Group-Theoretical Classification of Superconducting States

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Outline

- Pairing and superconductivity
  - Bloch *vs* Wannier *vs* orbital bases
  - Separation of variables, **d**-vector, etc.
  - Mean-field description
- Quick overview of group theory
  - common point groups
  - representations, character tables, projection operators
  - Landau approach to the transition
- Single-band superconductors (e.g. with C_{4v} symmetry)
  - Relation between nodal lines and symmetry
- Multi-band superconductors (e.g. Sr_2RuO_4)
- Superconductors with spin-orbit coupling

Pairing and superconductivity

Pairing operator :

annihilates an electron of spin σ at position $\mathbf{x}$

$$\hat{\Delta} = \int d^3\mathbf{x}\, d^3\mathbf{x}'\ \Delta_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}')\Psi_\sigma(\mathbf{x})\Psi_{\sigma'}(\mathbf{x}')$$

pairing function

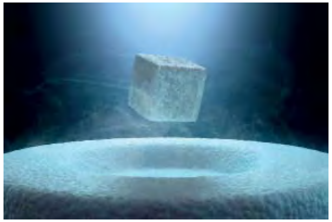
Antisymmetry imposes $\Delta_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') = -\,\Delta_{\sigma'\sigma}(\mathbf{x}'-\mathbf{x})$

Superconductivity : condensation of Cooper pairs : $\langle\hat{\Delta}\rangle \neq 0$

or rather

$$\int d^3y\ \Delta_{\sigma\sigma'}(\vec{y})\,\Psi_\sigma(\vec{x}'+\tfrac{1}{2}\vec{y})\,\Psi_{\sigma'}(\vec{x}'-\tfrac{1}{2}\vec{y})$$

$$\lim_{|\mathbf{x}-\mathbf{x}'|\to\infty} \langle \Delta^\dagger(\mathbf{x})\Delta(\mathbf{x}')\rangle \neq 0$$



In this talk : we do not care why…
(no discussion of mechanisms)

Bloch basis

annihilates an electron of spin σ & momentum $\mathbf{k}$ in band a

Bloch wavefunction

$$\Psi_\sigma(\mathbf{x}) = \sum_{\mathbf{k},a,\sigma} d_{a,\sigma}(\mathbf{k})\varphi_{\mathbf{k},a}(\mathbf{x}) \quad \text{where} \quad \{d_{a,\sigma}(\mathbf{k}), d^\dagger_{b,\sigma'}(\mathbf{k}')\} = (2\pi)^3\delta(\mathbf{k}-\mathbf{k}')\delta_{a,b}\delta_{\sigma,\sigma'}$$

$$H_0 = \sum_{\mathbf{k},a,\sigma} \varepsilon_a(\mathbf{k}) d^\dagger_{a,\sigma}(\mathbf{k}) d_{a,\sigma}(\mathbf{k})$$

band index

noninteracting Hamiltonian is diagonal

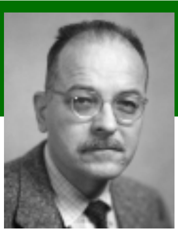
pairing function in the Bloch basis

$$\hat{\Delta} = \sum_{\mathbf{k},a,b,\sigma,\sigma'} \Delta_{a\sigma,b\sigma'}(\mathbf{k}) d_{a\sigma}(\mathbf{k}) d_{b\sigma'}(-\mathbf{k})$$

(assumes pair has no net momentum)

$$\Delta_{a\sigma,b\sigma'}(\mathbf{k}) = -\Delta_{b\sigma',a\sigma}(-\mathbf{k})$$

antisymmetry



Wannier basis

Interaction is diagonal

annihilates an electron of spin σ & orbital m at site $\mathbf{r}$

Wannier wavefunction

$$\Psi_\sigma(\mathbf{x}) = \sum_{\mathbf{r},m,\sigma} c_{\mathbf{r},m,\sigma} w_{m,\sigma}(\mathbf{x}-\mathbf{r}) \quad \text{where} \quad \{c_{\mathbf{r},m,\sigma}, c^\dagger_{\mathbf{r}',m',\sigma'}\} = \delta_{\mathbf{r},\mathbf{r}'}\delta_{m,m'}\delta_{\sigma,\sigma'}$$

annihilates an electron of spin σ, orbital m and momentum $\mathbf{k}$

$$H_0 = \sum_{\mathbf{r},\mathbf{r}',m,m',\sigma} t^{m,m'}_{\mathbf{r},\mathbf{r}'} c^\dagger_{\mathbf{r},m,\sigma} c_{\mathbf{r}',m',\sigma} = \sum_{\mathbf{k},m,m',\sigma} t^{m,m'}(\mathbf{k}) c^\dagger_{m,\sigma}(\mathbf{k}) c_{m',\sigma}(\mathbf{k})$$

orbital basis

(= Bloch basis if $N_b = 1$)

otherwise diagonalize $t^{m,m'}(\mathbf{k}) \longrightarrow \varepsilon_a(\mathbf{k})$ and $d_{a,\sigma}(\mathbf{k}) = \sum_m V_{a,m}(\mathbf{k}) c_{m,\sigma}(\mathbf{k})$

$\mathbf{k}$ - dependent unitary matrix

$$\hat{\Delta} = \sum_{\mathbf{r},\mathbf{r}',m,m',\sigma,\sigma'} \Delta_{\mathbf{r}m\sigma,\mathbf{r}'m'\sigma'} c_{\mathbf{r}m\sigma} c_{\mathbf{r}'m'\sigma'} \qquad \Delta_{\mathbf{r}m\sigma,\mathbf{r}'m'\sigma'} = -\Delta_{\mathbf{r}'m'\sigma',\mathbf{r}m\sigma}$$

pairing function in the Wannier basis

$$\hat{\Delta} = \sum_{\mathbf{k},m,m',\sigma,\sigma'} \Delta_{m\sigma,m'\sigma'}(\mathbf{k}) c_{m\sigma}(\mathbf{k}) c_{m'\sigma'}(-\mathbf{k}) \qquad \Delta_{m\sigma,m'\sigma'}(\mathbf{k}) = -\Delta_{m'\sigma',m\sigma}(-\mathbf{k})$$

pairing function in the orbital basis

Separation of variables

Orbital basis : $$\Delta_{m,\sigma;m',\sigma'}(\mathbf{k}) = \sum_{\alpha\beta\gamma} \psi_{\alpha\beta\gamma} f^{\alpha}(\mathbf{k}) O^{\beta}_{mm'} S^{\gamma}_{\sigma\sigma'}$$

pairing amplitudes

Bloch basis : $$\Delta_{a,\sigma;b,\sigma'}(\mathbf{k}) = \sum_{\alpha\beta\gamma} \chi_{\alpha\beta\gamma} f^{\alpha}(\mathbf{k}) B^{\beta}_{ab}(\mathbf{k}) S^{\gamma}_{\sigma\sigma'}$$

$$d_{a,\sigma}(\mathbf{k}) = \sum_{m} V_{a,m}(\mathbf{k}) c_{m,\sigma}(\mathbf{k})$$

The basis functions $f^{\alpha}(\mathbf{k})$, $O^{\beta}_{mm'}$, $B^{\beta}_{ab}(\mathbf{k})$, $S^{\gamma}_{\sigma\sigma'}$ must transform according to **irreducible representations** of the symmetry group

Spatial and spin parts

$$\Delta_{m,\sigma;m',\sigma'}(\mathbf{k}) = \sum_{\alpha\beta\gamma} \psi_{\alpha\beta\gamma} f^{\alpha}(\mathbf{k}) O^{\beta}_{mm'} S^{\gamma}_{\sigma\sigma'}$$

Spatial part : $f(\mathbf{k}) = \sum_{\mathbf{r}} f_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}}$ $(\alpha \rightarrow \mathbf{r})$

Spin part : $S_{\sigma\sigma'} = d_{\gamma}(\hat{\mathbf{d}}_{\gamma})_{\sigma\sigma'}$ $\hat{\mathbf{d}}_{\gamma} = i(\tau_{\gamma}\tau_2)$ « **d** » - vector

$$\hat{\mathbf{d}}_0 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad |\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle$$

spin 0
singlet (antisymmetric)

$$\hat{\mathbf{d}}_x = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad |\downarrow\downarrow\rangle - |\uparrow\uparrow\rangle$$

$$\hat{\mathbf{d}}_y = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} \qquad i\,(|\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle)$$

$$\hat{\mathbf{d}}_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle$$

spin 1
triplet (symmetric)

Mean field approximation

Bloch basis, spin singlet :

$$H_{MF} = \sum_{\mathbf{k},a,\sigma} \varepsilon_a(\mathbf{k}) d^\dagger_{a,\sigma}(\mathbf{k}) d_{a,\sigma}(\mathbf{k}) + \sum_{\mathbf{k},a,b} \bar{\Delta}_{ab}(\mathbf{k}) \left[d_{a\uparrow}(\mathbf{k}) d_{b\downarrow}(-\mathbf{k}) - d_{a\downarrow}(\mathbf{k}) d_{b\uparrow}(-\mathbf{k}) \right]$$

Nambu representation : $\Psi(\mathbf{k}) = \left(d_{1\uparrow}(\mathbf{k}), \ldots, d_{N_b\uparrow}(\mathbf{k}), d^\dagger_{1\downarrow}(-\mathbf{k}), \ldots, d^\dagger_{N_b\downarrow}(-\mathbf{k}) \right)$

$$H_{MF} = \sum_{\mathbf{k}} \Psi^\dagger(\mathbf{k}) \mathscr{H}(\mathbf{k}) \Psi(\mathbf{k})$$ where $$\mathscr{H}(\mathbf{k}) = \begin{pmatrix} \epsilon(\mathbf{k}) & \boldsymbol{\Delta}(\mathbf{k}) \\ \boldsymbol{\Delta}^\dagger(\mathbf{k}) & -\epsilon(-\mathbf{k}) \end{pmatrix}$$

$N_b \times N_b$ matrix

One band $(N_b = 1)$: eigenvalues $\xi(\mathbf{k}) = \pm \sqrt{\varepsilon^2(\mathbf{k}) + \Delta^2(\mathbf{k})}$

$\mathbf{k}-$dependent **gap function**

Many bands $(N_b > 1)$: more complicated

Group theory I

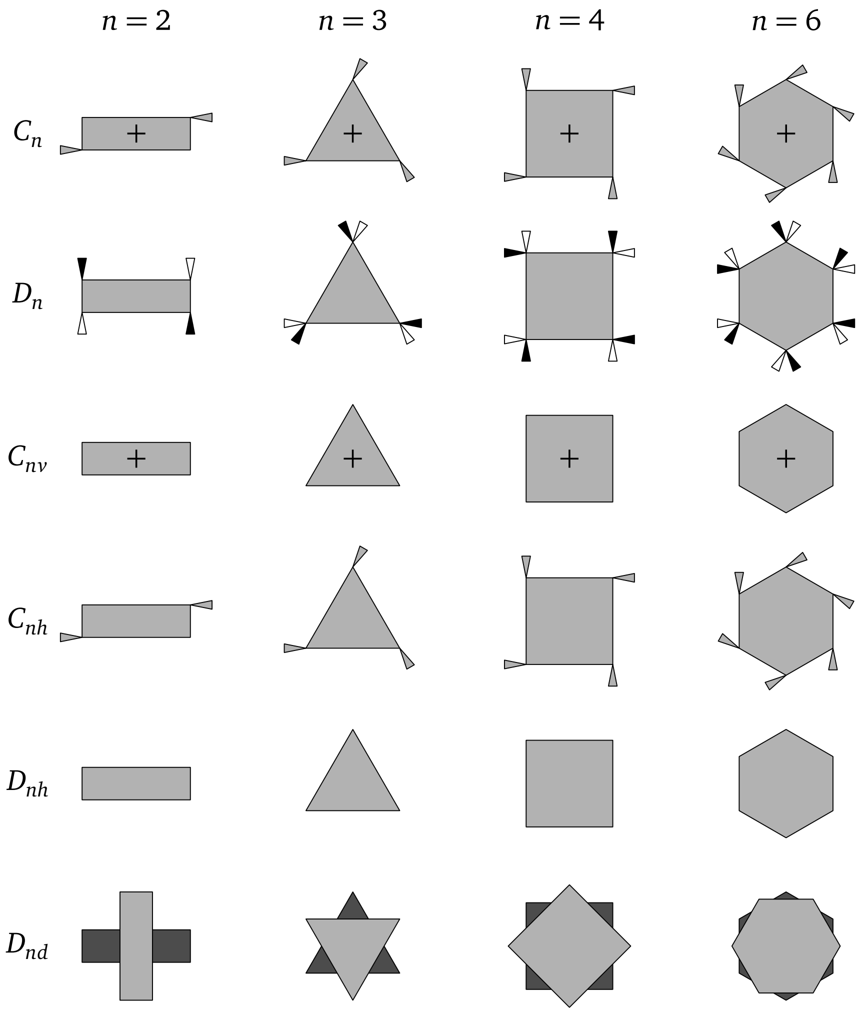
A **group** G is a set $\{a, b, c, \dots\}$ endowed with a multiplication law satisfying the following constraints:

1. Group multiplication is **associative**: $(ab)c = a(bc)$.
2. There is a **neutral element** e such that $ea = ae = a, \forall a \in G$
3. Each element a has an **inverse** a^{-1} such that $aa^{-1} = a^{-1}a = e$

It is implicit that if $a, b \in G$, then $ab \in G$ (**closure** under the group multiplication)

Most groups of interest for us are finite subgroups of the $O(3)$ (the group of orthogonal matrices of dimension 3)

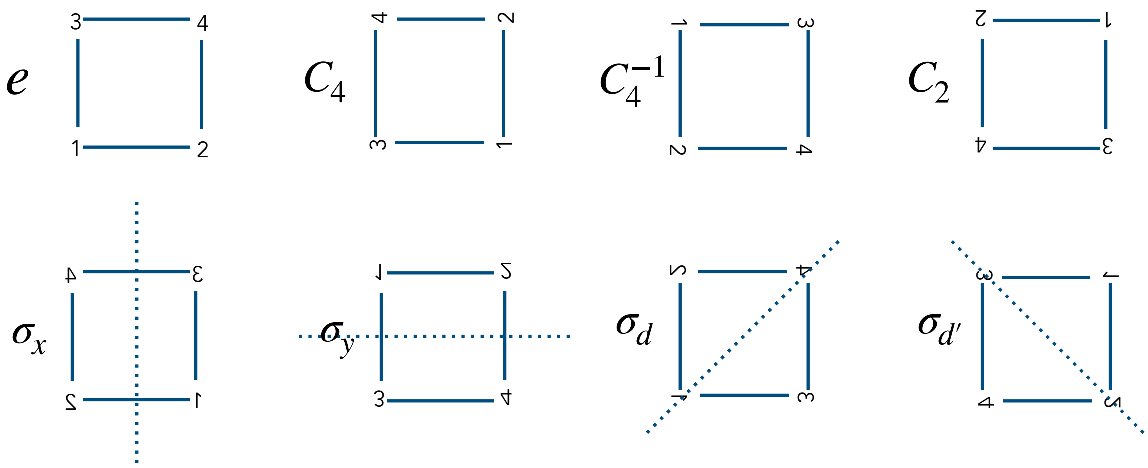
Common point groups



Example : C_{4v}

Table 1: *A simple example of group representation for C_{4v}: the matrices act on the coordinates (x,y). C_n is a rotation by $2\pi/n$ in the x-y plane. σ_x, σ_y, σ_d and $\sigma_{d'}$ are reflexions across the planes $x=0$, $y=0$, $x=-y$ and $x=y$, respectively.*

g	$R(g)$	g	$R(g)$	g	$R(g)$	g	$R(g)$
e	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	C_4	$\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$	C_4^{-1}	$\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	C_2	$\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}$
σ_x	$\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$	σ_y	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	σ_d	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\sigma_{d'}$	$\begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix}$



$$\mathscr{R} : G \to GL(d)$$

regular $d \times d$ matrices

$$a \to R(a) \qquad R(ab) = R(a)R(b)$$

Conjugacy classes : a and b are **conjugate** if $b = c^{-1}ac$ for some $c \in G$

a and b are then « the same type » of transformation

Reducible representation : $\exists$ basis such that $R(a) = R^{(1)}(a) \oplus R^{(2)}(a)$, $\forall a \in G$

$$R(a) = \begin{pmatrix} R^{(1)}(a) & 0 \\ 0 & R^{(2)}(a) \end{pmatrix}$$

We care about **irreducible** representations

Character tables : example of C_{4v}

Character of class in a representation : $\chi(a) = \mathrm{tr}\, R(a)$

	e	$2C_4$	C_2	$\sigma_{x,y}$	$\sigma_{d,d'}$	basis functions
A_1	1	1	1	1	1	1
A_2	1	1	1	-1	-1	$\mathscr{R}_z\ ,\ xy(x^2-y^2)$
B_1	1	-1	1	1	-1	x^2-y^2
B_2	1	-1	1	-1	1	xy
E	2	0	-2	0	0	$[\mathscr{R}_x, \mathscr{R}_y]\ ,\ [x,y]$

Orthogonality of rows :

$$\sum_{\mu}^{K} \frac{g_i}{g} \chi_i^{(\mu)*} \chi_j^{(\mu)} = \delta_{ij}$$

(sum over irreps)

Orthogonality of columns :

$$\sum_{i}^{K} \frac{g_i}{g} \chi_i^{(\nu)*} \chi_i^{(\mu)} = \delta_{\mu\nu}$$

(sum over classes)

g_i = *# of elements in class* i

g = *# of elements in group*

Character tables : simpler example of C_{2v}

		e	C_2	σ_x	σ_y	basis functions
even-even	A_1	1	1	1	1	$1\ ,\ z\ ,\ x^2+y^2$
odd-odd	A_2	1	1	−1	−1	$\mathscr{R}_z\ ,\ xy$
even-odd	B_1	1	−1	1	−1	$x\ ,\ \mathscr{R}_y\ ,\ xz$
odd-even	B_2	1	−1	−1	1	$y\ ,\ \mathscr{R}_x\ ,\ yz$

Tensor products of representations

e.g. momentum ↓ e.g. orbital ↓

$$\Delta_{m,\sigma;m',\sigma'}(\mathbf{k}) = \sum_{\alpha\beta\gamma} \psi_{\alpha\beta\gamma} f^{\alpha}(\mathbf{k}) O^{\beta}_{mm'} S^{\gamma}_{\sigma\sigma'}$$

$$R_{i\mu,j\nu}(a) = R^{(1)}_{ij}(a) R^{(2)}_{\mu\nu}(a) \quad \text{or} \quad R(a) = R^{(1)}(a) \otimes R^{(2)}(a)$$

$$R^{(\mu)} \otimes R^{(\nu)} = \bigoplus_{\rho} C^{\rho}_{\mu\nu} R^{(\rho)}$$

products of irreducible representations are generally **reducible** (Clebsch-Gordan series)

$$\chi_i(R^{(\mu)} \otimes R^{(\nu)}) = \chi_i^{(\mu)} \chi_i^{(\nu)} = \sum_{\rho} C^{\rho}_{\mu\nu} \chi_i^{(\rho)}$$

characters of tensor products are products of characters

$$C^{\rho}_{\mu\nu} = \sum_{i=1}^{K} \frac{g_i}{g} \chi_i^{*(\rho)} \chi_i^{(\mu)} \chi_i^{(\nu)}$$

from

$$\sum_{\mu}^{K} \frac{g_i}{g} \chi_i^{(\mu)*} \chi_j^{(\mu)} = \delta_{ij}$$

Projection operator :

$$P^{(\mu)} = \sum_{a \in G} \frac{d_{\mu}}{g} \chi^{(\mu)*}(a) R(a)$$

Projects states in the tensor product space onto the irreducible representation labelled μ

Schur's lemma

- Consider a reducible representation $R = R_1 \oplus R_2$, acting on space $V = V_1 \oplus V_2$
- Suppose the Hamiltonian obeys the symmetry : $HR(a) = R(a)H$
- If R_1 and R_2 are not equivalent, then $H = H_1 \oplus H_2$ is **block diagonal**

Main use of group theory : classification of energy levels and selection rules

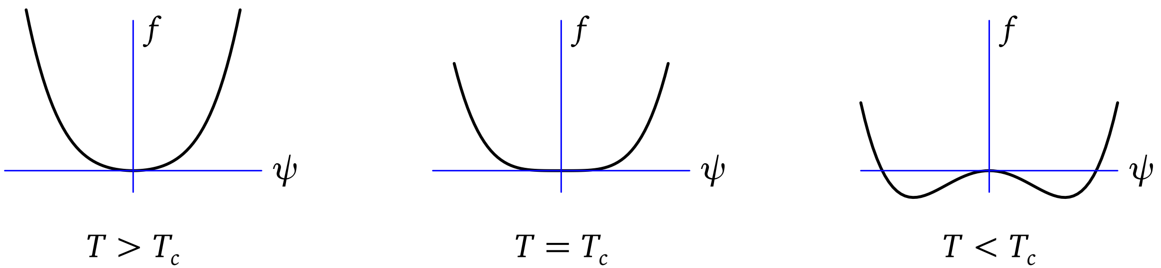
The Landau free energy

$$\Delta_{m,\sigma;m',\sigma'}(\mathbf{k}) = \sum_r \psi_r \, \Delta^{(r)}_{m,\sigma;m',\sigma'}(\mathbf{k})$$

single index r for the product basis functions

Landau free energy functional, compatible with the symmetries of the system :

$$f[\psi] = a_{rs}(T)\bar{\psi}_r\psi_s + b_{rspq}(T)\bar{\psi}_r\bar{\psi}_s\psi_p\psi_q + \cdots$$



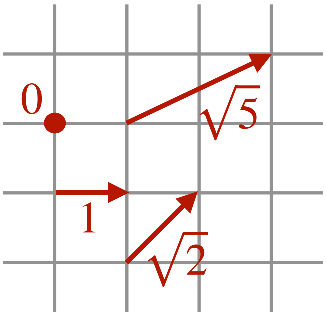
$a(T)$ is block-diagonal : $a(T) = \bigoplus_\mu a^{(\mu)}(T)$

$a(T)_{rs}$ can be viewed as an operator on the states, like a Hamiltonian

The representation with the first negative eigenvalue as T is lowered wins…

Single-band superconductor with C_{4v} symmetry

basis functions (spatial part) : $f^{\mathbf{r}}(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{r}}$



on-site pairing $|\mathbf{r}| = 0 : (1)$

first-neighbor pairing $|\mathbf{r}| = 1 : \left(e^{ik_x}, e^{ik_y}, e^{-ik_x}, e^{-ik_y}\right)$

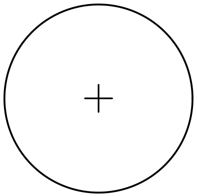
second-neighbor pairing $|\mathbf{r}| = \sqrt{2} : \left(e^{i(k_x+k_y)}, e^{i(k_x-k_y)}, e^{-i(k_x+k_y)}, e^{-i(k_x-k_y)}\right)$

	spin state	distance	gap functions	
A_1	singlet	0	1	« *s*-wave »
A_2	singlet	$\sqrt{5}$	$\sin k_x \ \sin k_y (\cos k_x - \cos k_y)$	« *f*-wave »
B_1	singlet	1	$\cos k_x - \cos k_y$	« *d*-wave »
B_2	singlet	$\sqrt{2}$	$\sin k_x \ \sin k_y$	« *d*-wave »
E	triplet	1	$[\sin k_x, \sin k_y]$	« *p*-wave »

$$P^{(\mu)} = \sum_{a\in G} \frac{d_\mu}{g} \chi^{(\mu)*}(a) R(a)$$

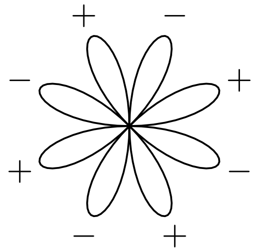
Single-band SC with C_4 symmetry : nodes

polar plots at constant $|\mathbf{k}|$



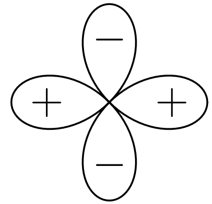
A_1

s



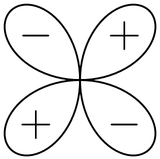
A_2

g



B_1

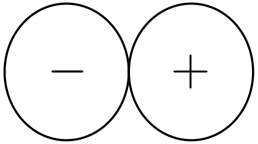
$d_{x^2-y^2}$



B_2

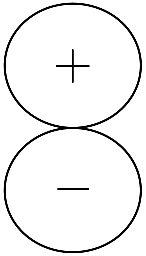
d_{xy}

E :



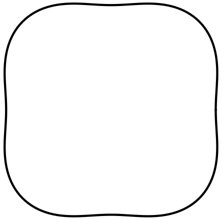
p_x

$\sin k_x$



p_y

$\sin k_y$



$|p_x \pm i p_y|$

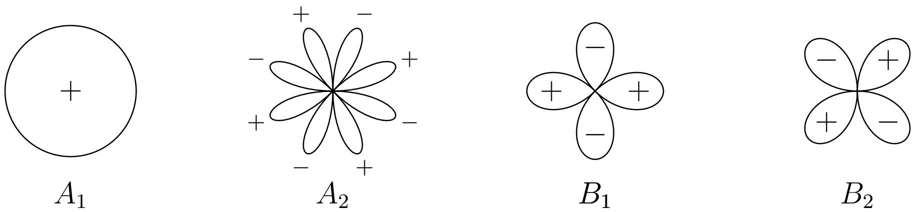
time-reversal symmetry breaking

Relation between nodes and symmetry

B_1 : The spatial part is odd under the diagonal mirror $\longrightarrow$ node at $\pm 45°$

B_2 : The spatial part is odd under σ_x and σ_y $\longrightarrow$ nodes along x and y

A_2 : The spatial part is odd under all mirrors $\longrightarrow$ nodes along x and y and at $\pm 45°$

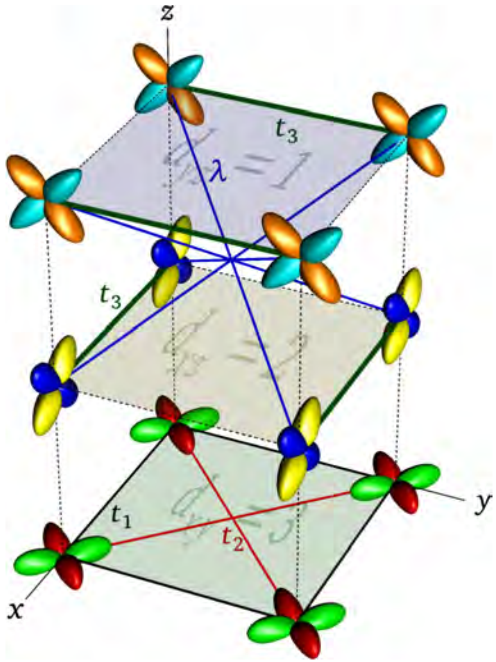


$$\xi(\mathbf{k}) = \pm\sqrt{\varepsilon^2(\mathbf{k}) + \Delta^2(\mathbf{k})}$$

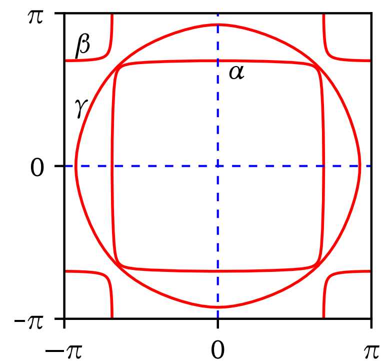
- In the one-band case : nodes are set by symmetry (i.e. representation).
- This is no longer true in the multi-band case.

	e	$2C_4$	C_2	$\sigma_{x,y}$	$\sigma_{d,d'}$	basis functions
A_1	1	1	1	1	1	1
A_2	1	1	1	−1	−1	$\mathcal{R}_z$, $xy(x^2-y^2)$
B_1	1	−1	1	1	−1	x^2-y^2
B_2	1	−1	1	−1	1	xy
E	2	0	−2	0	0	$[\mathcal{R}_x, \mathcal{R}_y]$, $[x,y]$

Sr_2RuO_4 (D_{4h} symmetry, 3 bands)



Ru t_{2g} orbitals : d_{yz} , d_{xz} , d_{xy}



$$c_{m,\sigma}(\mathbf{k}) \rightarrow c'_{m,\sigma}(\mathbf{k}) = \sum_{m'} U_{mm'}(g) c_{m',\sigma}(g\mathbf{k})$$

(no spin orbit coupling)

$$U(C_4) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad U(\sigma_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad U(\sigma_z) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

D_{4h} character table

		e	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_z	$\sigma_{x,y}$	$\sigma_{d,d'}$	basis functions
even	A_{1g}	1	1	1	1	1	1	1	1	1	1	1
	A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1	$\mathcal{R}_z\ ,\ xy(x^2-y^2)$
	B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1	x^2-y^2
	B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1	xy
	E_g	2	0	−2	0	0	2	0	−2	0	0	$[\mathcal{R}_x, \mathcal{R}_y]\ ,\ z[x,y]$
odd	A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1	$xyz(x^2-y^2)$
	A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	z
	B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1	xyz
	B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1	$z(x^2-y^2)$
	E_u	2	0	−2	0	0	−2	0	2	0	0	$[x,y]$

orbital part

$$\hat{\mathbf{a}}_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \hat{\mathbf{b}}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \hat{\mathbf{c}}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$\hat{\mathbf{a}}_y = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \hat{\mathbf{b}}_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \hat{\mathbf{c}}_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

$$\hat{\mathbf{a}}_z = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \hat{\mathbf{b}}_z = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \hat{\mathbf{c}}_z = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$O_{mn} = \mathbf{a} \cdot \hat{\mathbf{a}}_{mn} + \mathbf{b} \cdot \hat{\mathbf{b}}_{mn} + \mathbf{c} \cdot \hat{\mathbf{c}}_{mn}$$

$$O_{mm'} \rightarrow \sum_{n,n'} U_{mn}(g) U_{m'n'}(g) O_{nn'}$$ or $$O \rightarrow U(g) O U^T(g)$$

Sr_2RuO_4 : singlet pairing functions

irrep	pairing function
A_{1g}	$\hat{\mathbf{a}}_z$
	$\hat{\mathbf{a}}_x + \hat{\mathbf{a}}_y$
	$\hat{\mathbf{b}}_z xy$
	$z(\hat{\mathbf{b}}_x y - \hat{\mathbf{b}}_y x)$
A_{2g}	$\hat{\mathbf{a}}_z xy(x^2 - y^2)$
	$xy(\hat{\mathbf{a}}_x - \hat{\mathbf{a}}_y)$
	$\hat{\mathbf{b}}_z (x^2 - y^2)$
	$z(\hat{\mathbf{b}}_x x + \hat{\mathbf{b}}_y y)$
B_{1g}	$\hat{\mathbf{a}}_z (x^2 - y^2)$
	$\hat{\mathbf{a}}_x - \hat{\mathbf{a}}_y$
	$\hat{\mathbf{b}}_z xy(x^2 - y^2)$
	$z(\hat{\mathbf{b}}_x y + \hat{\mathbf{b}}_y x)$

irrep	pairing function
B_{2g}	$\hat{\mathbf{a}}_z xy$
	$xy(\hat{\mathbf{a}}_x + \hat{\mathbf{a}}_y)$
	$\hat{\mathbf{b}}_z$
	$z(\hat{\mathbf{b}}_x x - \hat{\mathbf{b}}_y y)$
E_g	$\hat{\mathbf{a}}_z z(x, y)$
	$z(\hat{\mathbf{a}}_x x, \hat{\mathbf{a}}_y y)$
	$z(\hat{\mathbf{a}}_x y, \hat{\mathbf{a}}_y x)$
	$\hat{\mathbf{b}}_z z(x, y)$
	$(\hat{\mathbf{b}}_x, \hat{\mathbf{b}}_y)$
A_{1u}	$\hat{\mathbf{c}}_z z$
	$\hat{\mathbf{c}}_x x + \hat{\mathbf{c}}_y y$

irrep	pairing function
A_{2u}	$\hat{\mathbf{c}}_z xyz(x^2 - y^2)$
	$\hat{\mathbf{c}}_x y - \hat{\mathbf{c}}_y x$
B_{1u}	$\hat{\mathbf{c}}_z z(x^2 - y^2)$
	$\hat{\mathbf{c}}_x x - \hat{\mathbf{c}}_y y$
B_{2u}	$\hat{\mathbf{c}}_z xyz$
	$\hat{\mathbf{c}}_x y + \hat{\mathbf{c}}_y x$
E_u	$\hat{\mathbf{c}}_z (x, y)$
	$z(\hat{\mathbf{c}}_x, \hat{\mathbf{c}}_y)$

$x \to \sin k_x$
$y \to \sin k_y$
$z \to \sin k_z$

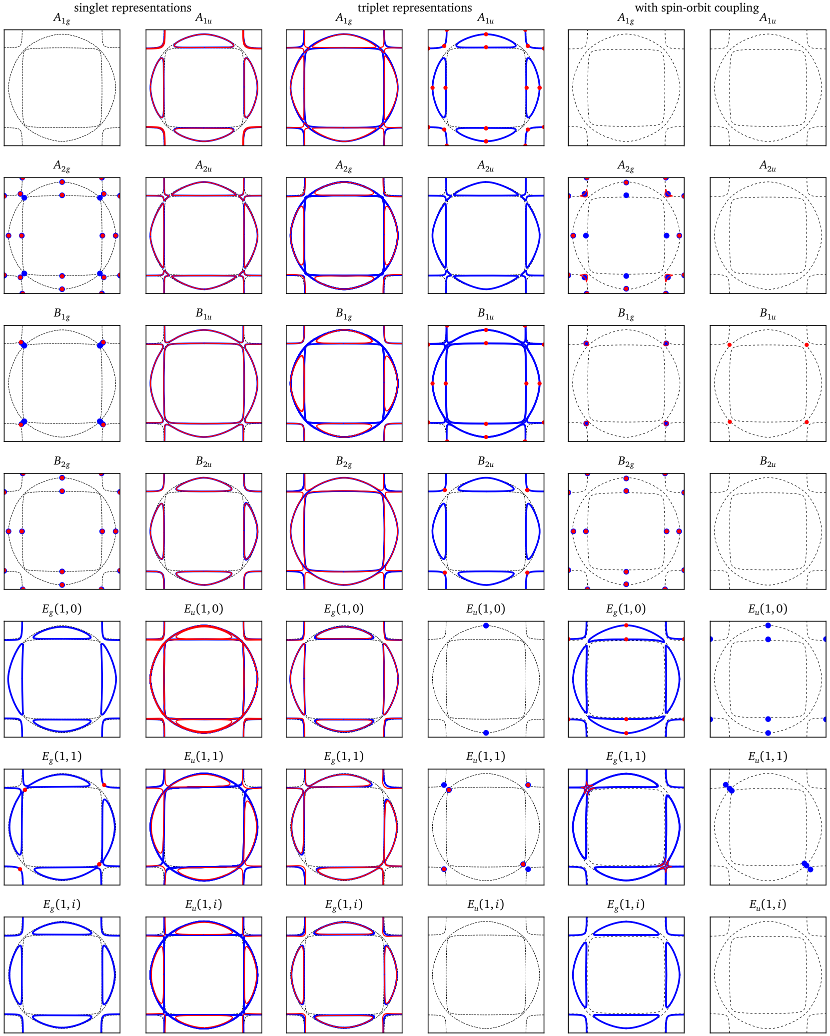
Sr_2RuO_4 : triplet pairing functions

irrep	pairing function
A_{1g}	$\hat{\mathbf{c}}_z xy(x^2-y^2)$
	$z(\hat{\mathbf{c}}_x y-\hat{\mathbf{c}}_y x)$
A_{2g}	$\hat{\mathbf{c}}_z$
	$z(\hat{\mathbf{c}}_x x+\hat{\mathbf{c}}_y y)$
B_{1g}	$\hat{\mathbf{c}}_z xy$
	$z(\hat{\mathbf{c}}_x y+\hat{\mathbf{c}}_y x)$
B_{2g}	$\hat{\mathbf{c}}_z(x^2-y^2)$
	$z(\hat{\mathbf{c}}_x x-\hat{\mathbf{c}}_y y)$
E_g	$\hat{\mathbf{c}}_z z(x,y)$
	$(\hat{\mathbf{c}}_x,\hat{\mathbf{c}}_y)$

irrep	pairing function
A_{1u}	$\hat{\mathbf{a}}_z xyz(x^2-y^2)$
	$xyz(\hat{\mathbf{a}}_x-\hat{\mathbf{a}}_y)$
	$\hat{\mathbf{b}}_z z(x^2-y^2)$
	$\hat{\mathbf{b}}_x x+\hat{\mathbf{b}}_y y$
A_{2u}	$\hat{\mathbf{a}}_z z$
	$z(\hat{\mathbf{a}}_x+\hat{\mathbf{a}}_y)$
	$\hat{\mathbf{b}}_z xyz$
	$\hat{\mathbf{b}}_x y-\hat{\mathbf{b}}_y x$
B_{1u}	$\hat{\mathbf{a}}_z xyz$
	$xyz(\hat{\mathbf{a}}_x+\hat{\mathbf{a}}_y)$
	$\hat{\mathbf{b}}_z z$
	$\hat{\mathbf{b}}_x x-\hat{\mathbf{b}}_y y$

irrep	pairing function
B_{2u}	$\hat{\mathbf{a}}_z z(x^2-y^2)$
	$z(\hat{\mathbf{a}}_x-\hat{\mathbf{a}}_y)$
	$\hat{\mathbf{b}}_z xyz(x^2-y^2)$
	$\hat{\mathbf{b}}_x y+\hat{\mathbf{b}}_y x$
E_u	$\hat{\mathbf{a}}_z(x,y)$
	$(\hat{\mathbf{a}}_x x,\hat{\mathbf{a}}_y y)$
	$(\hat{\mathbf{a}}_x y,\hat{\mathbf{a}}_y x)$
	$\hat{\mathbf{b}}_z(x,y)$
	$z(\hat{\mathbf{b}}_x,\hat{\mathbf{b}}_y)$

Sr_2RuO_4 : generic nodes



Nodes are not set by symmetry

Case of the diagonal mirror : $\Delta_\nu(k_x, k_y, k_z) \to \Delta'_\nu(k_x, k_y, k_z) = \mathscr{U}(\sigma_d)_{\nu\nu'}\Delta_{\nu'}(k_y, k_x, k_z)$

exchanged

this index labels basis vectors in orbital space

In B_{1g} representation : $\Delta'_\nu(k_x, k_y, k_z) = -\Delta_\nu(k_x, k_y, k_z)$

or $[\mathscr{U}(\sigma_d)\mathbf{\Delta}(k_x, k_x, k_z)]_\nu = -\Delta_\nu(k_x, k_x, k_z)$ along the diagonal

One-orbital case : $\mathscr{U} = 1$ and therefore $\Delta_\nu(k_x, k_x, k_z) = 0$

Case of Sr_2CuO_4 :

$\mathbf{\Delta}$ could be an eigenvector of $\mathscr{U}$ with eigenvalue -1, such as $\hat{\mathbf{a}}_x - \hat{\mathbf{a}}_y$

then no condition is imposed on $\Delta_\nu(k_x, k_x, k_z)$

Spin-orbit interaction

A model with Rashba spin-orbit coupling and C_{4v} symmetry (square lattice):

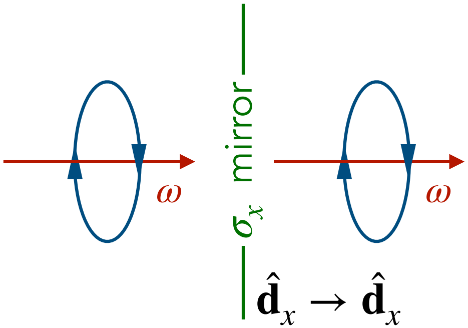
$$H_0 = \sum_{\mathbf{k}} C_{\mathbf{k}} \left[\varepsilon(\mathbf{k}) + \kappa(\tau_y \sin k_x - \tau_x \sin k_y) \right] C_{\mathbf{k}} \qquad \text{where} \qquad C_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow})$$

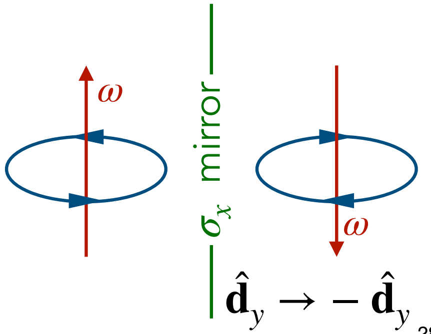
Spatial and spin transformations are intertwined : $\quad c_{\mathbf{r},\sigma} \to c'_{\mathbf{r},\sigma} = \sum_{\sigma'} S_{\sigma\sigma'}(g) c_{g\mathbf{r},\sigma'}$

In particular, for the $\frac{\pi}{2}$ rotation : $\quad S(C_4) = \cos\frac{\pi}{4} + i\sigma_z \sin\frac{\pi}{4} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1+i & 0 \\ 0 & 1-i \end{pmatrix}$

the reflexion σ_x maps (k_x, k_y) into $(-k_x, k_y)$. $\longrightarrow S^\dagger \tau_x S = \tau_x$ and $S^\dagger \tau_y S = -\tau_y$

Hence $S(\sigma_x) = i\tau_x$





Spin-orbit interaction (cont.)

Simplest basis functions compatible with this representation :

Irrep	Basis functions
A_1	$\hat{\mathbf{d}}_0$, $(\hat{\mathbf{d}}_x \sin k_y - \hat{\mathbf{d}}_y \sin k_x)$
A_2	$\hat{\mathbf{d}}_x \sin k_x + \hat{\mathbf{d}}_y \sin k_y$
B_1	$\hat{\mathbf{d}}_0(\cos k_x - \cos k_y)$, $\hat{\mathbf{d}}_x \sin k_y + \hat{\mathbf{d}}_y \sin k_x$
B_2	$\hat{\mathbf{d}}_x \sin k_x - \hat{\mathbf{d}}_y \sin k_y$
E_1	$\hat{\mathbf{d}}_z [\sin k_x, \sin k_y]$

Singlet and triplet functions may belong to the same representation

Under $\sigma_x : k_y \rightarrow k_y \, , \, k_x \rightarrow -k_x \, , \, \hat{\mathbf{d}}_x \rightarrow \hat{\mathbf{d}}_x \, , \, \hat{\mathbf{d}}_y \rightarrow -\hat{\mathbf{d}}_y$

Under $\sigma_d : k_y \rightarrow k_x \, , \, k_x \rightarrow k_y \, , \, \hat{\mathbf{d}}_x \rightarrow -\hat{\mathbf{d}}_y \, , \, \hat{\mathbf{d}}_y \rightarrow -\hat{\mathbf{d}}_x$

Under $C_4 : k_y \rightarrow -k_x \, , \, k_x \rightarrow k_y \, , \, \hat{\mathbf{d}}_x \rightarrow \hat{\mathbf{d}}_y \, , \, \hat{\mathbf{d}}_y \rightarrow -\hat{\mathbf{d}}_x$

	e	$2C_4$	C_2	$\sigma_{x,y}$	$\sigma_{d,d'}$	basis functions
A_1	1	1	1	1	1	1
A_2	1	1	1	−1	−1	$\mathcal{R}_z$, $xy(x^2-y^2)$
B_1	1	−1	1	1	−1	x^2-y^2
B_2	1	−1	1	−1	1	xy
E	2	0	−2	0	0	$[\mathcal{R}_x, \mathcal{R}_y]$, $[x,y]$

Conclusions

- Group theory allows a classification of pairing functions
  - Tools : projection operators and character tables !
- Weak coupling : the Bloch basis is more natural
- Intermediate to strong coupling : the orbital basis is more natural
- Multi-orbital case : nodes are not set by symmetry alone


Thank you!
Questions ?