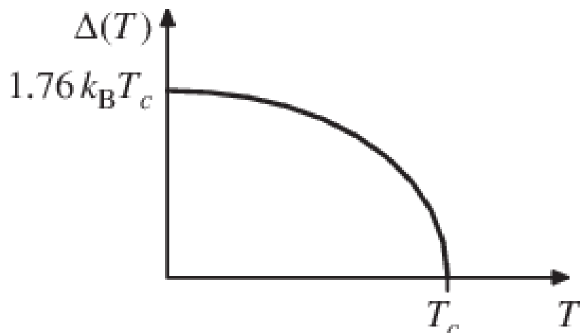
- The excitations of the superconductor relative to its ground state include both collective modes and single particle excitations
- The single particle excitations are fermionic, quasiparticles, mixing hole and electron character
- The precise form of the u_k and v_k functions enters differently as 'coherence factors' in various response functions, eg NMR or ultrasonic attenuation, confirming BCS predictions



Evidence for the BCS state

- The first predication was the existence of the energy gap Δ and the relation between Δ and T_c



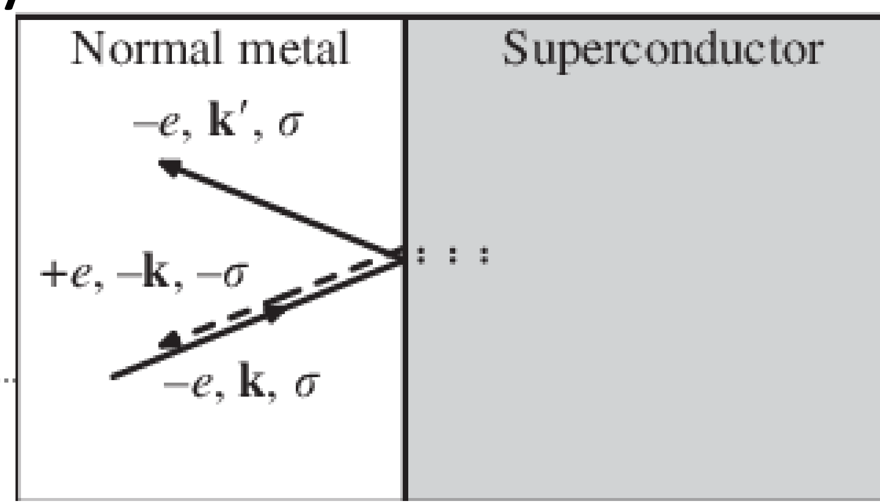


- The isotope effect showing changes of T_c with isotopic mass, M, also directly showed the role of the electron-phonon interaction

Evidence of the pair condensate

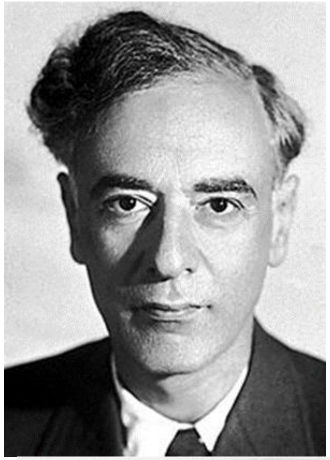
- Andreev scattering
- An electron tunnels into a superconductor, a hole of opposite spin is reflected back along a time revered trajectory
- 2e charge transferred
- Conductance peak

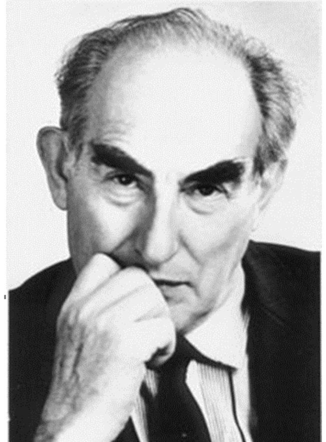
2x normal at energy < Δ



Ginzburg Landau theory of superconductivity

- Ginzburg and Landau proposed a phenomenological theory of superconductivity based on a complex order parameter Ψ(r)
- This is the ’order parameter’ for superconductivity
- It couples to a magnetic vector potential like a charge 2e quantum particle
- Gorkov later showed this Ψ(r) was equivalent to the BCS gap parameter, Δ, for the phase, corresponding to the pair condensate on BCS theory
- Predictions of the GL theory include the Abrikosov flux lattice explaining type II superconductivity





U(1) symmetry breaking

- The link between the BCS Δ and the GL ψ(r) shows that the phase transition is one of 2^{nd} order with symmetry breaking
- The Δ and ψ(r) parameters are complex
- The thermodynamic energy is determined by |Δ| and |ψ(r)| only. All phases exp(i ϑ) have equivalent ground state energy
- The energy depends on the (gauge invariant) gradient of the phase, and it is this which directly leads to the Meissner effect

$$F - F_0 \simeq |-i\hbar \partial \psi(r) - 2e A \psi(r)|^2$$

- This phase stiffness leads to the energy cost of a finite magnetic field inside the superconductor, hence to the Meissner effect

Gauge symmetry breaking

The theory lacked explicit 'gauge symmetry', which seemed to be an error
Nambu and Anderson saw this was essential to the Meissner effect

- Applying this idea in particle physics led to the Higgs mechanism, and the search for the Higgs boson at LHC
- An unexpected implication was the Josephson effect, $V = h\nu/(2e)$

BCS theory and the Higgs boson?

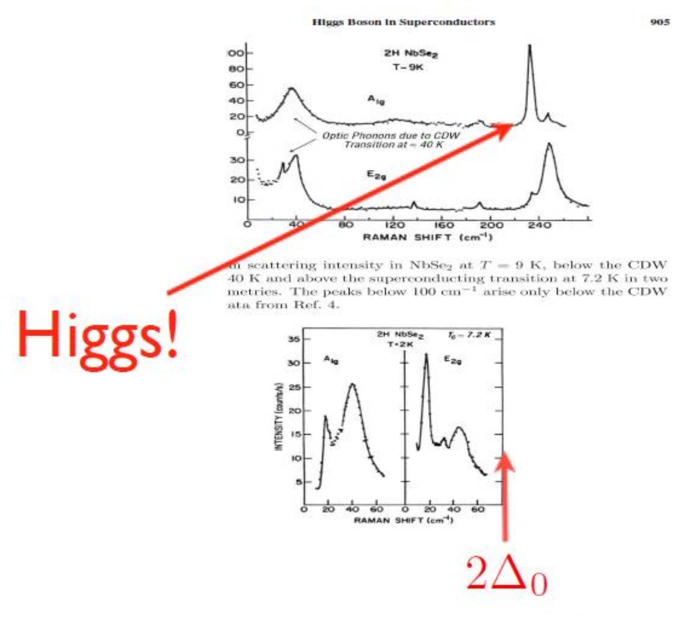
- Among the collective modes is an analogue of the Higgs boson
- Text and images below from a presentation by C.M.Varma Cargesse 2013.

Why is this the "Higgs"

Peter Higgs in "The Rise of the standard Model, Ed. (Hoddeson et al. 1997)

"The existence of the characteristic massive spin-zero modes had not been noticed by Anderson or by Englert and Brout. Indeed the theory of what particle physicists would call the Higgs mode in a superconductor was not published until 1981, after it had been detected in the Raman spectrum of superconducting NbSe(2)! (Ref. to expts. by Klein et al, and to theory by Littlewood and cmv)."

Why was the theory not done earlier for a superconductor?



End of Topic 1

- Any Questions?

Topic 2: Unconventional Superconductivty

- Discovery of High Tc superconductivity in cuprates
- Evidence for d-wave pairing in cuprates
- Spin triplet systems: superfluid 3-He, Sr_2RuO_4
- Non-centrosymmetric systems, eg CePt_3Si

More general symmetry breaking

- Nambu and Anderson recognized that BCS superconductivity corresponds to spontaneous breaking of U(1) gauge symmetry
- This was already implicit in the Landau Ginzburg theory, by the choice of a complex order parameter ψ, as a complex number
- But in general other types of symmetries can also be broken at the same T_c
  - Point group rotational symmetries (p or d-wave pairing)
  - Spin rotational symmetries (triplet pairing)
  - Time reversal symmetry breaking (chiral pairing)

More general types of Cooper pairing

- The BCS state pairs an up spin at k with a down spin at –k.
- This gives a spin singlet combination with zero centre of mass momentum
- This is readily generalized to k and spin dependent pairing states

$$F_{\alpha\beta}(\mathbf{k}) = \langle c_{-\mathbf{k}\alpha} c_{\mathbf{k}\beta} \rangle.$$

$$F(\mathbf{k}) = \begin{pmatrix} \langle c_{-\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} \rangle & \langle c_{-\mathbf{k}\uparrow} c_{\mathbf{k}\downarrow} \rangle \\ \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle & \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow} \rangle \end{pmatrix}.$$

$$\Delta^*_{\alpha\beta}(\mathbf{k}) = \sum_{\mathbf{k}'\gamma\delta} V_{\alpha\beta\gamma\delta}(\mathbf{k}, \mathbf{k}') \langle c_{-\mathbf{k}'\gamma} c_{\mathbf{k}'\delta} \rangle,$$

The generalized Nambu spinor

$$\begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & 0 & \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ 0 & \epsilon_{\mathbf{k}} - \mu & \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \\ \Delta^*_{\uparrow\uparrow}(\mathbf{k}) & \Delta^*_{\downarrow\uparrow}(\mathbf{k}) & -\epsilon_{\mathbf{k}} + \mu & 0 \\ \Delta^*_{\uparrow\downarrow}(\mathbf{k}) & \Delta^*_{\downarrow\downarrow}(\mathbf{k}) & 0 & -\epsilon_{\mathbf{k}} + \mu \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}\uparrow n} \\ u_{\mathbf{k}\downarrow n} \\ v_{\mathbf{k}\uparrow n} \\ v_{\mathbf{k}\downarrow n} \end{pmatrix} = E_{\mathbf{k}n} \begin{pmatrix} u_{\mathbf{k}\uparrow n} \\ u_{\mathbf{k}\downarrow n} \\ v_{\mathbf{k}\uparrow n} \\ v_{\mathbf{k}\downarrow n} \end{pmatrix}$$

The BCS energy gap function in general has 4 complex components, for spin up/down and particle/hole quasiparticle amplitudes.

It is also generally k dependent on the Fermi surface

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Constraints from Pauli symmetry

$$F_{\alpha\beta}(\mathbf{k}) = \langle c_{-\mathbf{k}\alpha} c_{\mathbf{k}\beta} \rangle$$
$$= -\langle c_{\mathbf{k}\beta} c_{-\mathbf{k}\alpha} \rangle$$
$$= -F_{\beta\alpha}(-\mathbf{k}).$$

$$\Delta_{\alpha\beta}(\mathbf{k}) = -\Delta_{\beta\alpha}(-\mathbf{k}).$$

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = i(\Delta_{\mathbf{k}} I + \mathbf{d}(\mathbf{k}) \cdot \sigma)\sigma_y,$$

$\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is a vector of the Pauli matrices, and I is the 2×2 unit

Singlet and triplet pairing symmetries

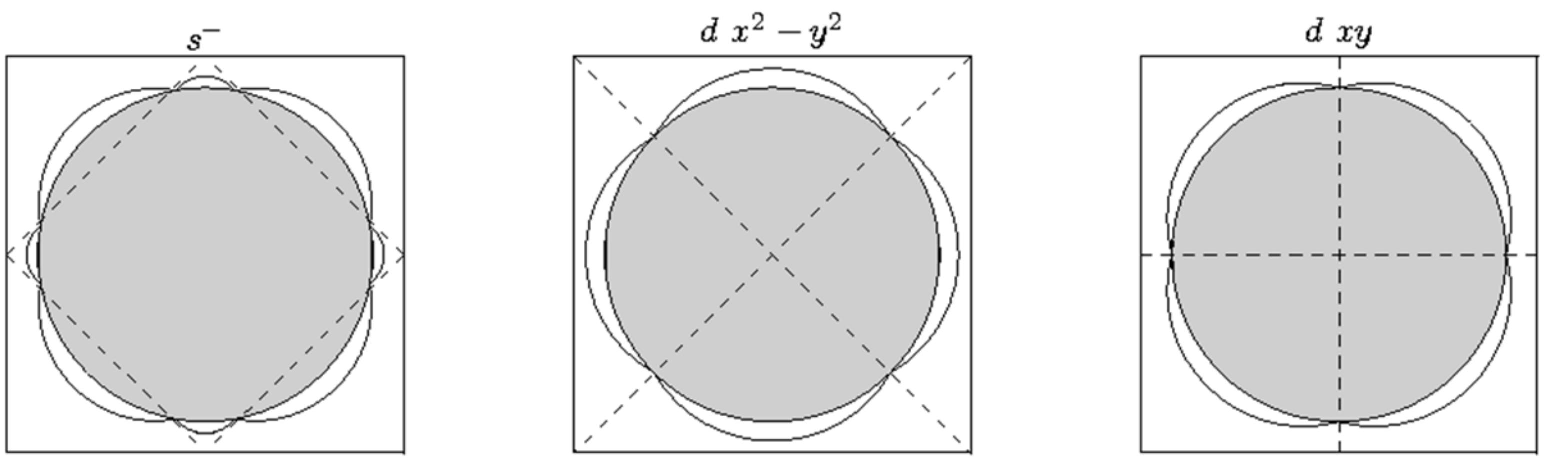
We can therefore have either singlet pairing, with a complex scalar order parameter obeying $\Delta_k = \Delta_{-k}$

Or triplet pairing with a complex 3 component vector order parameter obeying $\mathbf{d}_k = -\mathbf{d}_{-k}$

They are distinguished by spin rotational symmetry (ignoring spin-orbit coupling in the crystal) or by parity (replace r by -r)

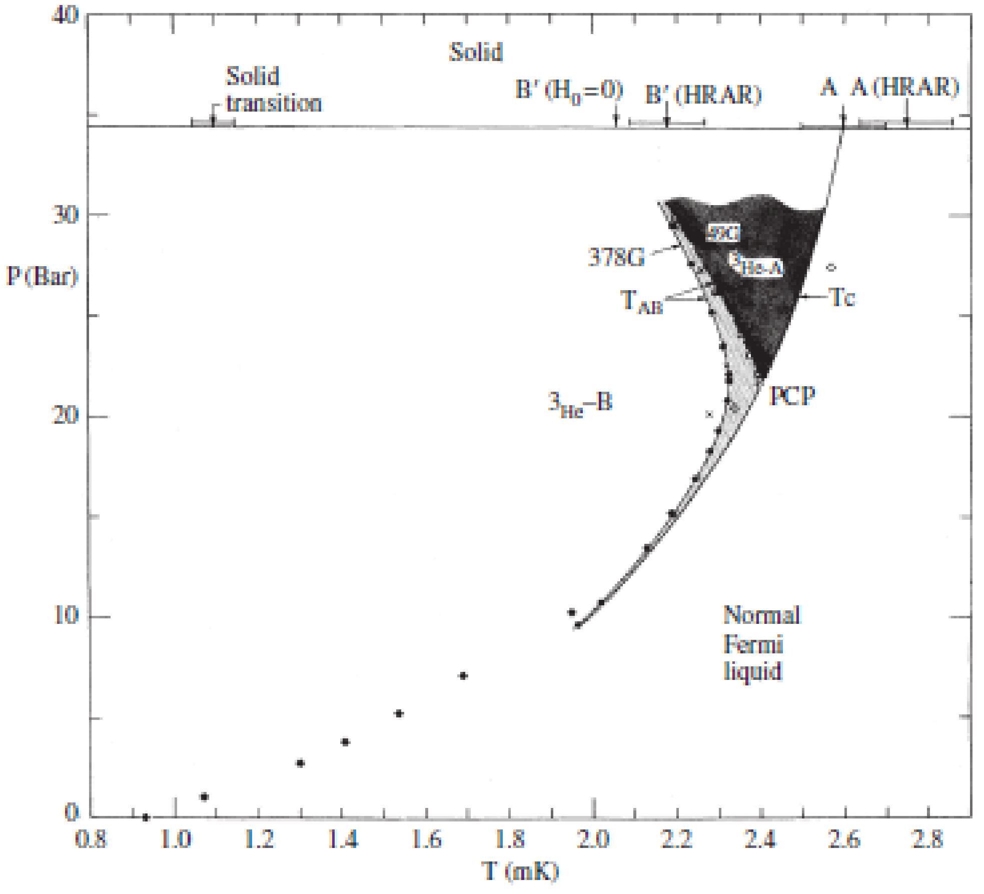
The interesting case of non-centro symmetric crystal systems with strong spin-orbit coupling allows both pairing types to co-exist

Possible gap nodes in singlet pairing states



Singlet pairing examples on a square (or tetragonal) crystal: s- (also called s+- by some) has full square symmetry, and may have nodes, while the d states have nodes required by symmetry for most Fermi surface shapes

Triplet pairing in superfluid helium-3



- Tony Leggett won the Nobel prize for his identification of the A and B phases of 3-He

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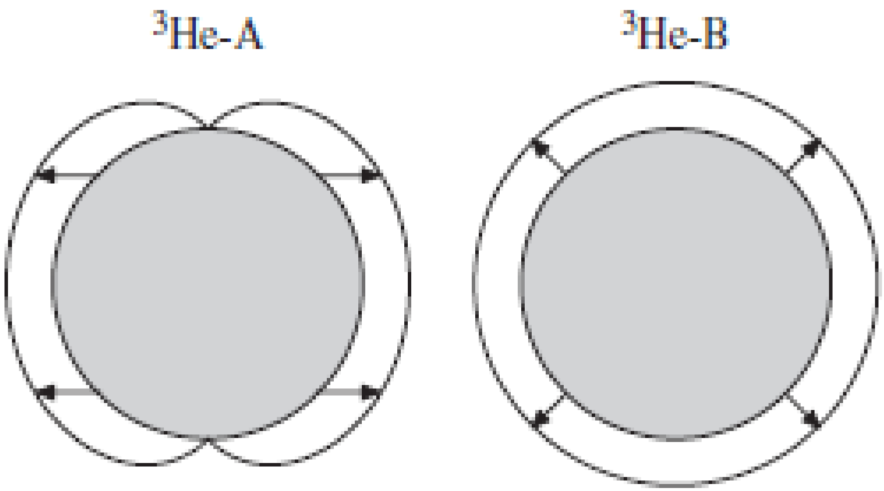
ABM and BW triplet p-wave states

ABM $\mathbf{d}_k=(0,0,k_x+ik_y)$
BW $\mathbf{d}_k=(k_x,k_y,k_z)$



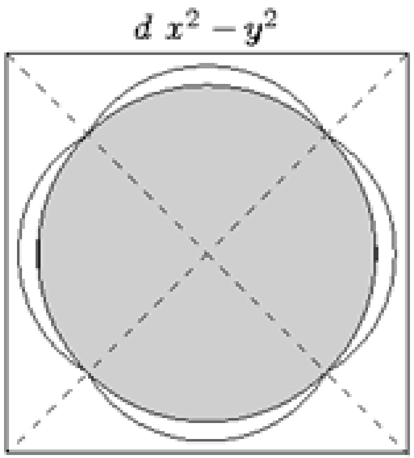
Note that the ABM state has point nodes in the gap, is chiral, and time reversal symmetry breaking (Time reversal means that the order parameter is complex, ψ* obeys the time reversed Schrodinger equation for ψ)

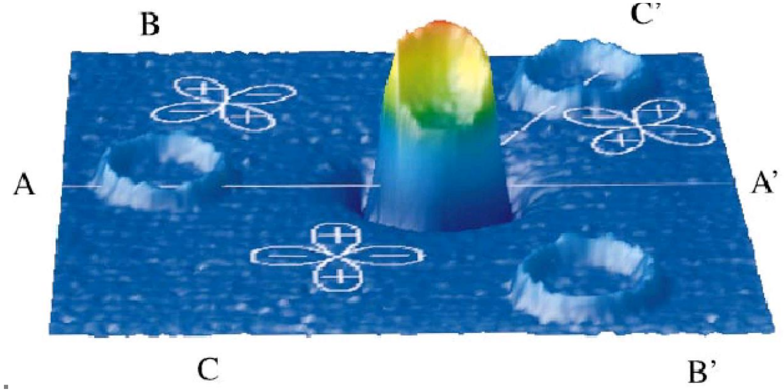
The new superconductors

- 2011 is the 100th anniversary of the 1911 discovery of superconductivity in Hg at 4.1K
- By the 1970's the highest transition temperatures achieved were around 23K in materials like Nb_3Ge
- In 1986 superconductivity at temperatures 38-135K was achieved in materials such as $La_{2-x}Ba_xCuO_4$, $YBa_2Cu_3O_7$

D-wave pairing in cuprate superconductors

- Until recently it was thought that non s-wave Cooper pairing was unusual and only occurred in a few materials
- But many superconductors are now believed to break additional symmetries
- Eg the high T_c cuprates have d x^2-y^2 pairing





Tsuei and Kirtley, Rev Mod Phys 2000

Evidence for gap nodes

- Power laws in low temperature properties, eg penetration depth
- Direct observations of gap structure with ARPES

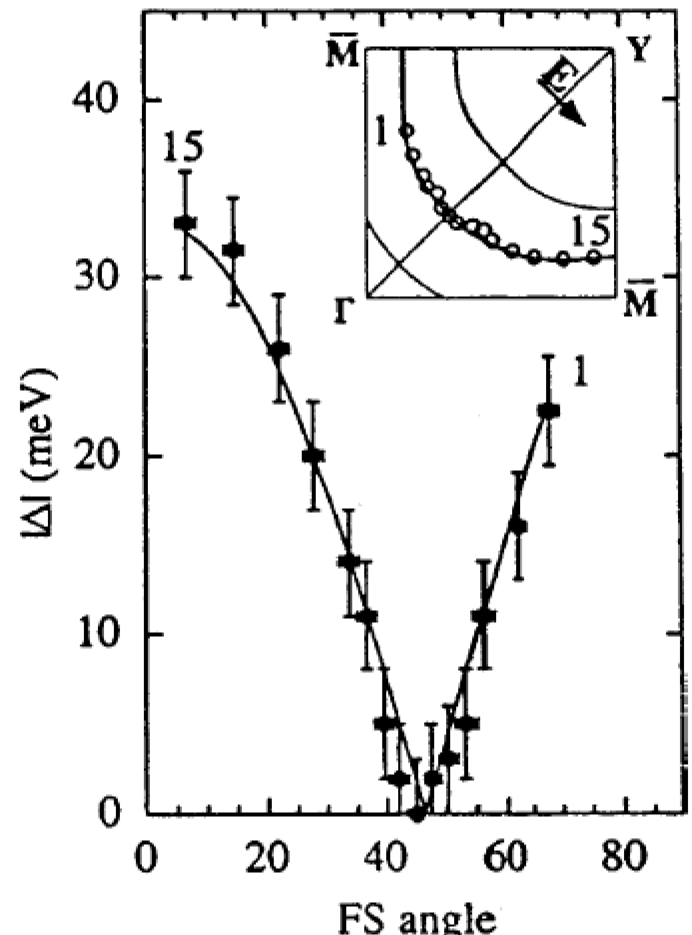


FIG. 4. Energy gap in Bi-2212: ●, measured with ARPES as a function of angle on the Fermi surface; solid curve, with fits to the data using a *d*-wave order parameter. Inset indicates the locations of the data points in the Brillouin zone. From Ding, Norman, *et al.* (1996).

Phase sensitive tunneling

- The Josephson effect is a coherent effect of tunnelling between two paired materials
- Wollman et al detected a sign change between tunneling from x and y faces of a crystal (pi-shift)
- Tsuei and Kirtley detected ½-integer flux in tricrystal rings and also ½- flux Abrikosov vortices in films grown on tricrystals

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Tsuei and Kirtley's experiment

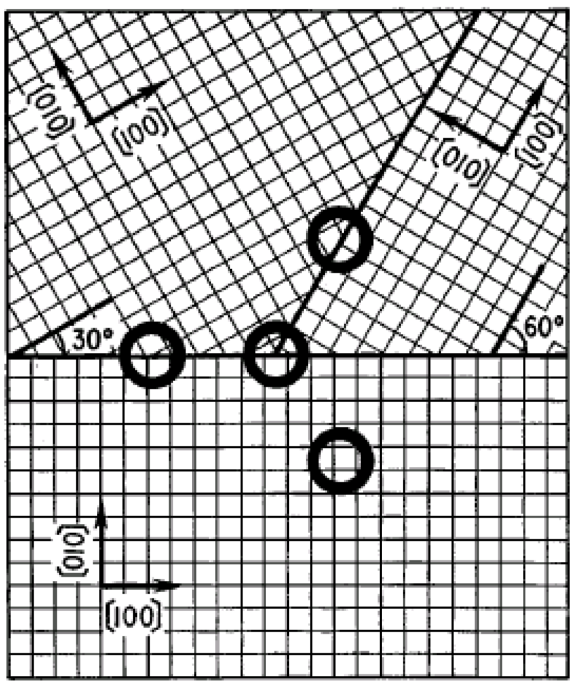
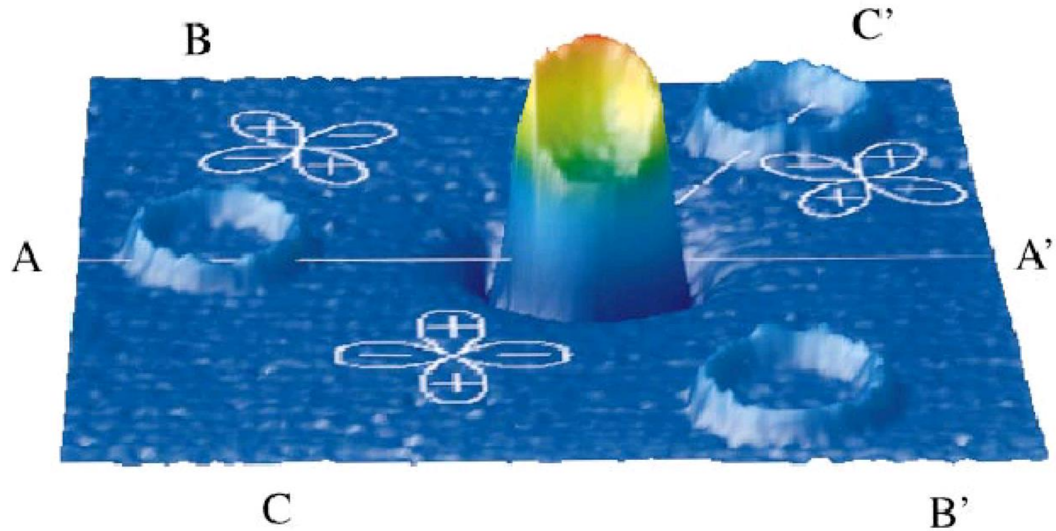


FIG. 11. Experimental configuration for the π-ring tricrystal experiment of Tsuei *et al.* (1994). The central, three-junction ring is a π ring, which should show half-integer flux quantization for a $d_{x^2-y^2}$ superconductor, and the two-junction rings and zero-junction ring are zero rings, which should show integer flux quantization, independent of the pairing symmetry.

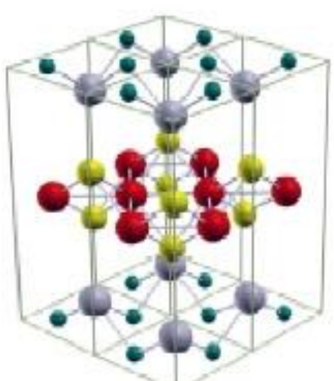


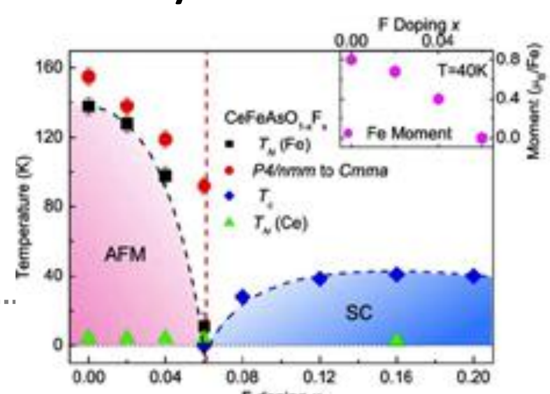
Rings crossing the grain boundaries twice have integer flux

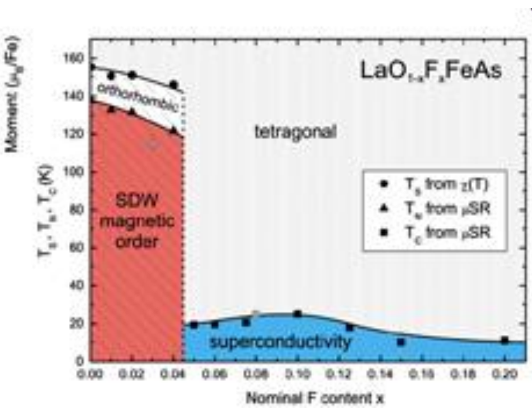
The ring at the centre always traps ½-flux

Other high temperature superconductors

- MgB_2 and K_3C_{60} both seem to have a full s-wave like gap, H3S is also assumed to be electron-phonon driven and so s-wave pairing
- Borocarbides, 2-d organics shown evidence for gap nodes, and may be d-wave (still controversial)
- The iron based pnictide materials are likely to be s-, which can be derived from similar models to cuprates for the relevant Fermi surface geometry



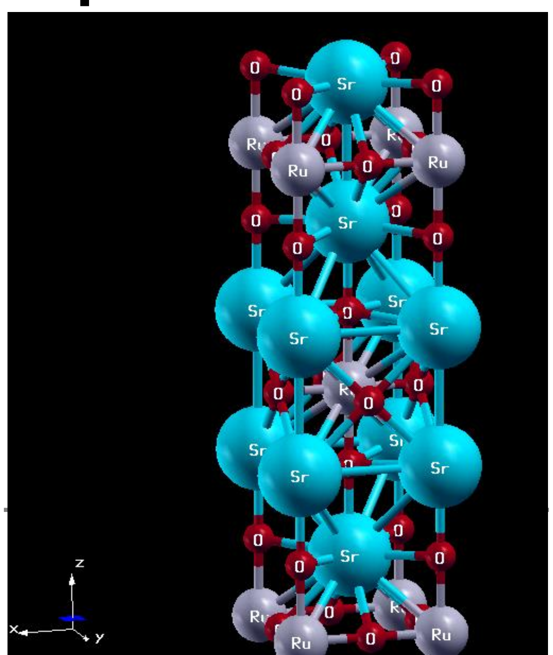




(images from physics.aps.org)

Triplet Superconductivity in Sr_2RuO_4

A 1.5K superconductor discovered by Prof Y. Maeno, Kyoto
Structurally it is isomorphic to La_2CuO_4 the parent of the high Tc compounds

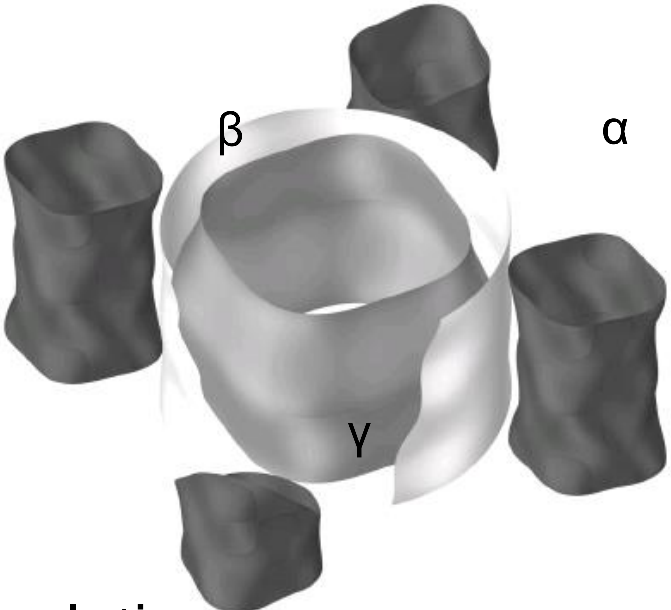


•Sigrist and Rice predicted spin triplet pairing driven by ferromagnetic spin fluctuations

•A solid state analogue of the ABM state of ^3He?

The Fermi surface in Sr_2RuO_4

There are three cylindrical Fermi surface sheets, measured with great accuracy by Bergman and Mackenzie



These agree well with LDA band calculations, and are derived from the Ru 4d T_{2g} multiplet of d states |xz›, |yz› (giving αβ) and $|x^2\text{-}y^2\rangle$ (giving γ)

Non-magnetic impurity scattering

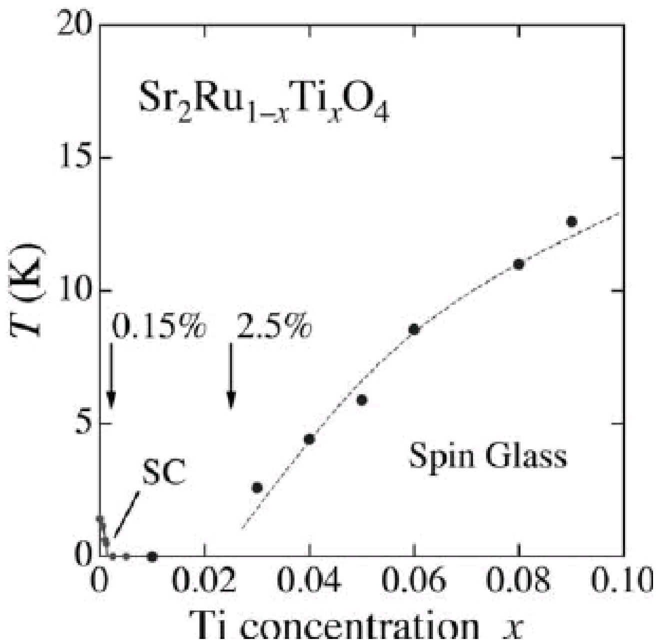
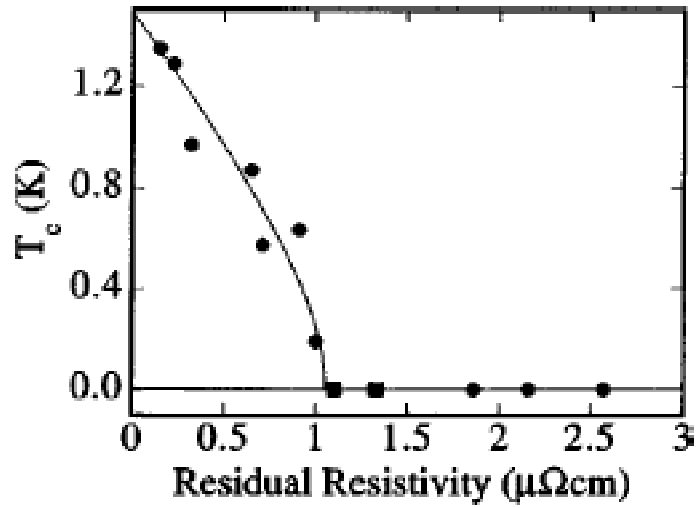


Fig. 4. Temperature-concentration phase diagram of $Sr_2Ru_{1-x}Ti_xO_4$. The superconductivity with $T_c = 1.5$ K is quickly suppressed by Ti substitution. The nonmagnetic Ti impurity induces a magnetic transition at $x \sim 2.5\%$.



S-wave superconductors are protected against non-magnetic impurity scattering (Anderson's theorem), but unconventional superconductors are not

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A solid state analogue of ^{3}He-A?

TABLE I: Irreducible representations of even and odd parity in a tetragonal crystal. The symbols X, Y Z represent any functions transforming as x, y and z under crystal point group operations, while I represents any function which is invariant under all point group symmetries.

Rep.	symmetry	Rep.	symmetry
A_{1g}	I	A_{1u}	$XYZ(X^2-Y^2)$
A_{2g}	$XY(X^2-Y^2)$	A_{2u}	Z
B_{1g}	X^2-Y^2	B_{1u}	XYZ
B_{2g}	XY	B_{2u}	$Z(X^2-Y^2)$
E_g	$\{XZ,YZ\}$	E_u	$\{X,Y\}$

In a tetragonal crystal group theory allows a set of d-wave pairing states or p-wave states similar to 3-He (Annett Adv. Phys 1990)

P-wave triplet states based on the E_u irreducible representation include an analogue of the ABM phase

$$\mathbf{d}_k=(\sin(k_x)+ i \sin(k_y))\mathbf{e}_z$$

This corresponds to the crystal analogue of $L_z=1$, $S_z=0$ (|↑↓+↓↑>) triplet pairing

Spin susceptibilities and the chiral symmetry state

The well known result for the spin-susceptibility of the ABM state of ^{3}He was found by Leggett

$$\hat{\chi}_s(T) = \chi_n \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & Y(T) \end{bmatrix}.$$

where Y(T) is the Yosida function

In 3-He the c-axis can rotate freely,
But for Sr_2RuO_4 the spin-orbit coupling pins the d-vector to the c-axis,

Therefore the susceptibility is independent of temperature below T_c for magnetic fields in the a-b plane

Experimental spin susceptibility for a-b plane oriented fields

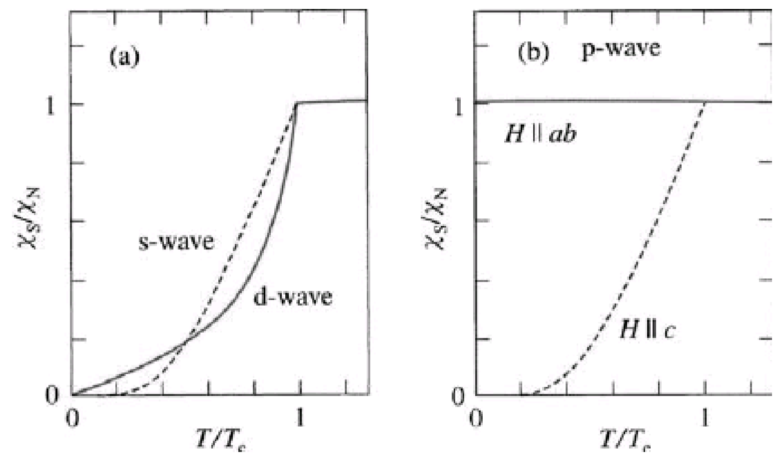


Fig. 1. The expected spin susceptibility of (a) spin-singlet superconductors and (b) spin-triplet superconductor with pure spin-basis component.

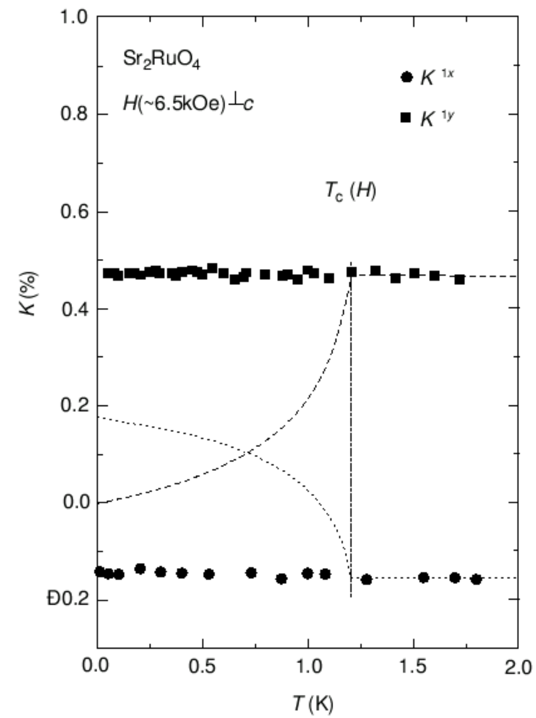


Figure 3 Temperature dependence of K^{1x} and K^{1y} at low temperatures. Broken lines below T_c indicate the calculation for the spin-singlet d-wave state in two dimensions with $d_{x^2-y^2}$ symmetry, using the parameters $\Delta(\phi) = \Delta_0 \cos(2\phi)$ and $2\Delta_0 = 8k_B T_c$ which are compatible with those of $YBa_2Cu_3O_7$ (ref. 15). ϕ is the angle on the cylindrical Fermi surface of the CuO_2 plane.

NMR experiments by Ishida (Nature 1998) and later neutron scattering experiments by Duffy et al (PRL 2000) confirmed this consistency with the chiral state prediction

Spontaneous time reversal symmetry breaking in Sr_2RuO_4

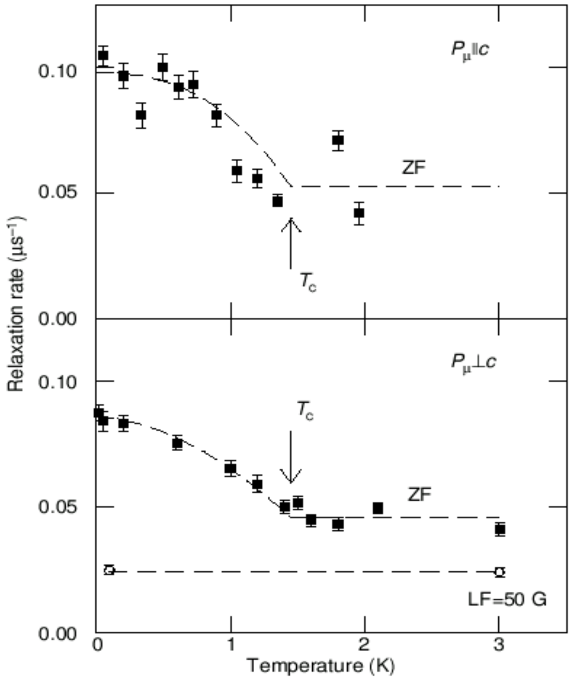


Figure 2 Zero-field (ZF) relaxation rate Λ for the initial muon spin polarization $\| c$ (top) and $\perp c$ (bottom). T_c from a.c.-susceptibility indicated by arrows. Circles in bottom figure give relaxation rate in $B_{LF} = 50$ G$\perp c$. Curves are guides to the eye.

Muon spin rotation, Luke et al Nature 1988

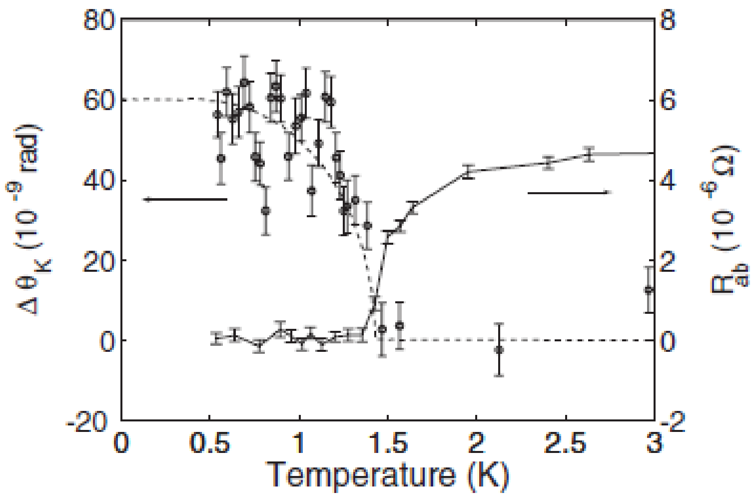
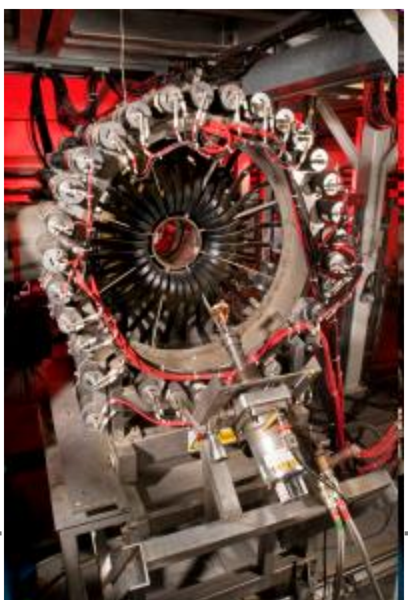


FIG. 2. Zero-field (earth field) measurement of Kerr effect (○) and *ab*-plane electrical resistance (dotted line). Dashed curve is a fit to a BCS gap temperature dependence.

Optical Kerr effect,
Xia et al, PRL 2006

Muon spin rotation experiments

Muons are produced preferentially in a single spin orientation (because of parity violation in the weak force).
Injected into a solid they precess in any local magnetic field before decaying.
The gamma detected from the decay is also dependent on the spin orientation, making it possible to determine the field B inside the material



MuSR spectrometer ISIS

The sudden change of internal B field at T_c indicates a magnetic transition, but at exactly the same temperature as superconductivity.
Hence the superconductivity is intrinisically magnetic and T breaking

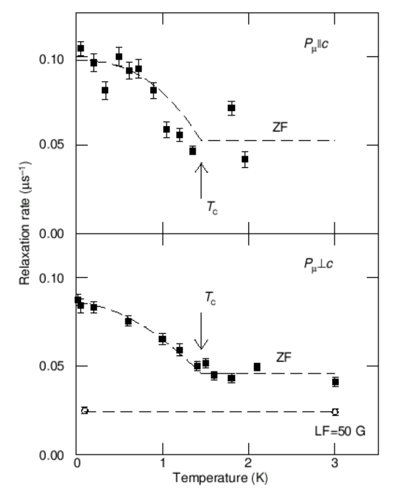


Figure 2 Zero-field (ZF) relaxation rate Λ for the initial muon spin polarization $\parallel c$ (top) and $\perp c$ (bottom). T_c from a.c.-susceptibility indicated by arrows. Circles in bottom figure give relaxation rate in $B_{LF} = 50\,G \perp c$. Curves are guides to the eye.

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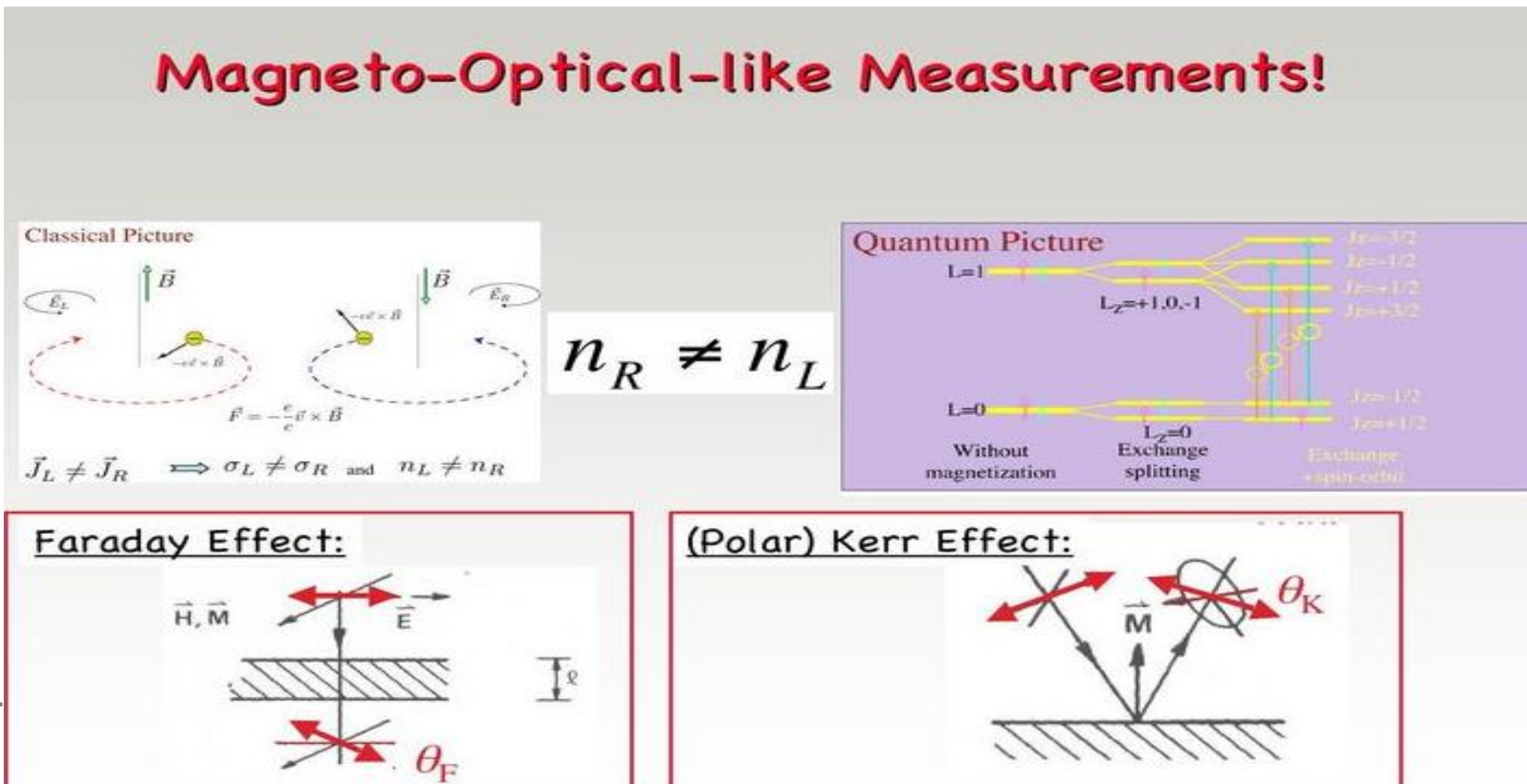
The polar Kerr effect

Dichroism: different refractive indices for left and right circular polarized light, leads to rotation of the plane of polarization of reflected light in magnetic materials



(Image from A. Kapitulnik talk Kavli UCSB 2007)

Non-centrosymmetric superconductivity

CePt3Si Bauer et al, Phys Rev Lett 92 027003 (2004)

Lack of inversion symmetry implies parity P is non-conserved
Singlet and triplet Cooper pairing must coexist

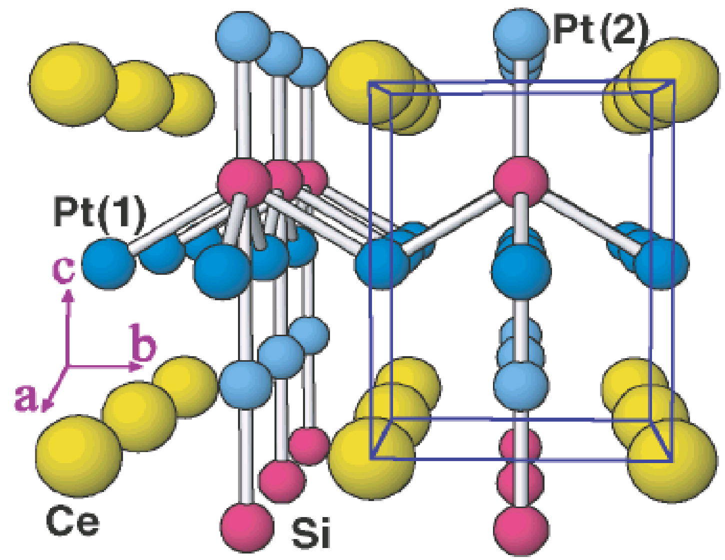


FIG. 1 (color online). Crystal structure of $CePt_3Si$. The bonds indicate the pyramidal coordination [Pt_5]Si around the Si atom. Origin shifted by (0.5, 0.5, 0.8532) for convenient comparison with the parent $AuCu_3$ structure.

Relativity for electrons in solids

Bloch's theorem

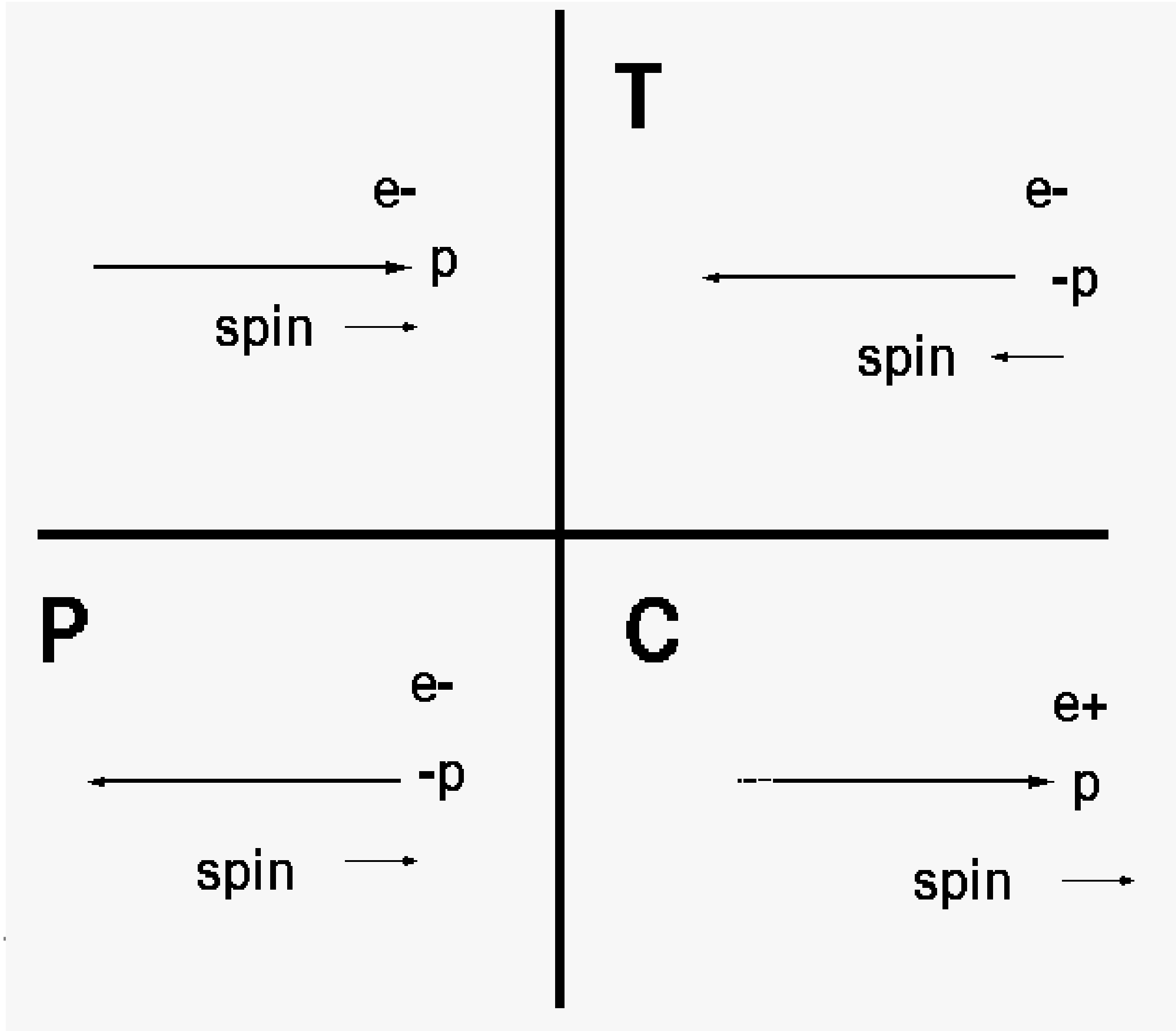
$$\hat{R}\psi(\vec{r}) = \psi(\vec{r}+\vec{R}) = e^{i\vec{k}.\vec{R}}\psi(\vec{r})$$

where $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ is a translational symmetry of the crystal and $\vec{k}$ is *crystal momentum* (usually in 1st Brillouin zone)

This applies *equally* for the Scrödinger and Dirac equation, in a periodic cystal potential,

$$V(\vec{r}) = V(\vec{r}+\vec{R})$$

C, P



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C, P and T symmetries in solids

C, P, T symmetries for electrons in crystals

$\hat{P}$ changes an electron $|\vec{k},\uparrow\rangle$ to $|-\vec{k},\uparrow\rangle$.

$\hat{T}$ changes an electron $|\vec{k},\uparrow\rangle$ to $|-\vec{k},\downarrow\rangle$.

The combination $\hat{P}\hat{T}$ implies that $|\vec{k},\uparrow\rangle$ is *degenerate* with $|\vec{k},\downarrow\rangle$. *Kramers degeneracy.*

$\hat{C}$ is normally not useful (except in crystals of antimatter!), but a form of $\hat{C}$ *particle-hole symmetry* can be useful exchanging positive energy electron states with negative energy hole states. But this is not an exact symmetry except in special cases (eg graphene).

Rashba spin-orbit coupling

In a non-centrosymmetric crystal structure like $CePt_3Si$ spin-orbit interactions break the Kramers degeneracy.

The Fermi surface splits into two spin-states, except at the two points (0,0,+/-kz)

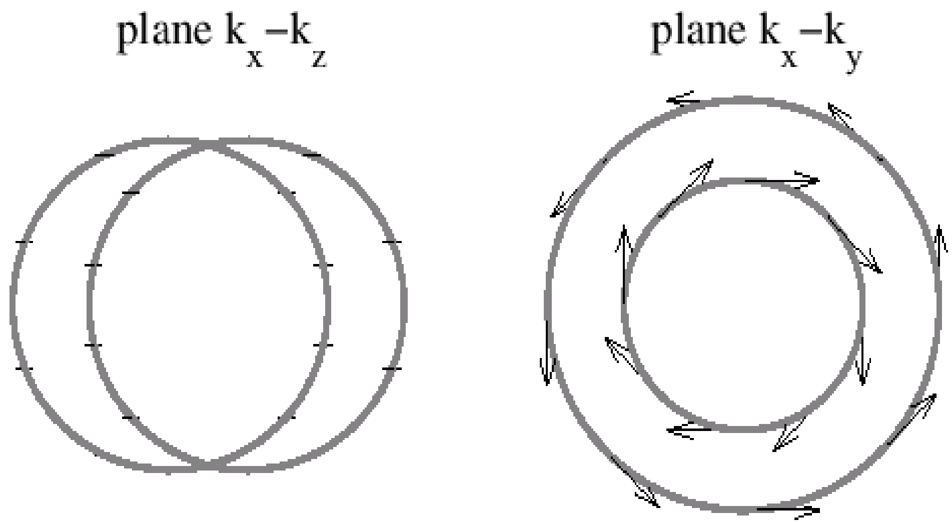


FIG. 1: Fermi surfaces for $g_{\mathbf{k}} \propto (k_y, -k_x, 0)$ as in $CePt_3Si$. The arrows show the structure of the quasi-particle spin. Only along the z-axis the spin degeneracy is preserved.

k

A model mixed s-p state which has a line node arising from the mixing

- Hayashi et al proposed the following model
- S and p pairing states exist on both Fermi surface sheets.
- The singlet gap Δ is constant, the triplet gap d_k lies parallel to the Rashba splitting vector g_k
- One sheet is nodeless, the other has two horizontal nodal lines of gap nodes
- This state has the full crystal symmetry (A_1 symmetric)

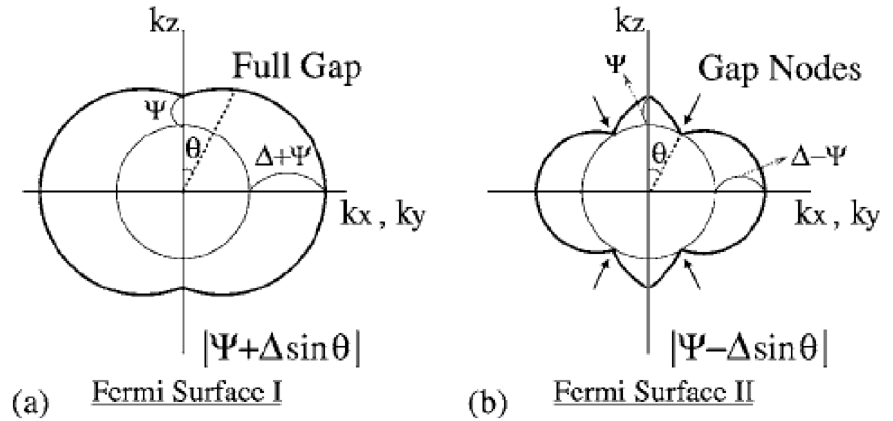


FIG. 1. Schematic figures of the gap structure on the Fermi surfaces. (a) On Fermi surface I, the gap is $|\Psi+\Delta \sin\theta|$. (b) On Fermi surface II, the gap is $|\Psi-\Delta \sin\theta|$. In these figures, it is assumed that both Ψ and Δ are real and positive, and $\Psi<\Delta$.

End of Topic 2

- Any Questions?

Topic 3: Unconventional Superconductivty II

- Group theory and symmetry classification
- Ginzburg Landau theory for unconventional order parameters

Symmetries to Consider

We can now use this to examine the effects of various symmetries which might be present

- time translational invariance (thermal equilibrium) $t \to t + T$
- gauge symmetry $\hat{\psi}^+_\sigma(\mathbf{r}, t) \exp i\theta(\mathbf{r})$
- crystal translational symmetry $\mathbf{r} \to \mathbf{r} + \mathbf{R}$
- crystal point group symmetries
- spin rotational symmetries (with/without spin orbit coupling)
- parity $\mathbf{r} \to -\mathbf{r}$, and time reversal $t \to -t$
- electron-hole symmetry (eg near ϵ_F)

Translation Symmetries

Superconducting states with finite condensate momentum $\mathbf{Q}$ exist, eg the Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state of a superconductor in a magnetic field, or CN Yang's eta-pairing ($\mathbf{Q} = (\pi, \pi)$ on a square lattice) (PRL 1989). But for simplicity let us from now on concentrate on zero total momentum pairing states of the form

$$c^+_{\mathbf{k}\sigma} c^+_{-\mathbf{k}\sigma'}.$$

We shall also assume a static time-independent external pairing field and response (but note "odd frequency pairing" observed in ferromagnet-superconductor multilayers).

Parity (Inversion) Symmetry

The majority of the 230 possible crystal space groups include inversion symmetry (parity). But interest has now grown in a number of non-centrosymmetric superconductors (eg $CePt_3Si$) which do not have inversion.
Note that for a system with inversion the normal state Fermi surface obeys *Kramers degeneracy*, $\epsilon_{\mathbf{k}\uparrow} = \epsilon_{\mathbf{k}\downarrow}$.
Without inversion Rashba type spin-orbit interactions break this degeneracy.
Time reversal symmetry (non-magnetic normal state) only requires $\epsilon_{\mathbf{k}\uparrow} = \epsilon_{-\mathbf{k}\downarrow}$.

Crystal SpaceGroup and Spin Symmetries

With these restrictions the pairing field is of the form

$$\Delta_{\sigma\sigma'}(\mathbf{k}) c^{+}_{\mathbf{k}\sigma} c^{+}_{-\mathbf{k}\sigma'} + h.c..$$

and this reduces the symmetries to consider to

- crystal point group symmetries (rotations, reflections)
- spin rotational symmetries (with/without spin orbit coupling)

In the presence of spin-obrit coupling the spin directions must be rotated together with the orbital degrees of freedome (eg $\mathbf{J} = \mathbf{L} + \mathbf{S}$). Spin-orbit interaction is always non-zero, but is possibly small, so we shall consider spin rotational symmetry, $SU(2)$, either combined with spatial rotations or separately.

Spin Symmetries and the Pauli principle

Consider first the spin indices in our external pairing potential. There are four possibilities $\uparrow\uparrow$, $\uparrow\downarrow$, $\downarrow\uparrow$ and $\downarrow\downarrow$
But from the form of our pairing field

$$\Delta_{\sigma\sigma'}(\mathbf{k})c^{+}_{\mathbf{k}\sigma}c^{+}_{-\mathbf{k}\sigma'} + h.c..$$

and the anticommutation of the fermi operators we see that

$$\Delta_{\uparrow\uparrow}(\mathbf{k}) = -\Delta_{\uparrow\uparrow}(-\mathbf{k})$$

and similarly for $\downarrow\downarrow$. Also, for $\uparrow\downarrow$ and $\downarrow\uparrow$ we find

$$\Delta_{\uparrow\downarrow}(\mathbf{k}) = -\Delta_{\downarrow\uparrow}(-\mathbf{k})$$

We can separate these into one combination which is even in **k**, and three which are odd. This is the usual separation into *singlet* and *triplet* pairing. It is simply the result of having two spin-half fermi particles

Singlet and triplet pairing states

It is convenient to separate the four spin components of the pairing field into a scalar $\Delta_{\mathbf{k}}$ and a vector $\mathbf{d}_{\mathbf{k}}$ as follows

$$\Delta_{\sigma\sigma'}(\mathbf{k}) = (\Delta_{\mathbf{k}} I + \sigma.\mathbf{d}_{\mathbf{k}})\mathbf{i}\sigma_{\mathbf{y}}$$

where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is a vector of Pauli matrices and I is the 2x2 unit matrix.
Explicitly for singlet pairing

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} 0 & \Delta_{\mathbf{k}} \\ -\Delta_{\mathbf{k}} & 0 \end{pmatrix}$$

where $\Delta_{\mathbf{k}} = \Delta_{-\mathbf{k}}$

Singlet and triplet pairing states (2)

And for triplet pairing

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_x + id_y & d_z \\ d_z & d_x + id_y \end{pmatrix}$$

where $\mathbf{d}_\mathbf{k} = -\mathbf{d}_{-\mathbf{k}}$
The fact that these are scalar and vectors under rotation (in spin-space) follows from the mappring of the $SU(2)$ group of spin $1/2$ particles to the $SO(3)$ rotation group in 3 dimensions.

Singlet and triplet pairing states (3)

Now consider our pairing susceptibility Γ as a response to pairing fields of singlet and triplet type. We can separate the pairing field $F_{\sigma\sigma'}(\mathbf{k})$ into singlet and triplet components in the same way as we did for the external pairing field.

Assuming that the crystal has no preferred spin orientations directions (weak spin-orbit) then it follows that the response function *must be invariant under spin rotation*. The scalar pairing field must lead to a scalar response and vice-versa

$$F(\mathbf{k}) = \sum_{\mathbf{k}'} \Gamma_s(\mathbf{k}, \mathbf{k}')\Delta_{\mathbf{k}'}$$

$$\mathbf{F}(\mathbf{k}) = \sum_{\mathbf{k}'} \Gamma_t(\mathbf{k}, \mathbf{k}')\mathbf{d}_{\mathbf{k}'}$$

These responses are independent; only one diverges at T_c.

Singlet and triplet pairing states (4)

We have now come to the fundamental symmetry principle which allows us to define different tyes of superconductor by symmetries.
As temperature is reduced, whichever of the pairing responses diverges first (highest T_c) will determine the type of the superconductivity present.
Notice that this argument is extremely general, but

- This argument applies only at T_c, where the response is *linear*. Below T_c non-linear response can lead to mixings of different symmetry types.
- We ignore "accidental" degeneracy.

It may be possible to construct a model Hamiltonian for which singelt and triplet pairing have the same T_c, but it would be unlikely that nature would do this.

Singlet and triplet pairing states (5)

We not need to assume zero spin-orbit coupling. The singlet and triplet order parameters are even/odd is sufficient to distinguish them.

The even pairing field $\Delta_{\mathbf{k}}$ can only lead to an even pairing amplitude and vice-versa. However in now the triplet response can be a tensor relation between vector $\mathbf{d}_{\mathbf{k}'}$ and the triplet pairing amplitude vector $\mathbf{F}(\mathbf{k})$,

$$F_i(\mathbf{k}) = \sum_{\mathbf{k}'} \Gamma_{ij}(\mathbf{k}, \mathbf{k}') d_{j\mathbf{k}'}$$

The princpal axes of the tensor will mean that not all directions for the triplet $\mathbf{d}_{\mathbf{k}}$ vector are equivalent, and one specific direction may have the highest T_c.

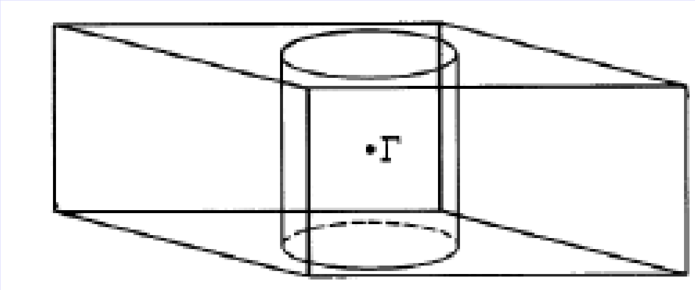
Sr_2RuO_4 is believed to be a spin triplet system with the $\mathbf{d}_{\mathbf{k}}$ vector pinned along the crystal c-axis (see lecture 1)

Crystal point group symmetries

A similar argument can be made for the **k** dependenes of the pairing within the crystal's Brillouin zone. Here the relevant classification is by *irreducible representations* of the crystal point group. The theory of representations is a whole course in itself, but the basic ideas are relatively straightforward.

The crystal will have a set of rotation axes (C_2, C_3, C_4 or C_6) and mirror planes (σ_v). Together these form a group.

These operations transform functions in the Brillouin zone $f(\mathbf{k})$ in different ways. Functions can be classified into components which are distinct by symmetry (eg even/odd).



Crystal point group symmetries (2)

The *character table* of the group lists the irreducible representations, and usually also the simplest functions which transform according to the symmetries. Eg for D_4 (tetragonal crystals)

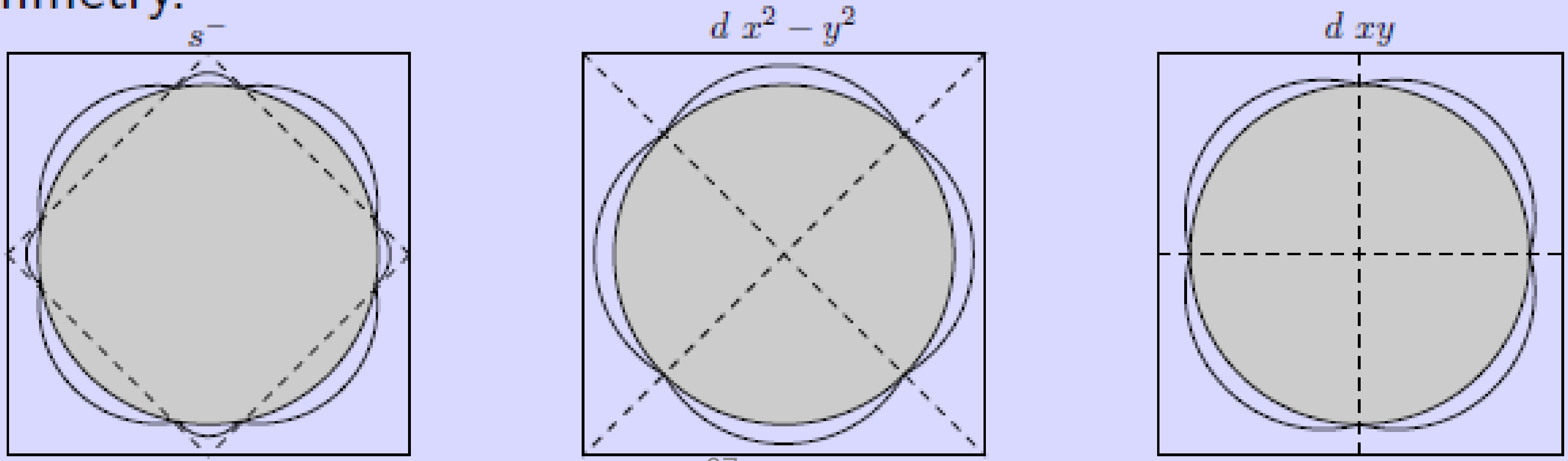
	E	C_2	$2C_4$	$2C_2'$	$2C_2''$	
A_1	1	1	1	1	1	const.
A_2	1	1	1	-1	-1	$xy(x^2 - y^2)$
B_1	1	1	-1	1	-1	xy
B_2	1	1	-1	-1	1	$x^2 - y^2$
E	2	-2	0	0	0	$\{x, y\}$

Crystal point group symmetries (3)

The gap function $\Delta_{\mathbf{k}}$ of the superconductor will transform as one of the irreducible representations of the point group, eg

$$\Delta_{\mathbf{k}} = \Delta f(\mathbf{k})$$

where $f(\mathbf{k})$ is a basis function for the relevant symmetry.
In many (not all) cases gap nodal points are required by symmetry.



A Ginzburg Landau approach

Let us now reformulate these symmetry arguments in terms of the Ginzburg Landau theory of superconductivity.

- This is valid near to T_c
- Assuming non accidental degneracy of order parameters we can determine the gap function at T_c and also below it.
- Agin this is general and does not assume any specific pairing model or a mean field (eg BCS) approximation.

A Ginzburg Landau approach (2)

The original Ginzburg Landau theory assumed a single complex order parameter, here η. The free energy in the superconducting state is

$$f_s - f_n = \frac{\hbar^2}{2m}|\nabla\eta|^2 + \alpha(T)|\eta|^2 + \frac{\beta}{2}|\eta|^4$$

where $\eta(\mathbf{r})$ is assumed to vary slowly on microscopic length scales ($\xi_0 >> a$). T_c is the temperature where $\alpha(T)$ becomes negative.

A magnetic vector potential can be included by the usual replacement

$$-i\hbar\nabla \to -i\hbar\nabla - 2e\mathbf{A}$$

signifying a charge $2e$ condensate.

A Ginzburg Landau approach (3)

This is true for s-wave superconductivity, and also for any system with a pairing in a *one-dimensional* irreducible representation of the symmetry group. For example $d_{x^2-y^2}$ pairing in the cuprates.
For a two, three or higher dimensional irreducible representation then we have a set of order parameters η_i, $i = 1, 2 \ldots$.
We must generalize the Ginzburg Landau theory to this case.
Again group theory helps us find the relevant terms.

A Ginzburg Landau approach (4)

Consider first the quadratic term. If there are multiple order parameters η_i then it might have the form

$$f_s - f_n = \sum_{ij} \alpha_{ij}(T)\eta_i^* \eta_j$$

where α_{ij} is a temperature dependent matrix.
But by the central defining principle of irreducible representations, any matrix can be decomposed by unitary transformations into a block diagonal form

$$\alpha_{ij} = \begin{pmatrix} \alpha^{\Gamma} & 0 & 0 \\ 0 & \alpha^{\Gamma'} & 0 \\ 0 & 0 & \dots \end{pmatrix}$$

where Γ, Γ' etc. are irreducible representations of the symmetry group.

A Ginzburg Landau approach (5)

The different irreducible representations will have distinct transition temperatures T_c, and again the one with the highest temperature determines the pairing symmetry.
Within a single irrep. Γ the matrix α^Γ is is just a constant times the identity matrix. Therefore the quadratic term must have the form

$$f_s - f_n = \alpha^\Gamma(T) \sum_i \eta_i^* \eta_i$$

where $\alpha^\Gamma(T)$ is positive for $T > T_c$ and negative for $T < T_c$.
If a second irreducible representation also becomes superconducting, this must (almost) always occur at a second phase transition $T_{c2} < T_c$. The heavy fermion system UPt_3 might be an example of this (Garg).

A Ginzburg Landau approach (6)

The nature of the state immediately below T_c is determined by the *quartic* terms in the Ginzburg Landau theory.
The form of these is again determined by goup theory, they are *quartic invariants* of the symmetry group.

$$f_s - f_n = \alpha^{\Gamma}(T) \sum_i \eta_i^* \eta_i + \frac{1}{2} \sum_{ijkl} \beta_{ijkl} \eta_i^* \eta_j^* \eta_k \eta_l$$

For example from the E representation of D_{4h}, we have to consider the product reresentation, and discover how many terms in the product are invariants of the full symmetry group:

$$E \times E \times E \times E = 4A_1 + \ldots$$

A Ginzburg Landau approach (7)

In this case one of the invariants is identically zero, and so there are three quartic terms. The minimum free energy is dependent on these parameters.

Three types of minima can occur

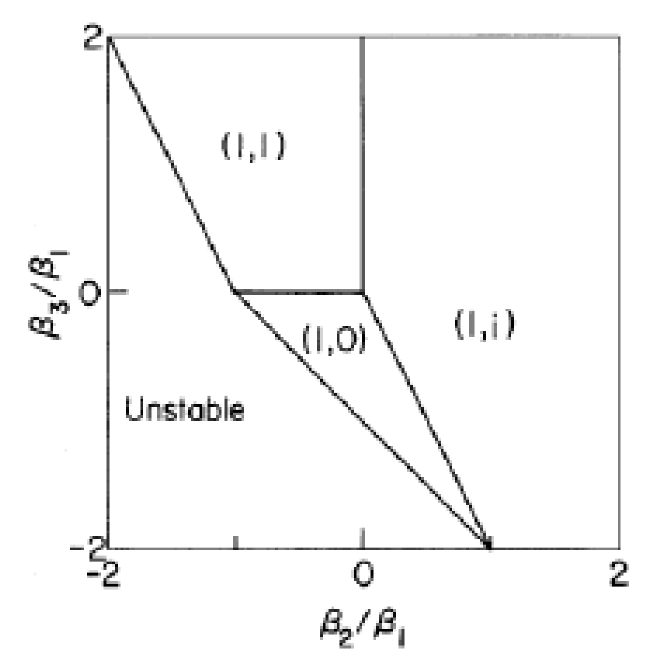
$\Delta_{\mathbf{k}} \sim k_x k_z$

$\Delta_{\mathbf{k}} \sim (k_x + k_y) k_z$

$\Delta_{\mathbf{k}} \sim (k_x + i k_y) k_z$

or for odd parity etc.

$\mathbf{d}_{\mathbf{k}} \sim k_x + i k_y$



Δ.

A Ginzburg Landau approach (8)

The form of the gradient terms is also determined by group theory:

$$f_s - f_n = \sum_{ijkl} \frac{\hbar^2}{2m_{ijkl}} \nabla_i \eta_j^* \nabla_i \eta_j + \alpha^\Gamma(T) \sum_i \eta_i^* \eta_i + \frac{1}{2} \sum_{ijkl} \beta_{ijkl} \eta_i^* \eta_j^* \eta_k \eta_l$$

Now we also have to determine how ∇ decomposes into the irreducible representations of the group, eg in D_{4h}

$$(\nabla_x, \nabla_y) \sim E$$

$$\nabla_z \sim A_2$$

Example time reversal symmetry breaking in LaNiGa2

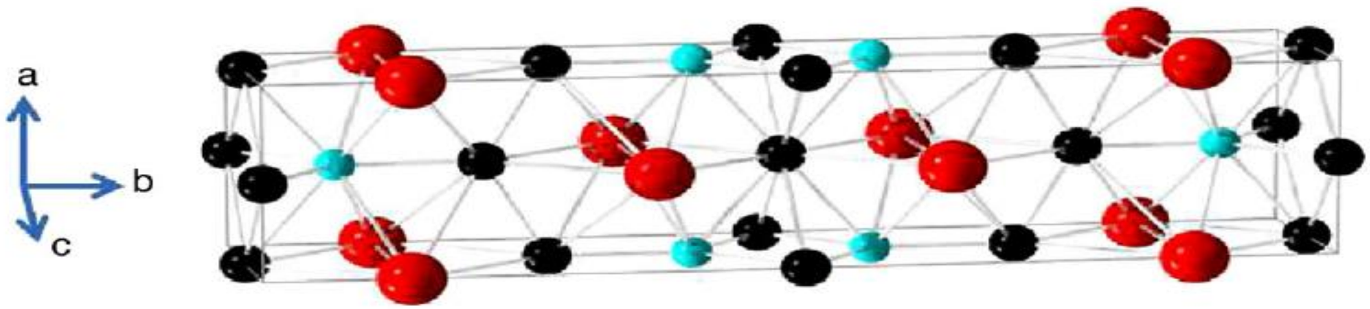


FIG. 1 (color online). The orthorhombic crystal structure of $LaNiGa_2$. The red spheres (largest) are La, blue spheres (smallest) are Ni, and the black spheres (medium) are Ga.

An orthorhombic crystal with point group D_{2h} (possessing inversion symmetry). It becomes superconducting at 2.1K

Muon spin relaxation in LaNiGa2

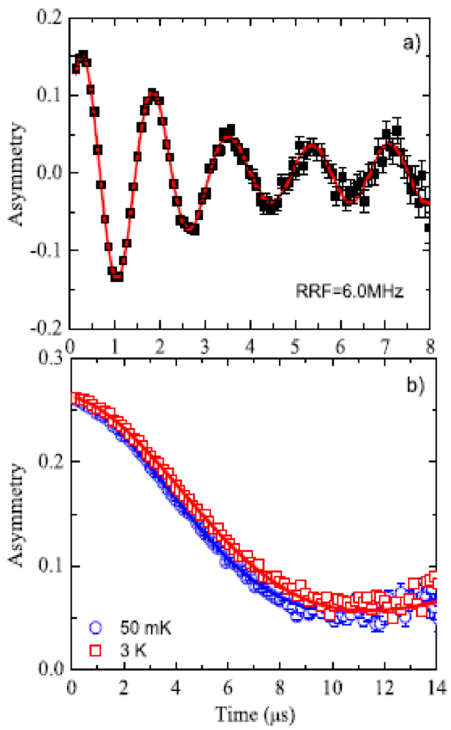


FIG. 2 (color online). The upper graph is a typical muon asymmetry spectra in $LaNiGa_2$ taken in a transverse field of 40 mT at 0.05 K (shown in the rotating reference frame (RRF) of 6.0 MHz. The line is a fit to the data using Eqn. (1). For clarity, only one of the two virtual detectors have been shown. The lower graph is the zero field μSR spectra for $LaNiGa_2$. The blue symbols are the data collected at 56 mK and the red symbols are the data collected at 3.0 K. The lines are a least squares fit to the data.

Evidence for TRSB in LaNiGa2

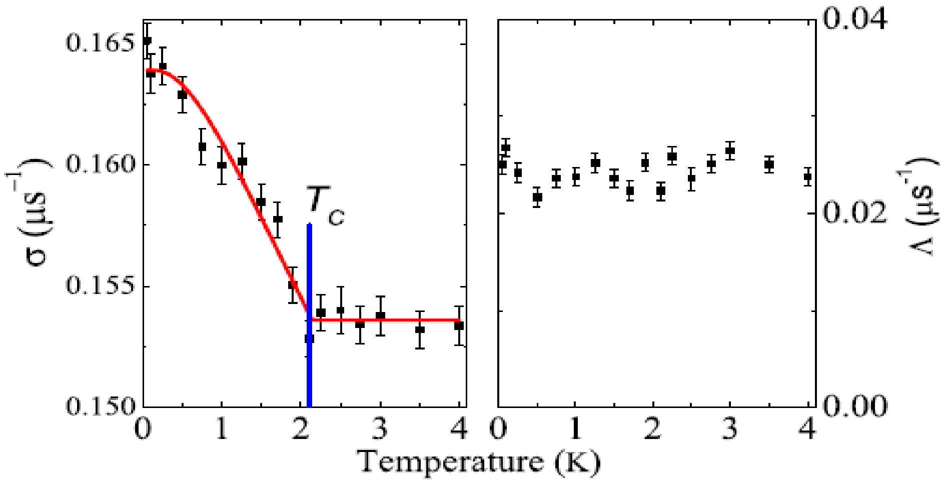


FIG. 4 (color online). The left graph shows the temperature dependence of σ, for $LaNiGa_2$ in zero-field, which clearly shows the spontaneous fields appearing at $T_c = 2.1$ K (shown has the vertical line). The line is fit to the data using an approximation [34] to the BCS order parameter for σ_e. The right graph shows the temperature dependence of the electronic relaxation rate, Λ, for $LaNiGa_2$ in zero-field, which shows no temperature dependence.

The symmetry is low and so only one-dimensional irreducible representations exist

$SO(3)\times D_{2h}$	Gap function (unitary)	Gap function (nonunitary)
$^1A_1$	$\Delta(\mathbf{k}) = 1$	$\cdots$
$^1B_1$	$\Delta(\mathbf{k}) = XY$	$\cdots$
$^1B_2$	$\Delta(\mathbf{k}) = XZ$	$\cdots$
$^1B_3$	$\Delta(\mathbf{k}) = YZ$	$\cdots$
$^3A_1$	$\mathbf{d}(\mathbf{k}) = (0, 0, 1)XYZ$	$\mathbf{d}(\mathbf{k}) = (1, i, 0)XYZ$
$^3B_1$	$\mathbf{d}(\mathbf{k}) = (0, 0, 1)Z$	$\mathbf{d}(\mathbf{k}) = (1, i, 0)Z$
$^3B_2$	$\mathbf{d}(\mathbf{k}) = (0, 0, 1)Y$	$\mathbf{d}(\mathbf{k}) = (1, i, 0)Y$
$^3B_3$	$\mathbf{d}(\mathbf{k}) = (0, 0, 1)X$	$\mathbf{d}(\mathbf{k}) = (1, i, 0)X$

D_{2h}	Gap function with strong SOC
A_1	$\mathbf{d}(\mathbf{k}) = (AX, BY, CZ)$
B_1	$\mathbf{d}(\mathbf{k}) = (AY, BX, CXYZ)$
B_2	$\mathbf{d}(\mathbf{k}) = (AZ, BXYZ, CX)$
B_3	$\mathbf{d}(\mathbf{k}) = (AXYZ, BZ, CY)$

The GL free energy for triplet pairing has just 2 possible quartic terms

The usual Landau free energy describing a triplet pairing instability in our system is of the form

$$F = a|\boldsymbol{\eta}|^2 + \frac{b}{2}|\boldsymbol{\eta}|^4 + b'|\boldsymbol{\eta} \times \boldsymbol{\eta}^*|^2 \qquad (5)$$

where $\boldsymbol{\eta}$ is the order parameter, which relates to the **d** vector through $\mathbf{d}(\mathbf{k}) = \boldsymbol{\eta}\Gamma(\mathbf{k})$ [the possible functional forms of $\Gamma(\mathbf{k})$ are given in Table I, upper].

The minimum energy state is unitary (0,0,1) if b'>0, and non-unitary (1,i,0) if b'<0.

The latter breaks time reversal symmetry

LaNiGa2 reference

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Nonunitary Triplet Pairing in the Centrosymmetric Superconductor $LaNiGa_2$

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Muon spin rotation and relaxation experiments on the centrosymmetric intermetallic superconductor $LaNiGa_2$ are reported. The appearance of spontaneous magnetic fields coincides with the onset of superconductivity, implying that the superconducting state breaks time reversal symmetry, similarly to noncentrosymmetric $LaNiC_2$. Only four triplet states are compatible with this observation, all of which are nonunitary triplets. This suggests that $LaNiGa_2$ is the centrosymmetric analogue of $LaNiC_2$. We argue that these materials are representatives of a new family of paramagnetic nonunitary superconductors.

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Conclusions

- The instability of the normal state due to formation of Cooper pairs is a form of a diverging response function
- Assuming no "accidental" degeneracy we can separate the response into different distinct symmetry channels
- The instability of the normal state is into a single *irreducible representation* of the full symmetry group
- Below T_c group theory determines the form of the quartic terms in the Ginzburg Landau expansion, and hence the possible ground states
- Extension to multiple coupled order parameters is also possible

End of Topic 3

- Any Questions?