Spin Space Group in a Nutshell

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Outline

• Rotating a scalar field and a vector field

• Symmetry of spin-ordered state
  o Rotation of positions and spins
  o Spin space groups vs. magnetic space group

• Formalism of spin space group
  o Definition of spin space group
  o Spin point group symbols

• Summary and references

• Application to altermagnetism ⇒ Akash’s presentation
How rotation changes a field?

Case of a scalar field

\[ R: f(r) \rightarrow f(R^{-1}r) \]

- electron density
- nuclear density
- Coulomb potential
etc...

\[ f(r) = f'(Rr) \]

i.e.,

\[ f(R^{-1}r) = f'(r) \]
How rotation changes a field?

Case of a vector field

\[ R: v(r) \rightarrow R v(R^{-1} r) \]

- \( R^{-1} r \): global positional change
- \( Rv \): local vector rotation

In general...
- \( N \)-th-rank polar tensor field
  \[ R: T_{lmn\ldots}(r) \rightarrow R_{il} R_{jm} R_{kn\ldots} T_{lmn\ldots}(R^{-1} r) \]
- \( N \)-th-rank axial tensor field
  \[ R: T_{lmn\ldots}(r) \rightarrow \det(R) R_{il} R_{jm} R_{kn\ldots} T_{lmn\ldots}(R^{-1} r) \]
Spin-ordered state

Spin-ordered crystals

= nuclear density (scalar field) + spin arrangement (axial vector field)
Symmetry of a spin-ordered state

Which symmetry operation does this spin-ordered state have?

\[ \rho(r) \rightarrow \rho(R^{-1}r) \]

\[ M(r) \rightarrow R_{C_{4z}} M(R^{-1}r) \]

- 2-step interpretation
  - Coordination space, \( r \): \n    - \( \rho(r) \rightarrow \rho(R^{-1}r) \)
    - \( M(r) \rightarrow M(R^{-1}r) \)
  - Spin space, \( M \):
    - \( \rho(r) : \) no change
    - \( M(R^{-1}r) \rightarrow R_{C_{4z}} M(R^{-1}r) \)
Symmetry of a spin-ordered state

This spin-ordered state has $\{4|4\}$ symmetry

- For magnetic space groups, coordination- and spin-part operations are always the same (i.e., locked or coupled)

- What about **decoupling** (or **unlocking**) them, such as $\{2|4\}$?
  
  $\Rightarrow$ the key idea of spin space group
Decoupled symmetry operations

Which symmetry operation does this spin-ordered state have?

\[ \rho(r) \rightarrow \rho(R_{C_{4z}}^{-1}r) \]
\[ M(r) \rightarrow R_{C_{2z}} M(R_{C_{4z}}^{-1}r) \]

Decoupled
Spin space group vs. magnetic space group

Spin Space Group
A group of symmetry operations like \{a\|b\} (decoupled or unlocked)
Used when no (or negligible) spin-orbital coupling
∵ if SOC is strong, coordination (r, orbital) and spin (M) cannot be decoupled

Magnetic Space Group
A group of symmetry operations like \{a\|a\} (coupled or locked)
Used when spin-orbital coupling is strong
Brief mathematical introduction

Describing operations in spin space

Rotations

3D rotation group, $\text{SO}(3)$
- Special Orthogonal in 3D
- Determinant = 1
  - proper rotation $C_2, C_3, C_4, C_6, C_n$
  - improper rotation $m, i, \text{etc.}$

Time reversal

Order-2 group, \{E, $T'$\}
- E: identity
- $T'$: time reversal, spin flip

Operations acting in the spin space, $g_s$, are elements of $\text{SO}(3) \otimes \{E, T'\}$

$$g_s \in \text{SO}(3) \otimes \{E, T'\}$$

I am still thinking which the spin is treated as, a time-dependent axial vector or spinor...
If as an axial vector, how it is justified?
Brief mathematical introduction

Describing operations in coordination space

operations acting in the coordination space

| elements of the space group of the nonmagnetic structure, $G_0$

- spin part $\{b\}$ has no impact on the nuclear structure
- the coordination part $\{a\}$ must keep the nuclear structure so that the $\{b||a\}$ leaves the system unchanged
Brief mathematical introduction

Spin space groups are every subgroups of

\[ G_0 \otimes \text{SO}(3) \otimes \{E, T\}, \]

- coordination
- spin rotation
- time reversal (spin flip)

which keep the spin-ordered system unchanged. The operations are denoted as follows

\[ \{g_s \parallel g|t\} \]

- spin part
- coordination part

\[ g_s \in \text{SO}(3) \otimes \{E, T\} \]

\[ \{g|t\} \in G_0 \]

Seitz notation
- \( g \): space-rotation part
- \( t \): partial translation part

\[ \{g|t\}r = R(g)r + t \]

NOTE: \{ || \} and \{ | \} are the different symbols!!!
Brief mathematical introduction

How it acts on a field

**scaler field** \( \{g_s \parallel g \parallel t\} : \rho(r) \longrightarrow \{g \parallel t\} \rho(r) = \rho \left( R(g^{-1})(r - t) \right) \)

**vector field** \( \{g_s \parallel g \parallel t\} : M(r) \longrightarrow R(g_s)M \left( R(g^{-1})(r - t) \right) \)

Product

\[ \{g_s \parallel g \parallel t\}\{g'_s \parallel g' \parallel t'\} = \{g_s g'_s \parallel gg' | R(g) t' + t\} \]

Inverse element

\[ \{g_s \parallel g \parallel t\}^{-1} = \{g_s^{-1} \parallel g^{-1} \parallel - R(g^{-1}) t\} \]
Spin point group symbols

\[
\begin{align*}
\begin{array}{cccc}
2 & 4 & / & 1 \\
2 & m & & 1 \\
\end{array}
\end{align*}
\]

\{C_{2z} \parallel C_{4z}\} \quad \{E \parallel m_z\} \quad \{C_{2z} \parallel m_x\} \quad \{E \parallel m_{[110]}\}

- **Green part** ⇒ Point-group symmetry of nuclear structure (ignoring spin arrangement)
- **Superscript** ⇒ Spin part of the symmetry operation
Using an appropriate group for your system

![Diagram showing magnetic and spin orders with space and double space groups](image)

FIG. 1. Four-quadrant diagram describing the symmetry of solids. The general single-electron Hamiltonians, space groups, and their representative group elements are shown for each quadrant. Compared with the conventional crystallographic groups, the key characteristic of spin group is the partial decoupling between spatial rotation $C_n(\theta)$ and spin rotation $U_m(\varphi)$, where $m$ and $n$ denote the rotation axes, and the real scalars $\varphi$ and $\theta$ are the rotation angles. For the materials with SOC, i.e., the quadrants III and IV, the spatial and spin rotations are completely locked. For example, a spatial rotation by $2\pi/3$ requires a simultaneous spin rotation by $2\pi/3$ along the same axis. For the materials without SOC, the spin and spatial rotations are completely or partially decoupled, which implies that one symmetry operation could be composed of a spin and a spatial rotation with different rotation axes and angles. For the nonmagnetic case (quadrant II), we can either consider spatial rotation only or add a totally unconstrained spin rotation, which constitutes a SO(3) group for spin. For magnetic cases (quadrant I), spin rotation is constrained by the magnetic orders of the system, which allows more operations that are disallowed by SOC but less than the full SO(3) group. The schematic plot in quadrant I shows that, for a specific magnetic order, we can have a symmetry operation that is composed of a spatial rotation of $2\pi/3$ and a spin rotation of $4\pi/3$ along the same axis. Such operations are written as $\{U_m(\varphi)|C_n(\theta)\}$ where the spatial and spin rotation axes and angles could be different.
Summary

Non-magnetic without SOC

- Single-particle mean-field Hamiltonian
  \[ H_0 = \frac{p^2}{2m} + V(r) \]
- Symmetry
  Space group operation, \(|a|\)

Nonmagnetic system with SOC

- Single-particle mean-field Hamiltonian
  \[ H = H_0 + \frac{1}{2mc^2} (\nabla V(r) \times p) \cdot \sigma \]
- Symmetry
  Double space group, \(|a||a|\)
  \(a \in\) space group operation \(\otimes\) \(|E, R|\)
  \(R: 2\pi\) rotation \((R^2 = E)\)

Magnetic system without SOC

- Single-particle mean-field Hamiltonian
  \[ H = H_0 + M(r) \cdot \sigma \]
- Symmetry
  Spin space group, \(|b||a|\)
  \(a \in\) space group operation
  \(b \in SO(3) \otimes\) \(|E, \mathcal{T}|\)

Magnetic system with SOC

- Single-particle mean-field Hamiltonian
  \[ H = H_0 + \frac{1}{2mc^2} (\nabla V(r) \times p) \cdot \sigma + M(r) \cdot \sigma \]
- Symmetry
  Magnetic double space group, \(|a||a|\)
  \(a \in\) magnetic space group operation \(\otimes\) \(|E, R|\)
References

Original papers

- https://doi.org/10.1107/S2053273323009257: algorithm for spin space group assignment
- *Physica*, **76**, 538–554: paper by Litvin about spin space group

Textbooks

- “Space Groups for Solid State Scientist”, Burns and Glazer: for fundamentals of space group
- “Group theory”, Dresselhaus: for fundamentals of (double) group theory
- “Modern Quantum Mechanics”, Sakurai: for fundamentals of spin