Symmetry of Magnetically Induced Currents

MAGIC 2022 | Peterhouse, Cambridge, UK

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13th September 2022

Introduction

Overview

- Symmetry and pseudo-symmetry *groups* in magnetic fields
- *Unitary* representation analysis on *linear spaces*
- *Wavefunction* and *current density* symmetries
  - *Relationships* between wavefunction and current density symmetries
  - Symmetry *descent* and symmetry *breaking* in magnetic fields

Groups in magnetic fields

The electronic Hamiltonian

- For an N_e-electron system in a *uniform* magnetic field $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{r})$, consider the **Schrödinger–Pauli Hamiltonian** in atomic units:

$$\hat{\mathscr{H}} = \frac{1}{2}\sum_{k=1}^{N_\mathrm{e}} \left|-\hat{\boldsymbol{p}}_k + \boldsymbol{A}(\boldsymbol{r}_k)\right|^2 + \sum_{k=1}^{N_\mathrm{e}} v_\mathrm{ext}(\boldsymbol{r}_k) + \frac{1}{2}\sum_{k\neq l}^{N_\mathrm{e}} \frac{1}{|\boldsymbol{r}_k - \boldsymbol{r}_l|} + \frac{g_s}{2}\sum_{k=1}^{N_\mathrm{e}} \boldsymbol{B}\cdot\hat{\boldsymbol{s}}_k$$

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external potential

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electron–electron interaction

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spin Zeeman interaction

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Zero-field Hamiltonian, $\hat{\mathscr{H}}_0(v_\mathrm{ext})$

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$$\begin{aligned}
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&= \frac{1}{2}\sum_{k=1}^{N_\mathrm{e}} \hat{p}_k^2 + \sum_{k=1}^{N_\mathrm{e}} v_\mathrm{ext}(\boldsymbol{r}_k) + \frac{1}{2}\sum_{k\neq l}^{N_\mathrm{e}} \frac{1}{|\boldsymbol{r}_k - \boldsymbol{r}_l|} + \boldsymbol{A}(\boldsymbol{r}_k)\cdot\hat{\boldsymbol{p}}_k + \frac{g_s}{2}\sum_{k=1}^{N_\mathrm{e}} \boldsymbol{B}\cdot\hat{\boldsymbol{s}}_k + \frac{1}{2}A^2(\boldsymbol{r}_k) \\
&= \hat{\mathscr{H}}_0(v_\mathrm{ext}) + \boldsymbol{A}(\boldsymbol{r}_k)\cdot\hat{\boldsymbol{p}}_k + \frac{g_s}{2}\sum_{k=1}^{N_\mathrm{e}} \boldsymbol{B}\cdot\hat{\boldsymbol{s}}_k + \frac{1}{2}A^2(\boldsymbol{r}_k).
\end{aligned}$$

- How does each term transform *spatially* and *temporally*?

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Tensor transformations

- Let $\boldsymbol{v}$ be a rank-k Cartesian tensor in three dimensions.

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Tensor transformations

- Let $\boldsymbol{v}$ be a rank-k Cartesian tensor in three dimensions.
- *Spatially*, let $u \in \mathrm{O}(3)$ be any **proper** or **improper rotation** that acts on an orthogonal basis $\{\boldsymbol{e}_i\}$ spanning $\mathbb{R}^3$ according to

$$\hat{u}\boldsymbol{e}_i = \boldsymbol{e}_j\, U_{ji}.$$

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$\boldsymbol{U}$: representation matrix for u in $\{\boldsymbol{e}_i\}$

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To consider the *linear* action of u on $\boldsymbol{v}$, let $\boldsymbol{v}' = \hat{u}\boldsymbol{v}$.

- $\boldsymbol{v}$ is a **polar** tensor if

$$v'_{ab\ldots k} = U_{ap}U_{bq}\ldots U_{kz}\, v_{pq\ldots z}.$$

- $\boldsymbol{v}$ is an **axial** tensor if

$$v'_{ab\ldots k} = |\boldsymbol{U}|U_{ap}U_{bq}\ldots U_{kz}\, v_{pq\ldots z}.$$

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+1 for proper rotations, −1 for improper rotations

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Tensor transformations

- Let $\boldsymbol{v}$ be a rank-k Cartesian tensor in three dimensions.
- *Temporally*, let θ be the **time reversal** that acts on an orthogonal basis $\{\omega_1, \omega_2\}$ of a two-component spinor according to

$$\hat{\theta}\begin{bmatrix}\omega_1 & \omega_2\end{bmatrix} = \begin{bmatrix}\omega_2^* & -\omega_1^*\end{bmatrix}.$$

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To consider the *antilinear* action of θ on $\boldsymbol{v}$, let $\boldsymbol{v}'' = \hat{\theta}\boldsymbol{v}$.

  - $\boldsymbol{v}$ is a **time-even** tensor ($\boldsymbol{i}$-tensor) if

$$\boldsymbol{v}'' = \boldsymbol{v}.$$

  - $\boldsymbol{v}$ is a **time-odd** tensor ($\boldsymbol{c}$-tensor) if

$$\boldsymbol{v}'' = -\boldsymbol{v}.$$

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Tensor classifications

- There are *four* types of tensors under spatial-temporal transformations.
  - **polar time-even** tensors
    - position vectors $\boldsymbol{r}$
  - **polar time-odd** tensors
    - linear momentum vectors $\boldsymbol{p}$
    - magnetic vector potentials $\boldsymbol{A}$
    - current densities $\boldsymbol{j}$
  - **axial time-even** tensors
  - **axial time-odd** tensors
    - angular momentum vectors $\boldsymbol{l}$
    - magnetic field vectors $\boldsymbol{B}$

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Symmetry and pseudo-symmetry groups

Definition (symmetry group)

All transformations $\hat{T}$ that leave the electronic Hamiltonian $\hat{\mathscr{H}}$ invariant, *i.e.* $\hat{T}\hat{\mathscr{H}}\hat{T}^{-1} = \hat{\mathscr{H}}$, form the **symmetry group** of $\hat{\mathscr{H}}$. Such transformations are called **symmetry transformations**.

- Symmetry transformations impose *constraints* on the eigenfunctions of $\hat{\mathscr{H}}$ and properties calculated from them.

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Definition (pseudo-symmetry group)

Consider a term $\hat{\mathcal{H}}' \subset \hat{\mathcal{H}}$. All transformations $\hat{T}$ that leave $\hat{\mathcal{H}}'$ invariant but not the full $\hat{\mathcal{H}}$ form a **pseudo-symmetry group** of $\hat{\mathcal{H}}$. Such transformations are called **pseudo-symmetry transformations**.

- Pseudo-symmetry transformations provide ways to understand eigenfunctions of $\hat{\mathcal{H}}$ *(complicated)* from the perspective of $\hat{\mathcal{H}}'$ *(simpler)*.

Groups in magnetic fields

- Let us revisit the electronic Hamiltonian in a uniform magnetic field:

$$\hat{\mathscr{H}} = \hat{\mathscr{H}}_0(v_{\mathrm{ext}}) + \boldsymbol{A}(\boldsymbol{r}_k) \cdot \hat{\boldsymbol{p}}_k + \frac{g_s}{2} \sum_{k=1}^{N_{\mathrm{e}}} \boldsymbol{B} \cdot \hat{\boldsymbol{s}}_k + \frac{1}{2} A^2(\boldsymbol{r}_k).$$

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polar time-even

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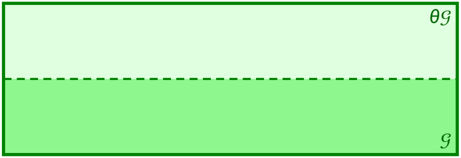
$\mathcal{G} + \theta\mathcal{G}$



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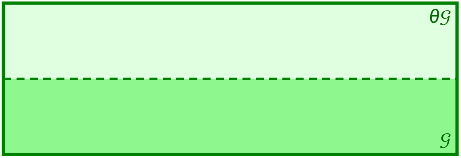
polar time-odd



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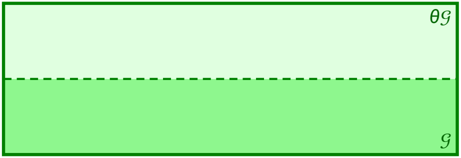

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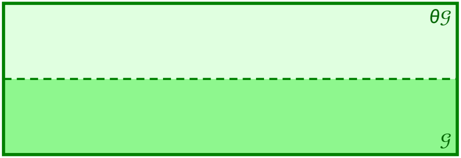

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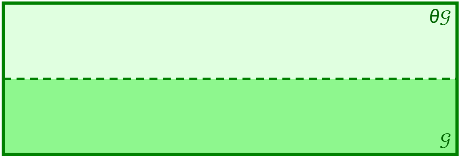
axial time-odd



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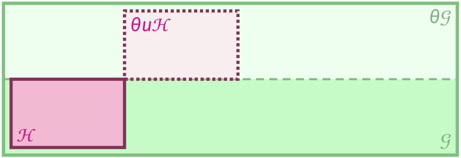
$\mathcal{H} + \theta u \mathcal{H}$

$(u \in \mathcal{G}, \hat{u}\boldsymbol{B} = -\boldsymbol{B})$



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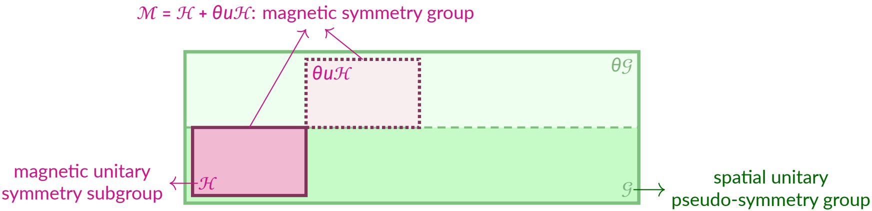

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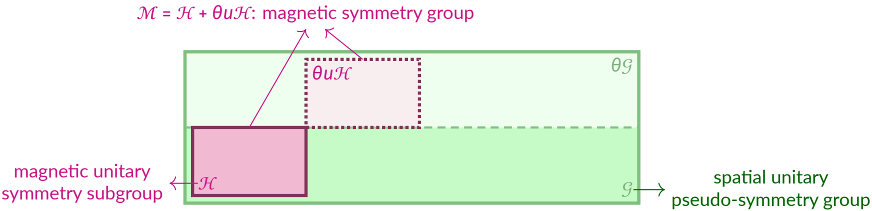
- If $\mathcal{M} = \mathcal{H} + \theta u \mathcal{H}$ is isomorphic to a **unitary group** $\mathcal{M}'$, we write $\mathcal{M} = \mathcal{M}'(\mathcal{H})$.



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