

Key symmetries of superconductivity Inversion and time reversal symmetry

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- *superconductivity:* general introduction
- Cooper pairing: symmetry aspects role of inversion and time reversal symmetry
- superconductivity in the absence of inversion and time reversal sym.
- lack of inversion symmetry: non-centrosymmetric superconductors and some of their physical properties

Superconductivity

Electrical resistance (1911)



London penetration depth

Field expulsion (1933)

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λ

Superconductivity

Electrical resistance (1911)





Superconductivity as a thermodynamic phase

Ginzburg-Landau theory (1950)

Superconductivity described by a complex macroscopic wave function

order parameter

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

Phenomenology of superconductivity

Superconductivity

Electrical resistance (1911)

Field expulsion (1933) Meissner-Ochsenfeld effect



Phenomenological point of view

Spontaneous symmetry breaking

2nd order phase transition from normal to superconducting state

spontaneous symmetry breaking

order parameter:

$$\Psi = |\Psi| e^{i\phi}$$

macroscopic wave function

$$|\Psi| = 0$$
 normal phase $T > T_c$

 $|\Psi| \neq 0$ superconducting phase $T < T_c$

$$\begin{split} & \text{Free energy expansion at } T_c \\ & F[\Psi] = a(T-T_c)|\Psi|^2 + b|\Psi|^4 \\ & a,b > 0 \quad \overset{\text{scalar under}}{\overset{\text{under}}{\underset{U(1)\text{-gauge operation}}{\text{sparse}}} \Psi \to \Psi e^{i\chi} \end{split}$$



2nd order phase transition from normal to superconducting state

spontaneous symmetry breaking



local U(1)-gauge invariance

Free energy functional

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

$$a, b, K > 0 \qquad \text{gradient} \quad \vec{D} = \frac{\hbar}{i} \vec{\nabla} + \frac{2e}{c} \vec{A} \qquad \text{vector potential} \quad \vec{A}$$

variational equations

$$\left\{a+2b|\Psi|^2-K\vec{D}^2\right\}\Psi=0 \qquad \quad \vec{\nabla}\times\vec{B}=\frac{4\pi}{c}\vec{J_s}$$

inhomogeneous oder parameter structures

supercurrent
$$\vec{J}_s = \frac{eK}{4\pi\hbar i} \left\{ \Psi^* (\vec{D}\Psi) - \Psi (\vec{D}\Psi)^* \right\}$$

London equation $\vec{\nabla}^2 \vec{B} + \lambda^{-2} \vec{B} = 0$

"massive photon"

Anderson-Higgs mechanism

etc

domain walls, vortices

local U(1)-gauge invariance



Microscopic point of view Cooper pairing of electrons

Microscopic theory of superconductivity

Bardeen-Cooper-Schrieffer (BCS) (1957)

 $-\vec{k}$

Superconducting state as a coherent state of electron Cooper pairs

$$\begin{split} |\Psi\rangle &= \prod_{\vec{k}} |\Phi_{\vec{k}}\rangle \quad \text{with} \quad |\Phi_{\vec{k}}\rangle = u_{\vec{k}} |0,0\rangle_{\vec{k}} + v_{\vec{k}} |1,1\rangle_{\vec{k}} \\ |0,0\rangle_{\vec{k}} \quad 0 \text{ electron} \\ |1,1\rangle_{\vec{k}} \quad 1 \text{ electron} \end{split} \text{ in each single-electron state} \quad \begin{cases} |+\vec{k}\uparrow\rangle \\ |-\vec{k}\downarrow\rangle \end{cases} \\ \\ \text{Cooper pairs} \\ \text{free adding / removing} \\ \text{of Cooper pairs} \\ \text{free adding / removing} \\ \text{of Cooper pairs} \\ \text{free adding / removing} \\ \text{of Cooper pairs} \\ \text{number of pairs} \\ \text{not fixed} \\ \end{split}$$

Microscopic theory of superconductivity

Bardeen-Cooper-Schrieffer (BCS) (1957)

Superconducting state as a coherent state of electron Cooper pairs

$$|\Psi
angle = \prod_{ec{k}} |\Phi_{ec{k}}
angle \qquad ext{with} \quad |\Phi_{ec{k}}
angle = u_{ec{k}} |0,0
angle_{ec{k}} + v_{ec{k}} |1,1
angle_{ec{k}}$$

pair wave function

 $|1,1\rangle_{\vec{k}} = c^{\dagger}_{\vec{k}\uparrow}c^{\dagger}_{-\vec{k}\downarrow}|0,0\rangle_{\vec{k}} \qquad \Psi_{\vec{k}} = \langle \Psi | c_{-\vec{k}\downarrow}c_{\vec{k}\uparrow} | \Psi \rangle = u_{\vec{k}}v_{\vec{k}}$



Pairing interaction - electron phonon (BCS)

Cooper pair formation (bound state of 2 electrons) needs attractive interaction







electron phonon interaction:



attractive interaction scattering between electron states
with degenerate energy

$$\varepsilon_{\vec{k}} = \varepsilon_{-\vec{k}}$$

Alternative mechanism for Cooper pairing

Pairing by magnetic fluctuations:



easily spin polarizable medium longer ranged interaction *pairing* for higher

angular momentum

Berk & Schrieffer (1966)



Cooper pair symmetry

Symmetry of pairs of identical electrons:

$$\Psi_{\vec{k}} = \langle c_{-\vec{k}s'} c_{\vec{k}s} \rangle = \underbrace{\phi(\vec{k})}_{\chi_{ss'}} \underbrace{\chi_{ss'}}_{\chi_{ss'}}$$

orbital spin



Pauli principle:

wave function totally antisymmetric under particle exchange

$$-\vec{k}\,s' \, \overbrace{\,\,}^{\,\,} \vec{k}\,s \quad \vec{k} \to -\vec{k} \qquad s \nleftrightarrow s'$$

even parity:	angular momentum L =0,2,4,, even	spin S=0 odd	spin singlet
odd parity:	L = 1,3,5,, odd	S=1 even	spin triplet

Cooper pair symmetry

Symmetry of pairs of identical electrons:

 $\Psi_{\vec{k}} = \langle c_{-\vec{k}s'} c_{\vec{k}s} \rangle = \phi(\vec{k}) \chi_{ss'}$ Classification Pauli p L = 0, S = 0: most symmetric "conventional pairing" wave fu under p = L > 0: lower symmetry "unconventional pairing"

 \vec{k} s

Fermi

sea

 $P_{tot}=0$

	angular momentum	spin		
even parity:	L =0,2,4,, even	S=0 odd	spin singlet	
odd parity:	$L = 1, 3, 5, \dots, $ odd	S=1 even	spin triplet	

Cooper pair symmetry

Symmetry of pairs of identical electrons:



 \vec{k} s

Anderson's Theorems (1959,1984)

Cooper pairs with total momentum $P_{tot}=0$ form from degenerate quasiparticle states.

How to guarantee existence of degenerate partners?

• Spin singlet pairing: time reversal symmetry $|\vec{k}\uparrow\rangle \longrightarrow \hat{T}|\vec{k}\uparrow\rangle = |-\vec{k}\downarrow\rangle \iff \epsilon_{\vec{k}\uparrow} = \epsilon_{-\vec{k}\downarrow}$ harmful: magnetic impurities, ferromagnetism, Zeemann fields (paramagnetic limiting)

• Spin triplet pairing: inversion symmetry $|\vec{k}\uparrow
angle \longrightarrow \hat{I}|\vec{k}\uparrow
angle = |-\vec{k}\uparrow
angle \longrightarrow \epsilon_{\vec{k}\uparrow} = \epsilon_{-\vec{k}\uparrow}$ harmful: crystal structure without inversion center Basic Model of systems without inversion center

Key symmetries and band structure



orbital and spin part distinctly treated

Electron spectrum:

$$\begin{split} \mathcal{H} &= \sum_{\vec{k},s} (\epsilon_{\vec{k}} - \mu) c_{\vec{k}s}^{\dagger} c_{\vec{k}s} + \alpha \sum_{\vec{k},s,s'} \vec{\lambda}_{\vec{k}} \cdot \{c_{\vec{k}s}^{\dagger} \vec{\sigma}_{ss'} c_{\vec{k}s'}\} \\ & \text{charge density} \qquad \text{spin density} \end{split}$$

Lack of time reversal symmetry



superconductivity in a ferromagnet



Electrons in a ferromagnet / magnetic field:

 $\epsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m} \quad \text{and Zeeman field} \quad \begin{aligned} -g\mu_B S_z \vec{M} \\ -g\mu_B S_z \vec{H} \end{aligned}$ $\rightarrow \quad \lambda_{\vec{k}} = \begin{cases} -g\mu_B \frac{\hbar}{2}M \\ -g\mu_B \frac{\hbar}{2}H \end{cases} \quad \rightarrow \quad \vec{\lambda}_{\vec{k}} = +\vec{\lambda}_{-\vec{k}} \end{aligned}$

Band structure - band splitting

$$\mathcal{H} = \sum_{\vec{k},s} \left(\frac{\hbar^2 \vec{k}^2}{2m} - \mu \right) c^{\dagger}_{\vec{k}+s} c_{\vec{k}+s} + \alpha \sum_{\vec{k},s,s'} \hat{z} \cdot (c^{\dagger}_{\vec{k}s} \vec{\sigma}_{ss'} c_{\vec{k}s'})$$



Band structure - band splitting

$$\mathcal{H} = \sum_{\vec{k},s} \left(\frac{\hbar^2 \vec{k}^2}{2m} - \mu \right) c^{\dagger}_{\vec{k}+s} c_{\vec{k}+s} + \alpha \sum_{\vec{k},s,s'} \hat{z} \cdot (c^{\dagger}_{\vec{k}s} \vec{\sigma}_{ss'} c_{\vec{k}s'})$$



Lack of inversion symmetry - non-centrosymmetric



motion of electron in electric field:

 $\epsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m} \quad \text{and special relativity} \quad \vec{B} = -\frac{\vec{v}_{\vec{k}}}{c} \times \vec{E} = \frac{\hbar E}{mc} (\vec{k} \times \hat{z})$ spin-orbit coupling: $-\mu_B \vec{B} \cdot \vec{S} = \frac{\hbar \mu_B E}{mc} (\vec{k} \times \hat{z}) \cdot \vec{S} = \alpha' \vec{\lambda}_{\vec{k}} \cdot \vec{S}$ Rashba-like spin-orbit coupling $\vec{\lambda}_{\vec{k}} = -\vec{\lambda}_{-\vec{k}}$

Band structure - band splitting

$$\mathcal{H} = \sum_{\vec{k},s} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c^{\dagger}_{\vec{k}s} c_{\vec{k}s} + \alpha \sum_{\vec{k},s,s'} (\vec{k} \times \hat{z}) (c^{\dagger}_{\vec{k}s} \vec{\sigma}_{ss'} c_{\vec{k}s'})$$



Band structure - band splitting

$$\mathcal{H} = \sum_{\vec{k},s} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c^{\dagger}_{\vec{k}s} c_{\vec{k}s} + \alpha \sum_{\vec{k},s,s'} (\vec{k} \times \hat{z}) (c^{\dagger}_{\vec{k}s} \vec{\sigma}_{ss'} c_{\vec{k}s'})$$



Superconducting phase

Superconducting phases

pair wave function
$$\hat{\Psi}_{\vec{k}} = \begin{pmatrix} \Psi_{\vec{k}\uparrow\uparrow} & \Psi_{\vec{k}\downarrow\downarrow} \\ \Psi_{\vec{k}\downarrow\uparrow} & \Psi_{\vec{k}\downarrow\downarrow} \end{pmatrix}$$

spin singlet, even parity $\hat{\Psi}_{ec{k}} = \left(egin{array}{cc} 0 & \psi(ec{k}) \ -\psi(ec{k}) & 0 \end{array}
ight)$ $=i\hat{\sigma}^{y}\psi(\vec{k})$ 1 configuration $\frac{\psi(\vec{k})}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ $\psi(-\vec{k}) = \psi(\vec{k})$

spin triplet, odd parity $\hat{\Psi}_{ec{k}} = egin{pmatrix} -d_x+id_y & d_z \ d_z & d_x+id_y \end{pmatrix}$ $= i \vec{d}(\vec{k}) \cdot \hat{\vec{\sigma}} \hat{\sigma}^y$ 3 configurations $\begin{cases} (-d_x(\vec{k}) + id_y(\vec{k}))|\uparrow\uparrow\rangle \\ \frac{d_z(\vec{k})}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ (d_x(\vec{k}) + id_y(\vec{k}))|\downarrow\downarrow\rangle \end{cases}$ $\vec{d}(-\vec{k}) = -\vec{d}(\vec{k})$

Superconducting phases

pair wave function
$$\hat{\Psi}_{\vec{k}} = \begin{pmatrix} \Psi_{\vec{k}\uparrow\uparrow} & \Psi_{\vec{k}\downarrow\downarrow} \\ \Psi_{\vec{k}\downarrow\uparrow} & \Psi_{\vec{k}\downarrow\downarrow} \end{pmatrix}$$

superconducting phase: bare $T_c = T_{c0}$ and $|\alpha \vec{\lambda}_{\vec{k}}| \sim k_B T_{c0}$



$$f(\rho) = \operatorname{Re}\sum_{n=1}^{\infty} \left(\frac{1}{2n-1+i\rho} - \frac{1}{2n-1}\right) \qquad \rho_{\vec{k}} = \frac{|\vec{\lambda}_{\vec{k}}|}{\pi k_B T_c} \qquad \hat{\lambda}_{\vec{k}} = \frac{\lambda_{\vec{k}}}{|\vec{\lambda}_{\vec{k}}|}$$

superconducting phase: bare $T_c = T_{c0}$ and $|\alpha \vec{\lambda}_{\vec{k}}| \sim k_B T_{c0}$



superconducting phase: bare $T_c = T_{c0}$ and $|lpha \vec{\lambda}_{\vec{k}}| \sim k_B T_{c0}$



superconducting phase: bare $T_c = T_{c0}$ and $|\alpha \vec{\lambda}_{\vec{k}}| \sim k_B T_{c0}$



$$\mathcal{H} = \sum_{\vec{k},s} (\epsilon_{\vec{k}} - \mu) c^{\dagger}_{\vec{k}s} c_{\vec{k}s} + \alpha \sum_{\vec{k},s,s'} \vec{\lambda}_{\vec{k}} \cdot \{c^{\dagger}_{\vec{k}s} \vec{\sigma}_{ss'} c_{\vec{k}s'}\}$$

time reversal symmetry breaking

$$lphaec{\lambda}_{ec{k}} = -\mu_Bec{H}$$

Zeeman coupling

inversion symmetry breaking

$$lpha \vec{\lambda}_{\vec{k}} = lpha (\vec{k} imes \hat{z})$$

Rashba spin-orbit coupling



$$\mathcal{H} = \sum_{\vec{k},s} (\epsilon_{\vec{k}} - \mu) c^{\dagger}_{\vec{k}s} c_{\vec{k}s} + \alpha \sum_{\vec{k},s,s'} \vec{\lambda}_{\vec{k}} \cdot \{c^{\dagger}_{\vec{k}s} \vec{\sigma}_{ss'} c_{\vec{k}s'}\}$$

time reversal symmetry breaking

$$lphaec{\lambda}_{ec{k}} = -\mu_Bec{H}$$

Zeeman coupling

inversion symmetry breaking

$$lpha \vec{\lambda}_{\vec{k}} = lpha (\vec{k} imes \hat{z})$$

Rashba spin-orbit coupling


Anderson theorem for perturbations

$$\mathcal{H} = \sum_{\vec{k},s} (\epsilon_{\vec{k}} - \mu) c^{\dagger}_{\vec{k}s} c_{\vec{k}s} + \alpha \sum_{\vec{k},s,s'} \vec{\lambda}_{\vec{k}} \cdot \{c^{\dagger}_{\vec{k}s} \vec{\sigma}_{ss'} c_{\vec{k}s'}\}$$

time reversal symmetry breaking

$$lphaec{\lambda}_{ec{k}} = -\mu_Bec{H}$$

Zeeman coupling

inversion symmetry breaking

$$lpha \vec{\lambda}_{\vec{k}} = lpha (\vec{k} imes \hat{z})$$

Rashba spin-orbit coupling



Structure of pairing state

Anderson theorem for perturbations - summary



Anderson theorem for perturbations - summary



Anderson theorem for perturbations - summary



Structure of pairing states

time reversal symmetry broken (e.g. magnetic field)

spin triplet state:	$\hat{\Psi}_{\vec{k}} = i\vec{d}(\vec{k})\cdot\hat{\vec{\sigma}}\hat{\sigma}^y$	with spin parallel to field
Cooper pair spin expectation	value $ec{d^*} imesec{d}\propto \langleec{S} angle eq 0$	$ec{d}(ec{k}) \perp ec{H}$

inversion symmetry broken (e.g. non-centrosymmetric crystal)

combination of spin singlet and spin triplet state: *mixed parity state*

$$\hat{\Psi}_{ec{k}} = \left\{ \psi(ec{k}) + ec{d}(ec{k}) \cdot \hat{ec{\sigma}}
ight\} i \hat{\sigma}^y$$
with
 $ec{\lambda}_{ec{k}} \parallel ec{d}(ec{k})$

Mixed parity states are *non-unitary*

unitary superconducting states: $\hat{\Psi}_{ec{k}}\hat{\Psi}^{\dagger}_{ec{k}}=|\Psi_{ec{k}}|^2\hat{\sigma}_0\propto~$ 2x2 unit matrix

$$\hat{\Psi}_{\vec{k}} = \left\{\psi(\vec{k}) + \vec{d}(\vec{k}) \cdot \hat{\vec{\sigma}}
ight\}i\hat{\sigma}^{y}$$



Non-centrosymmetric superconductors

Ce-based heavy Fermion superconductors



tetragonal crystal lattice

quantum critical point

Upper critical field

How to destroy Cooper pairs by a magnetic field?



Spin polarization - spin susceptibility



Paramagnetic limiting field

destruction of superconductivity due to Zeeman splitting of electron spins

Compare the two energies at T=0K

superconducting condensation energy

paramagnetic energy



paramagnetic limiting field

$$H_p = \frac{H_c(0)}{\sqrt{4\pi(\chi_p - \chi(0))}}$$

Paramagnetic limiting field

destruction of superconductivity due to Zeeman splitting of electron spin states

Compare the two energies at T=0K

superconducting condensation energy

paramagnetic energy



paramagnetic limiting field

$$H_p = \frac{H_c(0)}{\sqrt{4\pi(\chi_p - \chi(0))}}$$

Paramagnetic limiting field

destruction of superconductivity due to Zeeman splitting of electron spin states

Compare the two energies at T=0K

superconducting condensation energy

paramagnetic energy



paramagnetic limiting field

$$H_p = \frac{H_c(0)}{\sqrt{4\pi(\chi_p - \chi(0))}}$$

Paramagnetic limiting field - mixed parity state



Paramagnetic limiting field - mixed parity state



Upper critical field and paramagnetic limiting

CeRhSi₃





fits very well to theoretical expectations of paramagnetic limiting

Upper critical field and paramagnetic limiting



fits very well to theoretical expectations of paramagnetic limiting

Special features of mixed-parity states

intrinsic multi-band aspect

- twin boundaries
- surface states

Structure of the pair wave function

$$\hat{\Psi}(\vec{k}) = \left\{ \Delta_1 \psi(\vec{k}) + \Delta_2 \vec{d}(\vec{k}) \cdot \hat{\vec{\sigma}} \right\} i \hat{\sigma}^y$$

2 Fermi surfaces $\xi_{\vec{k}\pm} = \xi_{\vec{k}} \pm \alpha \left| \vec{k} \times \hat{z} \right|$



2 different pair wave functions:

$$\Psi_{\pm}(ec{k}) = \Delta_1 \psi(ec{k}) \pm \Delta_2 rac{ec{d}(ec{k}) \cdot ec{\lambda}_{ec{k}}}{|ec{\lambda}_{ec{k}}|}$$

non-centrosymmetric crystals can be twinned



Twin boundaries:



non-centrosymmetric crystals can be twinned



Twin boundaries:



non-centrosymmetric crystals can be twinned



Twin boundaries:



non-centrosymmetric crystals can be twinned



non-centrosymmetric crystals can be twinned



Quasiparticle tunneling multigap features and zero-bias anomalies



Quasiparticle tunneling multigap features and zero-bias anomalies



Quasiparticle tunneling

multigap features and zero-bias anomalies



Li_2Pd_3B & Li_2Pt_3B

Unequal twins



LaAIO₃ / SrTiO₃ Heterostructure

Environment for non-centrosymmetric superconductivity

LaAIO₃ / SrTiO₃ heterostructure



LaAlO₃ / SrTiO₃ heterostructure



LaAlO₃ / SrTiO₃ heterostructure



Reyren, Triscone, Mannhart et al. (2008)

LaAlO₃ / SrTiO₃ heterostructure



Reyren, Triscone, Mannhart et al. (2008)

Conclusions

• Cooper Pairing involves two key symmetries

{ time reversal inversion

 non-unitary states: spin polarized pairing mixed-parity pairing

lack of time reversal lack of inversion

- non-centrosymmetric superconductors with unconventional pairing
 - rich in phenomena with a complex phenomenology

 magnetoelectric phenomena connection to spintronics and multiferroics
 Edelstein, Mineev, Samokhin, Eschrig, ...
 Josephson effect phase sensitive probes Hayashi, Linder, Subdo, Borkje, ...
 Coexistence of magnetism and superconductivity at quantum critical points
 Yanase, Fujimoto, ...
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