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# Investigate the electronic structure of rare-earth materials with recognizing Breit Hamiltonian

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## Extended Abstract

### Introduction

Accurate modeling of core-electron spectroscopy in rare-earth and heavy-element systems requires quantum chemical methods that incorporate both relativistic effects and electron correlation. The Dirac-Coulomb Hamiltonian provides a foundational relativistic framework, but neglects magnetic and retardation interactions arising from the finite speed of light. For precise spectroscopic predictions, the Breit Hamiltonian—comprising the Gaunt (magnetic) and Gauge (retardation) terms—must be included.

### Methods

A fully adaptive, four-component Dirac-Coulomb-Breit Hamiltonian was implemented within a multiresolution analysis (MRA) framework using a multiwavelet basis. The multiwavelet approach employs dyadic scaling functions and their orthogonal complements, constructing a telescoping sequence of function spaces. The methodology involved:

1. Implementation of the Dirac-Coulomb mean-field equations.
2. Inclusion of the Gaunt term, which describes the magnetic interaction between electron current densities and increases computational cost by a factor of three due to its vector nature.
3. Reformulation of the Gauge term into a numerically stable expression utilizing only the inverse interelectronic distance operator, clarifying its relationship to the magnetic interaction.The accuracy of the multiwavelet implementation was governed by two parameters: a threshold (ε) and the polynomial order (k).

### Results

The multiwavelet implementation successfully calculated ground-state energies for two-electron, helium-like ions across a wide range of nuclear charges. Key findings include:

- The method's accuracy is independent of the chosen nuclear charge model.
- Multiwavelets can describe superheavy elements without being constrained by the boundary conditions that typically affect atomic orbital basis sets when solving the full four-component Dirac equation.
- For systems with only *s*-orbitals, the magnitude of the Gauge (retardation) correction was found to be identical to the magnetic (Gaunt) contribution, resulting in a ratio of EGauge/EMag=1*E*Gauge/*E*Mag=1. This equivalence breaks down in the presence of orbitals with higher angular momentum.

### Conclusion

This work demonstrates that the multiwavelet basis provides a robust, adaptive, and boundary-condition-free framework for relativistic quantum chemical calculations. The successful implementation of the full Dirac-Coulomb-Breit Hamiltonian and the quantitative analysis of the Gaunt and Gauge terms validate the multiwavelet approach as a powerful tool for future high-precision core-electron spectroscopy studies of strongly correlated systems, including f-element oxides and rare-earth materials.

**Key words:** Breit Hamiltonian, core-electron spectroscopy, rare-earth materials



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