Relativistic effects in atomic structure theory

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Why care about relativity in atomic physics?

- The first ever ‘tick’ of a nuclear clock was achieved last year
- A promising candidate for a nuclear clock is Th^{3+}
- Thorium is highly relativistic, so understanding the relativistic structure is important
- Aim of my project is to include relativistic effects into high-precision, all-orders calculations

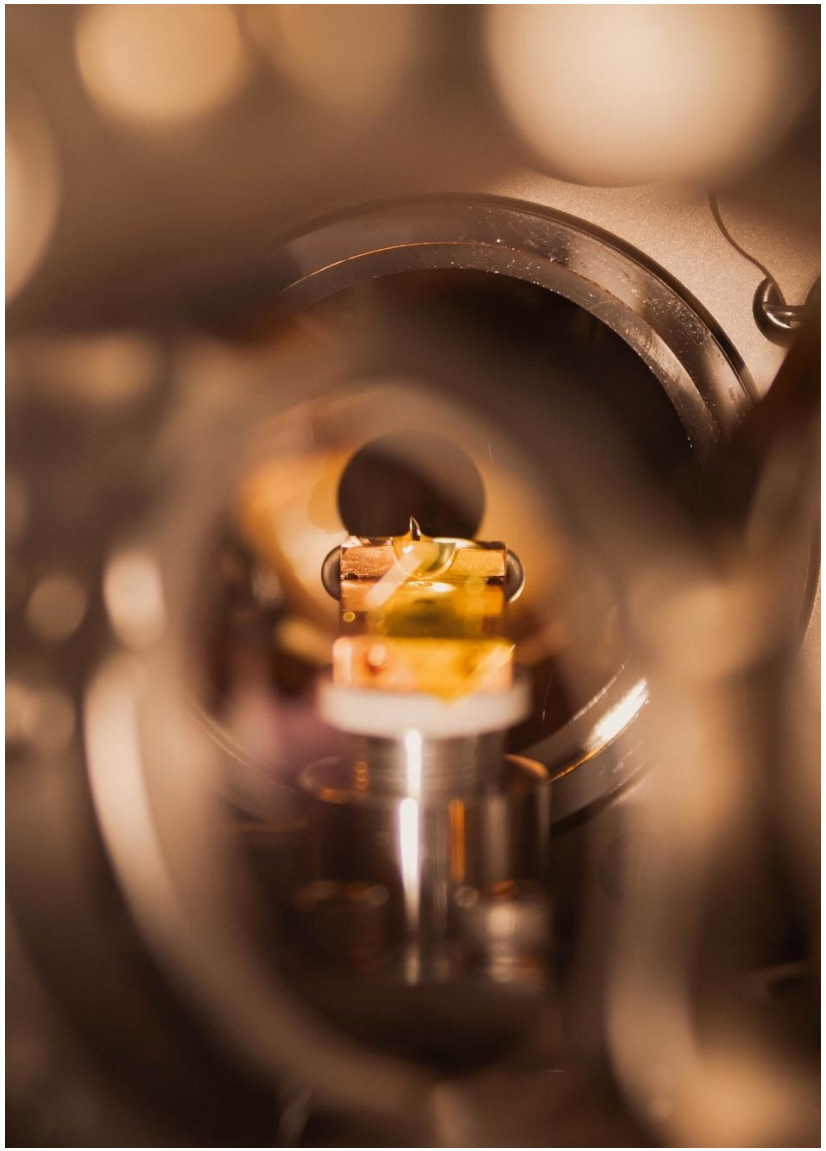
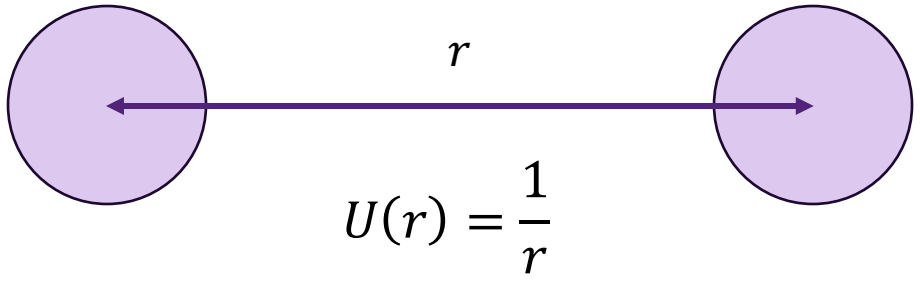


Figure: Calcium fluoride crystal which has been doped with thorium atoms. The crystal is probed with light from a vacuum ultraviolet (VUV) laser comb to determine the energy required to excite the nuclear ground state. Figure taken from The Washington Post.

Modelling atoms theoretically

- Atoms are too complicated to treat exactly
- Approximation methods and perturbation theory must be used for high accuracy calculations
- These calculations often start from the assumption that electron-electron interactions are purely Coulombic

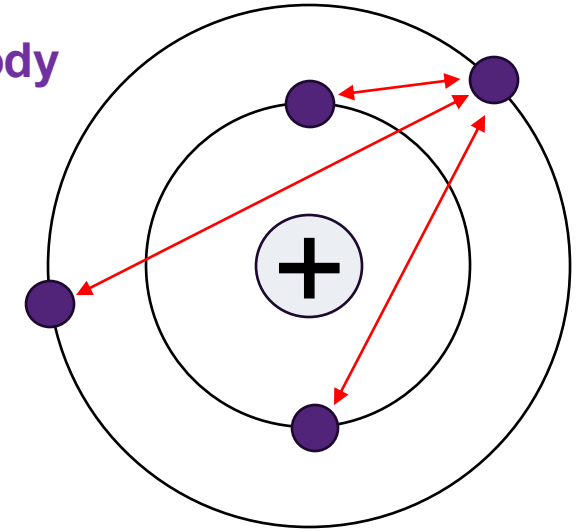


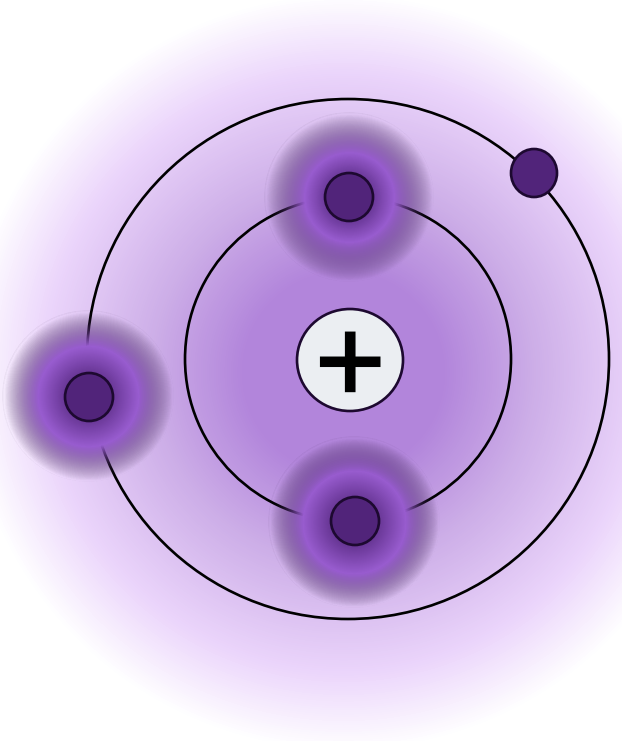
Completely non-relativistic

Hartree-Fock approximation

- Assume electrons move in a mean potential generated by all other electrons in atom
- Hartree-Fock is one choice for the mean potential; formed from just the Coulomb interaction
- Corrections beyond Hartree-Fock can be calculated using many-body perturbation theory
- MBPT normally done using Goldstone (standard) approach

Full many-body interactions





Mean-field approximation

The Coulomb interaction is not enough!

- The $6s$-$7s$ transition in caesium is forbidden due to parity conservation electromagnetically – weak interaction allows this to happen
- There was a 2.5σ tension between the SM and experiment using atomic structure calculations that used the Coulomb interaction
- Including relativistic corrections to the Coulomb interaction resolved this tension!

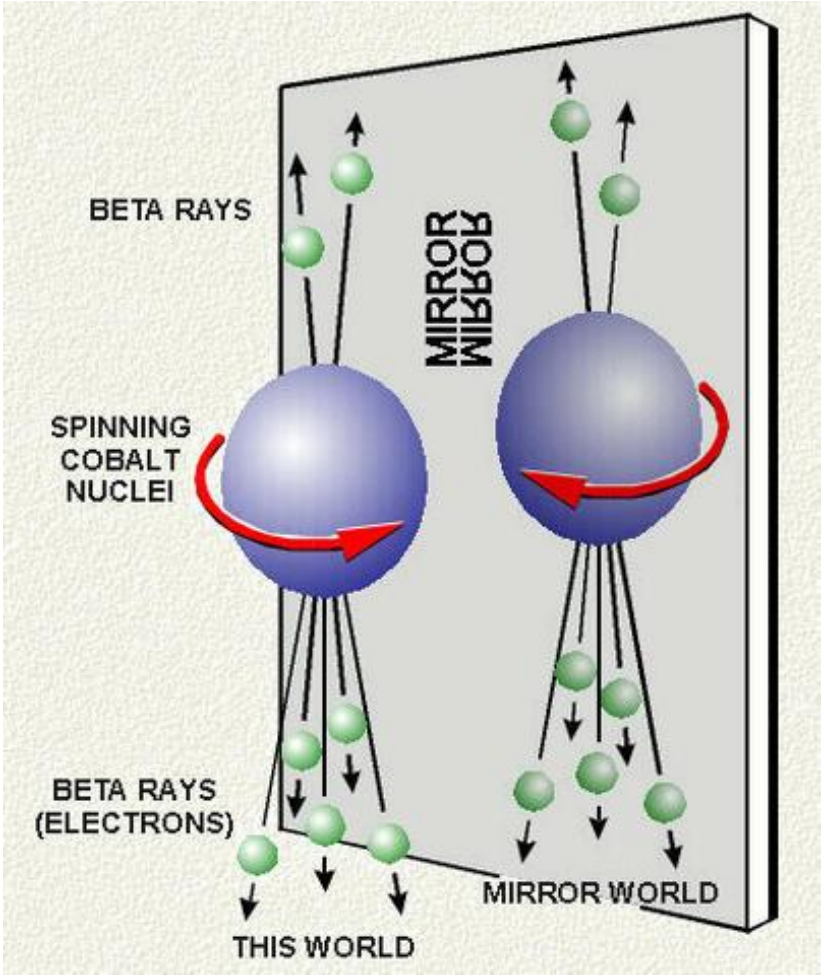
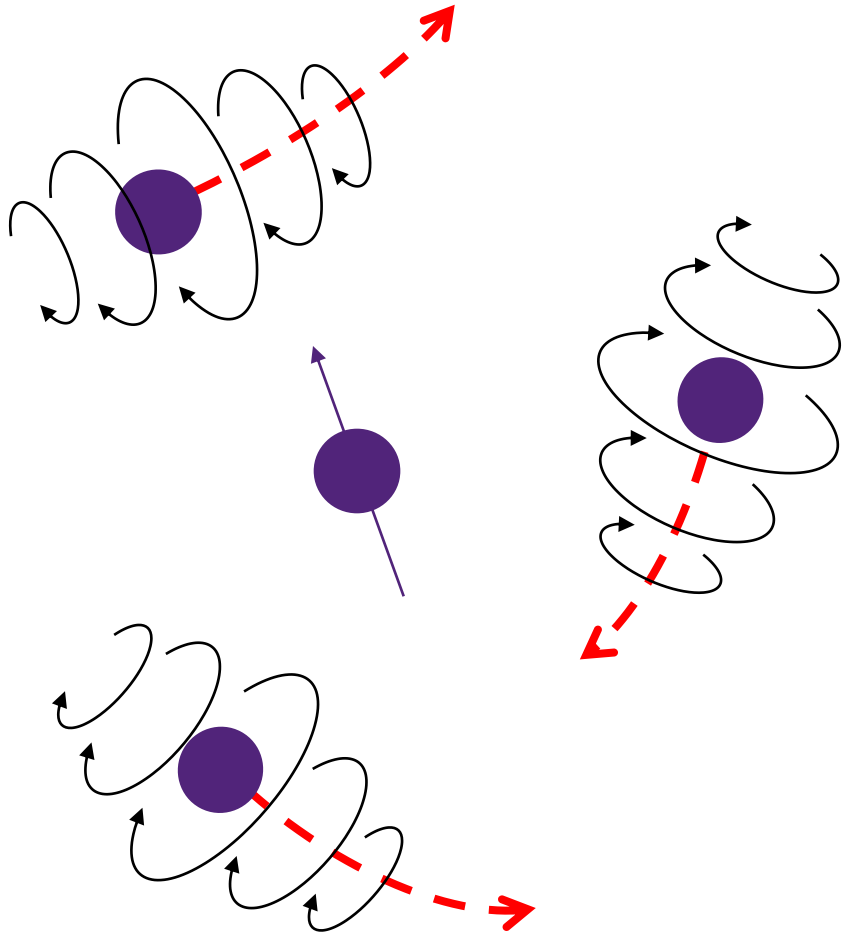


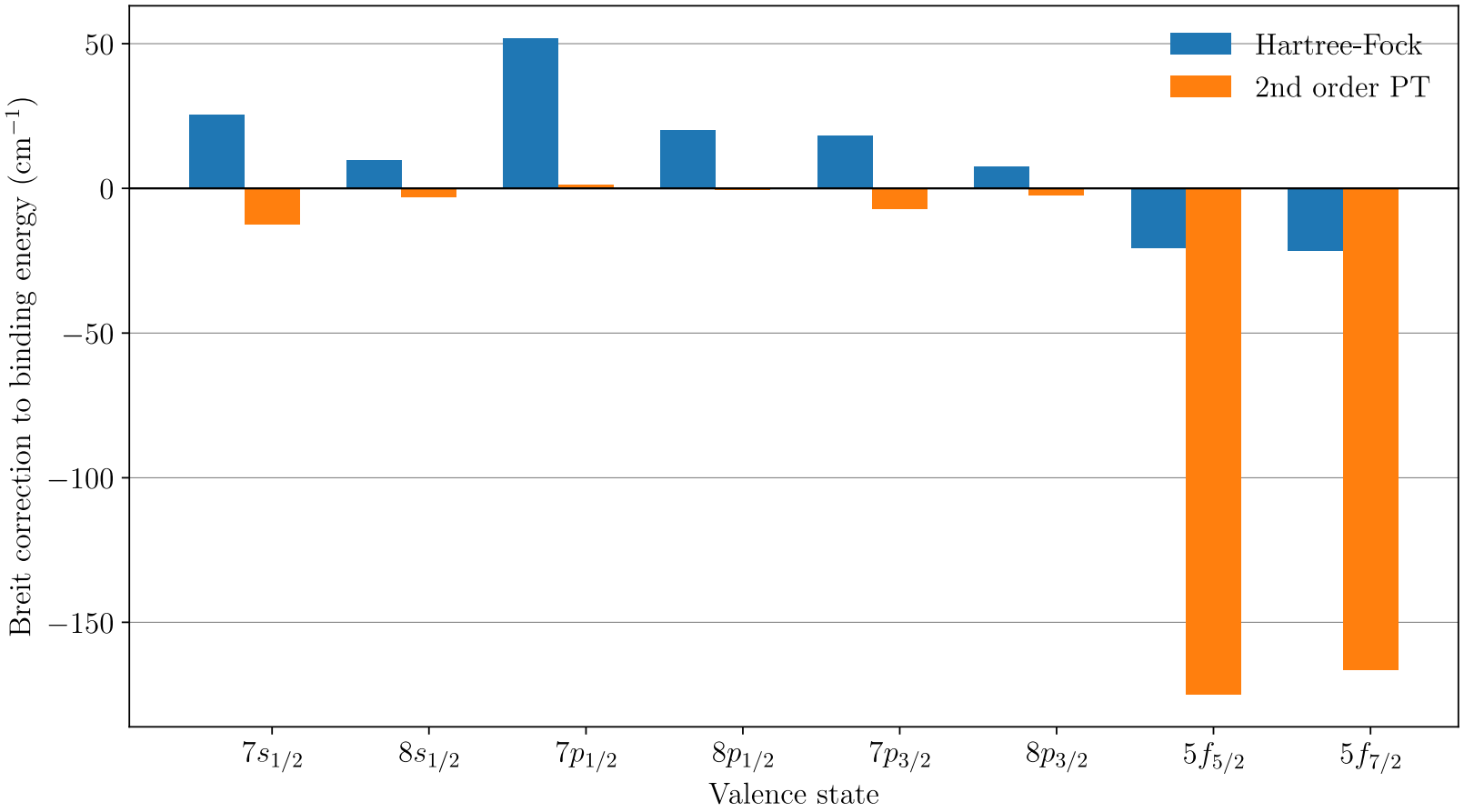
Figure: Cobalt atoms will preferentially eject beta particles in one direction relative to the nuclear spin, which isn't invariant under a parity transformation. Figure taken from NIST.

The Breit interaction

- The Coulomb interaction assumes electrons interact instantaneously
- Movement of electrons generates magnetic field
- The Breit interaction represents the coupling of electron spin to this magnetic field, plus retardation corrections from finite speed of light
- Currently can include Breit into Hartree-Fock and into 2nd order (Goldstone) MBPT



Breit contributions are significant at low orders of perturbation theory for heavy atoms. For singly-ionised radium:



Including Breit into perturbation theory is important, leading to important corrections even at 2nd order!

We have a problem

We want to include Breit into high-accuracy calculations

and

it makes a huge difference even at second order in perturbation theory, so we want to include it to higher orders

BUT

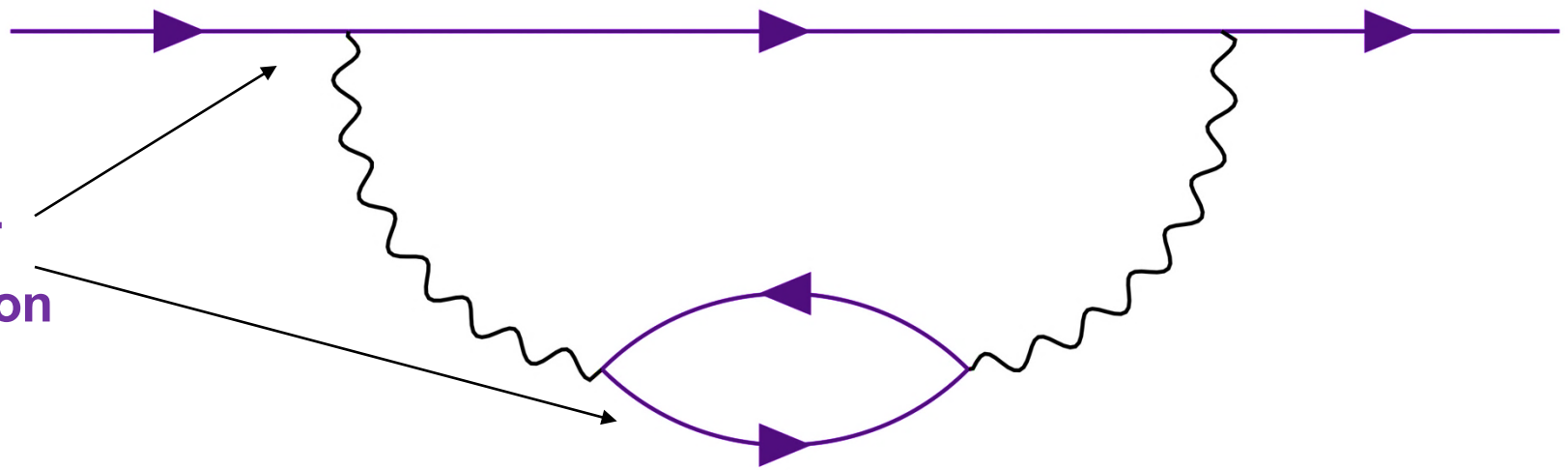
it's hard to go much further than second order with Goldstone perturbation theory

How can we get around this?

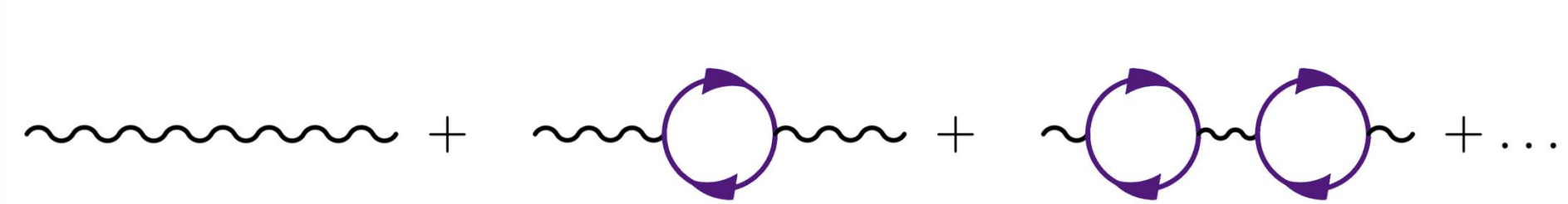
The Feynman method

- Instead of standard (Goldstone) method of MBPT, can use Feynman diagrams

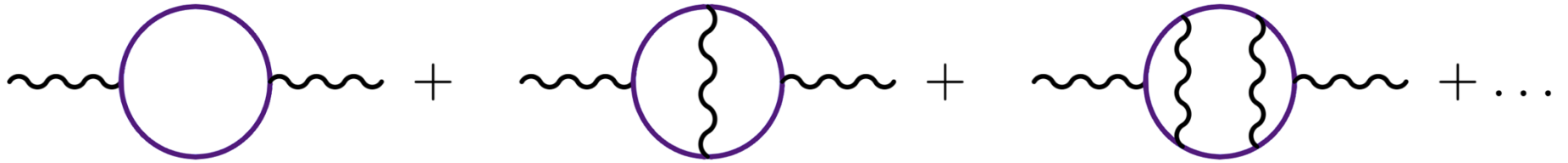
- Certain infinite series of diagrams can be summed exactly, including them to all orders of perturbation theory



In particular, the infinite series of diagrams,



and

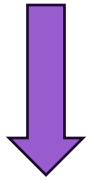


can be calculated **exactly** in the Feynman method!

Not currently possible to include Breit into the Feynman method

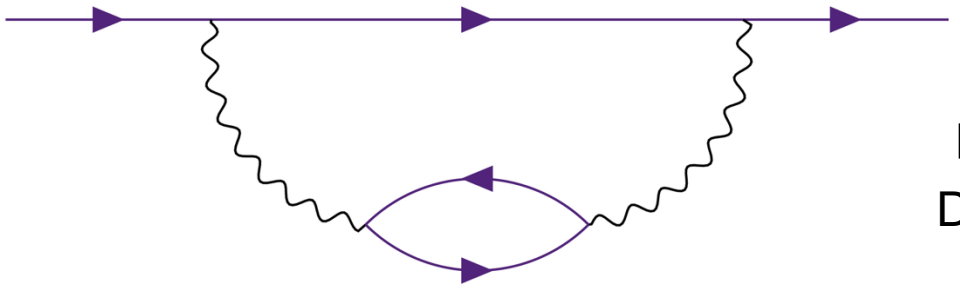
Goal:

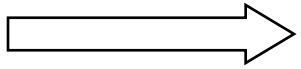
Include the Breit interaction into the Green's function



Breit can be included into all-orders calculations

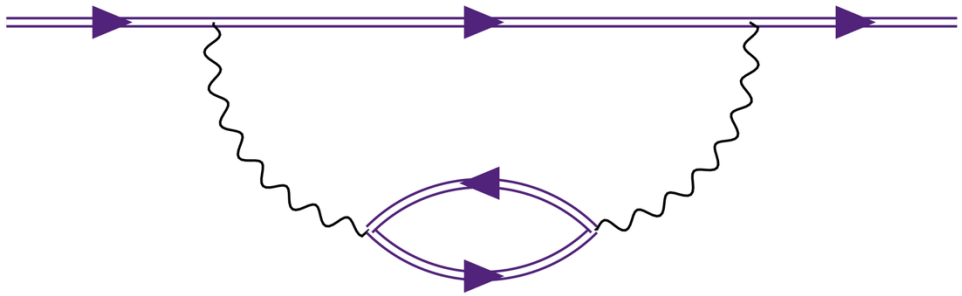
HF Green's function





Dyson equation

Breit + HF Green's function



Difficulties

- Coulomb interaction doesn't care about spin while Breit intrinsically does

Spin components

$$\hat{B}_{12} = -\frac{1}{2r}\left[\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 + \frac{(\boldsymbol{\alpha}_1 \cdot \boldsymbol{r})(\boldsymbol{\alpha}_2 \cdot \boldsymbol{r})}{r^2}\right]$$

- Turns out it is also highly sensitive to the spin structure of the rest of the Feynman diagram

- I have implemented Breit into the Feynman method and confirmed that it agrees with the Goldstone method at second order

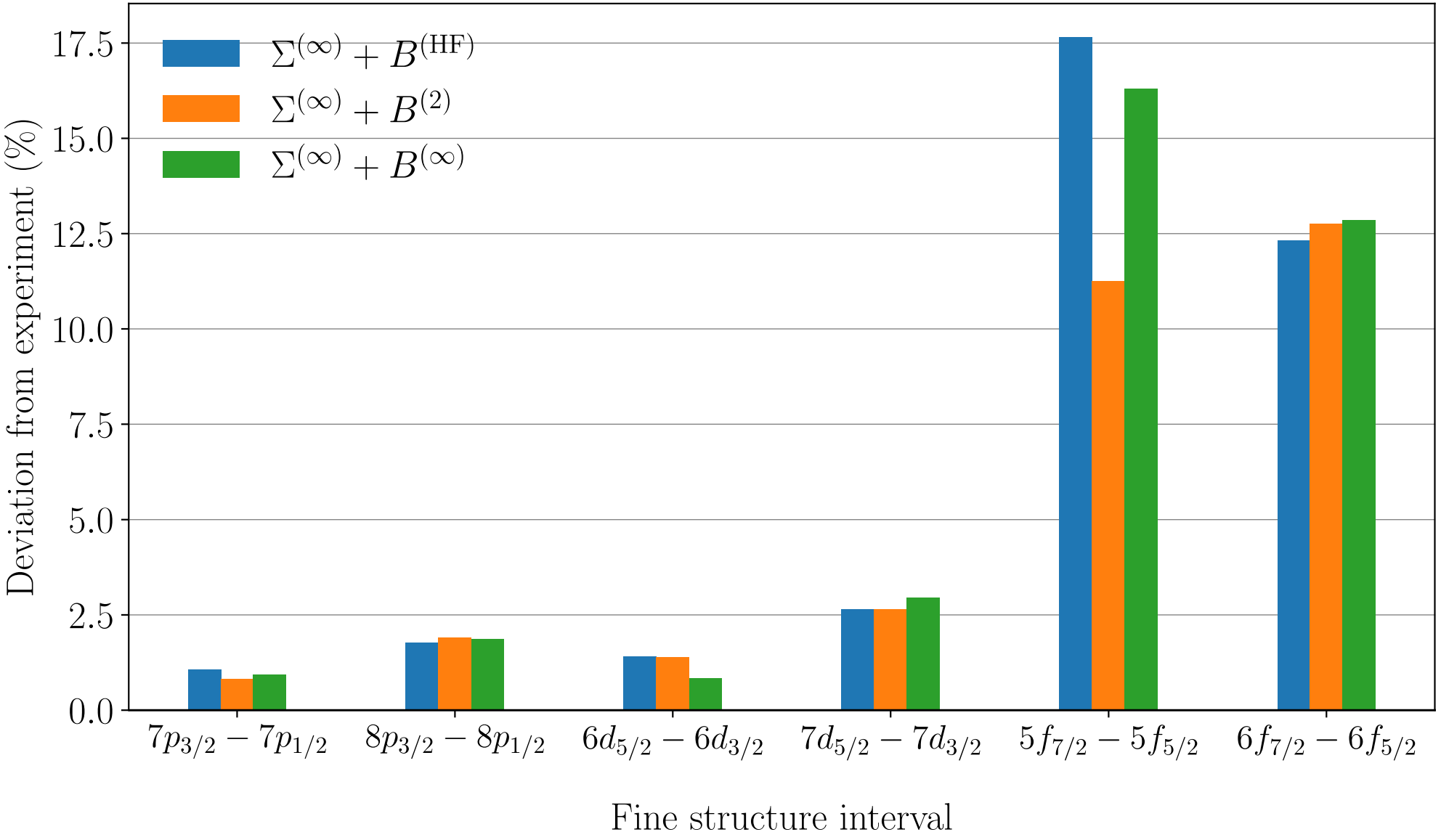
Fine structure

- Non-relativistically, states with same orbital angular momentum but different spin angular momentum are degenerate – relativity lifts this degeneracy

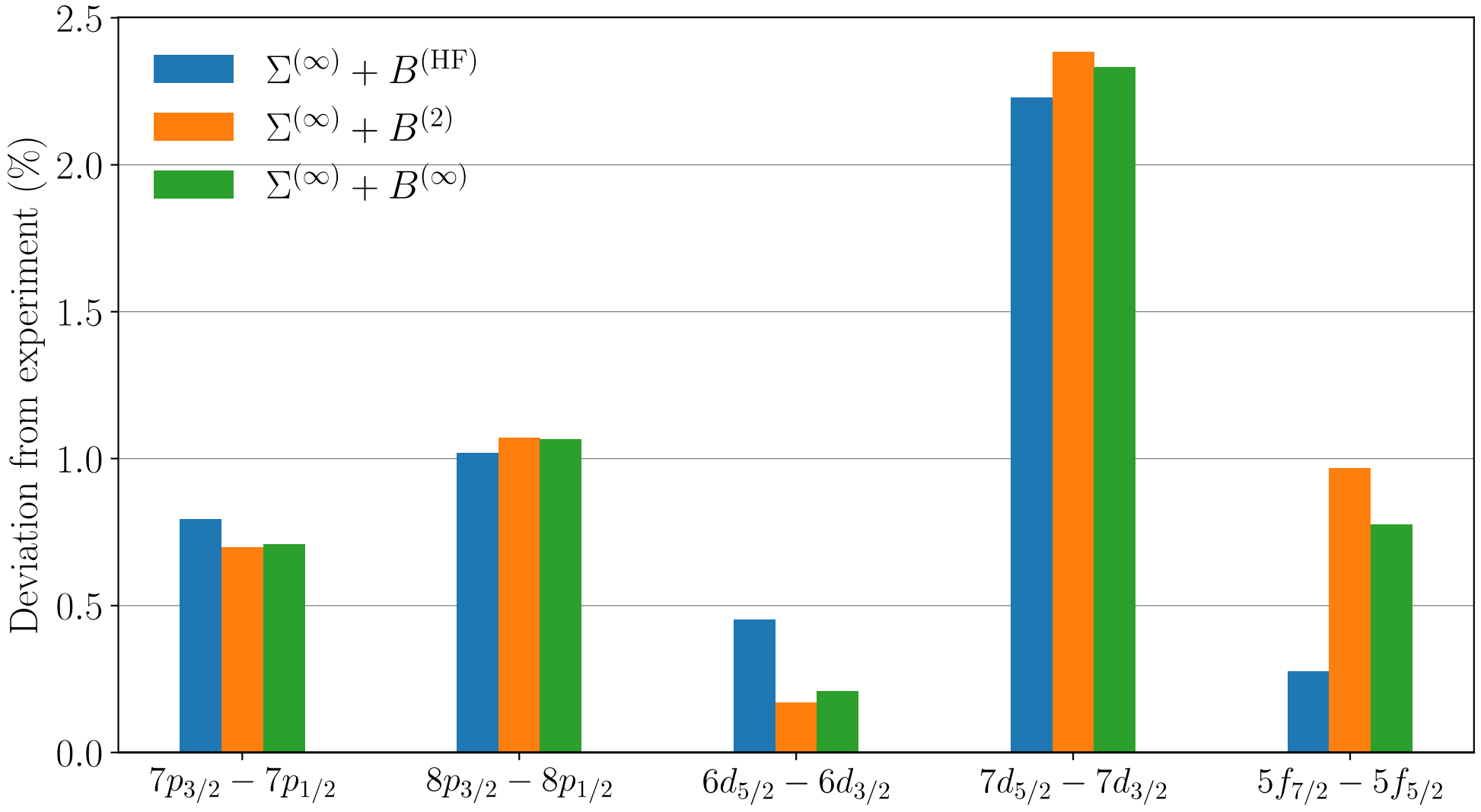
- Eg. the $7p_{3/2}$ and $7p_{1/2}$ states in caesium have an energy splitting referred to as the **fine structure interval**

- Can evaluate the fine structure interval with the inclusion of Breit at each level of perturbation theory

Radium


$\Sigma^{(\infty)} + B^{(\mathrm{HF})}$
$\Sigma^{(\infty)} + B^{(2)}$
$\Sigma^{(\infty)} + B^{(\infty)}$
Deviation from experiment (%)
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
$7p_{3/2} - 7p_{1/2}$
$8p_{3/2} - 8p_{1/2}$
$6d_{5/2} - 6d_{3/2}$
$7d_{5/2} - 7d_{3/2}$
$5f_{7/2} - 5f_{5/2}$
$6f_{7/2} - 6f_{5/2}$
Fine structure interval

Thorium


$\Sigma^{(\infty)} + B^{(\mathrm{HF})}$
$\Sigma^{(\infty)} + B^{(2)}$
$\Sigma^{(\infty)} + B^{(\infty)}$
Deviation from experiment (%)
0.0
0.5
1.0
1.5
2.0
2.5
$7p_{3/2} - 7p_{1/2}$
$8p_{3/2} - 8p_{1/2}$
$6d_{5/2} - 6d_{3/2}$
$7d_{5/2} - 7d_{3/2}$
$5f_{7/2} - 5f_{5/2}$
Fine structure interval

Next steps

- Try to include other relativistic effects (e.g. radiative corrections) into the calculation of fine structure intervals to see if this resolves problem
- Include frequency-dependence into the Breit interaction – should be negligible for small ions but becomes more important for heavy systems
- Calculate hyperfine structure constants
- Go beyond the Breit interaction

Thank you!