Phenomenological theories of unconventional superconductors

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Topics:

1. Overview of conventional Landau theory.
2. Group theory and Landau theory
3. Weak coupling theory determination of Landau theory
4. Homogeneous states: case study p+ip triplet in Sr_2RuO_4
5. Josephson coupling in d-wave
6. Spatial variations in the order parameter.

Special thanks to Manfred Sigrist for providing some powerpoint slides

Symmetry Breaking and Ginzburg-Landau theory

Phase transition with spontaneously broken symmetry : macroscopic wavefunction

Order parameter: $\Psi \begin{cases} = 0 & T > T_c \\ \neq 0 & T < T_c \end{cases}$

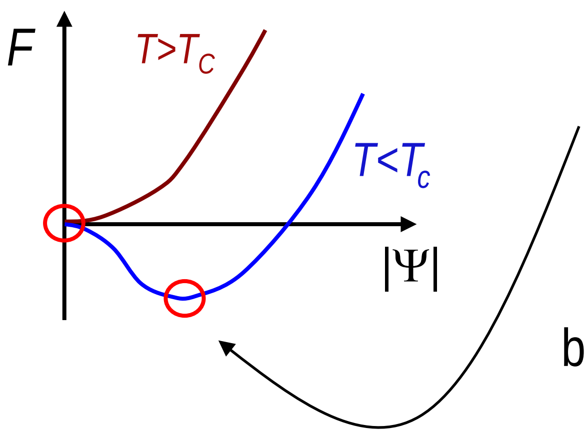
$\Psi = \Psi(\vec{r}, T) = |\Psi|\, e^{i\theta}$

Free energy functional:

$$F[\Psi, A] = \int d^3r \left[a(T)|\Psi|^2 + b|\Psi|^4 + K\left|\vec{D}\Psi\right|^2 + \frac{1}{8\pi}\left(\vec{\nabla}\times\vec{A}\right)^2 \right]$$

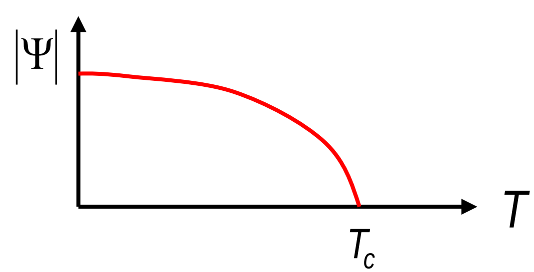
uniform phase: $a(T) = a'(T - T_c)$ $\boldsymbol{a', b} > 0$

$$|\Psi|^2 = \frac{a'(T_c - T)}{2b}$$



fixed phase

broken *U(1)* gauge symmetry



Ginzburg-Landau Free Energy

Free energy functional:
$$F\left[\Psi,\vec{A}\right]=\int d^3r\left[a(T)|\Psi|^2+b|\Psi|^4+K\left|\vec{D}\Psi\right|^2+\frac{1}{8\pi}\left(\vec{\nabla}\times\vec{A}\right)^2\right]$$

$$a(T)=a'(T-T_c)\qquad a',b,K>0\qquad \vec{D}=\vec{\nabla}+i\frac{2e}{\hbar c}\vec{A}\qquad \vec{B}=\vec{\nabla}\times\vec{A}$$

Ginzburg-Landau variational equations:

$$\left\{a+2b|\Psi|^2-K\vec{D}^2\right\}\Psi=0$$

$$\vec{\nabla}\times\vec{B}=\frac{4\pi}{c}\vec{J}_s$$

$$\vec{J}_s=\frac{e}{2hi}K\left\{\Psi^*\left(\vec{D}\Psi\right)-\Psi\left(\vec{D}\Psi\right)^*\right\}$$ supercurrent

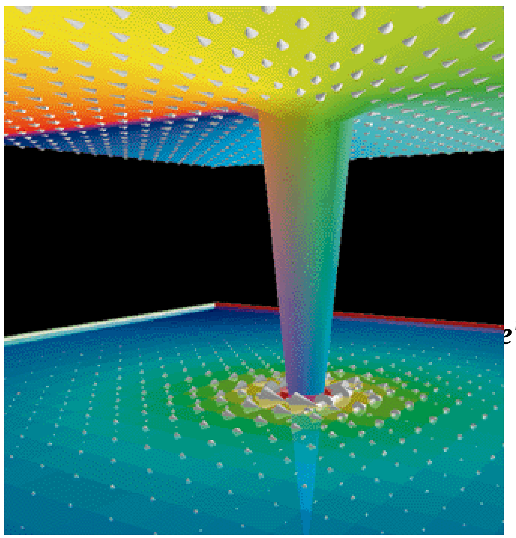
Ginzburg-Landau boundary conditions:

$$\boldsymbol{K}(\vec{\boldsymbol{n}}\cdot\vec{\boldsymbol{D}})\psi=0\qquad \vec{\boldsymbol{n}}\times(\vec{\boldsymbol{B}}-\vec{\boldsymbol{H}})=0$$

Standard Vortex

The free energy has a U(1) gauge invariance, allows order parameter solutions with phase winding.

Consider such a topological defect in the wave function: $\psi(\boldsymbol{r},\phi) = |\psi(\boldsymbol{r})|\, \boldsymbol{e}^{in\phi}$

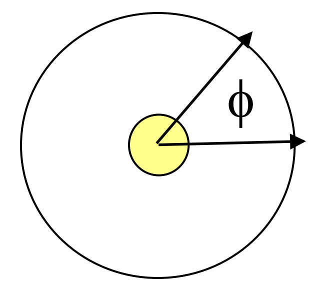


$e^{im\phi}$

$$\vec{j} = i\hbar[\psi(\nabla\psi)^* - \psi^*(\nabla\psi)] - \frac{2e}{c}|\psi|^2 \vec{A}$$

Far from the vortex core

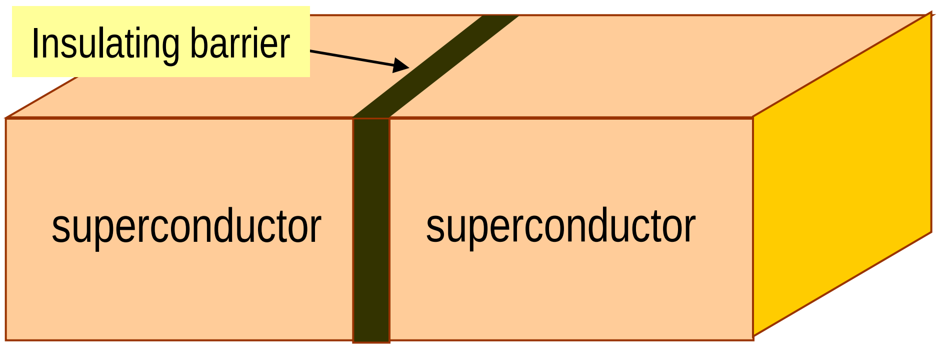
$$0 = |\psi|^2 [\hbar n \nabla\phi - \frac{2e}{c}\vec{A}]$$

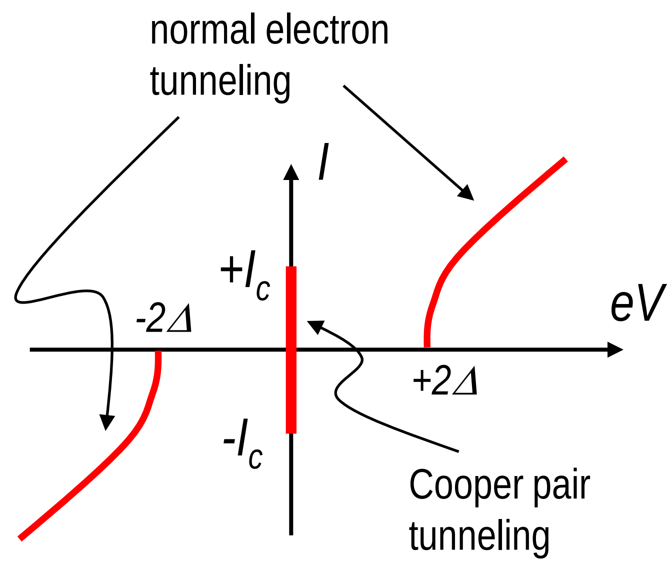


$$\oint \boldsymbol{A}\cdot \boldsymbol{dl} = \boldsymbol{n}\Phi_0 = \boldsymbol{n}\frac{\boldsymbol{hc}}{2\boldsymbol{e}}$$

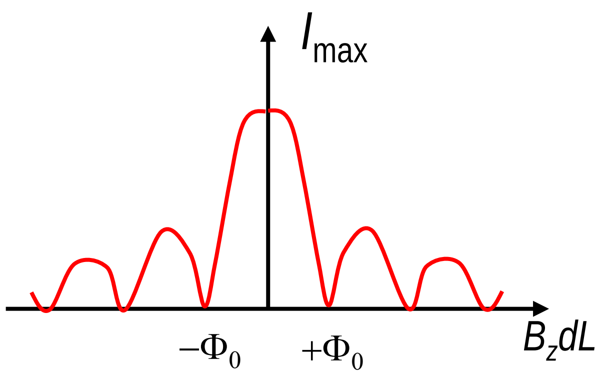
The flux contained by a vortex is quantized. Can also show that the energy of a vortex is finite.

Josephson Effect and Tunneling





Ic is suppressed by a magnetic field in the junction:



Ginzburg-Landau formulation - conventional superconductivity

Coupling term:

$$F_{12} = -\int_{\text{interface}} ds\, t\left\{\psi_1^*\psi_2 + \psi_1\psi_2^*\right\}$$

$$F = F_1 + F_2 + F_{12}$$

Standard boundary conditions:

$$\vec{n}\cdot K\left\{\vec{\nabla} - \frac{2ei}{\hbar c}\vec{A}\right\}\psi_a = 0$$

no current flows out of the superconductor
no bending of the order parameter

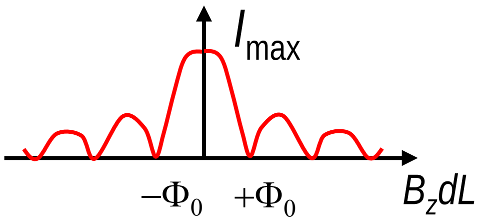
$a = 1,2$ $\quad \vec{n}$: normal vector

Effect of coupling:

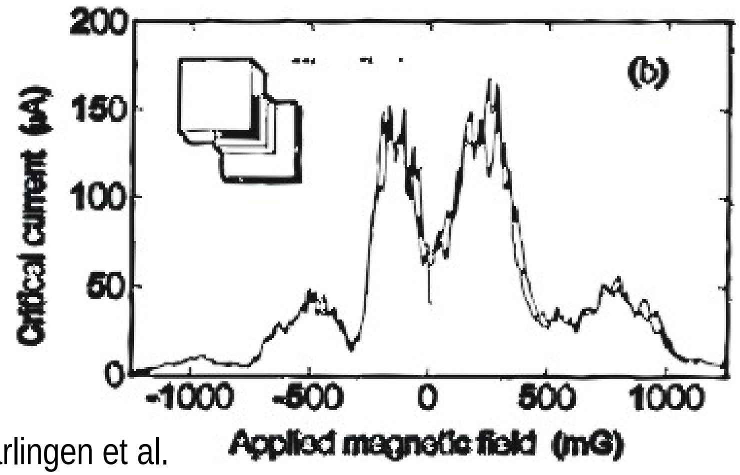
$$\vec{n}\cdot K\left\{\vec{\nabla} - \frac{2ei}{\hbar c}\vec{A}\right\}\psi_1 = -t\psi_2 \;\Rightarrow\; \Im\left[\vec{n}\cdot\psi_1^* K\left\{\vec{\nabla} - \frac{2ei}{\hbar c}\vec{A}\right\}\psi_1\right] = -t\Im\,\psi_1^*\psi_2$$

$$\vec{n}\cdot\vec{j} = -te\hbar i\left(\psi_1^*\psi_2 - \psi_2^*\psi_1\right) = 2te\hbar|\psi_1||\psi_2|\sin(\varphi_2 - \varphi_1)$$

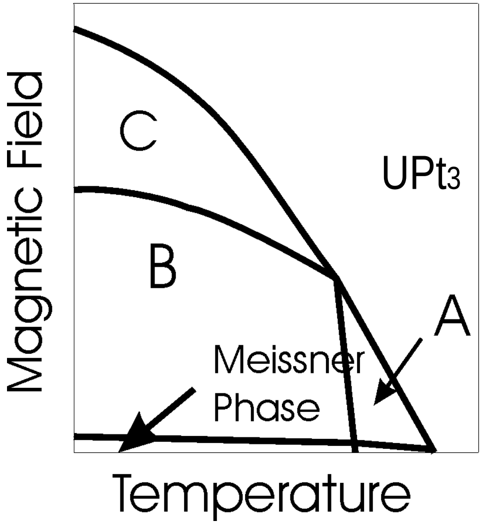
Can add a magnetic field through the junction and get

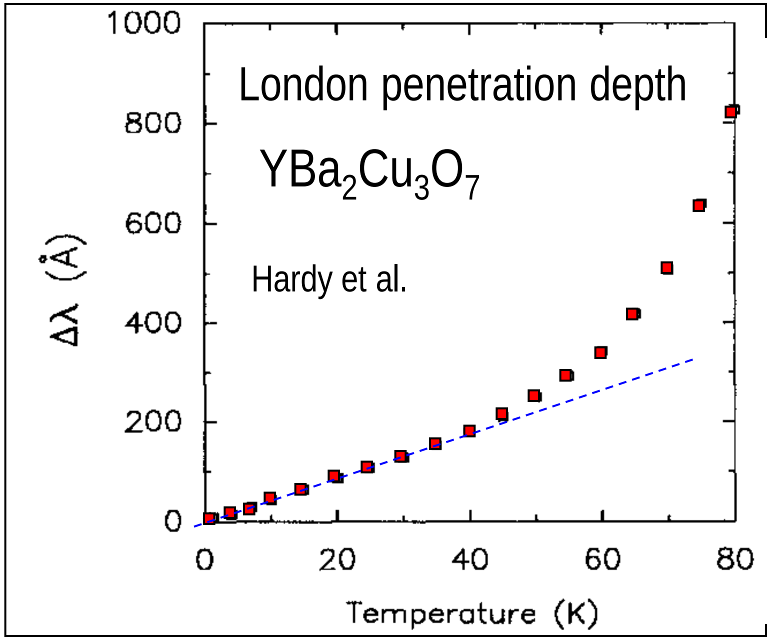


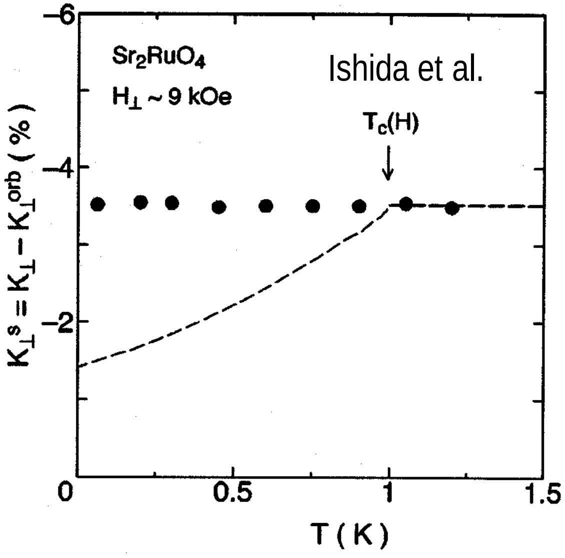
Unconventional behavior in many superconductors



Van Harlingen et al.





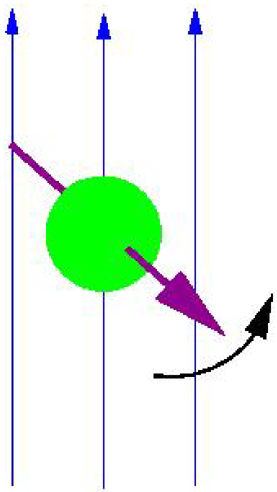


Broken Time Reversal: Sr_2RuO_4

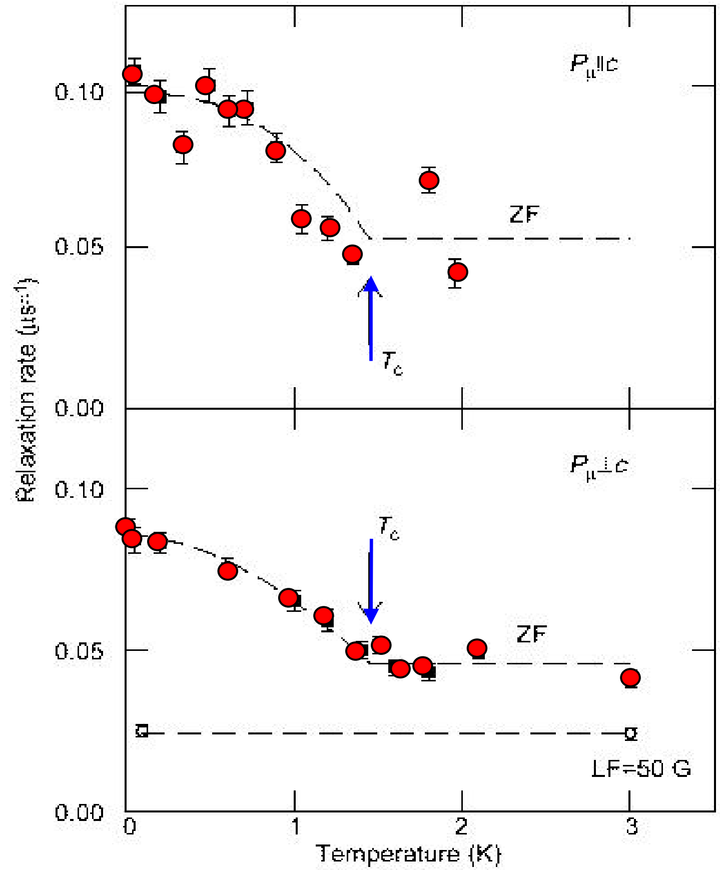
Zero-field muon spin relaxation

Muon spin depolarized by random
Internal field

Magnetism generated
by superconductivity
(0.1 - 1 Gauss)



B_{intern}



Luke, Uemura et al. (1998)

Also Polar Kerr effect (Xia, Kapitulnik, PRL 2006)
These experiments suggest px+ipy state

Landau Theory and Group Theory

Basis of order parameters

Landau: order parameters belong to irreducible representations of the normal state symmetry group

$$\psi(\vec{k}) = \sum_m \eta_m \psi_m(\vec{k})$$

$\{\psi_1(\vec{k})\psi_2(\vec{k})\ldots\}$ basis set of irred. rep.

Set up a free energy functional as a scalar function of η_m — transform according to the representation

$$F[\eta_m] = \int d^3r [a \sum_m |\eta_m|^2 + \sum_{m_1,\ldots m_4} b_{m_1,\ldots m_4} \eta^*_{m_1} \eta^*_{m_2} \eta_{m_3} \eta_{m_4}$$

Each irred. rep. has a different Tc!

invariant under all symmetry operations of rotations, time reversal and *U(1)*-gauge

$a = a'(T - T_c)$, $\quad \boldsymbol{b}_{\boldsymbol{m}1,\boldsymbol{m}2,\boldsymbol{m}3,\boldsymbol{m}4}$ real constant

Group Representations (REPS)

A REP of G is a mapping $D{:}G$ to nxn complex non-singular matrices.

Such that if $g_1\, g_2 = g_3$ then $D(g_1)D(g_2) = D(g_3)$

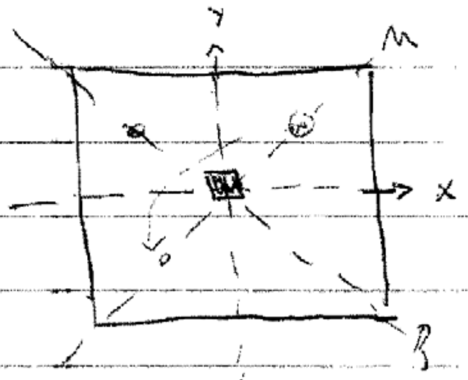
Example 1: let $G = \tilde{C}_4 \doteq C_4 = R(\hat{z}, \frac{\pi}{2})$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Example 2: $D(g)=1$ for all g in G.

Basis for this REP in C_4 or D_4 is $x^2+y^2+z^2$ (called A_{1g})

Example of a group



- $R(\hat{z}, \frac{\pi}{2}) = C_4$
- $R(\hat{x}, \pi) = C_{2x}$

$R(\hat{y}, \pi) = C_{2y}$

$R(\frac{\hat{x}+\hat{y}}{\sqrt{2}}, \pi) = C_{2m}^*$

$R(\frac{\hat{x}-\hat{y}}{\sqrt{2}}, \pi) = C_{2\beta}$

$$D_4 = \{ e, C_4, C_4^2, C_4^3, C_{2x}, C_{2y}, C_{2m}, C_{2\beta} \}$$

Note $C_{2\beta} = C_{2x} C_4$, in fact C_{2y}, C_{2m} can also be written in terms of C_{2x} and C_4

$$D_4 = gp(C_4, C_{2x}) : \quad C_4^4 = C_{2x}^2 = (C_{2x} C_4)^2 = e$$

└ generators

- Also $\tilde{C}_4 = gp(C_4) : C_4^4 = e$; $\tilde{C}_n = gp(C_n)$; $C_n^n = e$

Group Representations (REPS)

Equivalent REPS: Two REPS $D^{(1)}$ and $D^{(2)}$ are equivalent if $D^{(1)}(g)=SD^{(2)}(g)S^{-1}$ for all g in G (S does not depend upon g).

Character: Let $X(g)=Tr[D(g)]$ the set of $\{X(g)\}$ is the character of $D(g)$.

example: for $D_v(g)$:

$X_v(e)=3$, $X_v(C_4)=1$, $X_v(C_4^2)=-1$, $X_v(C_4^3)-1$

⇒

wo equivalent REPs have the came character *and*
wo REPS with the same character are equivalent.

Group Representations (REPS)

Reducible:

If $$D(g) = \begin{pmatrix} A(g) & 0 \\ 0 & B(g) \end{pmatrix}$$

then D(g) is reducible and D(g)=A(g)+B(g), otherwise D(g) is irreducible.

IRREPS are the building blocks of all REPS, in general:

$$D(g) = \sum_n a_n D^{(n)}(g)$$

IRREPS obey orthogonality conditions much like special functions.

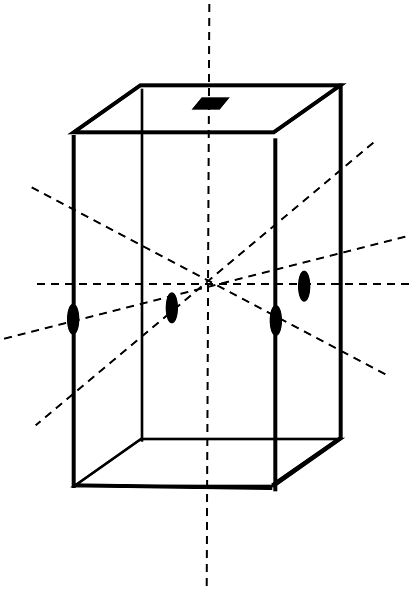
Specific example:

Superconductor with tetragonal crystal structure

Example of a tetragonal crystal with spin orbit coupling

Point group: D_{4h}

4 one-dim., 1 two-dim. representation



Character table for D_4

Γ	E	C_2	$2C_4$	$2C_2'$	$2C_2''$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

D_{4h} contains inversion

→ even and odd parity representations

Basis of order parameters

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Each irred. rep. has a different Tc!

invariant under all symmetry operations of rotations, time reversal and *U(1)*-gauge

$a = a'(T - T_c)$, $\boldsymbol{b}_{\boldsymbol{m}1,\boldsymbol{m}2,\boldsymbol{m}3,\boldsymbol{m}4}$ real constant

Construction of the Landau Energy:

Require invariance under all symmetry operations of the group.

Example: Consider E IRREP with basis and the following term in GL energy

$$\tilde{\beta}\eta_x^2\eta_x^*\eta_y^*$$

Under C_{2x} (η_x,η_y) becomes $(\eta_x,-\eta_y)$ so

$$\tilde{\beta}\eta_x^2\eta_x^*\eta_y^* \rightarrow -\tilde{\beta}\eta_x^2\eta_x^*\eta_y^* \qquad \tilde{\beta}=0$$

Ginzburg-Landau free energy functionals:

1-dimensional representations:

$$F[\Psi] = \int d^3r \left[a(T)|\Psi|^2 + b|\Psi|^4 \right]$$

like conventional SC

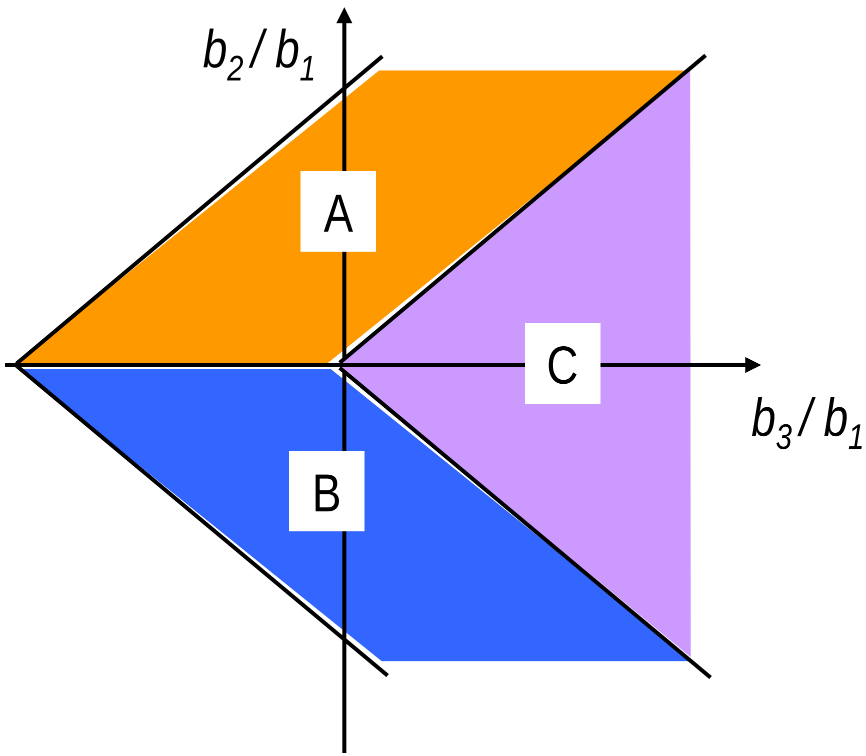
2-dimensional representations:

$$F[\vec{\eta}] = \int d^3r \left[a|\vec{\eta}|^2 + b_1|\vec{\eta}|^4 + \frac{b_2}{2}\left\{\eta_x^{*2}\eta_y^2 + \eta_x^2\eta_y^{*2}\right\} + b_3|\eta_x|^2|\eta_y|^2 \right]$$

Possible homogeneous superconducting phases

Higher-dimensional order parameters are "new": $\vec{\eta} = (\eta_x, \eta_y)$

$$F[\vec{\eta}] = \int d^3 r \left[a|\vec{\eta}|^2 + b_1 |\vec{\eta}|^4 + \frac{b_2}{2}\left\{ \eta_x^{*2}\eta_y^2 + \eta_x^2 \eta_y^{*2} \right\} + b_3 |\eta_x|^2 |\eta_y|^2 \right]$$



phase		broken symmetry
A	$(1, i)$	$U(1), \mathcal{K}$
B	$(1,1)$	$U(1), D_{4h} \rightarrow D_{2h}$
C	$(1,0)$	$U(1), D_{4h} \rightarrow D_{2h}$

$\mathcal{K}$ → magnetism

$D_{4h} \rightarrow D_{2h}$ → crystal deformation

Degeneracy: 2

domain formation possible

Ginzburg-Landau free energy: spatial variations

1-dimensional representations:

$$F\left[\eta,\vec{A}\right] = \int d^3r \left[a|\eta|^2 + b|\eta|^4 + K\left|\vec{D}\eta\right|^2 + \frac{1}{8\pi}\left(\vec{\nabla}\times\vec{A}\right)^2 \right]$$

$$a(T) = a'(T - T_c) \quad a', b, K > 0 \quad \vec{D} = \vec{\nabla} + i\frac{2e}{\hbar c}\vec{A} \quad \vec{B} = \vec{\nabla}\times\vec{A}$$

2-dimensional representations:

$$\begin{aligned} F\left[\vec{\eta},\vec{A}\right] = \int d^3r \Big[& a|\vec{\eta}|^2 + b_1|\vec{\eta}|^4 + \frac{b_2}{2}\left\{\eta_x^{*2}\eta_y^2 + \eta_x^2\eta_y^{*2}\right\} + b_3|\eta_x|^2|\eta_y|^2 \\ & + K_1\left\{|D_x\eta_x|^2 + |D_y\eta_y|^2\right\} + K_2\left\{|D_x\eta_y|^2 + |D_y\eta_x|^2\right\} + K_3\left\{|D_z\eta_x|^2 + |D_z\eta_y|^2\right\} \\ & + \left\{K_4(D_x\eta_x)^*(D_y\eta_y) + K_5(D_x\eta_y)^*(D_y\eta_x) + cc.\right\} + \frac{1}{8\pi}\left(\vec{\nabla}\times\vec{A}\right)^2 \Big] \end{aligned}$$

Important for understanding topological defects (domain walls, fractional vortices) and surface phenomena

Generalized BCS theory: Microscopic calculation of symmetry properties and gap functions

Generalized formulation of the BCS mean field theory

BCS Hamiltonian:

$$\mathcal{H} = \sum_{\vec{k},s} \xi_{\vec{k}} c^{\dagger}_{\vec{k}s} c_{\vec{k}s} + \frac{1}{2} \sum_{\vec{k},\vec{k}'} \sum_{s_1,s_2,s_3,s_4} V_{\vec{k},\vec{k}';s_1 s_2 s_3 s_4} c^{\dagger}_{\vec{k}s_1} c^{\dagger}_{-\vec{k}s_2} c_{-\vec{k}'s_3} c_{\vec{k}'s_4}$$

Mean field Hamiltonian:

$$\mathcal{H}_{mf} = \sum_{\vec{k},s} \xi_{\vec{k}} c^{\dagger}_{\vec{k}s} c_{\vec{k}s} - \frac{1}{2} \sum_{\vec{k},s_1,s_2} \left[\Delta_{\vec{k},s_1 s_2} c^{\dagger}_{\vec{k}s_1} c^{\dagger}_{-\vec{k}s_2} + \Delta^{*}_{\vec{k},s_1 s_2} c_{\vec{k}s_1} c_{-\vec{k}s_2} \right]$$

$$-\frac{1}{2} \sum_{\vec{k},\vec{k}'} \sum_{s_1,s_2,s_3,s_4} V_{\vec{k},\vec{k}';s_1 s_2 s_3 s_4} \langle c^{\dagger}_{\vec{k}s_1} c^{\dagger}_{-\vec{k}s_2} \rangle \langle c_{-\vec{k}'s_3} c_{\vec{k}'s_4} \rangle$$

Self-consistency equations:

$$\Delta_{\vec{k},ss'} = -\sum_{\vec{k}',s_3 s_4} V_{\vec{k},\vec{k}';ss's_3 s_4} \langle c_{\vec{k}'s_3} c_{-\vec{k}'s_4} \rangle$$

$$\Delta^{*}_{\vec{k},ss'} = -\sum_{\vec{k}'s_1 s_2} V_{\vec{k}',\vec{k};s_1 s_2 s's} \langle c^{\dagger}_{\vec{k}'s_1} c^{\dagger}_{-\vec{k}'s_2} \rangle$$

gap: 2x2-matrix

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} \Delta_{\vec{k}\uparrow\uparrow} & \Delta_{\vec{k}\uparrow\downarrow} \\ \Delta_{\vec{k}\downarrow\uparrow} & \Delta_{\vec{k}\downarrow\downarrow} \end{pmatrix}$$

Structure of the gap function in spin-space (parity and Pauli)

$$\Delta_{\vec{k},ss'} = -\sum_{\vec{k}',s_3s_4} V_{\vec{k},\vec{k}';ss's_3s_4} \langle c_{\vec{k}'s_3} c_{-\vec{k}'s_4} \rangle$$

$$\Delta^*_{\vec{k},ss'} = -\sum_{\vec{k}'s_1s_2} V_{\vec{k}',\vec{k};s_1s_2s's} \langle c^\dagger_{\vec{k}'s_1} c^\dagger_{-\vec{k}'s_2} \rangle$$

Gap function: 2x2 matrix in spin space

Even parity spin singlet

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} \Delta_{\vec{k},\uparrow\uparrow} & \Delta_{\vec{k},\uparrow\downarrow} \\ \Delta_{\vec{k},\downarrow\uparrow} & \Delta_{\vec{k},\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} 0 & \psi(\vec{k}) \\ -\psi(\vec{k}) & 0 \end{pmatrix} = i\hat{\sigma}_y \psi(\vec{k})$$

represented by scalar function $\psi(\vec{k}) = \psi(-\vec{k})$ even

Odd parity spin triplet

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} -d_x(\vec{k}) + i d_y(\vec{k}) & d_z(\vec{k}) \\ d_z(\vec{k}) & d_x(\vec{k}) + i d_y(\vec{k}) \end{pmatrix} = i\left(\vec{d}(\vec{k}) \cdot \hat{\vec{\sigma}}\right)\hat{\sigma}_y$$

represented by vector function $\vec{d}(\vec{k}) = -\vec{d}(-\vec{k})$ odd

Classification of gap functions

$$\mathcal{H}_{mf} = \sum_{\vec{k},s} \xi_{\vec{k}} c^\dagger_{\vec{k}s} c_{\vec{k}s} - \frac{1}{2} \sum_{\vec{k},s_1,s_2} \left[\Delta_{\vec{k},s_1 s_2} c^\dagger_{\vec{k}s_1} c^\dagger_{-\vec{k}s_2} + \Delta^*_{\vec{k},s_1 s_2} c_{\vec{k}s_1} c_{-\vec{k}s_2} \right]$$

$$-\frac{1}{2} \sum_{\vec{k},\vec{k}'} \sum_{s_1,s_2,s_3,s_4} V_{\vec{k},\vec{k}';s_1 s_2 s_3 s_4} \langle c^\dagger_{\vec{k}s_1} c^\dagger_{-\vec{k}s_2} \rangle \langle c_{-\vec{k}'s_3} c_{\vec{k}'s_4} \rangle$$

For a symmetry g of H: $$\boldsymbol{H}_{mf} = \boldsymbol{g}^{+} \boldsymbol{H}_{mf}\, \boldsymbol{g}$$

We know how the operators c transform under g and thus can deduce how the gap function transforms

Symmetry operations

Symmetries of normal phase: $G = \underbrace{G_o}_{\text{orbital rotation}} \times \underbrace{G_s}_{\text{spin rotation}} \times \underbrace{K}_{\text{time reversal}} \times \underbrace{U(1)}_{\text{gauge}}$

symmetry operation		
orbital rotation	$g c^{+}_{\vec{k}s} = c^{+}_{\hat{R}_o \vec{k}s}$	$\hat{R}_o$ orbital rotation
spin rotation	$g c^{+}_{\vec{k}s} = \sum_{s'} D_{ss'} c^{+}_{\vec{k}s'}$	$\hat{D} = e^{i\vec{\theta}\cdot\hat{\vec{\sigma}}/2}$
time reversal (antiunitary)	$\hat{K} c^{+}_{\vec{k}s} = \sum_{s'} (-i\hat{\sigma}_y)_{ss'} c_{-\vec{k}s'}$	
U(1) gauge	$\hat{\Phi} c^{+}_{\vec{k}s} = e^{i\phi/2} c^{+}_{\vec{k}s}$	

presence of strong spin-orbit coupling → spin and lattice rotation go together

Symmetry operations

Symmetries of normal phase: $G = G_o \times G_s \times K \times U(1)$

- G_o: orbital rotation
- G_s: spin rotation
- K: time reversal
- $U(1)$: gauge

Parity: $\psi(\vec{k}) = \psi(-\vec{k}) \quad \vec{d}(-\vec{k}) = -\vec{d}(\vec{k})$

symmetry operation	spin singlet	spin triplet
orbital rotation	$g_o\, \psi(\vec{k}) = \psi(\hat{R}_o \vec{k})$	$g_o\, \vec{d}(\vec{k}) = \vec{d}(\hat{R}_o \vec{k})$
spin rotation	$g_s\, \psi(\vec{k}) = \psi(\vec{k})$	$g_s\, \vec{d}(\vec{k}) = \hat{R}_s \vec{d}(\vec{k})$
time reversal	$\hat{K}\psi(\vec{k}) = \psi^*(\vec{k})$	$\hat{K}\, \vec{d}(\vec{k}) = \vec{d}^*(\vec{k})$
U(1) gauge	$\Phi\, \psi(\vec{k}) = e^{i\phi}\psi(\vec{k})$	$\Phi\, \vec{d}(\vec{k}) = e^{i\phi}\vec{d}(\vec{k})$

presence of strong spin-orbit coupling → spin and lattice rotation go together

Spin triplet pairing: $g\vec{d}(\vec{k}) = \hat{R}_s \vec{d}(\hat{R}_o \vec{k})$

identical 3D rotations $\begin{cases} \hat{R}_o \\ \hat{R}_s \end{cases}$

Example of a tetragonal crystal with spin orbit coupling

Point group: D_{4h}

4 one-dim., 1 two-dim. representation
even (g) / odd (u) parity

Γ	$\psi(\vec{k})$	Γ	$\vec{d}(\vec{k})$
A_{1g}	1	A_{1u}	$\hat{x}k_x + \hat{y}k_y$
A_{2g}	$k_x k_y (k_x^2 - k_y^2)$	A_{2u}	$\hat{y}k_x - \hat{x}k_y$
B_{1g}	$k_x^2 - k_y^2$	B_{1u}	$\hat{x}k_x - \hat{y}k_y$
B_{2g}	$k_x k_y$	B_{2u}	$\hat{y}k_x + \hat{x}k_y$
E_g	$\{k_x k_z, k_y k_z\}$	E_u	$\{\hat{z}k_x, \hat{z}k_y\}$ $\{\hat{x}k_z, \hat{y}k_z\}$

only one representation is relevant for the superconducting phase transition

Consequences of Symmetry Properties

1- Superconducting classes and symmetry imposed nodes:

$$D_4(D_2) = (E, C_2, 2e^{i\pi}C_4, 2e^{i\pi}U_2, 2U_2^{'})$$

Combined with $g_o\, \psi(\vec{k}) = \psi(\hat{R}_o \vec{k})$ yields nodes

2- Translational Invariance:

$$\vec{d}(\vec{k}+\vec{G}) = \vec{d}(\vec{k}) \quad \vec{d}(-\vec{k}) = -\vec{d}(\vec{k}) \quad \vec{d}(\vec{G}/2) = 0$$

BCS gives $\psi \xrightarrow{K} \psi^*$ K = time reversal

$\underline{d} \xrightarrow{K} \underline{d}^*$

and $\psi \xrightarrow{P} \psi$ P = parity

$\underline{d} \xrightarrow{P} -\underline{d}$

why no $\Delta \xrightarrow{K} -\Delta^*$?

Odd frequency pairing

Generalized BCS theory: Microscopic calculation of the Landau Energy

Generalized formulation of the BCS mean field theory

BCS Hamiltonian:

$$\mathcal{H} = \sum_{\vec{k},s} \xi_{\vec{k}} c^{\dagger}_{\vec{k}s} c_{\vec{k}s} + \frac{1}{2} \sum_{\vec{k},\vec{k}'} \sum_{s_1,s_2,s_3,s_4} V_{\vec{k},\vec{k}';s_1s_2s_3s_4} c^{\dagger}_{\vec{k}s_1} c^{\dagger}_{-\vec{k}s_2} c_{-\vec{k}'s_3} c_{\vec{k}'s_4}$$

Mean field Hamiltonian:

$$\mathcal{H}_{mf} = \sum_{\vec{k},s} \xi_{\vec{k}} c^{\dagger}_{\vec{k}s} c_{\vec{k}s} - \frac{1}{2} \sum_{\vec{k},s_1,s_2} \left[\Delta_{\vec{k},s_1s_2} c^{\dagger}_{\vec{k}s_1} c^{\dagger}_{-\vec{k}s_2} + \Delta^{*}_{\vec{k},s_1s_2} c_{\vec{k}s_1} c_{-\vec{k}s_2} \right]$$

$$-\frac{1}{2} \sum_{\vec{k},\vec{k}'} \sum_{s_1,s_2,s_3,s_4} V_{\vec{k},\vec{k}';s_1s_2s_3s_4} \langle c^{\dagger}_{\vec{k}s_1} c^{\dagger}_{-\vec{k}s_2} \rangle \langle c_{-\vec{k}'s_3} c_{\vec{k}'s_4} \rangle$$

Self-consistency equations:

$$\Delta_{\vec{k},ss'} = -\sum_{\vec{k}',s_3s_4} V_{\vec{k},\vec{k}';ss's_3s_4} \langle c_{\vec{k}'s_3} c_{-\vec{k}'s_4} \rangle$$

$$\Delta^{*}_{\vec{k},ss'} = -\sum_{\vec{k}'s_1s_2} V_{\vec{k}',\vec{k};s_1s_2s's} \langle c^{\dagger}_{\vec{k}'s_1} c^{\dagger}_{-\vec{k}'s_2} \rangle$$

gap: 2x2-matrix

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} \Delta_{\vec{k}\uparrow\uparrow} & \Delta_{\vec{k}\uparrow\downarrow} \\ \Delta_{\vec{k}\downarrow\uparrow} & \Delta_{\vec{k}\downarrow\downarrow} \end{pmatrix}$$

Generalized BCS theory

1 Bogolyubov transformation:

Mean field Hamiltonian: $$H_{mf} = \sum_{\vec{k}} C_{\vec{k}}^{+} \hat{X}_{\vec{k}} C_{\vec{k}} + K$$ $$\hat{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

with $C_{\vec{k}} = \begin{pmatrix} c_{\vec{k}\uparrow} \\ c_{\vec{k}\downarrow} \\ c_{-\vec{k}\uparrow}^{+} \\ c_{-\vec{k}\downarrow}^{+} \end{pmatrix}$ and $\hat{X}_{\vec{k}} = \frac{1}{2}\begin{pmatrix} \xi_{\vec{k}}\hat{\sigma}_0 & \hat{\Delta}_{\vec{k}} \\ \hat{\Delta}_{\vec{k}}^{+} & -\xi_{\vec{k}}\hat{\sigma}_0 \end{pmatrix}$

assumption: *unitary* $\hat{\Delta}_{\vec{k}}^{+}\hat{\Delta}_{\vec{k}} = \left|\Delta_{\vec{k}}\right|^2 \hat{\sigma}_0$

Unitary Bogolyubov transformation $\hat{U}_{\vec{k}} = \begin{pmatrix} \hat{u}_{\vec{k}} & \hat{v}_{\vec{k}} \\ \hat{v}_{-\vec{k}}^{*} & \hat{u}_{-\vec{k}}^{*} \end{pmatrix}, \quad \hat{U}_{\vec{k}}^{+}\hat{U}_{\vec{k}} = \hat{1}$ ⇒ $A_{\vec{k}} = \hat{U}_{\vec{k}}^{+} C_{\vec{k}}$

$$H_{mf} = \sum_{\vec{k}} A_{\vec{k}}^{+} \hat{E}_{\vec{k}} A_{\vec{k}} + K$$

$$\hat{E}_{\vec{k}} = \frac{1}{2}\begin{pmatrix} E_{\vec{k}}\hat{\sigma}_0 & 0 \\ 0 & -E_{\vec{k}}\hat{\sigma}_0 \end{pmatrix}$$

$$\hat{u}_{\vec{k}} = \frac{(E_{\vec{k}} + \xi_{\vec{k}})\hat{\sigma}_0}{\left\{2E_{\vec{k}}(E_{\vec{k}} + \xi_{\vec{k}})\right\}^{1/2}}, \quad \hat{v}_{\vec{k}} = \frac{-\hat{\Delta}_{\vec{k}}}{\left\{2E_{\vec{k}}(E_{\vec{k}} + \xi_{\vec{k}})\right\}^{1/2}}$$

$$E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + \left|\Delta_{\vec{k}}\right|^2}$$

Self-consistent gap equation

Bogolyubov transformation → Quasiparticle spectrum

$$E_{\vec{k}} = \sqrt{\xi_{\vec{k}}^2 + |\Delta_{\vec{k}}|^2} \qquad |\Delta_{\vec{k}}|^2 = \frac{1}{2}\mathrm{tr}\left(\hat{\Delta}_{\vec{k}}^{\dagger}\hat{\Delta}_{\vec{k}}\right)$$

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} \Delta_{\vec{k}\uparrow\uparrow} & \Delta_{\vec{k}\uparrow\downarrow} \\ \Delta_{\vec{k}\downarrow\uparrow} & \Delta_{\vec{k}\downarrow\downarrow} \end{pmatrix} \qquad A_{\vec{k}} = \hat{U}_{\vec{k}}^{+} C_{\vec{k}}$$

Self-consistency equation:

$$\Delta_{\vec{k},ss'} = -\sum_{\vec{k}',s_3s_4} V_{\vec{k},\vec{k}';ss's_3s_4} \langle c_{\vec{k}'s_3} c_{-\vec{k}'s_4} \rangle$$

$$\Delta^{*}_{\vec{k},ss'} = -\sum_{\vec{k}'s_1s_2} V_{\vec{k}',\vec{k};s_1s_2s's} \langle c^{\dagger}_{\vec{k}'s_1} c^{\dagger}_{-\vec{k}'s_2} \rangle$$

$$\Delta_{\vec{k},s_1s_2} = -\sum_{\vec{k}',s_3s_4} V_{\vec{k},\vec{k}';s_1s_2s_3s_4} \frac{\Delta_{\vec{k}',s_4s_3}}{2E_{\vec{k}}} \tanh\left(\frac{E_{\vec{k}}}{2k_BT}\right)$$

Transition temperature

Pairing interaction: $$V_{\vec{k},\vec{k}';s_1s_2s_3s_4} = J^0_{\vec{k},\vec{k}'}\hat{\sigma}^0_{s_1s_4}\hat{\sigma}^0_{s_2s_3} + J_{\vec{k},\vec{k}'}\hat{\vec{\sigma}}_{s_1s_4}\cdot\hat{\vec{\sigma}}_{s_2s_3}$$

density-density spin-spin

Self-consistence equation:

even parity spin singlet

$$\psi(\vec{k}) = -\sum_{\vec{k}'} \underbrace{(J^0_{\vec{k},\vec{k}'} - 3J_{\vec{k},\vec{k}'})}_{=v^s_{\vec{k},\vec{k}'}} \frac{\psi(\vec{k}')}{2E_{\vec{k}'}}\tanh\left(\frac{E_{\vec{k}'}}{2k_BT}\right)$$

$T \to T_c$

$$-\lambda\psi(\vec{k}) = -N(0)\langle v^s_{\vec{k},\vec{k}'}\psi(\vec{k}')\rangle_{\vec{k}',FS}$$

odd parity spin triplet

$$\vec{d}(\vec{k}) = -\sum_{\vec{k}'} \underbrace{(J^0_{\vec{k},\vec{k}'} + J_{\vec{k},\vec{k}'})}_{=v^t_{\vec{k},\vec{k}'}} \frac{\vec{d}(\vec{k}')}{2E_{\vec{k}'}}\tanh\left(\frac{E_{\vec{k}'}}{2k_BT}\right)$$

$T \to T_c$

$$-\lambda\vec{d}(\vec{k}) = -N(0)\langle v^t_{\vec{k},\vec{k}'}\vec{d}(\vec{k}')\rangle_{\vec{k}',FS}$$

eigenvalue λ ➡ $$k_BT_c = 1.14\epsilon_c e^{-1/\lambda}$$

From self-consistent gap equation to free energy

$$\psi(\vec{k}) = -\sum_{\vec{k}'} \underbrace{(J^0_{\vec{k},\vec{k}'} - 3J_{\vec{k},\vec{k}'})}_{= v^s_{\vec{k},\vec{k}'}} \frac{\psi(\vec{k}')}{2E_{\vec{k}'}} \tanh\left(\frac{E_{\vec{k}'}}{2k_B T}\right)$$

Go from the above gap equation to $\frac{\partial F}{\partial \eta_i^*}$ with

$$\boldsymbol{F}[\vec{\eta}] = \int \boldsymbol{d}^3\boldsymbol{r}\left[\boldsymbol{a}|\vec{\eta}|^2 + \boldsymbol{b}_1|\vec{\eta}|^4 + \frac{\boldsymbol{b}_2}{2}\left\{\eta_{\boldsymbol{x}}^{*2}\eta_{\boldsymbol{y}}^2 + \eta_{\boldsymbol{x}}^2\eta_{\boldsymbol{y}}^{*2}\right\} + \boldsymbol{b}_3|\eta_{\boldsymbol{x}}|^2|\eta_{\boldsymbol{y}}|^2\right]$$

Key Steps from BCS to GL

... m

key steps

i) let $V_{kk'} = \sum_r V_r \sum_m \psi_{rm}(k) \psi^*_{rm}(k')$ → this defines the correct basis functions

ii) $\frac{1}{2E} \tanh\left(\frac{\beta E}{2}\right) = \frac{1}{\beta} \sum_n \frac{1}{(\hbar\omega_n)^2 + E^2}$, allows for Taylor series $\frac{|\psi|^2}{\omega_n^2} \ll 1$ ≈

$\omega_n = (2n+1)\pi k_B T$

iii) $\sum_{k'} f_{k'} \ldots \rightarrow \int_{-\varepsilon_c}^{\varepsilon_c} d\xi\, N(\xi) \langle f_k \rangle_\xi \ldots \approx N(\varepsilon_F) \int_{-\varepsilon_c}^{\varepsilon_c} d\xi \langle f_k \rangle_{\varepsilon_F} \ldots$ → integral can be done.

finally get:

$$\lambda \psi(k) = \langle \psi_{rm}(k) \psi^*_{rm}(k') \psi(k') \rangle_{F.S.} + \text{const} \langle \psi_{rm}(k) \psi^*_{rm}(k) |\psi(k)|^2 \psi(k) \rangle_{F.S.}$$

iv) let $\psi(k) = \sum_m \eta_m \psi_{r,m}(k)$ use $\langle \psi_{rm}(k) \psi^*_{r'm'}(k) \rangle_{F.S.} = \delta_{mm'} \delta_{rr'}$

to get an equation for $\{\eta_m\}$ only compare to $\frac{\partial F}{\partial \eta^*_m} = 0$

Sr_2RuO_4 example:

$$\vec{d}(k) = \hat{z}[\eta_x f_x(k) + \eta_y f_y(k)]$$

$$\boldsymbol{F}[\vec{\eta}] = \int \boldsymbol{d}^3\boldsymbol{r}\left[\boldsymbol{a}|\vec{\eta}|^2 + \boldsymbol{b}_1|\vec{\eta}|^4 + \frac{\boldsymbol{b}_2}{2}\left\{\eta_{\boldsymbol{x}}^{*2}\eta_{\boldsymbol{y}}^2 + \eta_{\boldsymbol{x}}^2\eta_{\boldsymbol{y}}^{*2}\right\} + \boldsymbol{b}_3|\eta_{\boldsymbol{x}}|^2|\eta_{\boldsymbol{y}}|^2\right]$$

$$b_2 / b_1 = \gamma$$

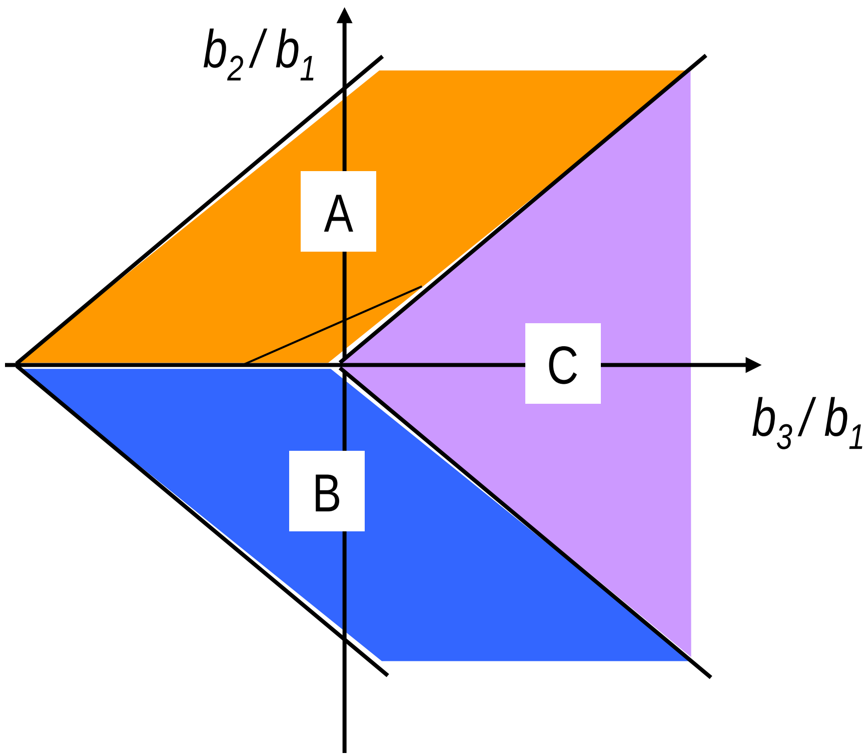
$$b_3 / b_1 = 2\gamma - 1 \qquad \left\langle (f_x^2 + f_y^2)^2 \right\rangle > 0 \qquad 0 \le \gamma \le 1$$

$$\gamma = \frac{< f_x^2 f_y^2 >}{< f_x^4 >}$$

Possible homogeneous superconducting phases

Higher-dimensional order parameters are interesting: $\vec{\eta} = (\eta_x, \eta_y)$

$$F[\vec{\eta}] = \int d^3 r \left[a|\vec{\eta}|^2 + b_1|\vec{\eta}|^4 + \frac{b_2}{2}\left\{\eta_x^{*2}\eta_y^2 + \eta_x^2\eta_y^{*2}\right\} + b_3|\eta_x|^2|\eta_y|^2 \right]$$

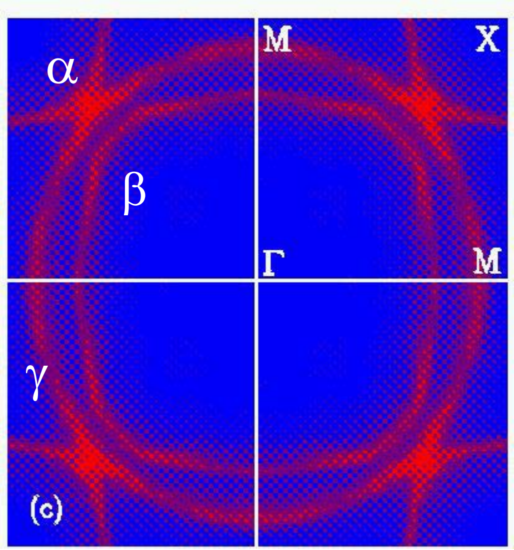


phase	$\psi(\vec{k})$	$\vec{d}(\vec{k})$	broken symmetry
A	$(k_x \pm ik_y)k_z$	$\hat{z}(k_x \pm ik_y)$	$U(1), \mathcal{K}$
B	$(k_x \pm k_y)k_z$	$\hat{z}(k_x \pm k_y)$	$U(1), D_{4h} \to D_{2h}$
C	k_xk_z, k_yk_z	$\hat{z}k_x, \hat{z}k_y$	$U(1), D_{4h} \to D_{2h}$

Chiral phase always wins (or ties) in weak coupling theory

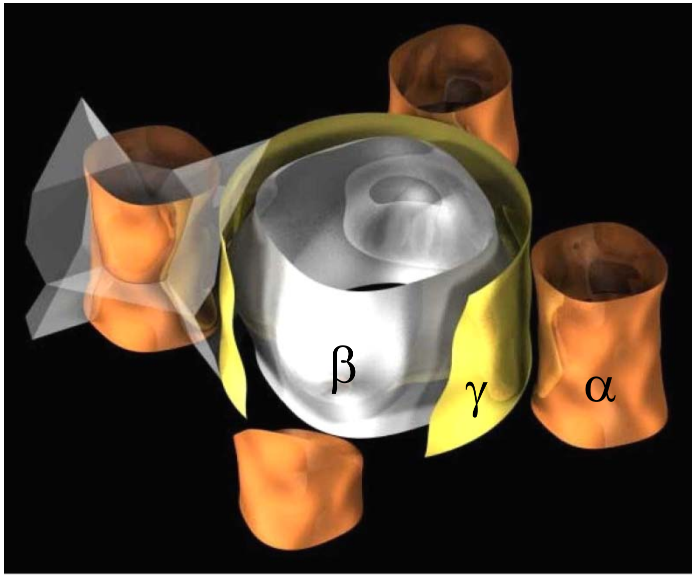
Fermi surfaces of Sr_2RuO_4

ARPES



Damascelli et al.

de Haas-van Alphen

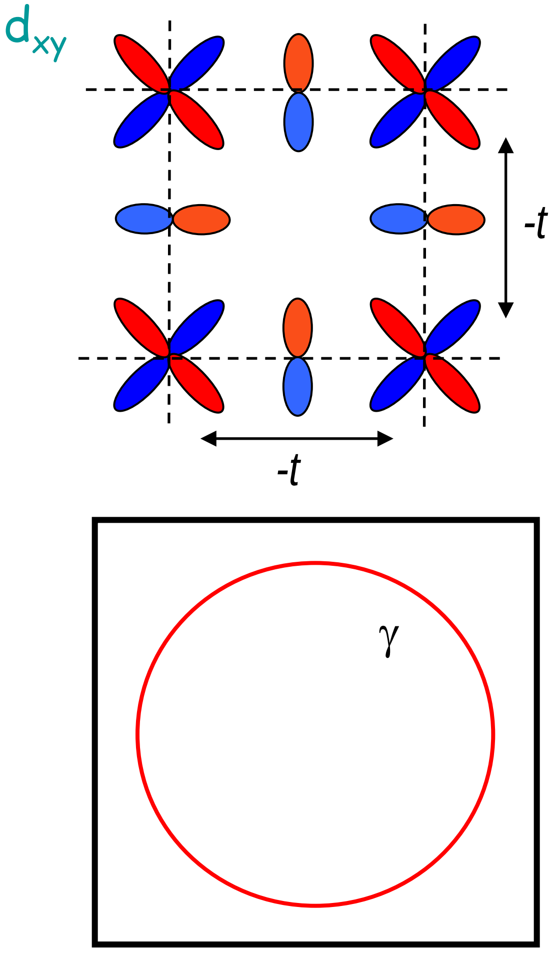


Bergemann et al.

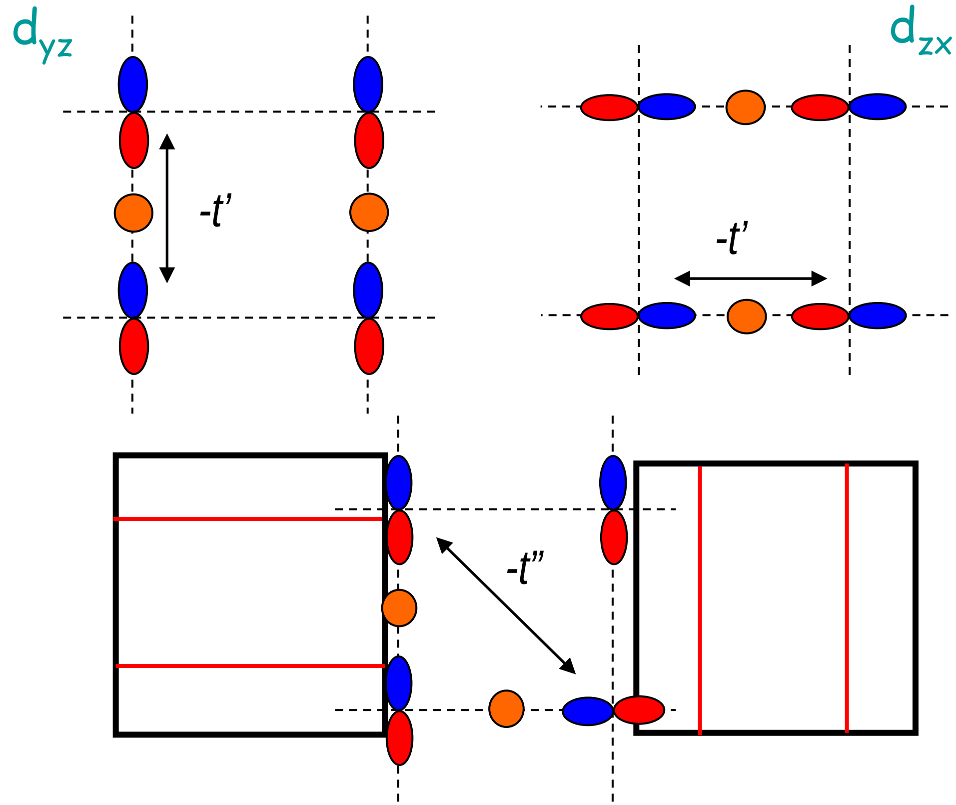
quasi-two-dimensional Fermi liquid

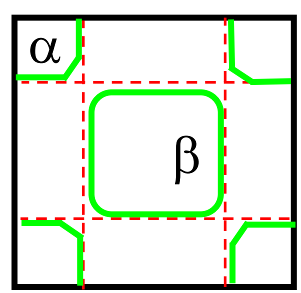
Agrees very well with bandstructure calculations   Oguchi, Singh

Electronic structure of t_{2g}-orbitals



electron-like

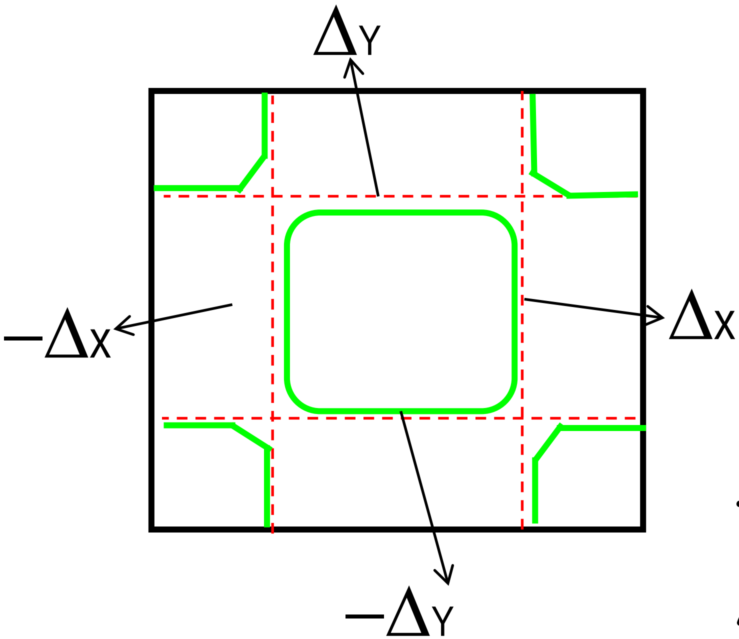




hole-like

electron-like

Pairing on the xz-yz orbitals



$$\gamma = \frac{< f_x^2 f_y^2 >}{< f_x^4 >}$$

$$\gamma \approx 0$$

Two phases nearly degenerate:

A: Δx=Δ and Δy=iΔ

B: Δx=Δy=Δ

Consider strain order parameter ε_{xy}:

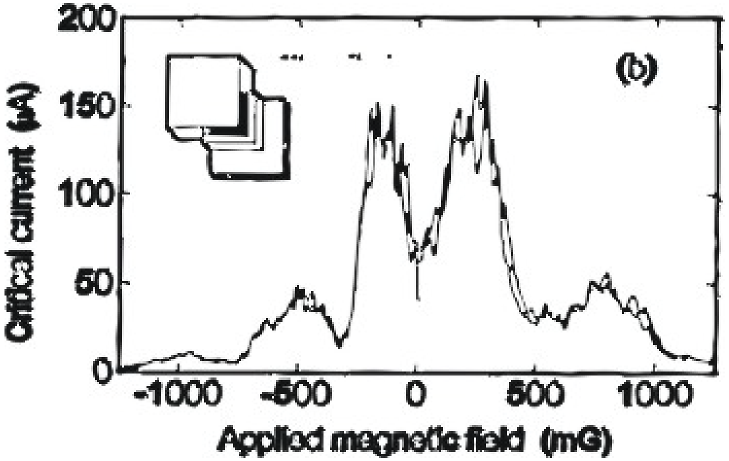
$$f_\varepsilon = \alpha_\varepsilon \varepsilon_{xy}^2 + g\varepsilon_{xy}(\eta_x^* \eta_y + \eta_y^* \eta_x)$$

$$\delta F = \frac{-g^2}{4\alpha_\varepsilon}(\eta_x^* \eta_y + \eta_y^* \eta_x)^2$$

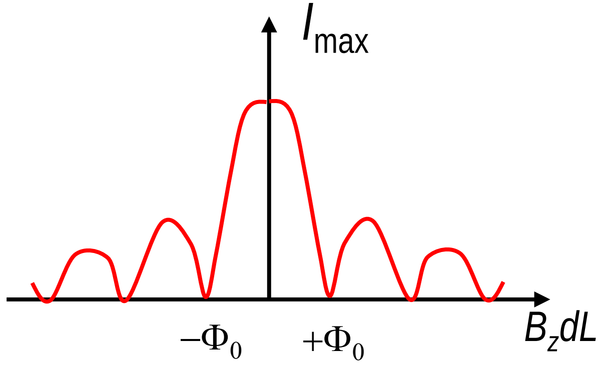
Favors B phase

Josephson effect: d-wave case

Josephson effect in cuprates

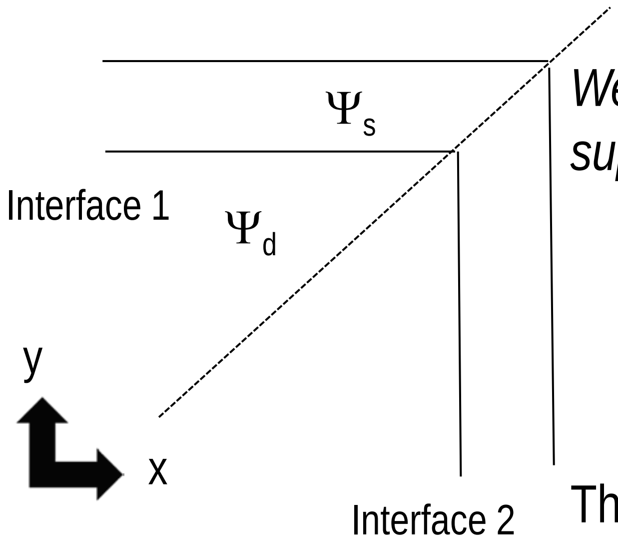


Van Harlingen et al.



S-wave prediction

Josephson Effect: d-wave



Weak link between d-wave (dx^2-y^2) and s-wave superconductor:

The coupling at the interface is:

$$F_{sd} = \varepsilon_1 \int dx[\psi_d \psi_s^* + \psi_d \psi_s^*] + \varepsilon_2 \int dy[\psi_d \psi_s^* + \psi_d \psi_s^*]$$

The only symmetry of D4h that survives the inclusion of boundaries is the two-fold rotation axis.

This mirror symmetry yields a relationship between ε_1 and ε_2.

Thanks