Symmetry of Magnetically Induced Currents

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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 $\boldsymbol{B}$, consider the Schrödinger–Pauli Hamiltonian:

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

E. I. Tellgren et al. J. Chem. Phys. 148.2 (January 2018), p. 024101.

T. J. P. Irons, A. Garner and A. M. Teale. Chemistry (MDPI). 3.3 (August 2021), pp. 916–934.